

# Atlas of the High-Temperature Water Vapor Spectrum in the 3000 to 4000 cm<sup>-1</sup> Region

A. S. Pine\* and M. J. Coulombe

*Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Massachusetts 02173*

and

C. Camy-Peyret and J-M. Flaud

*Laboratoire de Physique Moléculaire et d'Optique Atmosphérique, Bâtiment 221, Campus d'Orsay 91405. Orsay, France*

An atlas of the high-temperature (1200 K) absorption spectrum of water vapor in the 3000 to 4000 cm<sup>-1</sup> region is presented. The infrared spectrum was recorded at Doppler-limited resolution using a tunable difference-frequency laser spectrometer. The spectral region scanned encompasses the strong OH stretching fundamentals,  $\nu_1$  and  $\nu_3$ , and the bending overtone,  $2\nu_2$ , as well as associated hot bands. Almost all the lines have been assigned using a model Hamiltonian which yields very satisfactory agreement between calculated and observed line positions for  $J$  up to 27 or  $K_a$  up to 14. The calculated eigenvectors applied to the transition moment operator predict the measured line intensities quite closely. This work should serve as a reference for analyzing spectra from high-temperature sources such as combustion exhausts and cool stars.

Key words: difference-frequency laser; Doppler-limited resolution; high temperatures; infrared spectrum; OH stretching fundamentals; water vapor.

## Contents

|                                     | Page |  | Page |
|-------------------------------------|------|--|------|
| 1. Introduction.....                | 413  | 7. References.....   | 420  |
| 2. Experimental Considerations..... | 414  | <b>List of Tables</b>  |      |
| 2.1. Spectrometer.....              | 414  | 1. Summary of the hot water vapor bands<br>observed between 2965 and 4005 cm <sup>-1</sup> .....                                     | 418  |
| 2.2. Sample and Cell.....           | 415  | 2. Observed and calculated hot water vapor<br>transition wavenumbers and intensities<br>between 2965 and 4005 cm <sup>-1</sup> ..... | 421  |
| 3. Results.....                     | 416  |  |      |
| 4. Analysis and Discussion.....     | 417  |  |      |
| 5. Conclusions.....                 | 419  |  |      |
| 6. Acknowledgement .....            | 420  |  |      |

## 1. Introduction

The infrared spectrum of water vapor at ordinary temperatures ( $\sim 300$  K) is quite well known, with the high-resolution Fourier transform interferometer study by Camy-Peyret, Flaud, Guelachvili, and Amiot [1]<sup>1</sup> being perhaps the most complete and precise to date. Since water vapor is an oxidation product of the burning of hydrocarbons and other fuels and is present

in the atmospheres of cool stars, an accurate knowledge of its high-temperature infrared spectrum is an aid in combustion diagnostics and in astrophysical studies. At high temperatures the most extensive study is the H<sub>2</sub>O emission spectrum from an H<sub>2</sub>/O<sub>2</sub> flame by Flaud, Camy-Peyret, and Maillard [2], also recorded on a Fourier transform instrument. Temperatures in the flame reached 2900 K, which are much higher than can be obtained in absorption cell experiments. However the complex temperature distribution in the flame and its atmospheric pressure operation create some uncertainties in measurements of line intensities and positions. Thus it seems important to have a comprehensive, low-pressure absorption spectrum at intermediate temperatures to bridge the gap between the cold water and flame measurements.

We present here an atlas of the high-temperature absorption spectrum of water vapor recorded in the

<sup>1</sup> Figures in brackets indicate literature references at the end of this paper.

\* Present address: Molecular Spectroscopy Division, National Bureau of Standards, Washington, DC 20234.

© 1983 by the U.S. Secretary of Commerce on behalf of the United States. This copyright is assigned to the American Institute of Physics and the American Chemical Society.

Reprints available from ACS; see Reprint List at back of issue.

3000 to 4000  $\text{cm}^{-1}$  region with Doppler-limited resolution using a tunable difference-frequency laser spectrometer. This spectral region contains the strong  $\nu_1$  and  $\nu_3$  OH stretching fundamentals and the  $2\nu_2$  bending overtone. At the temperature of these measurements ( $\sim 1200$  K) the  $\nu_2$  vibration is highly excited so that many hot band lines as well as higher rotational levels are observed. This study thus makes it possible to extend the hot band and high  $J, K_a$  rotational assignments of  $\text{H}_2\text{O}$  and to have precision wavenumbers and transition intensities which can be used for reference and which can be helpful in refining theoretical models to improve predictive capabilities.

## 2. Experimental Considerations

### 2.1. Spectrometer

The tunable laser difference-frequency spectrometer used to record the Doppler-limited spectrum of high-temperature water vapor is based on mixing of a cw single-mode argon and a tunable dye laser in the nonlinear optical crystal  $\text{LiNbO}_3$ . The infrared beat frequency generated in the  $\text{LiNbO}_3$  crystal is split into sample and reference beams for ratio recording to eliminate amplitude fluctuations due to the incident lasers. Details on the visible-to-infrared conversion efficiency, spectral coverage, phasematching requirements, drift compensation, extended scan range, stabilization, and linear scan control of the difference-frequency spectrometer appear in references [3-6].

In the present experiment the difference-frequency spectrometer was tuned over the range from 4005  $\text{cm}^{-1}$  to 2965  $\text{cm}^{-1}$  to encompass the entire fundamental  $\nu_1$  and  $\nu_3$  bands and the overtone  $2\nu_2$  of water vapor. This coverage of more than 1000  $\text{cm}^{-1}$  at ultrahigh resolution (instrumental line-width  $\sim 3 \times 10^{-4}$   $\text{cm}^{-1}$ , Doppler line-width  $\sim 2 \times 10^{-2}$   $\text{cm}^{-1}$ ) is the most extensive continuous scan yet achieved with a tunable infrared laser. The spectrum was recorded in 3.75  $\text{cm}^{-1}$  segments overlapped at 3.0  $\text{cm}^{-1}$  intervals. Each segment required 5 minutes to scan using a time constant of 40 ms chosen to provide good signal-to-noise ratio ( $\sim 300:1$ ) and a full response to sharp spectral features. The data were digitized at a 20 Hz rate ( $\sim 6 \times 10^4$   $\text{cm}^{-1}$  grid) and stored on magnetic tape for subsequent computer processing.

A microprocessor-based tape data logger was specially constructed for this experiment for dedicated, reliable, high-density mass storage with a local memory buffer and manual baseline digitizer feature. The manual baseline digitizer feature was incorporated to correct for pathological baseline variations due to strong atmospheric water vapor absorptions which occur within the  $\text{H}_2\text{O}$  range scanned. It was not possible to evacuate the infrared section of the difference-frequency spectrometer; however, open atmospheric paths were reduced by inserting cells filled with dry  $\text{N}_2$  gas. In addition, the experiment was conducted in the winter months for lowest humidity since the laboratory

air-conditioning does not significantly reduce the humidity in the summer. Some  $\text{H}_2\text{O}$  lines are so strong though, that even a few centimeters of atmospheric path absorbs most of the light in the sample and reference beams, creating a very noisy spectrum.

The residual baseline variations in principle could be treated in various ways. Ideally, one would record both a full cell and an empty cell trace for normalization. However, the hot water cell could not be readily evacuated, since it was sealed off, and the vapor pressure was regulated through a temperature-controlled side-arm ice reservoir. Also this normalization method would have doubled the data recording time and storage requirements which would be prohibitive due to the extensive spectral coverage. A second normalization method would be to balance the open atmospheric paths in the sample and reference beams so that the ratio recording would eliminate the atmospheric background variation. Unfortunately the high-temperature sample cell geometry required a minimum open path of  $\sim 20$  cm, and this long a path in the reference beam would have caused the ratio-denominator to approach zero for too many lines. Thirdly, numerical methods could have been used to estimate the baseline by distinguishing between sharp Doppler-limited low pressure transitions and slow background variations due to broad atmospheric absorptions. This is our usual approach for generating baselines for molecular spectra outside the  $\text{H}_2\text{O}$  region. However, the algorithm does not work satisfactorily for the strong, relatively sharp, baseline variations due to

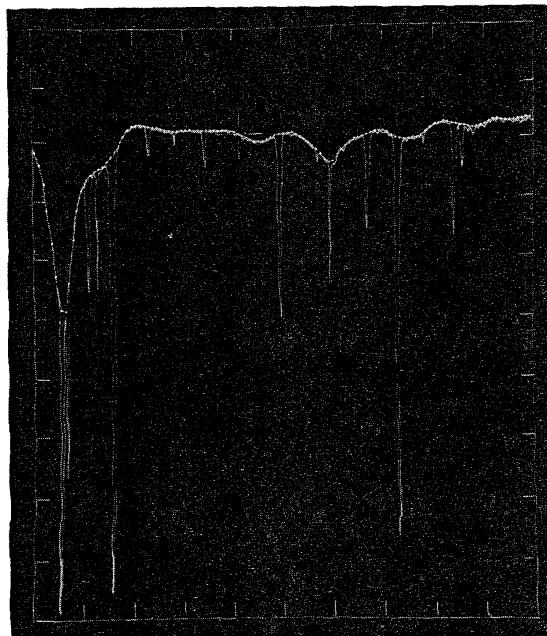


FIGURE 1. Display of tape logger data acquisition system showing interactive baseline digitizer on sample transmission trace. The dotted curve on the baseline is entered manually and the baseline is linearly interpolated.

atmospheric water vapor absorptions which were of course in exact coincidence with many of the lines under investigation. For all these practical reasons we chose to determine the baselines interactively with a manual baseline digitizer incorporated in the data logger electronics using a storage CRT display. An example of the sampled baseline on a transmission trace is shown in figure 1.

The observed signal-to-noise ratio of  $\sim 300:1$  was limited in this experiment by background noise generated by the high-temperature sample cell. For ordinary room-temperature cells the instrumental signal-to-noise ratio is  $\sim 1000:1$ . The hot cell creates two excess noise sources—thermal background radiation and atmospheric convection currents. Since the oven and cell walls at 1200 K are glowing red hot it is necessary to prevent this radiation from reaching the sample detector. This was accomplished by extending the hot cell windows outside the oven and optically masking the walls by focusing and spatially filtering the infrared laser beam. This was found to be more effective than spectral filtering using a broadband tunable interference wedge which caused additional attenuation. Convection currents in the heated air outside the hot cell windows created excess noise by shifting the infrared beam around on the active detector surface. This problem was reduced by inserting draft-shielding tubes against the cell windows. Evacuable antechambers would have been preferable but were prohibited by the oven configuration.

Transition wavenumbers were obtained by linear interpolation between fringes of a high-finesse scan calibration interferometer monitoring the visible lasers [4-6]. This interferometer was referenced to a Lamb-dip stabilized He/Ne laser which maintained the calibration and resestability to  $\sim 5 \times 10^{-4} \text{ cm}^{-1}$  during the entire course of the experiment ( $\sim 1$  month). The calibration of the index wavenumber, free-spectral-range and dispersion of the interferometer was accomplished by reference to the room-temperature  $\text{H}_2\text{O}$  Fourier-transform study by Camy-Peyret et al. [1]. Here, cold water spectral excerpts were recorded about every 100  $\text{cm}^{-1}$ . Clean, isolated reference lines were selected and the Fabry-Perot fringes were least-squares fit to a parabola. The correct interorder number could be estimated from previous precision measurements [4] of the free-spectral-range and were verified by the continuous scan of the high-temperature  $\text{H}_2\text{O}$  spectrum. The fit resulted in a calibration curve of

$$\sigma_N = \sigma_0 - N \times (\text{FSR} - N \times \text{DISP})$$

where  $N$  is the interorder number,  $\sigma_0 = 4005.19963 \text{ cm}^{-1}$ ,  $\text{FSR} = 0.0500316 \text{ cm}^{-1}$  and  $\text{DISP} = 1.6136 \times 10^{-10} \text{ cm}^{-1}$ . The dispersion (variation of the free-spectral-range) is quite noticeable over the extensive tuning range covered in this experiment ( $N_{\max} \sim 21000$ ). It results principally from wavelength-dependent phase shifts in the double-stack broadband multidilectric

reflective coatings of the scan calibration interferometer and to a lesser extent from the dispersion of air over the dye laser tuning range.

## 2.2. Sample and Cell

The absorption cell used in this experiment, schematically shown in figure 2, was a 4.1 cm diameter fused quartz tube with 3 mm thick GE125 fused quartz Brewster angle windows glass blown on to the ends of the tube. These windows are relatively water-free, exhibiting only  $\sim 3\%$  broadband absorption between 3600 and 3700  $\text{cm}^{-1}$ . A  $\sim 10$ -cm-long quartz side arm was blown onto the tube near one end for pump-out, fill and seal-off and for containing the sample reservoir during the experiment. The cell was approximately 130 cm long with the ends protruding equally from either side of the 90 cm long tube furnace.

The Marshall furnace consisted of a 30 cm and a 60 cm section mounted end-to-end with a 5.1 cm bore and a 6.5 cm insulating wall. The furnace was rated at 1100 °C and was operated at  $\sim 927^\circ\text{C}$  during this experiment. Temperature was measured with two platinum/platinum-13% rhodium thermocouples and a digital readout (Doric 412A Trendicator, nominal calibration accuracy  $\pm 0.6^\circ\text{C}$ ). Temperature was maintained manually  $\pm 1^\circ\text{C}$  using Variac controls on the ac power to the ovens after about a 3 h warm-up each day. The measured temperature profile is also shown in figure 2. There is a slight drop in temperature at the junction of the two ovens and much larger gradients near the ends of the oven. The cell extends through the gradient region out to room temperature in

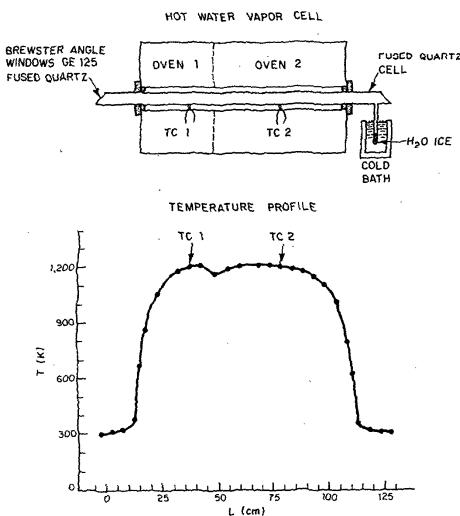


FIGURE 2. Sample cell schematic and temperature profile. During scan, thermocouples monitored temperatures at peaks of profile at TC1 and TC2; ovens were controlled individually.

order to avoid the excess noise problems associated with hot windows as discussed previously.

The water vapor pressure is maintained constant throughout the cell by controlling the temperature of the  $\text{H}_2\text{O}$  ice reservoir in the side arm. The cold bath contained a ~40% ethylene glycol in water antifreeze solution adequate for cooling to below  $-20^\circ\text{C}$  by passing cold liquid nitrogen boil-off gas through an immersed copper coil. The antifreeze was temperature regulated with an immersed resistance heater to  $\pm 0.2^\circ\text{C}$ . For the spectral region above  $\sim 3270 \text{ cm}^{-1}$  where the water vapor absorptions are strongest, the bath temperature was  $-20 \pm 0.2^\circ\text{C}$  corresponding to a vapor pressure of  $0.776 \pm 0.015 \text{ Torr}$  ( $1 \text{ Torr} = 133.3 \text{ Pa}$ ). Below  $3270 \text{ cm}^{-1}$  a reservoir temperature of  $-10 \pm 0.2^\circ\text{C}$ , corresponding to a vapor pressure of  $1.95 \pm 0.04 \text{ Torr}$ , was used to enhance the weaker transitions. In both ranges the cell was double-passed to increase the absorption.

The water sample itself was freshly distilled and deionized ( $\rho > 18 \text{ M}\Omega \text{ cm}$ ) before filling the cell. Nevertheless both  $\text{CO}_2$  and  $\text{CH}_4$  impurity lines are observed in the spectrum. These impurity lines were easily recognized by their distinctive patterns and they were sparse enough that there was little interference with the water spectrum. It is believed that the  $\text{CO}_2$  was present in the initial water sample due to absorption from the air since the amount of  $\text{CO}_2$  increases with the amount of time between distillation and cell filling. The  $\text{CH}_4$  only appears after cycling to high temperatures and may involve degassing from the

cell walls. A bake-out of the cell under vacuum, however, did not eliminate the methane.

It should also be noted that we initially tried some metal cells constructed of inert, high-temperature alloys, Monel 400 and Inconel 600. Metal cells would be more convenient for attaching flanges and demountable IR windows. However, the water vapor reacted with the hot metal walls at temperatures above  $\sim 550^\circ\text{C}$  and consequently the spectrum disappeared. Plating the cells with rhodium and platinum did not prevent this oxidation. For the much higher temperatures desired for this experiment, the metal cells were abandoned in favor of quartz.

### 3. Results

A small part of the high-temperature water vapor spectrum recorded between  $4005$  and  $2965 \text{ cm}^{-1}$  is presented in figure 3 in two overlapping  $12.75 \text{ cm}^{-1}$  panels including the transmission trace region appearing in figure 1. The spectral intensity scale is normalized according to Beer's law,

$$I(\sigma) = (pL)^{-1} \ln(B(\sigma)/S(\sigma)),$$

where  $p$  is the vapor pressure in Torr,  $L (= 252 \text{ cm})$  is the double-passed cell length,  $B(\sigma)$  is the baseline corresponding to the empty cell transmission, and  $S(\sigma)$  is the water vapor transmission spectrum. Even though the pressure is uniform throughout the cell, these intensities must be corrected for the variation of number

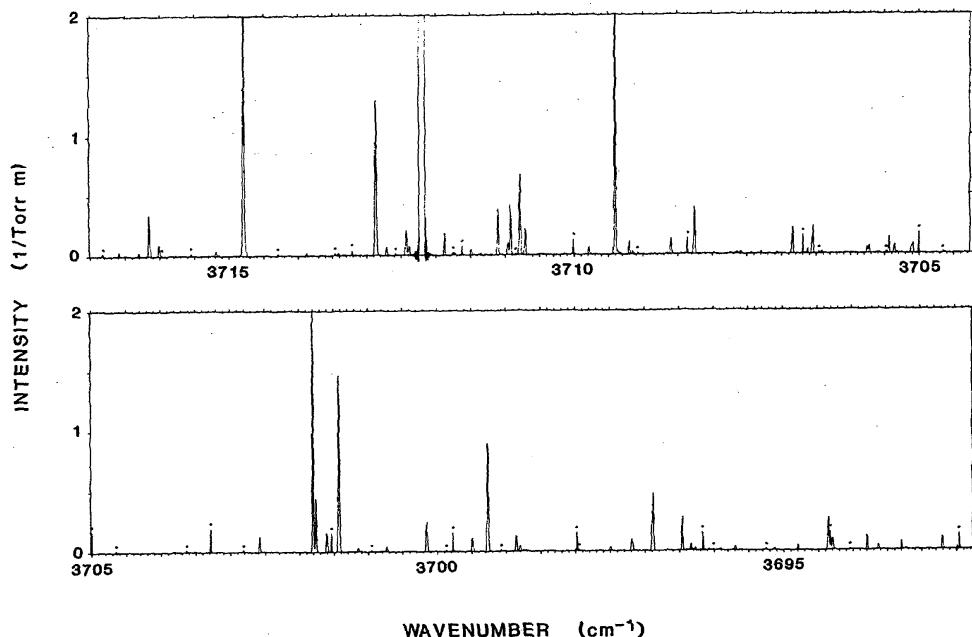


FIGURE 3. Portion of intensity spectrum of high-temperature  $\text{H}_2\text{O}$ .  $\text{CO}_2$  impurity lines are designated by an asterisk. The transmission trace of fig. 1 appears near  $3700 \text{ cm}^{-1}$ .

density, Doppler width, and lower state populations due to the temperature gradients in the cell. For example, high-temperature lines not seen at room temperature (i.e., hot band and high  $J$  transitions) have a shorter effective cell length ( $\sim 136$  cm) and twice the Doppler width than at 300 K. Such linewidth variation is readily observed throughout the spectrum and helps to distinguish the hot lines. Lines seen at both high and low temperatures have a complex line-shape corresponding to the sum of Gaussians weighted by the temperature distribution. Therefore one must proceed with care in analyzing these intensity data to derive transition moments. This problem is similar to that encountered in atmospheric and plume modeling, which are also plagued by complex pressure, density, and temperature distributions. In the present case these distributions have been measured from the vapor pressure at the cold bath temperature and the cell temperature profile shown in figure 2 and used to calculate the composite line intensities.

Impurity lines in the spectrum are not reported in this paper. Those arising from the  $v_1 + v_3$  and  $2v_2 + v_3$  combination bands of CO<sub>2</sub> and their associated hot bands are confined to the 3753 to 3554 cm<sup>-1</sup> region. They were easily distinguished from water vapor lines by their narrower Doppler width as befitting a heavier molecule. Lines due to the  $v_3$  band of CH<sub>4</sub> fall below 3200 cm<sup>-1</sup>. The noisy regions of the spectrum occur locally near very strong atmospheric water vapor absorptions and arise because of the low light level incident on the reference detector.

The instrumental precision of the difference-frequency spectrometer is dominated by the least reading (or digitizing grid) and is  $\sim 6 \times 10^{-4}$  cm<sup>-1</sup>. The performance here may be somewhat degraded because of the water vapor sample itself. Here the Doppler

widths are relatively large because of the light molecule and high temperatures. The background is noisier than usual due to black body thermal emission from the hot cell walls and to the hot air convection currents moving the infrared beam around outside the cell. Also the atmospheric water vapor absorption creates a pathological baseline that causes noise and distortion near strong lines.

The wavenumber scale in the spectrum is calibrated against the cold water spectrum of Camy-Peyret et al. [1] as mentioned earlier. A comparison of the transition wavenumbers measured here with those also observed in the room temperature spectrum of ref. [1] is given in figure 4. Here we find 949 coincident unblended lines, not saturated in the present data nor hand-measured or calculated in the previous, for which the average deviation is  $-0.5 \times 10^{-4}$  cm<sup>-1</sup> and the rms deviation is  $8.3 \times 10^{-4}$  cm<sup>-1</sup>. The rms deviation, of course, reflects the random errors in both sets of data. Since a precision of better than  $5 \times 10^{-4}$  cm<sup>-1</sup> is claimed for the cold water spectrum [1] itself, the present high-temperature spectrum appears to have a slightly lower precision in accordance with the instrumental difficulties discussed in the preceding paragraph.

#### 4. Analysis and Discussion

To assign the very rich spectrum of hot water vapor recorded with the tunable laser difference-frequency spectrometer, we have combined the experimental results obtained at room temperature [1] and at flame temperatures [2] together with the recent compilation of ref. [7] and new calculations performed by extrapolating the available energy levels and transition moments for the high-temperature conditions of our experiment. These new line positions and intensities were computed using the methods extensively described in ref. [7]. Almost all the observed lines were assigned and a summary of the different bands involved together with the number of lines belonging to each band is given in table 1. A total number of 15 cold and hot bands of H<sub>2</sub><sup>16</sup>O have been observed and also a few lines of H<sub>2</sub><sup>18</sup>O and H<sub>2</sub><sup>17</sup>O. The highest lower state energy level is as high as 7533.7 cm<sup>-1</sup> and lines with  $J$  up to 27 or  $K_a$  up to 14 have been assigned.

A complete listing of the experimental transition wavenumbers and intensities along with the rotational and vibrational assignments and the calculated wavenumbers and intensities for significant lines at  $T=1200$  K is presented in table 2. There are a number of lines that appear in the spectral recording that are not listed because the peak finding algorithm rejects lines that are too weak, too strong, or too broad. The weak lines are eliminated in order to discriminate against noise; the strongest lines are completely saturated and the broad lines are usually blends or shoulders whose frequencies would not be determined accurately by the program. In these cases, calculated line positions, assignments, and intensities are given in order to provide the most complete compilation.

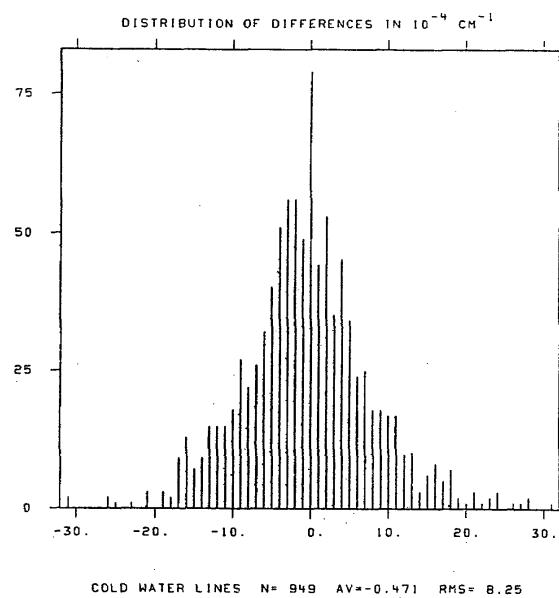


FIGURE 4. Comparison of transition wavenumber differences (in  $10^{-4}$  cm<sup>-1</sup>) for cold water. Present data minus ref. [1].

TABLE 1. Hot water vapor spectrum between 2965 and 4005  $\text{cm}^{-1}$ 

|                            |      |
|----------------------------|------|
| Number of observed lines   | 2279 |
| Number of calculated lines | 2735 |
| Number of unassigned lines | 74   |

| Summary of the bands observed |                  |               |     |                                 |   |   |   |
|-------------------------------|------------------|---------------|-----|---------------------------------|---|---|---|
| ISO                           | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | N   | $\nu_0$<br>( $\text{cm}^{-1}$ ) | $\sigma_{\min}$<br>( $\text{cm}^{-1}$ ) | $\sigma_{\max}$<br>( $\text{cm}^{-1}$ ) | $\Sigma k_{\sigma}^N(1000 \text{ K})$<br>( $\text{cm}^{-1}/\text{molecule cm}^{-2}$ ) |
| 161                           | 0 0 1            | 0 0 0         | 970 | 3755.930                        | 2973.723                                | 4004.705                                | 0.61 $\times 10^{-17}$  |
| 161                           | 1 0 0            | 0 0 0         | 605 | 3657.053                        | 2967.443                                | 4001.282                                | 0.58 $\times 10^{-18}$  |
| 161                           | -0 1 -1          | -0 1 0        | 147 | 3736.522                        | 3176.742                                | 4002.841                                | 0.57 $\times 10^{-18}$  |
| 161                           | 0 2 0            | 0 0 0         | 283 | 3151.630                        | 2966.007                                | 3990.216                                | 0.57 $\times 10^{-19}$  |
| 161                           | 0 2 1            | 0 2 0         | 106 | 3719.891                        | 3283.753                                | 3963.066                                | 0.32 $\times 10^{-19}$  |
| 161                           | 1 1 0            | 0 1 0         | 86  | 3640.228                        | 3082.251                                | 3961.121                                | 0.18 $\times 10^{-19}$  |
| 161                           | 0 0 2            | 0 0 1         | 74  | 3689.117                        | 3317.280                                | 3863.725                                | 0.20 $\times 10^{-19}$  |
| 161                           | 1 0 1            | 1 0 0         | 52  | 3592.769                        | 3189.137                                | 3837.458                                | 0.73 $\times 10^{-20}$  |
| 181                           | 0 0 1            | 0 0 0         | 49  | 3741.567                        | 3446.944                                | 3889.645                                | 0.38 $\times 10^{-20}$  |
| 161                           | 0 3 0            | 0 1 0         | 34  | 3072.046                        | 2966.735                                | 3424.031                                | 0.25 $\times 10^{-20}$  |
| 161                           | 0 3 1            | 0 3 0         | 8   | 3707.055                        | 3457.382                                | 3892.009                                | 0.30 $\times 10^{-21}$  |
| 161                           | 0 1 2            | 0 1 1         | 6   | 3668.871                        | 3442.173                                | 3786.688                                | 0.20 $\times 10^{-21}$  |
| 161                           | 2 0 0            | 1 0 0         | 4   | 3544.488                        | 3378.911                                | 3753.655                                | 0.19 $\times 10^{-21}$  |
| 171                           | 0 0 1            | 0 0 0         | 4   | 3748.318                        | 3648.879                                | 3896.484                                | 0.74 $\times 10^{-22}$  |
| 161                           | 1 2 0            | 0 2 0         | 3   | 3623.464                        | 3284.131                                | 3588.704                                | 0.88 $\times 10^{-22}$  |
| 161                           | 1 1 1            | 1 1 0         | 3   | 3572.026                        | 3467.501                                | 3706.852                                | 0.70 $\times 10^{-22}$  |
| 161                           | 1 0 1            | 0 0 1         | 1   | 3493.892                        | 3263.265                                | 3263.265                                | 0.16 $\times 10^{-22}$  |

ISO: isotopic species, 161, 171, and 181 stand, respectively, for  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$

$v'_1 v'_2 v'_3$ ,  $v_1 v_2 v_3$ : vibrational quantum numbers of the upper and lower levels of the band

N: number of transitions for each band

$\nu_0$ : band center in  $\text{cm}^{-1}$

$\sigma_{\min}$ : lower wavenumber for each band in  $\text{cm}^{-1}$

$\sigma_{\max}$ : higher wavenumber for each band in  $\text{cm}^{-1}$

$\Sigma k_{\sigma}^N(1000 \text{ K})$ : sum of all the calculated intensities at 1000 K for the lines belonging to a given band. Because this sum is performed over a finite spectral interval ( $2965$ – $4005 \text{ cm}^{-1}$ ) and because of an intensity cut-off in the experiment this sum is not to be taken as the total band intensity but is quoted here to give an idea of the relative importance in the interval of the different bands observed. It is not a very significant quantity for the weakest bands.

In table 2 the DIFF column is the wavenumber difference in  $10^{-4} \text{ cm}^{-1}$  for the present data minus prior literature values. The prior references are coded in the column labelled C. C stands for the cold water data of Camy-Peyret, Flaud, Guelachvili, and Amiot [1]; A and B are their theoretical and hand-measured values, respectively. S represents the very strong cold water lines (peak intensity  $>2(\text{Torr m})^{-1}$ ) which were somewhat saturated in the present transmission spectra, so their wavenumbers and intensities are not given reliably. H designates the high-temperature flame-spectra water emission lines observed by Flaud, Camy-Peyret, and Maillard [2]. D represents calculated asymmetry  $K$ -doublets or other blends not experimentally resolvable at the Doppler limit.

The distribution of differences between the present and the flame data (labelled H) is shown in figure 5 where the average deviation for the 533 lines compared is  $-5.2 \times 10^{-4} \text{ cm}^{-1}$  and the rms deviation is  $36.9 \times 10^{-4} \text{ cm}^{-1}$ . Assuming that the calibration precision is consistent for the high and the low  $J$  and  $K_a$  lines in the

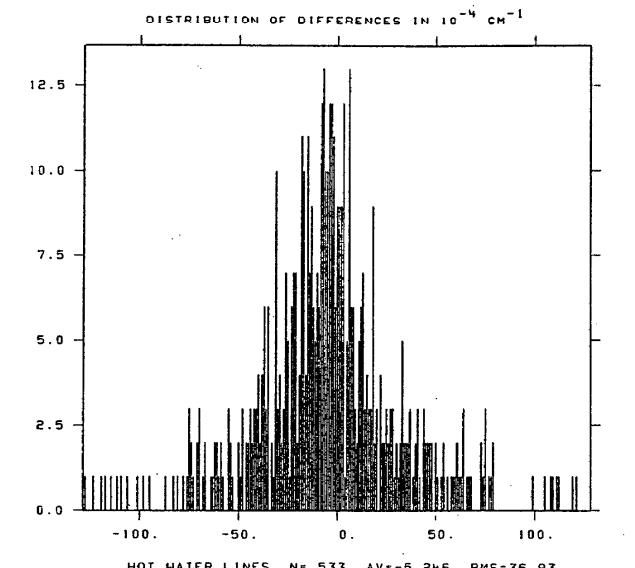


FIGURE 5. Comparison of transition wavenumber differences (in  $10^{-4} \text{ cm}^{-1}$ ) for hot water. Present data minus ref. [2].

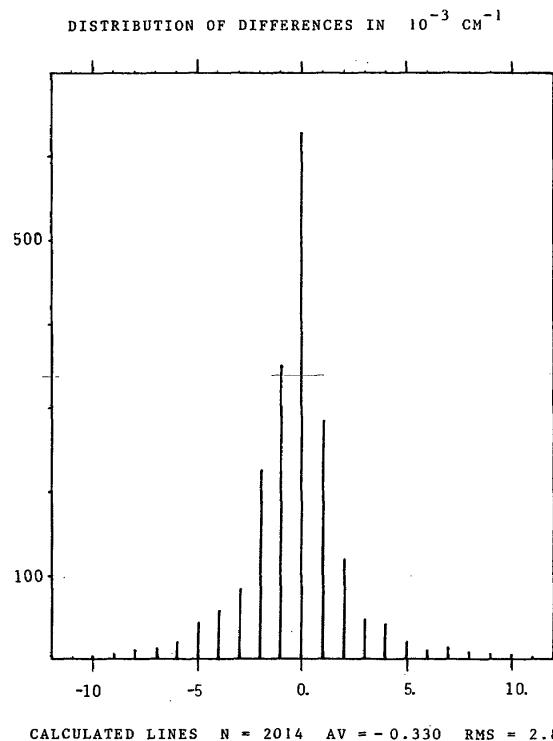


FIGURE 6. Comparison of observed minus calculated transition wavenumbers (in  $10^{-3} \text{ cm}^{-1}$ ) for present  $\text{H}_2\text{O}$  data and model.

present study, it appears that the flame spectra precision suffered from even larger linewidths and possible pressure shifts due to operation under atmospheric conditions. Thus the present high-temperature absorption data should provide more reliable ( $<1 \times 10^{-3} \text{ cm}^{-1}$ ) calibration references for hot  $\text{H}_2\text{O}$  sources and model calculations.

The agreement between the line positions observed in this work and the predicted ones is shown in figure 6. The predicted line positions are based both on the energy levels of ref. [2] and on calculated ones. Here 2014 unblended hot and cold lines are included yielding average and rms deviations of  $-3.3 \times 10^{-4}$  and  $28.0 \times 10^{-4} \text{ cm}^{-1}$ , respectively, with the high  $J$ ,  $K_a$  lines dominating the discrepancies. This agreement is very satisfactory, considering the convergence difficulties at high  $J$  and  $K_a$  usually encountered with  $\text{H}_2\text{O}$  theories.

The eigenvectors from the same model Hamiltonian used for the energy level and transition wavenumber calculation are used to compute the transition intensities for comparison with experiment. The peak intensity (in  $(\text{Torr m})^{-1} = (7.6 \text{ atm cm})^{-1}$ ) for an unblended line in the Doppler regime is calculated as a composite over the temperature distribution,

$$I_{\text{calc}}(\sigma_0) = (7.6L)^{-1} \int_0^L dx (\ln 2/\pi)^{1/2} N_0 k_\sigma^N(T) T_o / (T \gamma_D(T)).$$

Here  $\sigma_0$  is the peak wavenumber,  $N_0 = 2.686754 \times 10^{19}$  molecules/ $\text{cm}^3 \cdot \text{atm}$  is Loschmidt's number,  $T_o = 273.15 \text{ K}$

and  $k_\sigma^N(T)$  is the calculated line intensity (in  $\text{cm}^{-1}/\text{molecule cm}^{-2}$ ) at the local temperature  $T$ .  $\gamma_D(T)$  (in  $\text{cm}^{-1}$ ) is the Doppler half width,

$$\gamma_D(T) = 3.58 \times 10^{-7} \sigma_0 (T/M)^{1/2},$$

where  $M$  is the molecular weight (in amu). The calculated line intensities are listed in table 2 as  $S_{\text{calc}}$  for a reference temperature of  $T_{\text{ref}} = 1000 \text{ K}$ . They scale with temperature according to

$$k_\sigma^N(T) = k_\sigma^N(T_{\text{ref}}) \exp[-(E''/k_B)(T^{-1} - T_{\text{ref}}^{-1})] [Z(T_{\text{ref}})/Z(T)]$$

where  $E''$  is the lower state energy, also listed in table 2, and  $Z(T)$  is the partition function.

Replacing the integral by a sum over a finite number of layers of thickness  $\Delta x_i$  at different temperature  $T_i$  we have

$$I_{\text{calc}}(\sigma_0) = \sum_i 2\Delta x_i (\ln 2/\pi)^{1/2} N_0 k_\sigma^N(T_i) T_o / (7.6L T_i \gamma_D(T_i)),$$

the factor of 2 arising from double passing the cell. The temperature profile of figure 2 shows the values  $T_i$  as dots at layer intervals of  $\sim 5 \text{ cm}$ .

A statistical analysis of the relative differences  $\delta I/I = |I_{\text{calc}} - I_{\text{obs}}|/I_{\text{obs}}$  between the observed and calculated peak intensities gives for 1728 isolated lines with  $I_{\text{obs}} > 0.007 \text{ (Torr m)}^{-1}$  the following results:

$$\begin{aligned} 0 \% &< \delta I/I &< 8 \% & 39.9 \% \text{ (of the lines)} \\ 8 \% &< \delta I/I &< 15 \% & 26.1 \% \\ 15 \% &< \delta I/I &< 30 \% & 25.2 \% \\ 30 \% &< \delta I/I && 8.8 \% \end{aligned}$$

These results are very satisfactory and show the quality of the model for calculating intensities for temperature up to 1200 K.

## 5. Conclusions

Using a tunable laser difference-frequency spectrometer, the hot water vapor absorption spectrum has been recorded between 2965 and 4005  $\text{cm}^{-1}$  with an instrumental resolution of  $3 \times 10^{-4} \text{ cm}^{-1}$ . The analysis of this very rich spectrum has been performed with the aid of previous experimental results and with a new calculation of water line positions and intensities appropriate to the temperatures ( $< 1200 \text{ K}$ ) of this experiment. Almost all the lines have been assigned and lines with  $J$  as high as 27 or  $K_a$  as high as 14 have been observed. Also, the agreement between the observed and calculated spectra for the line positions as well as for the line intensities shows that the model developed to perform the calculation can be used with good confidence.

## 6. Acknowledgement

The Lincoln Laboratory portion of this work was supported by the Air Force Office of Scientific Research, ESD Contract F19628-80-C-002.

## 7. References

- [1] Camy-Peyret, C., Flaud, J.-M., Guelachvili, G., and Amiot, C., *Mol. Phys.* **26**, 825 (1973).

- [2] Flaud, J.-M., Camy-Peyret, C., and Maillard, J. P., *Mol. Phys.* **32**, 499 (1976).
- [3] Pine, A. S., *J. Opt. Soc. Amer.* **64**, 1683 (1974).
- [4] Pine, A. S., *J. Opt. Soc. Amer.* **66**, 97 (1976).
- [5] Pine, A. S., in "Laser Spectroscopy III" (J. L. Hall and J. L. Carlsten, Eds.), pp. 376 (Springer-Verlag, New York, 1977).
- [6] Coulombe, M. J., and Pine, A. S., *Appl. Opt.* **18**, 1505 (1979).
- [7] Flaud, J.-M., Camy-Peyret, C., and Toth, R. A., *Water vapour line parameters from microwave to medium infrared*, Pergamon Press (1981).

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 2966.007               | 2966.0064             | -6     | C 0.287D-21       | 756.725  | 5    | 3      | 2      | 6   | 4     | 3     | 0 2 0            | 0 0 0         | 161 | 0.023            | 0.023             |
| 2966.735               | 2966.7337             |        | 0.762D-22         | 2309.731 | 6    | 2      | 5      | 7   | 1     | 6     | 0 3 0            | 0 1 0         | 161 | 0.003            | 0.003             |
| 2966.833               | 2966.8341             |        | 0.676D-22         | 1293.634 | 10   | 1      | 10     | 10  | 2     | 9     | 0 2 0            | 0 0 0         | 161 | 0.004            | 0.003             |
| 2967.443               | 2967.4400             | -8     | H 0.171D-21       | 4172.148 | 13   | 10     | 3      | 14  | 11    | 4     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.010             |
| 2967.443               |                       |        | D 0.569D-22       | 4172.148 | 13   | 10     | 4      | 14  | 11    | 3     | 1 0 0            | 0 0 0         | 161 |                  | 0.003             |
| 2967.984               | 2967.9841             |        | 0.695D-22         | 816.694  | 6    | 2      | 4      | 7   | 3     | 5     | 0 2 0            | 0 0 0         | 161 | 0.005            | 0.005             |
| 2969.516               | 2969.5158             |        | 0.289D-21         | 1293.634 | 9    | 1      | 8      | 10  | 2     | 9     | 0 2 0            | 0 0 0         | 161 | 0.014            | 0.013             |
| 2970.533               | 2970.5320             | -16    | H 0.630D-22       | 4665.969 | 15   | 9      | 6      | 16  | 10    | 7     | 1 0 0            | 0 0 0         | 161 | 0.003            | 0.004             |
| 2971.714               | 2971.7158             |        | 0.386D-22         | 2818.398 | 8    | 3      | 6      | 9   | 2     | 7     | 0 3 0            | 0 1 0         | 161 | 0.003            | 0.002             |
| 2972.053               | 2972.0533             |        | 0.279D-22         | 2426.195 | 12   | 1      | 11     | 13  | 4     | 10    | 1 0 0            | 0 0 0         | 161 | 0.004            | 0.001             |
| 2973.252               | 2973.2534             | 11     | C 0.209D-21       | 508.812  | 4    | 2      | 3      | 5   | 3     | 2     | 0 2 0            | 0 0 0         | 161 | 0.024            | 0.026             |
| 2973.723               | 2973.7212             |        | 0.140D-21         | 3824.994 | 14   | 6      | 8      | 15  | 8     | 7     | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.007             |
| 2974.589               | 2974.5886             | -14    | C 0.172D-21       | 920.211  | 8    | 0      | 8      | 9   | 1     | 9     | 0 2 0            | 0 0 0         | 161 | 0.013            | 0.011             |
| 2974.829               | 2974.8305             |        | 0.115D-21         | 2414.725 | 12   | 4      | 9      | 13  | 3     | 10    | 0 2 0            | 0 0 0         | 161 | 0.005            | 0.005             |
| 2975.083               | 2975.0837             | -2     | C 0.518D-21       | 920.169  | 8    | 1      | 8      | 9   | 0     | 9     | 0 2 0            | 0 0 0         | 161 | 0.034            | 0.032             |
| 2975.224               | 2975.2225             |        | 0.987D-22         | 1293.019 | 9    | 2      | 8      | 10  | 1     | 9     | 0 2 0            | 0 0 0         | 161 | 0.005            | 0.005             |
| 2975.300               |                       |        | D 0.614D-22       | 2254.284 | 9    | 7      | 3      | 10  | 8     | 2     | 0 2 0            | 0 0 0         | 161 |                  | 0.003             |
| 2975.301               | 2975.2938             |        | 0.184D-21         | 2254.283 | 9    | 7      | 2      | 10  | 8     | 3     | 0 2 0            | 0 0 0         | 161 | 0.009            | 0.008             |
|                        | 2975.3795             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.007             |
| 2977.479               |                       |        | D 0.721D-22       | 4350.602 | 12   | 12     | 0      | 13  | 13    | 1     | 1 0 0            | 0 0 0         | 161 |                  | 0.004             |
| 2977.479               | 2977.4768             | -18    | H 0.216D-21       | 4350.602 | 12   | 12     | 1      | 13  | 13    | 0     | 1 0 0            | 0 0 0         | 161 | 0.013            | 0.013             |
| 2977.943               | 2977.9426             | -9     | C 0.234D-21       | 648.979  | 5    | 2      | 3      | 6   | 3     | 4     | 0 2 0            | 0 0 0         | 161 | 0.021            | 0.022             |
| 2979.072               | 2979.0701             |        | 0.161D-21         | 1690.665 | 10   | 3      | 8      | 11  | 2     | 9     | 0 2 0            | 0 0 0         | 161 | 0.007            | 0.007             |
| 2979.750               | 2979.7481             |        | 0.176D-21         | 3464.885 | 13   | 6      | 8      | 14  | 8     | 7     | 0 0 1            | 0 0 0         | 161 | 0.008            | 0.009             |
| 2980.241               | 2980.2403             |        | 0.118D-21         | 888.632  | 5    | 4      | 2      | 6   | 5     | 1     | 0 2 0            | 0 0 0         | 161 | 0.008            | 0.008             |
| 2980.388               | 2980.3879             | 7      | C 0.355D-21       | 888.599  | 5    | 4      | 1      | 6   | 5     | 2     | 0 2 0            | 0 0 0         | 161 | 0.022            | 0.023             |
| 2980.677               | 2980.6755             |        | 0.160D-21         | 3032.690 | 11   | 7      | 5      | 12  | 9     | 4     | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.007             |
| 2981.145               | 2981.1437             | -1     | C 0.329D-21       | 1216.194 | 6    | 5      | 2      | 7   | 6     | 1     | 0 2 0            | 0 0 0         | 161 | 0.017            | 0.016             |
| 2981.174               | 2981.1706             |        | 0.109D-21         | 1216.189 | 6    | 5      | 1      | 7   | 6     | 2     | 0 2 0            | 0 0 0         | 161 | 0.004            | 0.005             |
| 2981.238               | 2981.2394             |        | 0.612D-22         | 1742.307 | 1    | 1      | 0      | 2   | 2     | 1     | 0 3 0            | 0 1 0         | 161 | 0.003            | 0.003             |
| 2981.360               | 2981.3631             |        | 0.127D-21         | 1920.769 | 4    | 1      | 4      | 5   | 0     | 5     | 0 3 0            | 0 1 0         | 161 | 0.007            | 0.005             |
| 2982.451               | 2982.4526             |        | 0.105D-21         | 1080.386 | 8    | 1      | 7      | 9   | 2     | 8     | 0 2 0            | 0 0 0         | 161 | 0.005            | 0.006             |
| 2983.314               | 2983.3149             |        | 0.106D-21         | 1821.599 | 3    | 0      | 3      | 4   | 1     | 4     | 0 3 0            | 0 1 0         | 161 | 0.006            | 0.004             |
| 2984.212               | 2984.2115             | -2     | C 0.277D-22       | 315.779  | 3    | 1      | 3      | 4   | 2     | 2     | 0 2 0            | 0 0 0         | 161 | 0.004            | 0.005             |
|                        | 2987.0117             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.004             |
| 2987.526               | 2987.5245             | 0      | C 0.346D-21       | 610.341  | 4    | 3      | 2      | 5   | 4     | 1     | 0 2 0            | 0 0 0         | 161 | 0.033            | 0.035             |
| 2987.739               | 2987.7384             | -11    | H 0.977D-22       | 4427.117 | 15   | 8      | 7      | 16  | 9     | 8     | 1 0 0            | 0 0 0         | 161 | 0.005            | 0.006             |
| 2988.197               | 2988.1905             |        | 0.940D-22         | 1590.691 | 7    | 6      | 2      | 8   | 7     | 1     | 0 2 0            | 0 0 0         | 161 | 0.004            | 0.004             |
|                        | 2988.2393             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.010             |
| 2988.287               | 2988.2875             |        | 0.278D-21         | 1590.690 | 7    | 6      | 1      | 8   | 7     | 2     | 0 2 0            | 0 0 0         | 161 | 0.011            | 0.012             |
| 2988.613               | 2988.6114             | -16    | C 0.116D-21       | 610.114  | 4    | 3      | 1      | 5   | 4     | 2     | 0 2 0            | 0 0 0         | 161 | 0.011            | 0.012             |
| 2989.596               |                       |        | D 0.893D-22       | 4087.981 | 12   | 11     | 1      | 13  | 12    | 2     | 1 0 0            | 0 0 0         | 161 |                  | 0.005             |
| 2989.596               | 2989.5969             | -23    | H 0.268D-21       | 4087.981 | 12   | 11     | 2      | 13  | 12    | 1     | 1 0 0            | 0 0 0         | 161 | 0.017            | 0.015             |
| 2989.624               | 2989.6238             |        | 0.908D-22         | 1079.080 | 9    | 0      | 9      | 9   | 1     | 8     | 0 2 0            | 0 0 0         | 161 | 0.006            | 0.005             |
|                        | 2989.7151             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.005             |
| 2990.676               | 2990.6724             |        | 0.615D-22         | 3465.060 | 13   | 6      | 7      | 14  | 8     | 6     | 0 0 1            | 0 0 0         | 161 | 0.003            | 0.003             |
| 2991.255               | 2991.2553             | 25     | H 0.113D-21       | 3360.598 | 14   | 4      | 11     | 15  | 5     | 10    | 1 0 0            | 0 0 0         | 161 | 0.005            | 0.006             |
| 2991.971               | 2991.9707             | 5      | C 0.889D-22       | 503.968  | 4    | 2      | 2      | 5   | 3     | 3     | 0 2 0            | 0 0 0         | 161 | 0.011            | 0.011             |
| 2992.653               | 2992.6542             | 10     | C 0.326D-21       | 1079.080 | 8    | 2      | 7      | 9   | 1     | 8     | 0 2 0            | 0 0 0         | 161 | 0.018            | 0.017             |
| 2993.736               | 2993.7352             | -17    | C 0.323D-21       | 885.600  | 7    | 1      | 6      | 8   | 2     | 7     | 0 2 0            | 0 0 0         | 161 | 0.021            | 0.021             |
| 2994.446               | 2994.4469             | 2      | C 0.555D-21       | 744.163  | 7    | 0      | 7      | 8   | 1     | 8     | 0 2 0            | 0 0 0         | 161 | 0.045            | 0.044             |
| 2994.715               | 2994.7208             | -1     | H 0.248D-21       | 3831.174 | 12   | 10     | 3      | 13  | 11    | 2     | 1 0 0            | 0 0 0         | 161 | 0.015            | 0.013             |
| 2994.715               |                       |        | D 0.826D-22       | 3831.173 | 12   | 10     | 2      | 13  | 11    | 3     | 1 0 0            | 0 0 0         | 161 |                  | 0.004             |
| 2995.455               | 2995.4556             | 7      | C 0.186D-21       | 744.064  | 7    | 1      | 7      | 8   | 0     | 8     | 0 2 0            | 0 0 0         | 161 | 0.016            | 0.015             |
| 2996.396               | 2996.3926             |        | 0.517D-22         | 1962.508 | 11   | 0      | 11     | 12  | 3     | 10    | 1 0 0            | 0 0 0         | 161 | 0.003            | 0.002             |
| 2997.292               | 2997.2872             | -42    | H 0.109D-21       | 4283.305 | 14   | 9      | 6      | 15  | 10    | 5     | 1 0 0            | 0 0 0         | 161 | 0.007            | 0.006             |
| 2997.301               |                       |        | D 0.362D-22       | 4283.301 | 14   | 9      | 5      | 15  | 10    | 6     | 1 0 0            | 0 0 0         | 161 |                  | 0.002             |
| 2998.972               | 2998.9717             |        | 0.582D-22         | 1437.969 | 9    | 3      | 7      | 10  | 2     | 8     | 0 2 0            | 0 0 0         | 161 | 0.003            | 0.003             |
| 2999.151               | 2999.1578             |        | 0.250D-21         | 2009.805 | 8    | 7      | 2      | 9   | 8     | 1     | 0 2 0            | 0 0 0         | 161 | 0.012            | 0.010             |
| 2999.151               |                       |        | D 0.834D-22       | 2009.805 | 8    | 7      | 1      | 9   | 8     | 2     | 0 2 0            | 0 0 0         | 161 |                  | 0.003             |
| 2999.6080              |                       |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.009             |
| 3001.1913              |                       |        |                   |          |      |        |        |     |       |       |                  |               |     |                  | 0.004             |
| 3003.474               | 3003.4748             | 3      | C 0.105D-21       | 709.609  | 6    | 1      | 5      | 7   | 2     | 6     | 0 2 0            | 0 0 0         | 161 | 0.009            | 0.009             |
| 3003.838               | 3003.8375             | -4     | C 0.937D-22       | 383.842  | 3    | 2      | 2      | 4   | 3     | 1     | 0 2 0            | 0 0 0         | 161 | 0.014            | 0.016             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3004.687               | 3004.6868             | 7 C    | 0.431D-21         | 742.076  | 4    | 4      | 1      | 5   | 5     | 0     | 0 2 0          | 0 0 0       | 161 | 0.034            | 0.034             |
| 3004.754               | 3004.7527             |        | 0.631D-22         | 2271.712 | 6    | 2      | 5      | 6   | 3     | 4     | 0 3 0          | 0 1 0       | 161 | 0.003            | 0.003             |
| 3004.987               | 3004.9836             |        | 0.577D-22         | 1962.508 | 12   | 2      | 11     | 12  | 3     | 10    | 0 2 0          | 0 0 0       | 161 | 0.002            | 0.002             |
| 3005.445               |                       | D      | 0.137D-21         | 1045.059 | 5    | 5      | 1      | 6   | 6     | 0     | 0 2 0          | 0 0 0       | 161 |                  | 0.007             |
| 3005.455               | 3005.4548             | 9 C    | 0.408D-21         | 1045.058 | 5    | 5      | 0      | 6   | 6     | 1     | 0 2 0          | 0 0 0       | 161 | 0.025            | 0.022             |
|                        | 3007.6932             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.003            |                   |
| 3008.278               | 3008.2779             |        | 0.175D-21         | 2740.420 | 10   | 7      | 3      | 11  | 9     | 2     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.008             |
| 3009.652               | 3009.6543             | 24 C   | 0.115D-21         | 885.600  | 8    | 1      | 8      | 8   | 2     | 7     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3010.232               | 3010.2321             | -2 C   | 0.304D-21         | 382.517  | 3    | 2      | 1      | 4   | 3     | 2     | 0 2 0          | 0 0 0       | 161 | 0.044            | 0.050             |
| 3011.030               | 3011.0261             |        | 0.235D-21         | 3127.862 | 12   | 6      | 6      | 13  | 8     | 5     | 0 0 1          | 0 0 0       | 161 | 0.009            | 0.011             |
| 3011.277               | 3011.2775             | -2 C   | 0.112D-21         | 882.891  | 7    | 2      | 6      | 8   | 1     | 7     | 0 2 0          | 0 0 0       | 161 | 0.008            | 0.007             |
| 3012.076               | 3012.0645             |        | 0.234D-21         | 2471.254 | 9    | 8      | 1      | 10  | 9     | 2     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.010             |
| 3012.076               |                       | D      | 0.781D-22         | 2471.254 | 9    | 8      | 2      | 10  | 9     | 1     | 0 2 0          | 0 0 0       | 161 |                  | 0.003             |
| 3012.233               | 3012.2305             |        | 0.329D-21         | 1394.814 | 6    | 6      | 1      | 7   | 7     | 0     | 0 2 0          | 0 0 0       | 161 | 0.022            | 0.014             |
| 3012.345               | 3012.3431             |        | 0.122D-21         | 1394.814 | 6    | 6      | 0      | 7   | 7     | 1     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.005             |
| 3012.377               | 3012.3762             | -4 C   | 0.137D-21         | 488.134  | 3    | 3      | 1      | 4   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.018             |
| 3012.531               | 3012.5308             | -4 C   | 0.412D-21         | 488.108  | 3    | 3      | 0      | 4   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.054            | 0.054             |
| 3012.543               |                       |        | 0.299D-21         | 552.912  | 5    | 1      | 4      | 6   | 2     | 5     | 0 2 0          | 0 0 0       | 161 |                  | 0.034             |
| 3013.573               | 3013.5716             | -17 C  | 0.189D-21         | 586.479  | 6    | 0      | 6      | 7   | 1     | 7     | 0 2 0          | 0 0 0       | 161 | 0.019            | 0.020             |
| 3014.488               | 3014.4886             | 16 H   | 0.161D-21         | 4045.316 | 14   | 8      | 7      | 15  | 9     | 6     | 1 0 0          | 0 0 0       | 161 | 0.007            | 0.009             |
| 3015.616               | 3015.6155             | 1 C    | 0.572D-21         | 586.243  | 6    | 1      | 6      | 7   | 0     | 7     | 0 2 0          | 0 0 0       | 161 | 0.059            | 0.060             |
| 3017.100               | 3017.1036             |        | 0.900D-22         | 2392.594 | 7    | 1      | 6      | 7   | 2     | 5     | 0 3 0          | 0 1 0       | 161 | 0.004            | 0.004             |
|                        | 3018.8241             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.015            |                   |
| 3019.099               | 3019.0961             |        | 0.822D-22         | 3244.601 | 14   | 2      | 12     | 15  | 4     | 11    | 0 0 1          | 0 0 0       | 161 | 0.003            | 0.004             |
| 3019.213               |                       | D      | 0.134D-21         | 3766.388 | 11   | 11     | 1      | 12  | 12    | 0     | 1 0 0          | 0 0 0       | 161 |                  | 0.007             |
| 3019.213               | 3019.2121             | 6 H    | 0.402D-21         | 3766.388 | 11   | 11     | 0      | 12  | 12    | 1     | 1 0 0          | 0 0 0       | 161 | 0.023            | 0.021             |
| 3021.771               |                       | D      | 0.117D-21         | 3512.401 | 11   | 10     | 2      | 12  | 11    | 1     | 1 0 0          | 0 0 0       | 161 |                  | 0.006             |
| 3021.771               | 3021.7693             | -15 H  | 0.351D-21         | 3512.401 | 11   | 10     | 1      | 12  | 11    | 2     | 1 0 0          | 0 0 0       | 161 | 0.020            | 0.017             |
| 3022.366               | 3022.3646             | -17 C  | 0.933D-22         | 416.209  | 4    | 1      | 3      | 5   | 2     | 4     | 0 2 0          | 0 0 0       | 161 | 0.012            | 0.014             |
| 3022.665               | 3022.6651             |        | 0.174D-21         | 1201.922 | 8    | 3      | 6      | 9   | 2     | 7     | 0 2 0          | 0 0 0       | 161 | 0.008            | 0.008             |
| 3023.151               | 3023.1494             |        | 0.330D-21         | 1789.041 | 7    | 7      | 0      | 8   | 8     | 1     | 0 2 0          | 0 0 0       | 161 | 0.016            | 0.013             |
| 3023.152               |                       | D      | 0.110D-21         | 1789.041 | 7    | 7      | 1      | 8   | 8     | 0     | 0 2 0          | 0 0 0       | 161 |                  | 0.004             |
|                        | 3023.8101             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.012            |                   |
| 3024.162               | 3024.1526             |        | 0.853D-22         | 1690.665 | 11   | 1      | 10     | 11  | 2     | 9     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3024.368               |                       | D      | 0.597D-22         | 3922.325 | 13   | 9      | 5      | 14  | 10    | 4     | 1 0 0          | 0 0 0       | 161 |                  | 0.003             |
| 3024.370               | 3024.3695             | -3 H   | 0.179D-21         | 3922.324 | 13   | 9      | 4      | 14  | 10    | 5     | 1 0 0          | 0 0 0       | 161 | 0.011            | 0.010             |
| 3025.414               | 3025.4189             |        | 0.485D-22         | 2764.699 | 8    | 3      | 6      | 8   | 4     | 5     | 0 3 0          | 0 1 0       | 161 | 0.003            | 0.002             |
| 3025.761               | 3025.7603             | -8 C   | 0.139D-21         | 212.156  | 2    | 1      | 2      | 3   | 2     | 1     | 0 2 0          | 0 0 0       | 161 | 0.029            | 0.035             |
|                        | 3026.9610             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.003            |                   |
| 3027.013               | 3027.0146             | -36 H  | 0.498D-22         | 2144.047 | 10   | 2      | 8      | 11  | 6     | 5     | 0 0 1          | 0 0 0       | 161 | 0.002            | 0.002             |
| 3027.125               | 3027.1271             |        | 0.677D-22         | 1731.898 | 2    | 1      | 2      | 3   | 0     | 3     | 0 3 0          | 0 1 0       | 161 | 0.003            | 0.003             |
|                        | 3027.3157             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.002            |                   |
| 3027.782               | 3027.7825             |        | 0.228D-21         | 3264.338 | 13   | 5      | 9      | 14  | 7     | 8     | 0 0 1          | 0 0 0       | 161 | 0.010            | 0.011             |
| 3028.238               | 3028.2365             |        | 0.126D-21         | 2124.953 | 11   | 1      | 10     | 12  | 4     | 9     | 1 0 0          | 0 0 0       | 161 | 0.005            | 0.005             |
| 3028.913               | 3028.9050             |        | 0.852D-22         | 1813.224 | 10   | 4      | 7      | 11  | 3     | 8     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3029.910               | 3029.9098             |        | 0.475D-22         | 709.609  | 7    | 1      | 7      | 7   | 2     | 6     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.004             |
| 3030.726               | 3030.7268             | 3 C    | 0.339D-21         | 285.419  | 2    | 2      | 1      | 3   | 3     | 0     | 0 2 0          | 0 0 0       | 161 | 0.060            | 0.071             |
| 3031.734               | 3031.7342             | -2 C   | 0.548D-21         | 447.252  | 5    | 0      | 5      | 6   | 1     | 6     | 0 2 0          | 0 0 0       | 161 | 0.072            | 0.078             |
| 3031.957               | 3031.9563             | 0 C    | 0.321D-21         | 704.214  | 6    | 2      | 5      | 7   | 1     | 6     | 0 2 0          | 0 0 0       | 161 | 0.028            | 0.027             |
| 3031.991               | 3031.9903             | -12 C  | 0.115D-21         | 285.219  | 2    | 2      | 0      | 3   | 3     | 1     | 0 2 0          | 0 0 0       | 161 | 0.021            | 0.024             |
| 3032.140               | 3032.1409             |        | 0.282D-21         | 2813.515 | 11   | 6      | 6      | 12  | 8     | 5     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.012             |
| 3032.500               | 3032.4986             |        | 0.935D-22         | 1772.413 | 3    | 0      | 3      | 3   | 1     | 2     | 0 3 0          | 0 1 0       | 161 | 0.004            | 0.004             |
| 3033.535               | 3033.5386             |        | 0.801D-22         | 2130.495 | 5    | 2      | 3      | 5   | 3     | 2     | 0 3 0          | 0 1 0       | 161 | 0.003            | 0.003             |
| 3034.177               | 3034.1764             |        | 0.946D-22         | 2813.533 | 11   | 6      | 5      | 12  | 8     | 4     | 0 0 1          | 0 0 0       | 161 | 0.003            | 0.004             |
| 3034.264               | 3034.2650             | 7 C    | 0.263D-21         | 300.362  | 3    | 1      | 2      | 4   | 2     | 3     | 0 2 0          | 0 0 0       | 161 | 0.044            | 0.053             |
| 3034.395               | 3034.3953             | 6 C    | 0.151D-21         | 704.214  | 7    | 0      | 7      | 7   | 1     | 6     | 0 2 0          | 0 0 0       | 161 | 0.012            | 0.013             |
| 3035.783               | 3035.7822             | -12 C  | 0.185D-21         | 446.697  | 5    | 1      | 5      | 6   | 0     | 6     | 0 2 0          | 0 0 0       | 161 | 0.023            | 0.026             |
| 3035.972               | 3036.0024             |        | 0.309D-21         | 2225.468 | 8    | 8      | 1      | 9   | 8     | 2     | 0 2 0          | 0 0 0       | 161 | 0.014            | 0.013             |
| 3035.972               |                       | D      | 0.103D-21         | 2225.468 | 8    | 8      | 0      | 9   | 8     | 1     | 0 2 0          | 0 0 0       | 161 |                  | 0.004             |
| 3036.070               | 3036.0693             |        | 0.122D-21         | 2053.969 | 5    | 1      | 4      | 5   | 2     | 3     | 0 3 0          | 0 1 0       | 161 | 0.005            | 0.005             |
| 3036.222               | 3036.2225             |        | 0.163D-21         | 2471.254 | 9    | 7      | 3      | 10  | 9     | 2     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3036.232               |                       | D      | 0.543D-22         | 2471.254 | 9    | 7      | 2      | 10  | 9     | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.002             |
| 3037.097               | 3037.0992             |        | 0.112D-21         | 1446.129 | 10   | 2      | 9      | 10  | 3     | 8     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.005             |
| 3037.099               |                       | D      | 0.283D-22         | 2392.594 | 6    | 3      | 4      | 7   | 2     | 5     | 0 3 0          | 0 1 0       | 161 |                  | 0.001             |

## HIGH-TEMPERATURE WATER VAPOR SPECTRUM

423

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |   |     |       |       |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|---|-----|-------|-------|
| 3037.580               | 3037.5801             |        | 0.859D-22         | 1819.337 | 3    | 1      | 2      | 3   | 2     | 1     | 0                | 3             | 0   | 0                | 1                 | 0 | 161 | 0.004 | 0.003 |
|                        | 3037.9034             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.003 |       |
| 3039.397               | 3039.3961             | 50     | H 0.165D-21       | 3824.994 | 14   | 7      | 8      | 15  | 8     | 7     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.008 | 0.009 |
| 3041.230               | 3041.2282             | -75    | H 0.588D-22       | 2572.140 | 7    | 3      | 4      | 7   | 4     | 3     | 0                | 3             | 0   | 0                | 1                 | 0 | 161 | 0.005 | 0.003 |
| 3041.234               | 3041.2282             | -75    | H 0.616D-22       | 3824.496 | 14   | 7      | 7      | 15  | 8     | 8     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.005 | 0.003 |
| 3041.429               | 3041.4309             |        | 0.155D-21         | 2275.373 | 11   | 2      | 9      | 12  | 5     | 8     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.007 | 0.006 |
| 3041.955               | 3041.9499             | -6     | H 0.260D-21       | 3685.403 | 13   | 8      | 5      | 14  | 9     | 6     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.013 | 0.013 |
| 3042.266               | 3042.2670             |        | 0.635D-22         | 2246.888 | 12   | 0      | 12     | 13  | 2     | 11    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.003 | 0.003 |
| 3042.328               | 3042.3358             |        | 0.954D-22         | 2462.876 | 7    | 2      | 5      | 7   | 3     | 4     | 0                | 3             | 0   | 0                | 1                 | 0 | 161 | 0.003 | 0.004 |
|                        | 3043.2250             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.003 |       |
| 3045.699               | 3045.6957             |        | 0.183D-21         | 2533.793 | 12   | 3      | 10     | 13  | 4     | 9     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.008 | 0.008 |
| 3047.236               | 3047.2313             |        | 0.135D-21         | 2918.244 | 13   | 3      | 11     | 14  | 5     | 10    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.005 | 0.006 |
| 3047.375               | 3047.3721             | -31    | H 0.345D-21       | 3629.095 | 14   | 6      | 9      | 15  | 7     | 8     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.017 | 0.017 |
| 3047.737               | 3047.7248             | -117   | H 0.228D-21       | 3472.880 | 14   | 5      | 10     | 15  | 6     | 9     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.011 | 0.011 |
|                        | 3048.0299             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.017 |       |
| 3048.549               |                       | D      | 0.163D-21         | 3216.185 | 10   | 10     | 0      | 11  | 11    | 1     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.008 |       |
| 3048.550               | 3048.5515             | 19     | H 0.488D-21       | 3216.185 | 10   | 10     | 1      | 11  | 11    | 0     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.027 | 0.023 |
| 3048.673               | 3048.6728             | 0      | C 0.165D-21       | 326.625  | 4    | 0      | 4      | 5   | 1     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.028 | 0.031 |
| 3048.947               | 3048.9468             | -6     | C 0.170D-21       | 552.912  | 6    | 1      | 6      | 6   | 2     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.018 | 0.019 |
| 3049.044               | 3049.0448             | 5      | C 0.827D-22       | 206.301  | 2    | 1      | 1      | 3   | 2     | 2     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.017 | 0.021 |
| 3050.073               | 3050.0734             |        | 0.639D-22         | 1640.508 | 1    | 0      | 1      | 1   | 0     | 0     | 0                | 3             | 0   | 0                | 1                 | 0 | 161 | 0.003 | 0.003 |
| 3050.703               | 3050.7032             |        | 0.519D-22         | 982.912  | 7    | 3      | 5      | 8   | 2     | 6     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.003 | 0.003 |
| 3051.740               | 3051.7345             | -55    | H 0.283D-21       | 3583.372 | 12   | 9      | 4      | 13  | 10    | 3     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.016 | 0.014 |
| 3051.740               |                       | D      | 0.944D-22         | 3583.372 | 12   | 9      | 3      | 13  | 10    | 4     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.005 |       |
|                        | 3051.7677             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.004 |       |
| 3054.197               | 3054.1938             |        | 0.187D-21         | 3084.835 | 13   | 4      | 10     | 14  | 6     | 9     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.008 | 0.009 |
| 3054.459               | 3054.4803             |        | 0.714D-22         | 2983.414 | 13   | 4      | 10     | 14  | 5     | 9     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.003 | 0.003 |
| 3055.610               | 3055.6097             | -3     | C 0.904D-22       | -542.906 | -5   | 2      | 4      | 6   | 1     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.009 | 0.010 |
| 3056.356               | 3056.3561             | -8     | C 0.499D-21       | 325.348  | 4    | 1      | 4      | 5   | 0     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.091 | 0.094 |
| 3057.146               | 3057.1466             | 2      | C 0.634D-22       | 542.906  | 6    | 0      | 6      | 6   | 1     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.007 | 0.007 |
| 3057.602               | 3057.5982             |        | 0.110D-21         | 2927.076 | 12   | 5      | 8      | 13  | 7     | 7     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.005 | 0.005 |
| 3057.908               | 3057.9065             |        | 0.322D-22         | 2552.858 | 6    | 4      | 3      | 6   | 5     | 2     | 0                | 3             | 0   | 0                | 1                 | 0 | 161 | 0.003 | 0.001 |
| 3058.560               | 3058.5575             |        | 0.106D-21         | 2522.263 | 10   | 6      | 5      | 11  | 8     | 4     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.005 | 0.004 |
| 3059.258               | 3059.2590             |        | 0.318D-21         | 2522.267 | 10   | 6      | 4      | 11  | 8     | 3     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.014 | 0.013 |
| 3059.723               | 3059.7230             |        | 0.760D-22         | 1690.665 | 10   | 1      | 10     | 11  | 2     | 9     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.003 | 0.003 |
| 3059.929               | 3059.9288             | -2     | C 0.664D-22       | 136.164  | 1    | 1      | 1      | 2   | 2     | 0     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.017 | 0.020 |
| 3061.228               | 3061.2292             | -9     | C 0.170D-21       | 1201.922 | 9    | 1      | 8      | 9   | 2     | 7     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.009 | 0.008 |
| 3062.283               | 3062.2828             |        | 0.515D-22         | 2414.725 | 13   | 2      | 11     | 13  | 3     | 10    | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.002 | 0.002 |
| 3064.404               | 3064.4037             | -6     | C 0.416D-21       | 224.838  | 3    | 0      | 3      | 4   | 1     | 4     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.093 | 0.101 |
| 3064.493               |                       | D      | 0.362D-22         | 2225.468 | 8    | 7      | 2      | 9   | 9     | 1     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.001 |       |
| 3064.494               | 3064.4897             |        | 0.109D-21         | 2225.468 | 8    | 7      | 1      | 9   | 9     | 0     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.005 | 0.004 |
| 3064.563               | 3064.5638             | -13    | H 0.128D-21       | 4006.071 | 15   | 6      | 9      | 16  | 7     | 10    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.007 | 0.007 |
| 3065.617               | 3065.6173             | -6     | C 0.188D-21       | 1006.116 | 8    | 2      | 7      | 8   | 3     | 6     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.011 | 0.010 |
| 3066.271               | 3066.2708             | 0      | C 0.636D-22       | 416.209  | 5    | 1      | 5      | 5   | 2     | 4     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.009 | 0.010 |
| 3066.413               | 3066.4096             | 61     | H 0.947D-22       | 3465.060 | 13   | 7      | 7      | 14  | 8     | 6     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.004 | 0.005 |
| 3067.012               | 3067.0118             | 0      | C 0.239D-21       | 134.902  | 1    | 1      | 0      | 2   | 2     | 1     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.067 | 0.074 |
| 3067.139               | 3067.1325             | -95    | H 0.297D-21       | 3464.885 | 13   | 7      | 6      | 14  | 8     | 7     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.015 | 0.014 |
| 3068.932               | 3068.9345             |        | 0.636D-22         | 2124.953 | 12   | 3      | 10     | 12  | 4     | 9     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.003 | 0.003 |
| 3069.508               |                       | D      | 0.150D-21         | 3266.538 | 13   | 5      | 8      | 14  | 7     | 7     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.007 |       |
| 3069.516               | 3069.5157             | -5     | H 0.402D-21       | 3347.780 | 12   | 8      | 5      | 13  | 9     | 4     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.025 | 0.019 |
| 3069.524               |                       | D      | 0.134D-21         | 3347.777 | 12   | 8      | 4      | 13  | 9     | 5     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.006 |       |
|                        | 3074.8632             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.003 |       |
|                        | 3077.0069             |        |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.009 |       |
| 3077.473               | 3077.4734             | 2      | C 0.745D-22       | 816.694  | 7    | 2      | 6      | 7   | 3     | 5     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.006 | 0.005 |
| 3077.939               | 3077.9374             | -9     | C 0.134D-21       | 222.052  | 3    | 1      | 3      | 4   | 0     | 4     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.031 | 0.033 |
| 3079.346               | 3079.3451             | -3     | H 0.430D-21       | 3266.762 | 11   | 9      | 2      | 12  | 10    | 3     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.027 | 0.020 |
| 3079.346               |                       | D      | 0.143D-21         | 3266.762 | 11   | 9      | 3      | 12  | 10    | 2     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.007 |       |
| 3079.529               | 3079.5290             | 0      | C 0.237D-21       | 399.457  | 5    | 0      | 5      | 5   | 1     | 4     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.037 | 0.037 |
| 3079.683               | 3079.6828             | -1     | C 0.109D-21       | 142.278  | 2    | 0      | 2      | 3   | 1     | 3     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.030 | 0.033 |
| 3079.924               | 3079.9261             |        | 0.783D-22         | 982.912  | 8    | 1      | 7      | 8   | 2     | 6     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.005 | 0.004 |
| 3080.874               | 3080.8639             | -98    | H 0.673D-22       | 3624.163 | 14   | 6      | 8      | 15  | 7     | 9     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.004 | 0.003 |
| 3081.342               | 3081.3417             | -3     | C 0.198D-21       | 300.362  | 4    | 1      | 4      | 4   | 2     | 3     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.037 | 0.039 |
| 3082.251               | 3082.2522             |        | 0.518D-22         | 4510.895 | 10   | 8      | 3      | 11  | 9     | 2     | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.003 | 0.003 |
|                        | 3082.252              | D      | 0.173D-22         | 4510.895 | 10   | 8      | 2      | 11  | 9     | 3     | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.001 |       |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3082.556               | 3082.5561             | 12     | C 0.124D-21       | 782.410  | 6    | 3      | 4      | 7   | 2     | 5     | 0 2 0          | 0 0 0       | 161 | 0.010            | 0.009             |
| 3082.607               | 3082.6061             | -9     | C 0.195D-21       | 399.457  | 4    | 2      | 3      | 5   | 1     | 4     | 0 2 0          | 0 0 0       | 161 | 0.029            | 0.030             |
| 3083.303               | 3083.3029             |        | 0.584D-22         | 1985.788 | 10   | 2      | 8      | 11  | 5     | 7     | 1 0 0          | 0 0 0       | 161 | 0.003            | 0.002             |
| 3085.359               | 3085.3588             |        | 0.322D-21         | 2254.283 | 9    | 6      | 4      | 10  | 8     | 3     | 0 0 1          | 0 0 0       | 161 | 0.013            | 0.013             |
| 3085.512               | 3085.5071             |        | 0.473D-21         | 2927.939 | 12   | 5      | 7      | 13  | 7     | 6     | 0 0 1          | 0 0 0       | 161 | 0.021            | 0.021             |
| 3085.688               | 3085.6897             |        | 0.436D-21         | 2612.801 | 11   | 5      | 7      | 12  | 7     | 6     | 0 0 1          | 0 0 0       | 161 | 0.018            | 0.018             |
| 3086.133               | 3086.1333             |        | 0.134D-21         | 2414.725 | 12   | 1      | 11     | 13  | 3     | 10    | 0 0 1          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3087.192               | 3087.1915             | -6     | C 0.247D-21       | 648.979  | 6    | 2      | 5      | 6   | 3     | 4     | 0 2 0          | 0 0 0       | 161 | 0.024            | 0.023             |
| 3088.320               | 3088.3184             | -42    | H 0.178D-22       | 6172.004 | 24   | 1      | 24     | 25  | 0     | 25    | 1 0 0          | 0 0 0       | 161 | 0.004            | 0.001             |
| 3088.401               | 3088.4016             |        | 0.132D-21         | 1581.336 | -10  | 3      | 8      | 10  | 4     | 7     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.005             |
| 3088.411               |                       |        | D 0.697D-22       | 4442.719 | 12   | 5      | 8      | 13  | 6     | 7     | 1 1 0          | 0 1 0       | 161 |                  | 0.004             |
| 3088.965               | 3088.9680             | 12     | H 0.159D-22       | 6147.789 | 23   | 1      | 22     | 24  | 2     | 23    | 1 0 0          | 0 0 0       | 161 | 0.002            | 0.001             |
| 3090.485               | 3090.4826             |        | 0.107D-21         | 3360.598 | 14   | 3      | 11     | 15  | 5     | 10    | 0 0 1          | 0 0 0       | 161 | 0.005            | 0.005             |
| 3092.427               | 3092.4317             |        | 0.124D-21         | 1813.224 | 11   | 2      | 9      | 11  | 3     | 8     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.005             |
| 3092.852               | 3092.8595             | 78     | H 0.141D-21       | 3101.436 | 13   | 5      | 9      | 14  | 6     | 8     | 1 0 0          | 0 0 0       | 161 | 0.008            | 0.006             |
| 3092.854               |                       |        | D 0.154D-22       | 6062.145 | 22   | 3      | 20     | 23  | 2     | 21    | 1 0 0          | 0 0 0       | 161 |                  | 0.001             |
| 3093.573               | 3093.5692             | -67    | H 0.454D-21       | 3127.862 | 12   | 7      | 6      | 13  | 8     | 5     | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.021             |
| 3093.690               | 3093.6893             | -1     | C 0.603D-22       | 206.301  | 3    | 1      | 3      | 3   | 2     | 2     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.015             |
| 3093.758               | 3093.7637             |        | 0.103D-21         | 2748.106 | 12   | 4      | 9      | 13  | 6     | 8     | 0 0 1          | 0 0 0       | 161 | 0.004            | 0.004             |
| 3093.816               | 3093.8194             | -33    | H 0.154D-21       | 3127.808 | 12   | 7      | 5      | 13  | 8     | 6     | 1 0 0          | 0 0 0       | 161 | 0.008            | 0.007             |
| 3094.548               | 3094.5477             | 0      | C 0.821D-22       | 503.968  | 5    | 2      | 4      | 5   | 3     | 3     | 0 2 0          | 0 0 0       | 161 | 0.009            | 0.010             |
| 3095.945               | 3095.9448             | -3     | C 0.245D-21       | 79.496   | 1    | 0      | 1      | 2   | 1     | 2     | 0 2 0          | 0 0 0       | 161 | 0.077            | 0.087             |
| 3096.056               | 3096.0536             |        | 0.557D-22         | 1340.886 | 9    | 3      | 7      | 9   | 4     | 6     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.002             |
| 3096.926               | 3096.9266             | 3      | C 0.317D-21       | 782.410  | 7    | 1      | 6      | 7   | 2     | 5     | 0 2 0          | 0 0 0       | 161 | 0.025            | 0.023             |
| 3097.292               |                       |        | D 0.199D-21       | 3032.691 | 11   | 8      | 4      | 12  | 9     | 3     | 1 0 0          | 0 0 0       | 161 |                  | 0.009             |
| 3097.297               | 3097.2943             | 6      | H 0.598D-21       | 3032.690 | 11   | 8      | 3      | 12  | 9     | 4     | 1 0 0          | 0 0 0       | 161 | 0.035            | 0.027             |
| 3097.999               | 3097.9997             |        | 0.708D-22         | 2586.529 | 12   | 3      | 10     | 13  | 5     | 9     | 0 0 1          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3098.815               | 3098.8163             |        | 0.747D-22         | 1282.919 | 8    | 4      | 5      | 9   | 3     | 6     | 0 2 0          | 0 0 0       | 161 | 0.005            | 0.003             |
|                        | 3099.4173             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.003             |
| 3099.512               | 3099.5067             |        | 0.911D-22         | 1962.508 | 11   | 1      | 11     | 12  | 3     | 10    | 0 0 1          | 0 0 0       | 161 | 0.004            | 0.004             |
| 3099.548               | 3099.5473             | -3     | C 0.211D-21       | 382.517  | 4    | 2      | 3      | 4   | 3     | 2     | 0 2 0          | 0 0 0       | 161 | 0.034            | 0.034             |
| 3099.801               | 3099.8000             | -7     | C 0.971D-22       | 275.497  | 4    | 0      | 4      | 4   | 1     | 3     | 0 2 0          | 0 0 0       | 161 | 0.019            | 0.020             |
| 3101.043               | 3101.0412             | 58     | H 0.310D-21       | 3264.338 | 13   | 6      | 7      | 14  | 7     | 8     | 1 0 0          | 0 0 0       | 161 | 0.014            | 0.014             |
| 3101.156               | 3101.1555             | -4     | C 0.268D-21       | 136.761  | 2    | 1      | 2      | 3   | 0     | 3     | 0 2 0          | 0 0 0       | 161 | 0.067            | 0.081             |
| 3101.431               | 3101.4269             |        | 0.170D-21         | 2613.104 | 11   | 5      | 6      | 12  | 7     | 5     | 0 0 1          | 0 0 0       | 161 | 0.006            | 0.007             |
| 3101.878               | 3101.8766             | -8     | C 0.198D-21       | 1122.709 | 8    | 3      | 6      | 8   | 4     | 5     | 0 2 0          | 0 0 0       | 161 | 0.010            | 0.010             |
| 3102.059               | 3102.0629             |        | 0.601D-22         | 4329.324 | 11   | 6      | 5      | 12  | 7     | 6     | 1 1 0          | 0 1 0       | 161 | 0.003            | 0.003             |
| 3102.461               | 3102.4600             | -18    | C 0.442D-22       | 285.219  | 3    | 2      | 2      | 3   | 3     | 1     | 0 2 0          | 0 0 0       | 161 | 0.008            | 0.013             |
|                        | 3102.7251             |        |                   |          |      |        |        |     |       |       |                |             |     |                  |                   |
| 3103.015               | 3103.0153             | -2     | C 0.125D-21       | 134.902  | 2    | 1      | 2      | 2   | 2     | 1     | 0 2 0          | 0 0 0       | 161 | 0.029            | 0.038             |
| 3105.871               | 3105.8698             | -2     | C 0.720D-22       | 927.744  | 7    | 3      | 5      | 7   | 4     | 4     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.004             |
| 3106.068               | 3106.0693             |        | 0.613D-22         | 1538.150 | 10   | 2      | 8      | 10  | 3     | 7     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.002             |
| 3106.070               |                       |        | D 0.154D-22       | 5748.125 | 20   | 5      | 16     | 21  | 4     | 17    | 1 0 0          | 0 0 0       | 161 |                  | 0.001             |
| 3107.152               | 3107.1499             | -12    | H 0.626D-21       | 2972.824 | 10   | 9      | 2      | 11  | 10    | 1     | 1 0 0          | 0 0 0       | 161 | 0.032            | 0.028             |
| 3107.152               |                       |        | D 0.209D-21       | 2972.824 | 10   | 9      | 1      | 11  | 10    | 2     | 1 0 0          | 0 0 0       | 161 |                  | 0.009             |
| 3107.330               | 3107.3300             | -6     | C 0.141D-21       | 285.419  | 3    | 2      | 1      | 3   | 3     | 0     | 0 2 0          | 0 0 0       | 161 | 0.025            | 0.029             |
| 3108.241               | 3108.2406             | -8     | C 0.213D-21       | 756.725  | 6    | 3      | 4      | 6   | 4     | 3     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.016             |
| 3109.379               | 3109.3774             | -4     | C 0.602D-22       | 610.114  | 5    | 3      | 3      | 5   | 4     | 2     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3109.759               | 3109.7582             | 0      | C 0.113D-21       | 488.108  | 4    | 3      | 2      | 4   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.013            | 0.014             |
| 3109.908               | 3109.9198             |        | 0.714D-22         | 4240.941 | 9    | 8      | 1      | 10  | 9     | 2     | 1 1 0          | 0 1 0       | 161 | 0.004            | 0.004             |
|                        | 3109.908              |        | D 0.238D-22       | 4240.941 | 9    | 8      | 2      | 10  | 9     | 1     | 1 1 0          | 0 1 0       | 161 |                  | 0.001             |
| 3110.308               | 3110.3100             | 21     | C 0.134D-21       | 602.774  | 6    | 1      | 5      | 6   | 2     | 4     | 0 2 0          | 0 0 0       | 161 | 0.013            | 0.013             |
| 3110.593               | 3110.5911             | -26    | C 0.380D-22       | 488.134  | 4    | 3      | 1      | 4   | 4     | 0     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.005             |
| 3112.097               | 3112.0976             | 10     | C 0.822D-22       | 383.842  | 4    | 2      | 2      | 4   | 3     | 1     | 0 2 0          | 0 0 0       | 161 | 0.012            | 0.013             |
| 3112.184               | 3112.1839             | 4      | C 0.375D-22       | 275.497  | 3    | 2      | 2      | 4   | 1     | 3     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.008             |
| 3112.391               | 3112.3890             | -9     | C 0.186D-21       | 610.341  | 5    | 3      | 2      | 5   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.017            | 0.018             |
| 3112.548               | 3112.5422             |        | 0.929D-22         | 2009.805 | 8    | 6      | 3      | 9   | 8     | 2     | 0 0 1          | 0 0 0       | 161 | 0.005            | 0.004             |
| 3112.588               | 3112.5879             |        | 0.279D-21         | 2009.805 | 8    | 6      | 2      | 9   | 8     | 1     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3112.670               | 3112.6708             |        | 0.174D-21         | 2321.814 | 10   | 5      | 6      | 11  | 7     | 5     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3112.694               | 3112.7029             |        | 0.401D-21         | 2629.337 | 12   | 4      | 9      | 13  | 5     | 8     | 1 0 0          | 0 0 0       | 161 | 0.015            | 0.017             |
| 3113.126               | 3113.1238             |        | 0.200D-21         | 1813.224 | 10   | 2      | 9      | 11  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.008            | 0.008             |
| 3113.579               | 3113.5795             |        | 0.107D-21         | 1446.129 | 9    | 0      | 9      | 10  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.005            | 0.004             |
| 3114.181               | 3114.1823             |        | 0.688D-22         | 2275.373 | 12   | 4      | 9      | 12  | 5     | 8     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3114.493               | 3114.4931             | 3      | C 0.559D-22       | 37.137   | 0    | 0      | 0      | 1   | 1     | 1     | 0 2 0          | 0 0 0       | 161 | 0.018            | 0.022             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|-----|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3115.877               | 3115.8762             | -9     | C 0.334D-21       | 173.365  | 3   | 0      | 3      | 3   | 1     | 2     | 0 2 0          | 0 0 0       | 161 | 0.076            | 0.091             |
| 3116.013               | 3116.0121             | -17    | C 0.762D-22       | 757.780  | 6   | 3      | 3      | 6   | 4     | 2     | 0 2 0          | 0 0 0       | 161 | 0.005            | 0.006             |
| 3116.624               | 3116.6218             | -21    | C 0.258D-21       | 1282.919 | 9   | 2      | 7      | 9   | 3     | 6     | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3118.110               | 3118.1104             | 6      | C 0.332D-21       | 508.812  | 5   | 2      | 3      | 5   | 3     | 2     | 0 2 0          | 0 0 0       | 161 | 0.038            | 0.040             |
| 3118.944               | 3118.9437             | -4     | C 0.457D-21       | 446.511  | 5   | 1      | 4      | 5   | 2     | 3     | 0 2 0          | 0 0 0       | 161 | 0.058            | 0.063             |
| 3118.981               | 3118.9803             |        | 0.162D-21         | 1718.719 | 9   | 2      | 7      | 10  | 5     | 6     | 1 0 0          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3119.182               | 3119.1817             | -4     | C 0.617D-22       | 136.164  | 2   | 1      | 1      | 2   | 2     | 0     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.019             |
|                        | 3119.7520             |        |                   |          |     |        |        |     |       |       |                |             |     | 0.003            |                   |
| 3120.193               | 3120.1917             |        | 0.555D-21         | 2321.905 | 10  | 5      | 5      | 11  | 7     | 4     | 0 0 1          | 0 0 0       | 161 | 0.020            | 0.022             |
| 3120.890               | 3120.8902             |        | 0.229D-21         | 2813.533 | 11  | 7      | 5      | 12  | 8     | 4     | 1 0 0          | 0 0 0       | 161 | 0.009            | 0.010             |
| 3120.964               | 3120.9646             | 7      | H 0.691D-21       | 2813.515 | 11  | 7      | 4      | 12  | 8     | 5     | 1 0 0          | 0 0 0       | 161 | 0.030            | 0.030             |
| 3121.599               | 3121.5993             | 1      | C 0.251D-21       | 931.237  | 7   | 3      | 4      | 7   | 4     | 3     | 0 2 0          | 0 0 0       | 161 | 0.014            | 0.015             |
| 3121.911               | 3121.9083             | -31    | H 0.319D-21       | 2927.939 | 12  | 6      | 7      | 13  | 7     | 6     | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.014             |
| 3122.470               | 3122.4701             | -3     | C 0.343D-21       | 212.156  | 3   | 1      | 2      | 3   | 2     | 1     | 0 2 0          | 0 0 0       | 161 | 0.072            | 0.084             |
| 3122.796               | 3122.7955             | -1     | C 0.148D-21       | 315.779  | 4   | 1      | 3      | 4   | 2     | 2     | 0 2 0          | 0 0 0       | 161 | 0.024            | 0.028             |
| 3123.067               | 3123.0672             | -10    | C 0.111D-21       | 1050.158 | 8   | 2      | 6      | 8   | 3     | 5     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.006             |
| 3123.130               | 3123.1309             | 5      | C 0.128D-21       | 661.549  | 6   | 2      | 4      | 6   | 3     | 3     | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3123.342               | 3123.3415             |        | 0.996D-22         | 3472.880 | 14  | 4      | 10     | 15  | 6     | 9     | 0 0 1          | 0 0 0       | 161 | 0.004            | 0.005             |
| 3123.418               | 3123.4096             |        | 0.121D-21         | 1718.719 | 10  | 4      | 7      | 10  | 5     | 6     | 0 2 0          | 0 0 0       | 161 | 0.004            | 0.005             |
| 3124.201               | 3124.1970             | -11    | H 0.156D-21       | 2927.076 | 12  | 6      | 6      | 13  | 7     | 7     | 1 0 0          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3125.019               | 3125.0186             |        | 0.818D-22         | 1731.898 | 3   | 1      | 2      | 3   | 0     | 3     | 0 3 0          | 0 1 0       | 161 | 0.004            | 0.003             |
| 3125.132               | 3125.1319             | 1      | C 0.383D-21       | 842.357  | 7   | 2      | 5      | 7   | 3     | 4     | 0 2 0          | 0 0 0       | 161 | 0.025            | 0.025             |
| 3125.186               | 3125.1830             | -55    | H 0.857D-21       | 2740.420 | 10  | 8      | 3      | 11  | 9     | 2     | 1 0 0          | 0 0 0       | 161 | 0.045            | 0.036             |
| 3125.188               |                       |        | D 0.286D-21       | 2740.420 | 10  | 8      | 2      | 11  | 9     | 3     | 1 0 0          | 0 0 0       | 161 | 0.012            |                   |
| 3126.003               | 3126.0016             | -11    | C 0.409D-22       | 70.091   | 1   | 1      | 1      | 2   | 0     | 2     | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.015             |
| 3126.567               | 3126.5701             | 15     | C 0.159D-21       | 1255.167 | 8   | 4      | 5      | 8   | 5     | 4     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3126.785               | 3126.7852             | -1     | C 0.109D-21       | 95.176   | 2   | 0      | 2      | 2   | 1     | 1     | 0 2 0          | 0 0 0       | 161 | 0.030            | 0.037             |
| 3126.911               |                       |        | D 0.892D-22       | 742.076  | 5   | 4      | 1      | 5   | 5     | 0     | 0 2 0          | 0 0 0       | 161 | 0.007            |                   |
| 3126.916               | 3126.9156             | 13     | C 0.139D-21       | 888.599  | 6   | 4      | 3      | 6   | 5     | 2     | 0 2 0          | 0 0 0       | 161 | 0.014            | 0.009             |
| 3126.924               |                       |        | D 0.532D-22       | 1059.647 | 7   | 4      | 4      | 7   | 5     | 3     | 0 2 0          | 0 0 0       | 161 | 0.003            |                   |
| 3127.420               | 3127.4174             | -19    | C 0.465D-22       | 888.632  | 6   | 4      | 2      | 6   | 5     | 1     | 0 2 0          | 0 0 0       | 161 | 0.002            | 0.003             |
| 3127.850               | 3127.8515             |        | 0.561D-22         | 1677.063 | 3   | 0      | 3      | 2   | 1     | 2     | 0 3 0          | 0 1 0       | 161 | 0.002            | 0.002             |
| 3128.104               | 3128.1001             |        | 0.846D-22         | 1131.776 | 8   | 3      | 5      | 8   | 4     | 4     | 0 2 0          | 0 0 0       | 161 | 0.003            | 0.004             |
| 3128.310               | 3128.3102             |        | 0.845D-22         | 4038.404 | 10  | 6      | 5      | 11  | 7     | 4     | 1 1 0          | 0 1 0       | 161 | 0.004            |                   |
| 3128.559               | 3128.5591             | 4      | C 0.162D-21       | 1059.835 | 7   | 4      | 3      | 7   | 5     | 2     | 0 2 0          | 0 0 0       | 161 | 0.009            | 0.008             |
| 3129.597               | 3129.5991             |        | 0.488D-21         | 2433.803 | 11  | 4      | 8      | 12  | 6     | 7     | 0 0 1          | 0 0 0       | 161 | 0.018            | 0.020             |
| 3129.910               |                       |        | D 0.332D-22       | 3997.511 | 9   | 7      | 3      | 10  | 8     | 2     | 1 1 0          | 0 1 0       | 161 | 0.002            |                   |
| 3129.913               | 3129.9230             |        | 0.996D-22         | 3997.511 | 9   | 7      | 2      | 10  | 8     | 3     | 1 1 0          | 0 1 0       | 161 | 0.007            | 0.005             |
| 3130.394               | 3130.3971             |        | D 0.203D-21       | 2124.953 | 11  | 2      | 10     | 12  | 4     | 9     | 0 0 1          | 0 0 0       | 161 | 0.009            | 0.008             |
| 3130.402               |                       |        | D 0.366D-22       | 1255.913 | 8   | 4      | 4      | 8   | 5     | 3     | 0 2 0          | 0 0 0       | 161 | 0.002            | 0.002             |
| 3131.351               | 3131.3493             | 16     | H 0.730D-21       | 2756.418 | 12  | 5      | 8      | 13  | 6     | 7     | 1 0 0          | 0 0 0       | 161 | 0.033            | 0.031             |
| 3132.161               | 3132.1598             | -4     | II 0.145D-22      | 7533.699 | 25  | 3      | 23     | 26  | 3     | 24    | 0 0 1          | 0 0 0       | 161 | 0.002            | 0.002             |
| 3133.070               | 3133.0685             | -15    | C 0.242D-21       | 42.372   | 1   | 0      | 1      | 1   | 1     | 0     | 0 2 0          | 0 0 0       | 161 | 0.076            | 0.094             |
| 3133.570               | 3133.5694             |        | 0.236D-21         | 1360.236 | 9   | 3      | 6      | 9   | 4     | 5     | 0 2 0          | 0 0 0       | 161 | 0.010            | 0.010             |
| 3134.498               | 3134.4984             |        | 0.155D-21         | 1477.297 | 9   | 4      | 5      | 9   | 5     | 4     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.006             |
| 3134.631               | 3134.6291             |        | 0.226D-21         | 1581.336 | 9   | 1      | 8      | 10  | 4     | 7     | 1 0 0          | 0 0 0       | 161 | 0.009            | 0.009             |
| 3135.095               |                       |        | D 0.291D-21       | 2701.890 | 9   | 9      | 1      | 10  | 10    | 0     | 1 0 0          | 0 0 0       | 161 | 0.012            |                   |
| 3135.096               | 3135.0969             | 14     | H 0.874D-21       | 2701.890 | 9   | 9      | 0      | 10  | 10    | 1     | 1 0 0          | 0 0 0       | 161 | 0.043            | 0.037             |
| 3135.382               | 3135.3808             |        | 0.150D-21         | 1899.008 | 11  | 3      | 8      | 11  | 4     | 7     | 0 2 0          | 0 0 0       | 161 | 0.005            | 0.006             |
| 3137.661               |                       |        | D 0.316D-22       | 3994.259 | 8   | 8      | 0      | 9   | 9     | 1     | 1 1 0          | 0 1 0       | 161 | 0.002            |                   |
| 3137.661               | 3137.6564             |        | 0.948D-22         | 3994.259 | 8   | 8      | 1      | 9   | 9     | 0     | 1 1 0          | 0 1 0       | 161 | 0.007            | 0.005             |
| 3138.145               | 3138.1404             | -68    | H 0.155D-21       | 3822.246 | 15  | 5      | 10     | 16  | 6     | 11    | 1 0 0          | 0 0 0       | 161 | 0.007            | 0.008             |
| 3139.018               | 3139.0128             | -22    | H 0.548D-22       | 5271.371 | 22  | 1      | 22     | 23  | 0     | 23    | 1 0 0          | 0 0 0       | 161 | 0.005            | 0.004             |
| 3139.018               |                       |        | D 0.183D-22       | 5271.371 | 22  | 0      | 22     | 23  | 1     | 23    | 1 0 0          | 0 0 0       | 161 | 0.001            |                   |
| 3139.109               | 3139.1139             | -37    | H 0.567D-21       | 2054.348 | 9   | 5      | 5      | 10  | 7     | 4     | 0 0 1          | 0 0 0       | 161 | 0.022            | 0.022             |
| 3139.115               |                       |        | D 0.232D-22       | 7210.551 | 23  | 5      | 19     | 24  | 5     | 20    | 0 0 1          | 0 0 0       | 161 | 0.002            |                   |
| 3139.525               | 3139.5240             | -10    | H 0.486D-22       | 5246.078 | 21  | 2      | 20     | 22  | 1     | 21    | 1 0 0          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3139.729               | 3139.7276             |        | 0.642D-22         | 4123.285 | 11  | 5      | 6      | 12  | 6     | 7     | 1 1 0          | 0 1 0       | 161 | 0.002            | 0.003             |
| 3140.021               | 3140.0195             |        | 0.174D-21         | 1789.041 | 7   | 6      | 2      | 8   | 8     | 1     | 0 0 1          | 0 0 0       | 161 | 0.006            | 0.007             |
| 3140.031               |                       |        | D 0.580D-22       | 1789.041 | 7   | 6      | 1      | 8   | 8     | 0     | 0 0 1          | 0 0 0       | 161 | 0.002            |                   |
| 3142.133               | 3142.1316             |        | 0.193D-21         | 2054.369 | 9   | 5      | 4      | 10  | 7     | 3     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.008             |
| 3142.780               | 3142.7798             | 2      | C 0.444D-22       | 173.365  | 2   | 2      | 1      | 3   | 1     | 2     | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.012             |
| 3142.860               | 3142.8637             | 41     | H 0.460D-22       | 5163.082 | 20  | 3      | 18     | 21  | 2     | 19    | 1 0 0          | 0 0 0       | 161 | 0.003            | 0.003             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |                 |                 |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|-----------------|-----------------|
|                        | 3145.1866             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.003            |                   |                 |                 |
| 3145.415               | 3145.4130             |        | 0.117D-21         | 1998.996 | 11   | 4      | 7      | 11  | 5     | 6     | 0                | 2             | 0   | 0                | 0                 | 161 0.004 0.005 |                 |
| 3145.895               | 3145.8945             |        | 0.331D-21         | 2275.373 | 11   | 3      | 9      | 12  | 5     | 8     | 0                | 0             | 1   | 0                | 0                 | 161 0.013 0.013 |                 |
|                        | 3146.5548             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.004            |                   |                 |                 |
|                        | 3148.1063             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.004            |                   |                 |                 |
| 3148.303               | 3148.2976             |        | 0.205D-21         | 2613.104 | 11   | 6      | 6      | 12  | 7     | 5     | 1                | 0             | 0   | 0                | 0                 | 161 0.008 0.009 |                 |
| 3148.353               | 3148.3508             | -20    | H 0.994D-21       | 2522.267 | 10   | 7      | 4      | 11  | 8     | 3     | 1                | 0             | 0   | 0                | 0                 | 161 0.039 0.041 |                 |
| 3148.374               |                       |        | 0.332D-21         | 2522.263 | 10   | 7      | 3      | 11  | 8     | 4     | 1                | 0             | 0   | 0                | 0                 | 161 0.014       |                 |
| 3149.259               | 3149.2599             | 9      | H 0.699D-21       | 2612.801 | 11   | 6      | 5      | 12  | 7     | 6     | 1                | 0             | 0   | 0                | 0                 | 161 0.028 0.029 |                 |
| 3149.537               |                       |        | D 0.248D-22       | 3360.598 | 15   | 4      | 11     | 15  | 5     | 10    | 0                | 2             | 0   | 0                | 0                 | 161 0.001       |                 |
| 3149.542               | 3149.5401             |        | 0.199D-21         | 2533.793 | 12   | 2      | 10     | 13  | 4     | 9     | 0                | 0             | 1   | 0                | 0                 | 161 0.007 0.008 |                 |
|                        | 3149.8940             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.004            |                   |                 |                 |
| 3151.356               | 3151.3555             | 4      | C 0.529D-22       | 446.511  | 4    | 3      | 2      | 5   | 2     | 3     | 0                | 2             | 0   | 0                | 0                 | 161 0.007 0.007 |                 |
| 3152.095               | 3152.1016             |        | 0.957D-22         | 1874.974 | 10   | 5      | 6      | 10  | 6     | 5     | 0                | 2             | 0   | 0                | 0                 | 161 0.004 0.004 |                 |
| 3152.281               | 3152.2811             |        | 0.669D-22         | 1045.058 | 6    | 5      | 2      | 6   | 6     | 1     | 0                | 2             | 0   | 0                | 0                 | 161 0.003 0.003 |                 |
| 3152.421               | 3152.4242             |        | 0.112D-21         | 1411.612 | 8    | 5      | 4      | 8   | 6     | 3     | 0                | 2             | 0   | 0                | 0                 | 161 0.008 0.005 |                 |
| 3152.722               | 3152.7255             |        | 0.374D-22         | 1411.647 | 8    | 5      | 3      | 8   | 6     | 2     | 0                | 2             | 0   | 0                | 0                 | 161 0.003 0.002 |                 |
| 3153.136               | 3153.1332             | -4     | H 0.118D-20       | 2471.254 | 9    | 8      | 1      | 10  | 9     | 2     | 1                | 0             | 0   | 0                | 0                 | 161 0.059 0.048 |                 |
| 3153.136               |                       |        | D 0.394D-21       | 2471.254 | 9    | 8      | 2      | 10  | 9     | 1     | 1                | 0             | 0   | 0                | 0                 | 161 0.016       |                 |
| 3153.280               | 3153.2808             |        | 0.108D-21         | 1631.384 | 9    | 5      | 4      | 9   | 6     | 3     | 0                | 2             | 0   | 0                | 0                 | 161 0.004 0.004 |                 |
| 3154.346               | 3154.3514             |        | 0.329D-22         | 1875.464 | 10   | 5      | 5      | 10  | 6     | 4     | 0                | 2             | 0   | 0                | 0                 | 161 0.002 0.001 |                 |
| 3155.380               | 3155.3801             | 6      | H 0.248D-22       | 7116.395 | 25   | 2      | 24     | 26  | 2     | 25    | 0                | 0             | 1   | 0                | 0                 | 161 0.004 0.002 |                 |
| 3155.617               | 3155.6182             |        | 0.117D-21         | 3770.713 | 9    | 6      | 3      | 10  | 7     | 4     | 1                | 1             | 0   | 0                | 1                 | 0               | 161 0.005 0.006 |
| 3156.326               | 3156.3282             | 8      | H 0.287D-22       | 7027.023 | 24   | 2      | 22     | 25  | 2     | 23    | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.004 0.003 |
| 3156.697               | 3156.6926             | -54    | H 0.350D-21       | 3084.835 | 13   | 5      | 8      | 14  | 6     | 9     | 1                | 0             | 0   | 0                | 0                 | 161 0.014 0.016 |                 |
| 3157.575               | 3157.5762             |        | 0.131D-21         | 3752.417 | 8    | 7      | 2      | 9   | 8     | 1     | 1                | 1             | 0   | 0                | 1                 | 0               | 161 0.007 0.006 |
| 3157.575               |                       |        | D 0.435D-22       | 3752.417 | 8    | 7      | 1      | 9   | 8     | 2     | 1                | 1             | 0   | 0                | 1                 | 0               | 161 0.002       |
| 3158.421               | 3158.4222             |        | 0.665D-22         | 3833.146 | 10   | 5      | 6      | 11  | 6     | 5     | 1                | 1             | 0   | 0                | 1                 | 0               | 161 0.004 0.003 |
| 3159.002               | 3159.0002             | -30    | H 0.351D-22       | 6889.730 | 23   | 4      | 20     | 24  | 4     | 21    | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.003 0.003 |
| 3159.345               | 3159.3446             | -19    | H 0.231D-22       | 7139.602 | 26   | 0      | 26     | 27  | 0     | 27    | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.004 0.002 |
| 3160.997               | 3160.9985             | -15    | H 0.385D-22       | 6197.461 | 18   | 11     | 7      | 19  | 11    | 8     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.003 0.003 |
| 3160.998               |                       |        | D 0.128D-22       | 6197.445 | 18   | 11     | 8      | 19  | 11    | 9     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.001       |
| 3162.084               | 3162.0841             |        | 0.128D-21         | 1690.665 | 10   | 0      | 10     | 11  | 2     | 9     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.005 0.005 |
| 3162.131               | 3162.1298             |        | 0.236D-21         | 2142.597 | 10   | 4      | 7      | 11  | 6     | 6     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.009 0.009 |
| 3163.164               | 3163.1654             | 14     | H 0.900D-22       | 2000.866 | 5    | 2      | 3      | 5   | 1     | 4     | 0                | 3             | 0   | 0                | 1                 | 0               | 161 0.007 0.004 |
| 3164.030               | 3164.0313             | -67    | H 0.391D-21       | 2437.501 | 11   | 5      | 7      | 12  | 6     | 6     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.021 0.016 |
| 3164.038               |                       |        | D 0.922D-22       | 4846.496 | 21   | 0      | 21     | 22  | 1     | 22    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.006       |
| 3164.038               |                       |        | D 0.307D-22       | 4846.496 | 21   | 1      | 21     | 22  | 0     | 22    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.002       |
| 3164.367               | 3164.3684             |        | 0.239D-21         | 2300.689 | 11   | 4      | 8      | 12  | 5     | 7     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.010 0.010 |
| 3164.491               |                       |        | D 0.271D-22       | 4820.645 | 20   | 1      | 19     | 21  | 2     | 20    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.002       |
| 3164.492               | 3164.4901             | -18    | H 0.813D-22       | 4820.645 | 20   | 2      | 19     | 21  | 1     | 20    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.006 0.005 |
| 3165.460               | 3165.4609             |        | 0.183D-21         | 1810.584 | 8    | 5      | 4      | 9   | 7     | 3     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.007 0.007 |
| 3166.456               | 3166.4559             |        | 0.552D-21         | 1810.589 | 8    | 5      | 3      | 9   | 7     | 2     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.022 0.021 |
|                        | 3167.0592             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.004            |                   |                 |                 |
| 3167.236               | 3167.2368             |        | 0.415D-22         | 885.600  | 7    | 3      | 4      | 8   | 2     | 7     | 0                | 2             | 0   | 0                | 0                 | 0               | 161 0.002 0.003 |
| 3167.536               | 3167.5376             | 28     | H 0.762D-22       | 4738.637 | 19   | 2      | 17     | 20  | 3     | 18    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.005 0.005 |
| 3167.542               |                       |        | D 0.254D-22       | 4738.625 | 19   | 3      | 17     | 20  | 2     | 18    | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.002       |
| 3167.911               | 3167.9098             | -9     | C 0.291D-22       | 224.838  | 3    | 2      | 1      | 4   | 1     | 4     | 0                | 2             | 0   | 0                | 0                 | 0               | 161 0.006 0.007 |
| 3169.269               | 3169.2729             |        | 0.521D-22         | 1920.769 | 5    | 1      | 4      | 5   | 0     | 5     | 0                | 3             | 0   | 0                | 1                 | 0               | 161 0.003 0.002 |
| 3169.820               | 3169.8208             | 18     | C 0.537D-22       | 552.912  | 5    | 3      | 2      | 6   | 2     | 5     | 0                | 2             | 0   | 0                | 0                 | 0               | 161 0.005 0.006 |
| 3170.077               | 3170.0769             |        | 0.168D-21         | 2748.106 | 12   | 5      | 7      | 13  | 6     | 8     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.008 0.007 |
| 3170.082               |                       |        | D 0.567D-22       | 1216.232 | 8    | 4      | 4      | 9   | 3     | 7     | 0                | 2             | 0   | 0                | 0                 | 0               | 161 0.003       |
| 3170.232               | 3170.2332             |        | 0.982D-22         | 1731.898 | 4    | 1      | 4      | 3   | 0     | 3     | 0                | 3             | 0   | 0                | 1                 | 0               | 161 0.006 0.004 |
|                        | 3172.1848             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.004            |                   |                 |                 |
| 3172.595               | 3172.5973             |        | 0.115D-21         | 3659.906 | 10   | 4      | 7      | 11  | 5     | 6     | 1                | 1             | 0   | 0                | 1                 | 0               | 161 0.004 0.006 |
| 3173.158               | 3173.1573             | -3     | C 0.511D-22       | 842.357  | 6    | 4      | 3      | 7   | 3     | 4     | 0                | 2             | 0   | 0                | 0                 | 0               | 161 0.003 0.003 |
|                        | 3174.7837             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.003            |                   |                 |                 |
| 3175.075               | 3175.0746             | 1      | H 0.977D-21       | 2321.905 | 10   | 6      | 5      | 11  | 7     | 4     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.037 0.039 |
| 3175.394               |                       |        | D 0.259D-22       | 5866.230 | 16   | 13     | 3      | 17  | 13    | 4     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.002       |
| 3175.402               | 3175.4016             | 44     | H 0.339D-21       | 2321.814 | 10   | 6      | 4      | 11  | 7     | 5     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.015 0.013 |
| 3175.901               |                       |        | D 0.459D-21       | 2254.284 | 9    | 7      | 3      | 10  | 8     | 2     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.018       |
| 3175.904               | 3175.8997             | 18     | H 0.138D-20       | 2254.283 | 9    | 7      | 2      | 10  | 8     | 3     | 1                | 0             | 0   | 0                | 0                 | 0               | 161 0.067 0.054 |
| 3176.742               | 3176.7390             |        | 0.524D-22         | 3101.124 | 7    | 4      | 4      | 8   | 6     | 3     | 0                | 1             | 1   | 0                | 1                 | 0               | 161 0.002 0.002 |
| 3177.037               | 3177.0394             | -14    | H 0.654D-22       | 5941.043 | 18   | 10     | 8      | 19  | 10    | 9     | 0                | 0             | 1   | 0                | 0                 | 0               | 161 0.005 0.005 |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3177.129               | 3177.1298             |             | 0.116D-21         | 2756.418 | 12   | 4      | 8      | 13  | 6     | 7     | 0 0 1            | 0 0 0         | 161 | 0.005            | 0.005             |
| 3177.263               | 3177.2579             |             | 0.495D-21         | 1899.008 | 10   | 3      | 8      | 11  | 4     | 7     | 1 0 0            | 0 0 0         | 161 | 0.020            | 0.019             |
| 3178.119               | 3178.1192             | -2          | C 0.238D-21       | 23.794   | 1    | 1      | 0      | 1   | 0     | 1     | 0 2 0            | 0 0 0         | 161 | 0.075            | 0.096             |
| 3178.956               | 3178.9559             |             | 0.103D-21         | 1538.150 | 9    | 2      | 8      | 10  | 3     | 7     | 1 0 0            | 0 0 0         | 161 | 0.004            | 0.004             |
| 3179.644               |                       | D 0.161D-22 | 6623.797          | 24       | 2    | 23     | 25     | 2   | 24    |       | 0 0 1            | 0 0 0         | 161 | 0.001            |                   |
| 3179.644               | 3179.6453             | -4          | H 0.483D-22       | 6623.797 | 24   | 1      | 23     | 25  | 1     | 24    | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.004             |
| 3180.387               | 3180.3791             | -75         | H 0.115D-21       | 6177.340 | 20   | 6      | 14     | 21  | 6     | 15    | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.009             |
| 3180.388               |                       | D 0.922D-22 | 5947.328          | 19       | 8    | 12     | 20     | 8   | 13    |       | 0 0 1            | 0 0 0         | 161 |                  | 0.007             |
|                        | 3180.4104             |             |                   |          |      |        |        |     |       |       |                  |               |     | 0.006            |                   |
| 3181.082               | 3181.0801             | -54         | H 0.157D-20       | 2225.468 | 8    | 8      | 1      | 9   | 9     | 0     | 1 0 0            | 0 0 0         | 161 | 0.074            | 0.062             |
| 3181.082               |                       | D 0.523D-21 | 2225.468          | 8        | 8    | 0      | 9      | 9   | 1     | 1     | 0 0 0            | 0 0 0         | 161 |                  | 0.021             |
|                        | 3181.6748             | 13          | H                 |          |      |        |        |     |       |       |                  |               |     | 0.002            |                   |
| 3182.278               | 3182.2788             |             | 0.600D-22         | 1006.116 | 7    | 4      | 3      | 8   | 3     | 6     | 0 2 0            | 0 0 0         | 161 | 0.002            | 0.003             |
| 3182.704               | 3182.7028             |             | 0.869D-22         | 1340.886 | 8    | 1      | 7      | 9   | 4     | 6     | 1 0 0            | 0 0 0         | 161 | 0.003            | 0.004             |
| 3182.816               | 3182.8191             |             | 0.153D-21         | 3526.630 | 8    | 6      | 3      | 9   | 7     | 2     | 1 1 0            | 0 1 0         | 161 | 0.007            | 0.007             |
| 3182.926               |                       | D 0.438D-22 | 2612.801          | 12       | 6    | 7      | 12     | 7   | 6     |       | 0 2 0            | 0 0 0         | 161 |                  | 0.002             |
| 3182.927               | 3182.9298             | 40          | H 0.675D-22       | 6400.980 | 22   | 3      | 19     | 23  | 3     | 20    | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.006             |
| 3183.489               |                       | D 0.150D-22 | 6647.500          | 25       | 0    | 25     | 26     | 0   | 26    |       | 0 0 1            | 0 0 0         | 161 |                  | 0.001             |
| 3183.489               | 3183.4889             | -8          | H 0.451D-22       | 6647.500 | 25   | 1      | 25     | 26  | 1     | 26    | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.004             |
| 3184.531               | 3184.5288             |             | 0.839D-22         | 1843.030 | 10   | 2      | 9      | 11  | 4     | 8     | 0 0 1            | 0 0 0         | 161 | 0.004            | 0.003             |
| 3184.824               | 3184.8240             | 1           | C 0.351D-22       | 37.137   | 2    | 0      | 2      | 1   | 1     | 1     | 0 2 0            | 0 0 0         | 161 | 0.010            | 0.014             |
| 3185.142               | 3185.1408             |             | 0.146D-21         | 1201.922 | 8    | 1      | 8      | 9   | 2     | 7     | 1 0 0            | 0 0 0         | 161 | 0.007            | 0.007             |
| 3185.210               |                       | D 0.549D-22 | 3530.958          | 7        | 7    | 1      | 8      | 8   | 0     |       | 1 1 0            | 0 1 0         | 161 |                  | 0.003             |
| 3185.210               | 3185.2090             |             | 0.165D-21         | 3530.958 | 7    | 7      | 0      | 8   | 8     | 1     | 1 1 0            | 0 1 0         | 161 | 0.009            | 0.008             |
| 3185.255               | 3185.2550             | 0           | C 0.102D-21       | 70.091   | 2    | 1      | 1      | 2   | 0     | 2     | 0 2 0            | 0 0 0         | 161 | 0.029            | 0.036             |
| 3186.274               | 3186.2709             | -13         | H 0.625D-22       | 5750.840 | 17   | 11     | 7      | 18  | 11    | 8     | 0 0 1            | 0 0 0         | 161 | 0.005            | 0.005             |
| 3186.275               |                       | D 0.208D-22 | 5750.844          | 17       | 11   | 6      | 18     | 11  | 7     |       | 0 0 1            | 0 0 0         | 161 |                  | -0.001            |
| 3186.694               | 3186.6907             | -38         | H 0.868D-22       | 6220.531 | 21   | 5      | 17     | 22  | 5     | 18    | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.007             |
| 3186.811               | 3186.8112             |             | 0.122D-21         | 3564.705 | 9    | 5      | 4      | 10  | 6     | 5     | 1 1 0            | 0 1 0         | 161 | 0.005            | 0.006             |
| 3187.531               | 3187.5341             | 46          | H 0.699D-21       | 2433.803 | 11   | 5      | 6      | 12  | 6     | 7     | 1 0 0            | 0 0 0         | 161 | 0.027            | 0.028             |
| 3188.835               |                       | D 0.502D-22 | 4438.750          | 20       | 0    | 20     | 21     | 1   | 21    |       | 1 0 0            | 0 0 0         | 161 |                  | 0.003             |
| 3188.836               | 3188.8379             | 9           | H 0.151D-21       | 4438.750 | 20   | 1      | 20     | 21  | 0     | 21    | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.008             |
| 3189.129               | 3189.1316             | -35         | H 0.207D-22       | 7025.977 | 18   | 7      | 11     | 19  | 7     | 12    | 0 1 1            | 0 1 0         | 161 | 0.003            | 0.002             |
| 3189.137               |                       | D 0.142D-22 | 7156.836          | 16       | 2    | 14     | 17     | 2   | 15    |       | 1 0 1            | 1 0 0         | 161 |                  | 0.001             |
| 3189.232               | 3189.2311             | -17         | H 0.132D-21       | 4412.316 | 19   | 1      | 18     | 20  | 2     | 19    | 1 0 0            | 0 0 0         | 161 | 0.009            | 0.007             |
| 3189.233               |                       | D 0.440D-22 | 4412.316          | 19       | 2    | 18     | 20     | 1   | 19    |       | 1 0 0            | 0 0 0         | 161 |                  | 0.002             |
| 3190.169               | 3190.1710             |             | 0.171D-21         | 1985.788 | 10   | 3      | 8      | 11  | 5     | 7     | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.007             |
| 3190.941               | 3190.9415             | 30          | H 0.162D-20       | 2144.047 | 10   | 5      | 6      | 11  | 6     | 5     | 1 0 0            | 0 0 0         | 161 | 0.059            | 0.063             |
|                        | 3191.1266             |             |                   |          |      |        |        |     |       |       |                  |               |     | 0.002            |                   |
| 3191.561               | 3191.5648             | 53          | H 0.107D-21       | 5702.781 | 18   | 9      | 9      | 19  | 9     | 10    | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.008             |
| 3191.972               | 3191.9720             |             | 0.452D-21         | 1590.690 | 7    | 5      | 3      | 8   | 7     | 2     | 0 0 1            | 0 0 0         | 161 | 0.016            | 0.018             |
| 3192.103               | 3192.1036             | 121         | H 0.910D-21       | 1874.974 | 9    | 4      | 6      | 10  | 6     | 5     | 0 0 1            | 0 0 0         | 161 | 0.033            | 0.035             |
| 3192.229               | 3192.2289             |             | 0.151D-21         | 1590.691 | 7    | 5      | 2      | 8   | 7     | 1     | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.006             |
|                        | 3193.2233             |             |                   |          |      |        |        |     |       |       |                  |               |     | 0.002            |                   |
| 3193.345               | 3193.3421             | -17         | H 0.128D-21       | 5987.875 | 20   | 5      | 15     | 21  | 5     | 16    | 0 0 1            | 0 0 0         | 161 | 0.008            | 0.010             |
| 3194.043               | 3194.0386             | -9          | H 0.522D-22       | 5591.113 | 16   | 12     | 4      | 17  | 12    | 5     | 0 0 1            | 0 0 0         | 161 | 0.005            | 0.004             |
| 3194.043               |                       | D 0.174D-22 | 5591.113          | 16       | 12   | 5      | 17     | 12  | 6     |       | 0 0 1            | 0 0 0         | 161 |                  | 0.001             |
|                        | 3194.6605             |             |                   |          |      |        |        |     |       |       |                  |               |     | 0.006            |                   |
| 3195.473               | 3195.4813             |             | 0.555D-22         | 2309.731 | 7    | 2      | 5      | 7   | 1     | 6     | 0 3 0            | 0 1 0         | 161 | 0.007            | 0.002             |
| 3195.604               | 3195.6076             | 35          | H 0.125D-21       | 5739.230 | 19   | 7      | 13     | 20  | 7     | 14    | 0 0 1            | 0 0 0         | 161 | 0.008            | 0.009             |
| 3196.093               | 3196.0931             | -5          | C 0.530D-22       | 0.0      | 1    | 1      | 1      | 0   | 0     | 0     | 0 2 0            | 0 0 0         | 161 | 0.018            | 0.023             |
| 3196.645               | 3196.6457             | 12          | C 0.129D-22       | 285.419  | 4    | 2      | 3      | 3   | 3     | 0     | 0 2 0            | 0 0 0         | 161 | 0.002            | 0.003             |
| 3197.865               | 3197.8644             | -7          | C 0.286D-21       | 136.761  | 3    | 1      | 2      | 3   | 0     | 3     | 0 2 0            | 0 0 0         | 161 | 0.068            | 0.084             |
|                        | 3199.0745             |             |                   |          |      |        |        |     |       |       |                  |               |     | 0.002            |                   |
| 3199.724               | 3199.7254             | 11          | C 0.352D-22       | 134.902  | 3    | 1      | 2      | 2   | 2     | 1     | 0 2 0            | 0 0 0         | 161 | 0.009            | 0.010             |
| 3200.832               | 3200.8348             |             | 0.121D-21         | 1920.769 | 6    | 1      | 6      | 5   | 0     | 5     | 0 3 0            | 0 1 0         | 161 | 0.006            | 0.005             |
| 3200.923               | 3200.9236             |             | 0.283D-21         | 2629.337 | 12   | 3      | 9      | 13  | 5     | 8     | 0 0 1            | 0 0 0         | 161 | 0.011            | 0.012             |
| 3200.964               | 3200.9711             |             | 0.749D-22         | 3940.521 | 11   | 4      | 7      | 12  | 5     | 8     | 1 1 0            | 0 0 1         | 161 | 0.004            | 0.004             |
| 3202.013               | 3202.0119             |             | 0.471D-21         | 2054.369 | 9    | 6      | 4      | 10  | 7     | 3     | 1 0 0            | 0 0 0         | 161 | 0.018            | 0.018             |
| 3202.101               | 3202.1042             | 12          | H 0.143D-20       | 2054.348 | 9    | 6      | 3      | 10  | 7     | 4     | 1 0 0            | 0 0 0         | 161 | 0.052            | 0.055             |
| 3202.536               | 3202.5388             | 26          | H 0.108D-21       | 5495.090 | 17   | 10     | 8      | 18  | 10    | 9     | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.007             |
| 3203.323               | 3203.3252             | -3          | H 0.169D-21       | 5492.082 | 18   | 8      | 10     | 19  | 8     | 11    | 0 0 1            | 0 0 0         | 161 | 0.011            | 0.011             |
| 3203.328               |                       | D 0.451D-22 | 1581.336          | 9        | 5    | 4      | 10     | 4   | 7     |       | 0 2 0            | 0 0 0         | 161 |                  | 0.002             |
| 3203.464               | 3203.4647             | -1          | C 0.183D-20       | 2009.805 | 8    | 7      | 2      | 9   | 8     | 1     | 1 0 0            | 0 0 0         | 161 | 0.088            | 0.070             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C   | $S_{\text{calc}}$ | $E''$          | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO   | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|----------|-------------------|----------------|------|--------|--------|-----|-------|-------|------------------|---------------|-------|------------------|-------------------|
| 3203.466               |                       | D        | 0.610D-21         | 2009.805       | 8    | 7      | 1      | 9   | 8     | 2     | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.023             |
| 3203.769               | 3203.7707             | -3       | H 0.916D-22       | 6147.789       | 23   | 2      | 22     | 24  | 2     | 23    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.009 0.007       |
| 3203.769               |                       | D        | 0.305D-22         | 6147.789       | 23   | 1      | 22     | 24  | 1     | 23    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.002             |
| 3204.332               |                       | D        | 0.348D-22         | 6062.148       | 22   | 3      | 20     | 23  | 3     | 21    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.003             |
| 3204.334               | 3204.3327             | -8       | H 0.104D-21       | 6062.145       | 22   | 2      | 20     | 23  | 2     | 21    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.010 0.008       |
|                        | 3205.7478             | -27      | H                 |                |      |        |        |     |       |       |                  |               |       | 0.004            |                   |
|                        | 3206.3337             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.005            |                   |
| 3206.732               | 3206.7283             | -23      | H 0.126D-21       | 5928.355       | 21   | 4      | 18     | 22  | 4     | 19    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.006 0.009       |
| 3207.490               | 3207.4875             | -7       | H 0.859D-22       | 6172.004       | 24   | 0      | 24     | 25  | 0     | 25    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.011 0.007       |
| 3207.490               |                       | D        | 0.286D-22         | 6172.004       | 24   | 1      | 24     | 25  | 1     | 25    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.002             |
|                        | 3207.5511             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.007            |                   |
| 3208.807               | 3208.8070             | -1       | H 0.119D-20       | 1998.996       | 10   | 4      | 7      | 11  | 5     | 6     | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.054 0.046       |
| 3208.810               |                       | D        | 0.314D-21         | 2142.597       | 10   | 5      | 5      | 11  | 6     | 6     | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.012             |
| 3209.746               | 3209.7461             | -4       | C 0.220D-21       | 79.496         | 3    | 0      | 3      | 2   | 1     | 2     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.060 0.075       |
| 3210.113               |                       | D        | 0.645D-22         | 3306.296       | 7    | 6      | 2      | 8   | 7     | 1     | 1 1 0            | 0 1 0         | 1 0 0 | 161              | 0.003             |
| 3210.116               | 3210.1126             |          | 0.193D-21         | 3306.296       | 7    | 6      | 1      | 8   | 7     | 2     | 1 1 0            | 0 1 0         | 1 0 0 | 161              | 0.010 0.009       |
|                        | 3210.2240             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.004            |                   |
|                        | 3210.6778             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.015            |                   |
| 3210.860               | 3210.8587             | -9       | H 0.164D-21       | 5748.125       | 20   | 4      | 16     | 21  | 4     | 17    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.011 0.012       |
|                        | 3211.3884             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.004            |                   |
| 3211.553               | 3211.5558             |          | 0.507D-21         | 1875.464       | 9    | 4      | 5      | 10  | 6     | 4     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.017 0.019       |
| 3211.584               | 3211.5860             |          | 0.244D-22         | 6682.004       | 14   | 3      | 11     | 15  | 3     | 12    | 1 0 1            | 1 0 0         | 1 0 0 | 161              | 0.003 0.002       |
| 3211.589               | 3211.5860             |          | 0.218D-22         | 6807.668       | 15   | 3      | 13     | 16  | 3     | 14    | 1 0 1            | 1 0 0         | 1 0 0 | 161              | 0.003 0.002       |
| 3211.618               | 3211.6204             |          | 0.970D-22         | 5324.660       | 16   | 11     | 5      | 17  | 11    | 6     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.007 0.006       |
| 3211.619               |                       | D        | 0.323D-22         | 5324.660       | 16   | 11     | 6      | 17  | 11    | 7     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.002             |
| 3212.249               | 3212.2469             |          | 0.156D-21         | 3321.013       | 8    | 5      | 4      | 9   | 6     | 3     | 1 1 0            | 0 1 0         | 1 0 0 | 161              | 0.007 0.007       |
| 3213.152               | 3213.1505             | -107D-21 | 2205.652          | -11 2 9 12 4 8 |      |        |        |     |       |       | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.005 0.004       |
| 3213.404               | 3213.4069             | -9       | H 0.239D-21       | 4048.252       | 19   | 0      | 19     | 20  | 1     | 20    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.017 0.012       |
| 3213.404               |                       | D        | 0.798D-22         | 4048.252       | 19   | 1      | 19     | 20  | 0     | 20    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.004             |
| 3213.639               | 3213.6383             |          | 0.486D-22         | 2904.672       | 8    | 2      | 7      | 9   | 3     | 6     | 1 1 0            | 0 1 0         | 1 0 0 | 161              | 0.002 0.002       |
| 3213.749               |                       | D        | 0.695D-22         | 4021.219       | 18   | 1      | 17     | 19  | 2     | 18    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.004             |
| 3213.750               | 3213.7502             | 6        | H 0.208D-21       | 4021.218       | 18   | 2      | 17     | 19  | 1     | 18    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.014 0.011       |
| 3214.033               | 3214.0341             |          | 0.287D-21         | 1813.224       | 10   | 1      | 9      | 11  | 3     | 8     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.011 0.011       |
| 3214.123               | 3214.1222             | -9       | C 0.224D-21       | 23.794         | 2    | 1      | 2      | 1   | 0     | 1     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.071 0.089       |
| 3214.558               | 3214.5616             | 5        | H 0.205D-21       | 5527.047       | 19   | 6      | 14     | 20  | 6     | 15    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.013 0.014       |
| 3215.087               | 3215.0870             | -26      | H 0.172D-22       | 7261.289       | 23   | 1      | 23     | 24  | 1     | 24    | 0 1 1            | 0 1 0         | 1 0 0 | 161              | 0.002 0.002       |
| 3215.320               | 3215.3199             |          | 0.183D-21         | 1446.129       | 9    | 1      | 9      | 10  | 3     | 8     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.008 0.007       |
| 3216.246               | 3216.2458             | 10       | H 0.190D-21       | 3940.590       | 17   | 2      | 15     | 18  | 3     | 16    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.009 0.010       |
| 3216.368               | 3216.3940             |          | 0.633D-22         | 3040.544       | 17   | 3      | 15     | 18  | 2     | 16    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.003 0.003       |
| 3216.523               | 3216.5226             | 5        | C 0.765D-22       | 222.052        | 4    | 1      | 3      | 4   | 0     | 4     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.015 0.018       |
| 3217.368               | 3217.3606             | -75      | H 0.594D-22       | 5256.141       | 17   | 9      | 8      | 18  | 9     | 9     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.004 0.004       |
| 3217.389               | 3217.3934             | 40       | H 0.814D-22       | 5513.266       | 19   | 5      | 14     | 20  | 5     | 15    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.004 0.006       |
| 3217.553               | 3217.5510             | -1       | H 0.177D-21       | 5255.445       | 17   | 9      | 9      | 18  | 9     | 10    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.010 0.011       |
| 3218.713               | 3218.7140             |          | 0.895D-22         | 1394.814       | 6    | 5      | 2      | 7   | 7     | 1     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.003 0.004       |
| 3218.759               | 3218.7596             | 49       | C 0.268D-21       | 1394.814       | 6    | 5      | 1      | 7   | 7     | 0     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.011 0.011       |
| 3218.959               | 3218.9416             |          | 0.455D-22         | 2522.267       | 11   | 7      | 4      | 11  | 8     | 3     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.004 0.002       |
| 3219.285               | 3219.2881             | -33      | H 0.734D-22       | 5183.590       | 15   | 12     | 4      | 16  | 12    | 5     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.006 0.005       |
| 3219.285               |                       | D        | 0.245D-22         | 5183.590       | 15   | 12     | 3      | 16  | 12    | 4     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.002             |
| 3219.384               | 3219.3838             | 0        | C 0.284D-21       | 173.365        | 3    | 2      | 1      | 3   | 1     | 2     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.062 0.075       |
|                        | 3220.0835             |          |                   |                |      |        |        |     |       |       |                  |               |       | 0.003            |                   |
| 3220.288               | 3220.2937             |          | 0.338D-21         | 1631.251       | 8    | 4      | 5      | 9   | 6     | 4     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.013 0.013       |
| 3220.442               | 3220.4425             | 0        | C 0.117D-21       | 275.497        | 4    | 2      | 2      | 4   | 1     | 3     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.020 0.024       |
| 3220.776               | 3220.7764             |          | 0.565D-22         | 2392.594       | 7    | 3      | 4      | 7   | 2     | 5     | 0 3 0            | 0 1 0         | 1 0 1 | 161              | 0.003 0.002       |
| 3221.293               | 3221.2935             |          | 0.169D-21         | 3810.940       | 16   | 4      | 13     | 17  | 3     | 14    | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.007 0.008       |
| 3222.039               | 3222.0339             | -8       | C 0.542D-22       | 95.176         | 2    | 2      | 0      | 2   | 1     | 1     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.014 0.018       |
| 3223.457               | 3223.4563             |          | 0.593D-22         | 1437.969       | 9    | 0      | 9      | 10  | 2     | 8     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.003 0.002       |
| 3225.559               | 3225.5614             | 27       | H 0.392D-22       | 5066.223       | 14   | 13     | 1      | 15  | 13    | 2     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.004 0.002       |
| 3225.706               | 3225.7059             | -4       | C 0.254D-21       | 1122.709       | 7    | 1      | 6      | 8   | 4     | 5     | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.012 0.012       |
| 3226.069               | 3226.0686             | 6        | C 0.168D-21       | 1006.116       | 7    | 0      | 7      | 8   | 3     | 6     | 1 0 0            | 0 0 0         | 0 0 0 | 161              | 0.008 0.009       |
| 3227.465               | 3227.4644             |          | 0.338D-21         | 399.457        | 5    | 2      | 3      | 5   | 1     | 4     | 0 2 0            | 0 0 0         | 0 0 0 | 161              | 0.045 0.050       |
| 3227.751               | 3227.7506             |          | D 0.563D-22       | 5688.504       | 22   | 2      | 21     | 23  | 2     | 22    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.004             |
| 3227.751               | 3227.7506             | -7       | H 0.169D-21       | 5688.504       | 22   | 1      | 21     | 23  | 1     | 22    | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.016 0.012       |
| 3228.068               | 3228.0658             | -37      | H 0.170D-21       | 5070.020       | 16   | 10     | 6      | 17  | 10    | 7     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.012 0.011       |
|                        | 3228.072              |          | D 0.568D-22       | 5070.000       | 16   | 10     | 7      | 17  | 10    | 8     | 0 0 1            | 0 0 0         | 0 0 0 | 161              | 0.004             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3228.170               | 3228.1683             | 3      | H 0.191D-21       | 5604.312 | 21   | 3      | 19     | 22  | 3     | 20    | 0 0 1          | 0 0 0       | 161 | 0.017            | 0.013             |
| 3228.173               |                       |        | D 0.638D-22       | 5604.309 | 21   | 2      | 19     | 22  | 2     | 20    | 0 0 1          | 0 0 0       | 161 |                  | 0.004             |
|                        | 3228.4654             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.003             |
| 3228.907               | 3228.9081             | -59    | H 0.326D-22       | 6804.469 | 20   | 2      | 18     | 21  | 2     | 19    | 0 1 1          | 0 1 0       | 161 | 0.003            | 0.003             |
| 3229.039               | 3229.0401             | 15     | C 0.192D-20       | 1810.589 | 8    | 6      | 3      | 9   | 7     | 2     | 1 0 0          | 0 0 0       | 161 | 0.071            | 0.073             |
| 3229.058               |                       |        | 0.642D-21         | 1810.584 | 8    | 6      | 2      | 9   | 7     | 3     | 1 0 0          | 0 0 0       | 161 |                  | 0.024             |
| 3229.900               | 3229.9006             | 1      | C 0.981D-22       | 70.091   | 3    | 1      | 3      | 2   | 0     | 2     | 0 2 0          | 0 0 0       | 161 | 0.029            | 0.034             |
| 3230.285               | 3230.2842             |        | 0.802D-21         | 1718.719 | 9    | 3      | 7      | 10  | 5     | 6     | 0 0 1          | 0 0 0       | 161 | 0.030            | 0.031             |
| 3230.333               | 3230.3346             |        | 0.124D-21         | 3383.266 | 9    | 4      | 5      | 10  | 5     | 6     | 1 1 0          | 0 1 0       | 161 | 0.006            |                   |
| 3230.420               | 3230.4201             | -7     | C 0.126D-20       | 1631.384 | 8    | 4      | 4      | 9   | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.048            | 0.049             |
| 3230.511               | 3230.5152             | 47     | H 0.230D-21       | 5471.863 | 20   | 3      | 17     | 21  | 3     | 18    | 0 0 1          | 0 0 0       | 161 | 0.016            | 0.015             |
| 3230.986               |                       |        | D 0.779D-21       | 1789.041 | 7    | 7      | 1      | 8   | 8     | 0     | 1 0 0          | 0 0 0       | 161 |                  | 0.030             |
| 3230.986               | 3230.9836             | 9      | C 0.234D-20       | 1789.041 | 7    | 7      | 0      | 8   | 8     | 1     | 1 0 0          | 0 0 0       | 161 | 0.113            | 0.089             |
| 3231.325               | 3231.3313             | -17    | H 0.275D-21       | 5035.117 | 17   | 8      | 10     | 18  | 8     | 11    | 0 0 1          | 0 0 0       | 161 | 0.018            | 0.017             |
| 3231.336               |                       |        | D 0.159D-21       | 5713.250 | 23   | 1      | 23     | 24  | 1     | 24    | 0 0 1          | 0 0 0       | 161 |                  | 0.011             |
| 3231.336               |                       |        | D 0.531D-22       | 5713.250 | 23   | 0      | 23     | 24  | 0     | 24    | 0 0 1          | 0 0 0       | 161 |                  | 0.004             |
| 3232.274               | 3232.2737             | -3     | C 0.273D-22       | 206.301  | 4    | 1      | 3      | 3   | 2     | 2     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.007             |
| 3232.756               | 3232.7565             | -14    | H 0.127D-20       | 1874.974 | 9    | 5      | 4      | 10  | 6     | 5     | 1 0 0          | 0 0 0       | 161 | 0.046            | 0.048             |
| 3232.885               | 3232.8889             |        | 0.216D-21         | 1875.464 | 9    | 5      | 5      | 10  | 6     | 4     | 1 0 0          | 0 0 0       | 161 | 0.008            | 0.008             |
| 3233.019               | 3233.0192             | 0      | C 0.108D-21       | 142.278  | 4    | 0      | 4      | 3   | 1     | 3     | 0 2 0          | 0 0 0       | 161 | 0.025            | 0.031             |
| 3233.484               | 3233.4836             |        | 0.116D-21         | 2180.644 | 8    | 1      | 8      | 7   | 0     | 7     | 0 3 0          | 0 1 0       | 161 | 0.005            | 0.004             |
| 3233.985               | 3233.9902             | -62    | H 0.288D-21       | 1616.452 | 9    | 3      | 7      | 10  | 4     | 6     | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.011             |
| 3233.997               |                       |        | D 0.496D-22       | 6525.059 | 18   | 4      | 14     | 19  | 4     | 15    | 0 1 1          | 0 1 0       | 161 |                  | 0.004             |
| 3234.368               | 3234.3704             | 13     | H 0.385D-21       | 5199.598 | 18   | 6      | 12     | 19  | 6     | 13    | 0 0 1          | 0 0 0       | 161 | 0.021            | 0.024             |
| 3234.614               | 3234.6099             | -61    | H 0.995D-22       | 5292.098 | 19   | 4      | 15     | 20  | 4     | 16    | 0 0 1          | 0 0 0       | 161 | 0.006            |                   |
| 3234.692               | 3234.6936             | 30     | H 0.325D-22       | 6474.707 | 14   | 2      | 12     | 15  | 2     | 13    | 1 0 1          | 1 0 0       | 161 | 0.003            | 0.003             |
| 3235.133               | 3235.1333             | 3      | H 0.275D-21       | 5294.035 | 19   | 5      | 15     | 20  | 5     | 16    | 0 0 1          | 0 0 0       | 161 | 0.015            | 0.018             |
| 3235.454               | 3235.4523             | -31    | H 0.353D-22       | 6351.855 | 13   | 4      | 10     | 14  | 4     | 11    | 1 0 1          | 1 0 0       | 161 | 0.002            | 0.003             |
| 3236.239               | 3236.2108             |        | 0.470D-22         | 3535.871 | 10   | 2      | 8      | 11  | 4     | 7     | 0 1 1          | 0 1 0       | 161 | 0.003            | 0.002             |
| 3236.400               | 3236.3996             | -14    | C 0.441D-21       | 1581.336 | 9    | 2      | 8      | 10  | 4     | 7     | 0 0 1          | 0 0 0       | 161 | 0.017            | 0.017             |
| 3236.649               | 3236.6492             | 2      | C 0.118D-21       | 79.496   | 2    | 2      | 1      | 2   | 1     | 2     | 0 2 0          | 0 0 0       | 161 | 0.032            | 0.040             |
| 3236.871               | 3236.8705             |        | 0.881D-22         | 2919.634 | 7    | 3      | 5      | 8   | 5     | 4     | 0 1 1          | 0 1 0       | 161 | 0.004            | 0.004             |
| 3236.971               | 3236.9725             |        | 0.235D-21         | 3141.047 | 8    | 4      | 5      | 9   | 5     | 4     | 1 1 0          | 0 1 0       | 161 | 0.011            | 0.010             |
| 3237.055               |                       |        | D 0.474D-22       | 4919.246 | 15   | 11     | 4      | 16  | 11    | 5     | 0 0 1          | 0 0 0       | 161 |                  | 0.003             |
| 3237.055               | 3237.0557             | 18     | H 0.142D-21       | 4919.246 | 15   | 11     | 5      | 16  | 11    | 6     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.009             |
| 3237.342               | 3237.3426             |        | 0.235D-21         | 3109.911 | 6    | 6      | 1      | 7   | 7     | 0     | 1 1 0          | 0 1 0       | 161 | 0.012            | 0.010             |
| 3237.343               |                       |        | D 0.782D-22       | 3109.911 | 6    | 6      | 0      | 7   | 7     | 1     | 1 1 0          | 0 1 0       | 161 |                  | 0.003             |
| 3237.733               | 3237.7396             | 64     | H 0.369D-21       | 3675.116 | 18   | 1      | 18     | 19  | 0     | 19    | 1 0 0          | 0 0 0       | 161 | 0.030            | 0.018             |
| 3237.733               |                       |        | D 0.123D-21       | 3675.116 | 18   | 0      | 18     | 19  | 1     | 19    | 1 0 0          | 0 0 0       | 161 |                  | 0.006             |
| 3238.024               | 3238.0262             | 1      | H 0.319D-21       | 3647.465 | 17   | 1      | 16     | 18  | 2     | 17    | 1 0 0          | 0 0 0       | 161 | 0.019            | 0.015             |
| 3238.026               |                       |        | D 0.106D-21       | 3647.463 | 17   | 2      | 16     | 18  | 1     | 17    | 1 0 0          | 0 0 0       | 161 |                  | 0.005             |
|                        | 3238.3501             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.009             |
| 3238.880               | 3238.8766             | -18    | H 0.309D-22       | 6823.215 | 22   | 0      | 22     | 23  | 0     | 23    | 0 1 1          | 0 1 0       | 161 | 0.004            | 0.003             |
| 3239.097               | 3239.0970             |        | 0.677D-22         | 3101.144 | 7    | 5      | 3      | 8   | 6     | 2     | 1 1 0          | 0 1 0       | 161 | 0.002            | 0.003             |
| 3239.214               | 3239.2134             |        | 0.204D-21         | 3101.124 | 7    | 5      | 2      | 8   | 6     | 3     | 1 1 0          | 0 1 0       | 161 | 0.008            | 0.009             |
| 3239.608               | 3239.6049             | 27     | H 0.177D-21       | 2586.529 | 12   | 4      | 8      | 13  | 5     | 9     | 1 0 0          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3240.107               | 3240.1071             | 1      | C 0.177D-21       | 325.348  | 5    | 1      | 4      | 5   | 0     | 5     | 0 2 0          | 0 0 0       | 161 | 0.028            | 0.031             |
| 3240.182               | 3240.1765             | -35    | H 0.959D-22       | 3567.234 | 16   | 2      | 14     | 17  | 3     | 15    | 1 0 0          | 0 0 0       | 161 | 0.004            |                   |
| 3240.487               | 3240.4923             | 33     | H 0.286D-21       | 3567.180 | 16   | 3      | 14     | 17  | 2     | 15    | 1 0 0          | 0 0 0       | 161 | 0.013            |                   |
| 3241.426               | 3241.4235             | -31    | H 0.457D-21       | 5052.664 | 18   | 5      | 13     | 19  | 5     | 14    | 0 0 1          | 0 0 0       | 161 | 0.025            | 0.028             |
| 3241.753               | 3241.7524             | -12    | H 0.597D-22       | 6134.898 | 16   | 7      | 9      | 17  | 7     | 10    | 0 1 1          | 0 1 0       | 161 | 0.004            | 0.005             |
| 3241.773               | 3241.7741             | 2      | C 0.901D-22       | 542.906  | 6    | 2      | 4      | 6   | 1     | 5     | 0 2 0          | 0 0 0       | 161 | 0.008            | 0.010             |
| 3242.697               | 3242.6966             | -8     | H 0.244D-21       | 3439.308 | 15   | 3      | 12     | 16  | 4     | 13    | 1 0 0          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3242.948               | 3242.9530             |        | 0.138D-21         | 2300.689 | 11   | 3      | 8      | 12  | 5     | 7     | 0 0 1          | 0 0 0       | 161 | 0.005            | 0.005             |
| 3243.045               | 3243.0449             | -8     | C 0.481D-21       | 1282.919 | 8    | 2      | 7      | 9   | 3     | 6     | 1 0 0          | 0 0 0       | 161 | 0.020            |                   |
| 3243.159               | 3243.1606             | -26    | H 0.285D-21       | 4830.895 | 16   | 9      | 7      | 17  | 9     | 8     | 0 0 1          | 0 0 0       | 161 | 0.015            | 0.017             |
| 3243.257               | 3243.2575             | -149   | H 0.948D-22       | 4830.598 | 16   | 9      | 8      | 17  | 9     | 9     | 0 0 1          | 0 0 0       | 161 | 0.004            | 0.006             |
| 3243.367               | 3243.3657             | 31     | H 0.325D-21       | 4833.203 | 17   | 7      | 11     | 18  | 7     | 12    | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.019             |
| 3244.179               | 3244.1743             | -45    | H 0.255D-22       | 6082.402 | 14   | 10     | 4      | 15  | 10    | 5     | 0 1 1          | 0 1 0       | 161 | 0.005            | 0.002             |
| 3244.406               | 3244.4063             | 2      | C 0.345D-22       | 382.517  | 5    | 2      | 3      | 4   | 3     | 2     | 0 2 0          | 0 0 0       | 161 | 0.005            | 0.005             |
| 3244.644               |                       |        | D 0.314D-22       | 4796.961 | 14   | 12     | 3      | 15  | 12    | 4     | 0 0 1          | 0 0 0       | 161 |                  | 0.002             |
| 3244.644               | 3244.6389             | 6      | H 0.943D-22       | 4796.961 | 14   | 12     | 2      | 15  | 12    | 3     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.006             |
| 3244.943               | 3244.9427             | 3      | C 0.365D-21       | 136.761  | 4    | 1      | 4      | 3   | 0     | 3     | 0 2 0          | 0 0 0       | 161 | 0.086            | 0.105             |
| 3245.402               | 3245.4024             | 2      | C 0.554D-22       | 142.278  | 3    | 2      | 2      | 3   | 1     | 3     | 0 2 0          | 0 0 0       | 161 | 0.013            | 0.016             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3246.553               | 3246.5555             |        | 0.601D-21         | 1724.707 | 9    | 4      | 6      | 10  | 5     | 5     | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.023             |
|                        | 3247.2960             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.011            |                   |
| 3247.363               | 3247.3635             | 12     | C 0.970D-21       | 1411.612 | 7    | 4      | 4      | 8   | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.038            | 0.039             |
| 3248.922               | 3248.9255             |        | 0.106D-21         | 2337.669 | 9    | 0      | 9      | 8   | 1     | 8     | 0 3 0          | 0 1 0       | 161 | 0.004            | 0.004             |
| 3249.199               | 3249.1963             | -31    | H 0.704D-21       | 2275.373 | 11   | 4      | 7      | 12  | 5     | 8     | 1 0 0          | 0 0 0       | 161 | 0.026            | 0.027             |
| 3249.472               | 3249.4733             |        | 0.656D-22         | 982.912  | 7    | 1      | 7      | 8   | 2     | 6     | 1 0 0          | 0 0 0       | 161 | 0.003            | 0.003             |
| 3249.680               | 3249.6760             | -21    | H 0.146D-22       | 5996.680 | 13   | 11     | 3      | 14  | 11    | 4     | 0 1 1          | 0 1 0       | 161 | 0.003            | 0.001             |
| 3250.294               | 3250.2944             | 19     | H 0.908D-22       | 5965.715 | 16   | 6      | 10     | 17  | 6     | 11    | 0 1 1          | 0 1 0       | 161 | 0.006            | 0.007             |
| 3251.504               | 3251.5080             |        | 0.349D-21         | 1411.647 | 7    | 4      | 3      | 8   | 6     | 2     | 0 0 1          | 0 0 0       | 161 | 0.013            | 0.014             |
| 3251.582               |                       |        | D 0.101D-21       | 5246.078 | 21   | 1      | 20     | 22  | 1     | 21    | 0 0 1          | 0 0 0       | 161 |                  | 0.006             |
| 3251.583               | 3251.5812             | -11    | H 0.303D-21       | 5246.078 | 21   | 2      | 20     | 22  | 2     | 21    | 0 0 1          | 0 0 0       | 161 | 0.027            | 0.019             |
| 3251.788               | 3251.7863             |        | 0.136D-21         | 2998.768 | 8    | 3      | 6      | 9   | 4     | 5     | 1 1 0          | 0 1 0       | 161 | 0.005            | 0.006             |
| 3251.883               |                       |        | D 0.114D-21       | 5163.090 | 20   | 3      | 18     | 21  | 3     | 19    | 0 0 1          | 0 0 0       | 161 |                  | 0.007             |
| 3251.889               | 3251.8880             | -5     | H 0.342D-21       | 5163.082 | 20   | 2      | 18     | 21  | 2     | 19    | 0 0 1          | 0 0 0       | 161 | 0.027            | 0.021             |
|                        | 3252.4192             | -8     | H                 |          |      |        |        |     |       |       |                |             |     | 0.005            |                   |
|                        | 3253.5849             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.005            |                   |
| 3253.683               |                       |        | D 0.856D-22       | 4665.977 | 15   | 10     | 5      | 16  | 10    | 6     | 0 0 1          | 0 0 0       | 161 |                  | 0.005             |
| 3253.685               | 3253.6818             | -1     | H 0.257D-21       | 4665.969 | 15   | 10     | 6      | 16  | 10    | 7     | 0 0 1          | 0 0 0       | 161 | 0.017            | 0.015             |
| 3253.941               | 3253.9430             | 7      | H 0.528D-22       | 6430.797 | 20   | 1      | 19     | 21  | 1     | 20    | 0 1 1          | 0 1 0       | 161 | 0.009            | 0.004             |
| 3253.941               |                       |        | D 0.176D-22       | 6430.797 | 20   | 2      | 19     | 21  | 2     | 20    | 0 1 1          | 0 1 0       | 161 |                  | 0.001             |
| 3254.033               | 3254.0375             | 41     | H 0.407D-21       | 5031.977 | 19   | 4      | 16     | 20  | 4     | 17    | 0 0 1          | 0 0 0       | 161 | 0.025            | 0.025             |
| 3254.148               | 3254.1483             | -1     | C 0.398D-21       | 224.838  | 5    | 0      | 5      | 4   | 1     | 4     | 0 2 0          | 0 0 0       | 161 | 0.077            | 0.091             |
| 3254.625               | 3254.6228             | -22    | B 0.472D-22       | 1908.017 | 4    | 3      | 2      | 4   | 2     | 3     | 0 3 0          | 0 1 0       | 161 | 0.002            | 0.002             |
| 3254.625               | 3254.6228             | -22    | B 0.170D-22       | 610.341  | 6    | 3      | 4      | 5   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.002            | 0.002             |
| 3255.029               |                       |        | D 0.959D-22       | 5271.371 | 22   | 1      | 22     | 23  | 1     | 23    | 0 0 1          | 0 0 0       | 161 |                  | 0.006             |
| 3255.029               | 3255.0293             | -14    | H 0.288D-21       | 5271.371 | 22   | 0      | 22     | 23  | 0     | 23    | 0 0 1          | 0 0 0       | 161 | 0.027            | 0.018             |
| 3255.033               |                       |        | D 0.263D-22       | 2688.080 | 9    | 2      | 7      | 9   | 1     | 8     | 0 3 0          | 0 1 0       | 161 |                  | 0.001             |
|                        | 3255.9988             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.006            |                   |
| 3256.083               |                       |        | D 0.829D-21       | 1590.691 | 7    | 6      | 2      | 8   | 7     | 1     | 1 0 0          | 0 0 0       | 161 |                  | 0.032             |
| 3256.085               | 3256.0837             | -16    | C 0.249D-20       | 1590.690 | 7    | 6      | 1      | 8   | 7     | 2     | 1 0 0          | 0 0 0       | 161 | 0.124            | 0.096             |
| 3256.244               | 3256.2444             | -15    | H 0.456D-21       | 4612.789 | 16   | 8      | 8      | 17  | 8     | 9     | 0 0 1          | 0 0 0       | 161 | 0.022            | 0.026             |
| 3257.087               | 3257.0730             | 7      | H 0.150D-21       | 4610.020 | 16   | 8      | 9      | 17  | 8     | 10    | 0 0 1          | 0 0 0       | 161 | 0.008            | 0.008             |
| 3257.226               | 3257.2254             | -7     | C 0.175D-21       | 224.838  | 4    | 2      | 3      | 4   | 1     | 4     | 0 2 0          | 0 0 0       | 161 | 0.034            | 0.040             |
| 3257.553               | 3257.5544             | 11     | H 0.293D-22       | 6095.508 | 17   | 4      | 13     | 18  | 4     | 14    | 0 1 1          | 0 1 0       | 161 | 0.003            | 0.002             |
| 3257.708               | 3257.7088             | -18    | H 0.169D-21       | 4855.145 | 18   | 5      | 14     | 19  | 5     | 15    | 0 0 1          | 0 0 0       | 161 | 0.010            | 0.010             |
| 3258.074               | 3258.0734             | 1      | C 0.145D-20       | 1631.384 | 8    | 5      | 4      | 9   | 6     | 3     | 1 0 0          | 0 0 0       | 161 | 0.055            | 0.055             |
| 3258.154               | 3258.1585             |        | 0.570D-21         | 1631.251 | 8    | 5      | 3      | 9   | 6     | 4     | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.022             |
| 3258.270               | 3258.2723             | -3     | H 0.532D-21       | 4851.824 | 18   | 4      | 14     | 19  | 4     | 15    | 0 0 1          | 0 0 0       | 161 | 0.030            | 0.031             |
| 3258.893               | 3258.8920             | -23    | H 0.438D-22       | 6267.035 | 15   | 1      | 15     | 16  | 1     | 16    | 1 0 1          | 1 0 0       | 161 | 0.004            | 0.003             |
| 3258.893               |                       |        | D 0.146D-22       | 6267.035 | 15   | 0      | 15     | 16  | 0     | 16    | 1 0 1          | 1 0 0       | 161 |                  | 0.001             |
| 3259.540               | 3259.5377             | -45    | H 0.570D-22       | 6028.859 | 12   | 3      | 9      | 13  | 3     | 10    | 1 0 1          | 1 0 0       | 161 | 0.004            | 0.004             |
| 3259.706               | 3259.7031             |        | 0.660D-22         | 2920.133 | 7    | 3      | 4      | 8   | 5     | 3     | 0 1 1          | 0 1 0       | 161 | 0.004            | 0.003             |
|                        | 3260.1844             |        |                   |          |      |        |        |     |       |       |                |             |     | 0.003            |                   |
| 3260.428               | 3260.4265             | -9     | C 0.139D-21       | 222.052  | 5    | 1      | 5      | 4   | 0     | 4     | 0 2 0          | 0 0 0       | 161 | 0.028            | 0.032             |
| 3261.016               | 3261.0144             |        | 0.277D-21         | 1985.788 | 10   | 4      | 6      | 11  | 5     | 7     | 1 0 0          | 0 0 0       | 161 | 0.010            | 0.010             |
| 3261.162               | 3261.1626             | -4     | H 0.596D-21       | 4638.648 | 17   | 6      | 12     | 18  | 6     | 13    | 0 0 1          | 0 0 0       | 161 | 0.031            | 0.034             |
| 3261.829               | 3261.8298             | 2      | H 0.552D-21       | 3319.451 | 17   | 0      | 17     | 18  | 1     | 18    | 1 0 0          | 0 0 0       | 161 | 0.033            | 0.025             |
| 3261.829               |                       |        | D 0.184D-21       | 3319.451 | 17   | 1      | 17     | 18  | 0     | 18    | 1 0 0          | 0 0 0       | 161 |                  | 0.008             |
| 3262.067               |                       |        | D 0.157D-21       | 3291.152 | 16   | 1      | 15     | 17  | 2     | 16    | 1 0 0          | 0 0 0       | 161 |                  | 0.007             |
| 3262.071               | 3262.0687             | -18    | H 0.472D-21       | 3291.149 | 16   | 2      | 15     | 17  | 1     | 16    | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.021             |
| 3262.426               | 3262.4252             | -3     | H 0.540D-22       | 6402.156 | 21   | 1      | 21     | 22  | 1     | 22    | 0 1 1          | 0 1 0       | 161 | 0.007            | 0.004             |
| 3262.426               |                       |        | D 0.180D-22       | 6402.156 | 21   | 0      | 21     | 22  | 0     | 22    | 0 1 1          | 0 1 0       | 161 |                  | 0.001             |
| 3262.518               | 3262.5171             | 1      | C 0.640D-22       | 927.744  | 6    | 1      | 5      | 7   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.003            | 0.004             |
| 3262.582               | 3262.5822             | -10    | H 0.195D-21       | 4534.961 | 14   | 11     | 3      | 15  | 11    | 4     | 0 0 1          | 0 0 0       | 161 | 0.013            | 0.011             |
| 3262.583               |                       |        | D 0.650D-22       | 4534.961 | 14   | 11     | 4      | 15  | 11    | 5     | 0 0 1          | 0 0 0       | 161 |                  | 0.004             |
| 3263.265               |                       |        | D 0.164D-22       | 5062.020 | 10   | 0      | 10     | 11  | 1     | 11    | 1 0 1          | 0 0 1       | 161 |                  | 0.001             |
| 3263.275               | 3263.2738             | -10    | C 0.194D-21       | 704.214  | 7    | 2      | 5      | 7   | 1     | 6     | 0 2 0          | 0 0 0       | 161 | 0.015            | 0.015             |
| 3263.388               | 3263.4249             |        | 0.124D-21         | 3083.854 | 14   | 3      | 11     | 15  | 4     | 12    | 1 0 0          | 0 0 0       | 161 | 0.004            | 0.005             |
| 3263.493               | 3263.4903             | -15    | H 0.420D-21       | 3211.214 | 15   | 2      | 13     | 16  | 3     | 14    | 1 0 0          | 0 0 0       | 161 | 0.018            | 0.018             |
| 3264.384               | 3264.3901             | 64     | H 0.138D-21       | 3211.056 | 15   | 3      | 13     | 16  | 2     | 14    | 1 0 0          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3264.387               |                       |        | D 0.261D-22       | 6273.238 | 17   | 5      | 12     | 18  | 5     | 13    | 0 1 1          | 0 1 0       | 161 |                  | 0.002             |
| 3265.092               | 3265.0921             | 2      | C 0.133D-21       | 300.362  | 5    | 1      | 4      | 4   | 2     | 3     | 0 2 0          | 0 0 0       | 161 | 0.022            | 0.025             |
| 3265.314               | 3265.3141             |        | 0.313D-22         | 2512.378 | 10   | 0      | 10     | 9   | 1     | 9     | 0 3 0          | 0 1 0       | 161 | 0.002            | 0.001             |
| 3265.567               | 3265.5699             | -4     | H 0.278D-21       | 4606.199 | 17   | 5      | 12     | 18  | 5     | 13    | 0 0 1          | 0 0 0       | 161 | 0.014            | 0.016             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3265.904               |                       | D      | 0.250D-21         | 2905.435 | 6    | 5      | 2      | 7   | 6     | 1     | 1 1 0            | 0 1 0         | 161 | 0.010            |                   |
| 3265.915               | 3265.9120             | -12    | H 0.723D-21       | 4428.109 | 16   | 7      | 9      | 17  | 7     | 10    | 0 0 1            | 0 0 0         | 161 | 0.041            | 0.039             |
| 3266.086               | 3266.0864             |        | 0.417D-21         | 1474.981 | 8    | 3      | 6      | 9   | 5     | 5     | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.016             |
| 3266.385               | 3266.3853             | -3     | C 0.462D-22       | 446.697  | 6    | 1      | 5      | 6   | 0     | 6     | 0 2 0            | 0 0 0         | 161 | 0.005            | 0.006             |
| 3266.681               | 3266.6836             | 39     | H 0.475D-22       | 5887.770 | 11   | 5      | 7      | 12  | 5     | 8     | 1 0 1            | 1 0 0         | 161 | 0.002            | 0.003             |
|                        | 3267.3754             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.008            |                   |
| 3267.484               | 3267.4835             | -3     | H 0.736D-21       | 4291.906 | 16   | 6      | 10     | 17  | 6     | 11    | 0 0 1            | 0 0 0         | 161 | 0.034            | 0.039             |
|                        | 3267.6235             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.003            |                   |
| 3268.408               |                       | D      | 0.507D-22         | 2161.286 | 6    | 3      | 4      | 6   | 2     | 5     | 0 3 0            | 0 1 0         | 161 | 0.002            |                   |
| 3268.414               | 3268.4134             |        | 0.609D-22         | 4564.113 | 15   | 1      | 14     | 16  | 2     | 15    | 1 1 0            | 0 1 0         | 161 | 0.005            | 0.003             |
| 3268.992               |                       | D      | 0.199D-22         | 4074.046 | 12   | 3      | 9      | 13  | 4     | 10    | 1 1 0            | 0 1 0         | 161 | 0.001            |                   |
| 3269.003               | 3269.0019             | -81    | H 0.146D-21       | 4427.258 | 15   | 9      | 6      | 16  | 9     | 7     | 0 0 1            | 0 0 0         | 161 | 0.006            | 0.008             |
| 3269.041               | 3269.0445             | 36     | H 0.437D-21       | 4427.117 | 15   | 9      | 7      | 16  | 9     | 8     | 0 0 1            | 0 0 0         | 161 | 0.017            | 0.024             |
| 3270.113               | 3270.1072             | -64    | H 0.105D-21       | 4431.637 | 13   | 12     | 2      | 14  | 12    | 3     | 0 0 1            | 0 0 0         | 161 | 0.005            | 0.006             |
| 3270.113               |                       | D      | 0.349D-22         | 4431.637 | 13   | 12     | 1      | 14  | 12    | 2     | 0 0 1            | 0 0 0         | 161 | 0.002            |                   |
| 3270.427               | 3270.4269             | 3      | C 0.232D-21       | 782.410  | 7    | 3      | 4      | 7   | 2     | 5     | 0 2 0            | 0 0 0         | 161 | 0.012            | 0.016             |
| 3271.020               | 3271.0198             | 1      | C 0.826D-22       | 602.774  | 6    | 3      | 3      | 6   | 2     | 4     | 0 2 0            | 0 0 0         | 161 | 0.009            | 0.008             |
|                        | 3271.0717             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.007            |                   |
|                        | 3271.4437             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.006            |                   |
| 3271.481               | 3271.4694             | -26    | H 0.210D-21       | 4409.312 | 16   | 7      | 10     | 17  | 7     | 11    | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.011             |
| 3271.673               | 3271.6758             | 17     | H 0.320D-21       | 3080.181 | 14   | 4      | 11     | 15  | 3     | 12    | 1 0 0            | 0 0 0         | 161 | 0.013            | 0.014             |
| 3271.890               | 3271.8903             | -4     | C 0.539D-22       | 326.625  | 5    | 2      | 4      | 5   | 1     | 5     | 0 2 0            | 0 0 0         | 161 | 0.007            | 0.009             |
| 3272.052               | 3272.0506             |        | 0.524D-21         | 1899.008 | 10   | 2      | 8      | 11  | 4     | 7     | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.020             |
| 3273.404               | 3273.4035             |        | 0.941D-21         | 1718.719 | 9    | 4      | 5      | 10  | 5     | 6     | 1 0 0            | 0 0 0         | 161 | 0.030            | 0.035             |
| 3273.427               | 3273.4273             | 3      | C 0.145D-21       | 326.625  | 6    | 0      | 6      | 5   | 1     | 5     | 0 2 0            | 0 0 0         | 161 | 0.020            | 0.025             |
| 3273.725               |                       | D      | 0.433D-22         | 5762.059 | 10   | 6      | 4      | 11  | 6     | 5     | 1 0 1            | 1 0 0         | 161 | 0.003            |                   |
| 3273.731               | 3273.7311             |        | 0.188D-21         | 2919.634 | 7    | 4      | 3      | 8   | 5     | 4     | 1 1 0            | 0 1 0         | 161 | 0.007            | 0.008             |
| 3273.774               | 3273.7737             | -3     | C 0.210D-21       | 42.372   | 2    | 2      | 1      | 1   | 1     | 0     | 0 2 0            | 0 0 0         | 161 | -0.061           | 0.078             |
| 3273.875               | 3273.8756             |        | 0.257D-21         | 1216.189 | 6    | 4      | 3      | 7   | 6     | 2     | 0 0 1            | 0 0 0         | 161 | 0.008            | 0.011             |
| 3274.637               | 3274.6411             |        | 0.496D-21         | 1998.996 | 10   | 3      | 7      | 11  | 5     | 6     | 0 0 1            | 0 0 0         | 161 | 0.020            | 0.019             |
| 3275.176               | 3275.1744             | -13    | C 0.787D-21       | 1216.194 | 6    | 4      | 2      | 7   | 6     | 1     | 0 0 1            | 0 0 0         | 161 | 0.030            | 0.034             |
| 3275.256               |                       | D      | 0.177D-21         | 4820.645 | 20   | 2      | 19     | 21  | 2     | 20    | 0 0 1            | 0 0 0         | 161 | 0.010            |                   |
| 3275.256               | 3275.2575             | 2      | H 0.530D-21       | 4820.645 | 20   | 1      | 19     | 21  | 1     | 20    | 0 0 1            | 0 0 0         | 161 | 0.036            | 0.031             |
| 3275.476               | 3275.4752             | -13    | H 0.593D-21       | 4738.637 | 19   | 3      | 17     | 20  | 3     | 18    | 0 0 1            | 0 0 0         | 161 | 0.034            | 0.034             |
| 3275.484               |                       | D      | 0.198D-21         | 4738.625 | 19   | 2      | 17     | 20  | 2     | 18    | 0 0 1            | 0 0 0         | 161 | 0.011            |                   |
| 3275.927               | 3275.9304             | 7      | H 0.958D-22       | 5970.941 | 18   | 2      | 16     | 19  | 2     | 17    | 0 1 1            | 0 1 0         | 161 | 0.007            | 0.007             |
| 3276.221               | 3276.2206             | 0      | C 0.231D-21       | 446.511  | 5    | 3      | 2      | 5   | 2     | 3     | 0 2 0            | 0 0 0         | 161 | 0.027            | 0.030             |
| 3276.511               | 3276.5108             | -3     | C 0.444D-21       | 325.348  | 6    | 1      | 6      | 5   | 0     | 5     | 0 2 0            | 0 0 0         | 161 | 0.068            | 0.078             |
|                        | 3277.2418             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.010            |                   |
| 3277.611               |                       | D      | 0.897D-22         | 6022.801 | 19   | 2      | 18     | 20  | 2     | 19    | 0 1 1            | 0 1 0         | 161 | 0.007            |                   |
| 3277.613               |                       | D      | 0.299D-22         | 6022.801 | 19   | 1      | 18     | 20  | 1     | 19    | 0 1 1            | 0 1 0         | 161 | 0.002            |                   |
| 3277.613               | 3277.6126             | -21    | H 0.360D-21       | 1718.719 | 9    | 6      | 3      | 10  | 5     | 6     | 0 2 0            | 0 0 0         | 161 | 0.022            | 0.014             |
| 3277.703               | 3277.7026             | 9      | H 0.705D-21       | 4608.227 | 18   | 3      | 15     | 19  | 3     | 16    | 0 0 1            | 0 0 0         | 161 | 0.032            | 0.039             |
| 3277.825               | 3277.8246             |        | 0.231D-21         | 4608.578 | 18   | 4      | 15     | 19  | 4     | 16    | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.013             |
| 3278.565               | 3278.5655             | 12     | H 0.506D-21       | 4846.496 | 21   | 1      | 21     | 22  | 1     | 22    | 0 0 1            | 0 0 0         | 161 | 0.038            | 0.030             |
| 3278.565               |                       | D      | 0.169D-21         | 4846.496 | 21   | 0      | 21     | 22  | 0     | 22    | 0 0 1            | 0 0 0         | 161 | 0.010            |                   |
| 3279.097               | 3279.0964             | 4      | C 0.252D-20       | 1477.297 | 8    | 4      | 5      | 9   | 5     | 4     | 1 0 0            | 0 0 0         | 161 | 0.088            | 0.099             |
| 3279.255               | 3279.2590             | 6      | H 0.663D-22       | 5862.344 | 12   | 2      | 10     | 13  | 2     | 11    | 1 0 1            | 1 0 0         | 161 | 0.006            | 0.005             |
| 3279.258               |                       | D      | 0.283D-22         | 5567.984 | 14   | 8      | 7      | 15  | 8     | 8     | 0 1 1            | 0 1 0         | 161 | 0.002            |                   |
| 3279.373               | 3279.3709             | -10    | H 0.367D-21       | 4283.305 | 14   | 10     | 4      | 15  | 10    | 5     | 0 0 1            | 0 0 0         | 161 | 0.018            | 0.019             |
| 3279.375               |                       | D      | 0.122D-21         | 4283.301 | 14   | 10     | 5      | 15  | 10    | 6     | 0 0 1            | 0 0 0         | 161 | 0.006            |                   |
| 3280.074               | 3280.0739             | 1      | C 0.611D-22       | 37.137   | 2    | 2      | 0      | 1   | 1     | 1     | 0 2 0            | 0 0 0         | 161 | 0.018            | 0.023             |
| 3280.891               | 3280.8931             | 18     | H 0.856D-21       | 4432.863 | 17   | 5      | 13     | 18  | 5     | 14    | 0 0 1            | 0 0 0         | 161 | 0.037            | 0.046             |
|                        | 3280.9850             |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.005            |                   |
| 3281.017               | 3281.0207             | 33     | H 0.152D-21       | 5680.555 | 16   | 4      | 12     | 17  | 4     | 13    | 0 1 1            | 0 1 0         | 161 | 0.008            | 0.010             |
| 3281.817               | 3281.8153             | 13     | H 0.309D-21       | 4427.160 | 17   | 4      | 13     | 18  | 4     | 14    | 0 0 1            | 0 0 0         | 161 | 0.014            | 0.017             |
| 3282.836               | 3282.8341             | 48     | H 0.529D-21       | 2746.024 | 13   | 3      | 10     | 14  | 4     | 11    | 1 0 0            | 0 0 0         | 161 | 0.019            | 0.021             |
| 3282.972               | 3282.9735             | -18    | H 0.702D-21       | 4206.332 | 15   | 8      | 8      | 16  | 8     | 9     | 0 0 1            | 0 0 0         | 161 | 0.028            | 0.036             |
| 3283.062               | 3283.0617             | 1      | C 0.308D-20       | 1394.814 | 6    | 6      | 1      | 7   | 7     | 0     | 1 0 0            | 0 0 0         | 161 | 0.146            | 0.123             |
| 3283.062               |                       | D      | 0.103D-20         | 1394.814 | 6    | 6      | 0      | 7   | 7     | 1     | 1 0 0            | 0 0 0         | 161 | 0.041            |                   |
| 3283.753               |                       | D      | 0.182D-22         | 6955.305 | 15   | 5      | 11     | 16  | 5     | 12    | 0 2 1            | 0 2 0         | 161 | 0.002            |                   |
| 3283.763               | 3283.7627             | -4     | C 0.142D-20       | 1360.236 | 8    | 3      | 6      | 9   | 4     | 5     | 1 0 0            | 0 0 0         | 161 | 0.050            | 0.058             |
| 3284.131               | 3284.1272             |        | 0.253D-22         | 4188.395 | 6    | 3      | 4      | 7   | 4     | 3     | 1 2 0            | 0 2 0         | 161 | 0.007            | 0.001             |
| 3284.190               | 3284.1947             | -53    | B 0.730D-21       | 1411.647 | 7    | 5      | 3      | 8   | 6     | 2     | 1 0 0            | 0 0 0         | 161 | 0.027            | 0.029             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$      | $J'$     | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |     |       |       |       |       |
|------------------------|-----------------------|--------|-------------------|------------|----------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|-----|-------|-------|-------|-------|
| 3284.224               | 3284.2253             | 10     | C                 | 0.227D-20  | 1411.612 | 7      | 5      | 2   | 8     | 6     | 3              | 1           | 0   | 0                | 0                 | 161 | 0.082 | 0.090 |       |       |
| 3284.561               | 3284.5737             |        |                   | 0.137D-21  | 5512.023 | 15     | 6      | 10  | 16    | 6     | 11             | 0           | 1   | 1                | 0                 | 161 | 0.007 | 0.009 |       |       |
| 3285.007               | 3285.0002             | 0      | H                 | 0.322D-21  | 4221.012 | 16     | 6      | 11  | 17    | 6     | 12             | 0           | 0   | 1                | 0                 | 0   | 161   | 0.013 | 0.017 |       |
| 3285.052               | 3285.0515             |        |                   | 0.212D-21  | 1340.886 | 8      | 2      | 7   | 9     | 4     | 6              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.009 | 0.009 |
| 3285.673               |                       |        | D                 | 0.267D-21  | 2981.363 | 16     | 0      | 16  | 17    | 1     | 17             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.011 |       |
| 3285.673               | 3285.6724             | -35    | H                 | 0.801D-21  | 2981.363 | 16     | 1      | 16  | 17    | 0     | 17             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.038 | 0.034 |
| 3285.759               | 3285.7587             | -25    | H                 | 0.918D-22  | 5998.164 | 20     | 0      | 20  | 21    | 0     | 21             | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.010 | 0.007 |
| 3285.759               |                       |        | D                 | 0.306D-22  | 5998.164 | 20     | 1      | 20  | 21    | 1     | 21             | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.002 |       |
| 3285.819               | 3285.8200             | -50    | H                 | 0.678D-21  | 2952.396 | 15     | 1      | 14  | 16    | 2     | 15             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.021 | 0.028 |
| 3285.831               |                       |        | D                 | -0.226D-21 | 2952.389 | 15     | 2      | 14  | 16    | 1     | 15             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.009 |       |
| 3286.169               | 3286.1696             | -4     | B                 | 0.244D-21  | 1201.922 | 8      | 0      | 8   | 9     | 2     | 7              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.007 | 0.011 |
|                        | 3287.2464             |        |                   |            |          |        |        |     |       |       |                |             |     |                  |                   |     |       |       | 0.007 |       |
| 3288.100               | 3288.0982             | -58    | H                 | 0.581D-21  | 2872.278 | 14     | 3      | 12  | 15    | 2     | 13             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.022 | 0.024 |
| 3288.203               | 3288.2039             | 17     | H                 | 0.244D-21  | 4172.148 | 13     | 11     | 3   | 14    | 11    | 4              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.012 | 0.013 |
| 3288.203               |                       |        | D                 | 0.814D-22  | 4172.148 | 13     | 11     | 2   | 14    | 11    | 3              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.004 |       |
| 3288.483               | 3288.4828             | 4      | C                 | 0.119D-21  | 212.156  | 3      | 3      | 0   | 3     | 2     | 1              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.019 | 0.028 |
| 3288.555               | 3288.5512             | -36    | H                 | 0.181D-21  | 2872.572 | 14     | 2      | 12  | 15    | 3     | 13             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.009 | 0.007 |
| 3288.918               | 3288.9193             | 8      | C                 | 0.138D-21  | 447.252  | 6      | 2      | 5   | 6     | 1     | 6              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.015 | 0.018 |
| 3290.199               | 3290.2011             | 8      | H                 | 0.146D-20  | 4174.285 | 16     | 5      | 11  | 17    | 5     | 12             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.060 | 0.075 |
|                        | 3290.3475             |        |                   |            |          |        |        |     |       |       |                |             |     |                  |                   |     |       |       | 0.005 |       |
| 3291.357               | 3291.3574             | 4      | C                 | 0.439D-21  | 447.252  | 7      | 0      | 7   | 6     | 1     | 6              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.051 | 0.057 |
| 3292.505               | 3292.5043             | -3     | C                 | 0.702D-22  | 95.176   | 3      | 2      | 2   | 2     | 1     | 1              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.018 | 0.022 |
| 3292.615               |                       |        | D                 | 0.977D-22  | 2733.965 | 5      | 5      | 1   | 6     | 6     | 0              | 1           | 1   | 0                | 0                 | 1   | 0     | 161   | 0.004 |       |
| 3292.617               | 3292.6199             |        |                   | 0.293D-21  | 2733.965 | 5      | 5      | 0   | 6     | 6     | 1              | 1           | 1   | 0                | 0                 | 1   | 0     | 161   | 0.012 | 0.012 |
| 3292.812               |                       |        | D                 | 0.105D-21  | 756.725  | 5      | 1      | 4   | 6     | 4     | 3              | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.007 |       |
| 3292.822               | 3292.8213             | -9     | C                 | 0.148D-21  | 446.697  | 7      | 1      | 7   | 6     | 0     | 6              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.018 | 0.019 |
| 3293.093               | 3293.0926             | -3     | C                 | 0.110D-21  | 586.243  | 7      | 1      | 6   | 7     | 0     | 7              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.008 | 0.011 |
| 3293.326               | 3293.3365             | -25    | H                 | 0.374D-21  | 4016.170 | 15     | 7      | 8   | 16    | 7     | 9              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.013 | 0.019 |
| 3293.426               | 3293.4284             |        |                   | 0.206D-22  | 5601.531 | 10     | 5      | 6   | 11    | 5     | 7              | 1           | 0   | 1                | 1                 | 0   | 0     | 161   | 0.009 | 0.001 |
| 3294.058               | 3294.0588             | 16     | C                 | 0.478D-21  | 1474.981 | 8      | 4      | 4   | 9     | 5     | 5              | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.016 | 0.019 |
| 3294.210               | 3294.2107             | 10     | C                 | 0.393D-22  | 206.301  | 3      | 3      | 1   | 3     | 2     | 2              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.011 | 0.009 |
| 3294.252               | 3294.2518             | -7     | H                 | 0.437D-22  | 5381.543 | 12     | 10     | 2   | 13    | 10    | 3              | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.006 | 0.003 |
| 3294.883               | 3294.8842             | -28    | H                 | 0.641D-21  | 4045.316 | 14     | 9      | 5   | 15    | 9     | 6              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.026 | 0.032 |
| 3294.893               |                       |        | D                 | 0.214D-21  | 4045.289 | 14     | 9      | 6   | 15    | 9     | 7              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.011 |       |
| 3296.645               | 3296.6451             | 2      | H                 | 0.105D-20  | 4006.071 | 15     | 7      | 9   | 16    | 7     | 10             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.040 | 0.052 |
| 3297.137               | 3297.1360             | -15    | H                 | 0.490D-21  | 3870.212 | 15     | 6      | 9   | 16    | 6     | 10             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.020 | 0.024 |
| 3297.504               | 3297.5037             | -4     | C                 | 0.179D-21  | 300.362  | 4      | 3      | 2   | 4     | 2     | 3              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.028 | 0.033 |
| 3298.107               | 3298.1072             | 3      | C                 | 0.181D-20  | 1255.167 | 7      | 3      | 5   | 8     | 5     | 4              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.069 | 0.077 |
| 3298.153               | 3298.1529             | -10    | H                 | 0.150D-21  | 5579.500 | 17     | 3      | 15  | 18    | 3     | 16             | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.007 | 0.010 |
| 3298.427               | 3298.4480             |        |                   | 0.130D-21  | 2739.446 | 13     | 4      | 10  | 14    | 3     | 11             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.005 |       |
| 3298.776               | 3298.7726             | -22    | H                 | 0.901D-21  | 4412.316 | 19     | 2      | 18  | 20    | 2     | 19             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.057 | 0.048 |
| 3298.777               |                       |        | D                 | 0.300D-21  | 4412.316 | 19     | 1      | 18  | 20    | 1     | 19             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.016 |       |
| 3298.914               |                       |        |                   | 0.333D-21  | 4331.094 | 18     | 3      | 16  | 19    | 3     | 17             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.018 |       |
| 3298.941               | 3298.9427             | 33     | H                 | 0.100D-20  | 4331.070 | 18     | 2      | 16  | 19    | 2     | 17             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.046 | 0.053 |
|                        | 3299.5255             |        |                   |            |          |        |        |     |       |       |                |             |     |                  |                   |     |       |       | 0.005 |       |
| 3299.869               | 3299.8669             | -23    | H                 | 0.242D-21  | 2426.195 | 12     | 3      | 9   | 13    | 4     | 10             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.011 | 0.009 |
| 3300.139               | 3300.1371             | 3      | H                 | 0.183D-21  | 5466.402 | 16     | 3      | 13  | 17    | 3     | 14             | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.013 | 0.012 |
| 3300.214               | 3300.2143             | -4     | C                 | 0.435D-21  | 1045.058 | 5      | 4      | 2   | 6     | 6     | 1              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.020 | 0.021 |
| 3301.100               |                       |        |                   | 0.395D-21  | 4201.285 | 17     | 3      | 14  | 18    | 3     | 15             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.020 |       |
| 3301.216               | 3301.2152             | 15     | H                 | 0.117D-20  | 4201.855 | 17     | 4      | 14  | 18    | 4     | 15             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.051 | 0.060 |
| 3301.937               | 3301.9369             | 2      | H                 | 0.864D-21  | 4438.750 | 20     | 0      | 20  | 21    | 0     | 21             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.060 | 0.047 |
| 3301.937               |                       |        | D                 | 0.288D-21  | 4438.750 | 20     | 1      | 20  | 21    | 1     | 21             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.016 |       |
| 3302.205               | 3302.2088             | -41    | H                 | 0.198D-21  | 5310.246 | 15     | 5      | 11  | 16    | 5     | 12             | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.014 | 0.013 |
| 3303.074               | 3303.0730             | -21    | C                 | 0.256D-21  | 1050.158 | 7      | 2      | 6   | 8     | 3     | 5              | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.008 | 0.013 |
| 3303.284               | 3303.2844             | 4      | C                 | 0.661D-22  | 416.209  | 5      | 3      | 3   | 5     | 2     | 4              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.008 | 0.009 |
| 3303.550               | 3303.5464             | -59    | H                 | 0.877D-22  | 5579.492 | 11     | 3      | 9   | 12    | 3     | 10             | 1           | 0   | 1                | 1                 | 0   | 0     | 161   | 0.006 | 0.006 |
| 3303.989               | 3303.9898             | 12     | H                 | 0.464D-21  | 4027.494 | 16     | 5      | 12  | 17    | 5     | 13             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.019 | 0.023 |
| 3304.136               | 3304.1393             | 1      | H                 | 0.222D-21  | 5152.969 | 14     | 6      | 8   | 15    | 6     | 9              | 0           | 1   | 1                | 0                 | 1   | 0     | 161   | 0.009 | 0.014 |
| 3305.139               |                       |        | D                 | 0.163D-21  | 3922.325 | 13     | 10     | 3   | 14    | 10    | 4              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.008 |       |
| 3305.140               | 3305.1391             | -109   | H                 | 0.489D-21  | 3922.324 | 13     | 10     | 4   | 14    | 10    | 5              | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.027 | 0.024 |
| 3305.200               | 3305.2004             | 1      | H                 | 0.159D-20  | 4017.909 | 16     | 4      | 12  | 17    | 4     | 13             | 0           | 0   | 1                | 0                 | 0   | 0     | 161   | 0.066 | 0.079 |
| 3307.186               | 3307.1865             | 3      | H                 | 0.488D-21  | 4291.906 | 16     | 7      | 10  | 17    | 6     | 11             | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.017 | 0.026 |
| 3308.077               | 3308.0774             | -5     | C                 | 0.109D-20  | 1255.913 | 7      | 4      | 4   | 8     | 5     | 3              | 1           | 0   | 0                | 0                 | 0   | 0     | 161   | 0.041 | 0.046 |
| 3308.321               | 3308.3201             | 7      | C                 | 0.140D-21  | 586.479  | 8      | 0      | 8   | 7     | 1     | 7              | 0           | 2   | 0                | 0                 | 0   | 0     | 161   | 0.014 | 0.013 |

## HIGH-TEMPERATURE WATER VAPOR SPECTRUM

433

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO   | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-------|------------------|-------------------|
| 3308.649               | 3308.6459             |             | 0.256D-21         | 5015.703 | 14   | 5      | 9      | 15  | 5     | 10    | 0 1 1            | 0 1 0         | 161   | 0.015            | 0.015             |
| 3308.699               | 3308.6990             | 2           | C 0.218D-21       | 173.365  | 4    | 2      | 3      | 3   | 1     | 2     | 0 2 0            | 0 0 0         | 161   | 0.047            | 0.056             |
| 3308.786               | 3308.7816             | -87         | H 0.105D-20       | 3824.994 | 14   | 8      | 6      | 15  | 8     | 7     | 0 0 1            | 0 0 0         | 161   | 0.042            | 0.050             |
| 3308.888               |                       | D 0.506D-22 | 5611.332          | 19       | 0    | 19     | 20     | 0   | 20    | 0     | 1 1 1            | 0 1 0         | 161   |                  | 0.003             |
| 3308.888               | 3308.8879             | 6           | H 0.152D-21       | 5611.332 | 19   | 1      | 19     | 20  | 1     | 20    | 0 1 1            | 0 1 0         | 161   | 0.013            | 0.010             |
| 3308.989               | 3308.9842             | 108         | H 0.350D-21       | 3824.496 | 14   | 8      | 7      | 15  | 8     | 8     | 0 0 1            | 0 0 0         | 161   | 0.014            | 0.017             |
| 3309.009               | 3309.0098             | 3           | C 0.420D-21       | 586.243  | 8    | 1      | 8      | 7   | 0     | 7     | 0 2 0            | 0 0 0         | 161   | 0.037            | 0.040             |
| 3309.259               | 3309.2556             | -37         | H 0.113D-20       | 2660.950 | 15   | 0      | 15     | 16  | 1     | 16    | 1 0 0            | 0 0 0         | 161   | 0.067            | 0.045             |
| 3309.259               |                       | D 0.375D-21 | 2660.950          | 15       | 1    | 15     | 16     | 0   | 16    | 1 0 0 | 0 0 0            | 161           |       | 0.015            |                   |
| 3309.261               |                       | D 0.314D-21 | 2631.282          | 14       | 1    | 13     | 15     | 2   | 14    | 1 0 0 | 0 0 0            | 161           |       | 0.012            |                   |
| 3309.367               |                       | 0.941D-21   | 2631.272          | 14       | 2    | 13     | 15     | 1   | 14    | 1 0 0 | 0 0 0            | 161           |       | 0.037            |                   |
| 3309.384               | 3309.3807             | 18          | H 0.152D-20       | 3822.246 | 15   | 6      | 10     | 16  | 6     | 11    | 0 0 1            | 0 0 0         | 161   | 0.070            | 0.073             |
| 3309.388               |                       | D 0.503D-22 | 2983.324          | 8        | 3    | 5      | 9      | 4   | 6     | 1 1 0 | 0 1 0            | 161           |       | 0.002            |                   |
| 3310.526               | 3310.5257             | -3          | C 0.290D-20       | 1216.194 | 6    | 5      | 2      | 7   | 6     | 1     | 1 0 0            | 0 0 0         | 161   | 0.146            | 0.125             |
| 3310.531               |                       | D 0.972D-21 | 1216.189          | 6        | 5    | 1      | 7      | 6   | 2     | 1 0 0 | 0 0 0            | 161           |       | 0.042            |                   |
| 3310.856               | 3310.8553             | -35         | H 0.783D-21       | 2551.486 | 13   | 2      | 11     | 14  | 3     | 12    | 1 0 0            | 0 0 0         | 161   | 0.028            | 0.031             |
| 3311.582               | 3311.5844             | 44          | H 0.260D-21       | 2550.883 | 13   | 3      | 11     | 14  | 2     | 12    | 1 0 0            | 0 0 0         | 161   | 0.008            | 0.010             |
| 3312.055               | 3312.0539             | -10         | C 0.188D-21       | 552.912  | 6    | 3      | 4      | 6   | 2     | 5     | 0 2 0            | 0 0 0         | 161   | 0.017            | 0.019             |
| 3313.253               | 3313.2529             | -1          | C 0.136D-21       | 79.496   | 3    | 2      | 1      | 2   | 1     | 2     | 0 2 0            | 0 0 0         | 161   | 0.035            | 0.045             |
| 3313.394               | 3313.3936             | -5          | C 0.271D-21       | 782.410  | 6    | 1      | 6      | 7   | 2     | 5     | 1 0 0            | 0 0 0         | 161   | 0.016            | 0.018             |
| 3313.930               | 3313.9270             | -22         | H 0.265D-21       | 3831.174 | 12   | 11     | 1      | 13  | 11    | 2     | 0 0 1            | 0 0 0         | 161   | 0.013            | 0.013             |
| 3313.930               |                       | D 0.882D-22 | 3831.173          | 12       | 11   | 2      | 13     | 11  | 3     | 0 0 1 | 0 0 0            | 161           |       | 0.004            |                   |
| 3314.105               | 3314.1045             | -6          | H 0.951D-21       | 2124.953 | 11   | 3      | 8      | 12  | 4     | 9     | 1 0 0            | 0 0 0         | 161   | 0.032            | 0.036             |
| 3315.043               | 3315.0444             |             | 0.316D-21         | 1477.297 | 8    | 3      | 5      | 9   | 5     | 4     | 0 0 1            | 0 0 0         | 161   | 0.009            | 0.012             |
| 3315.872               | 3315.8711             | -111        | H 0.553D-21       | 3360.598 | 14   | 6      | 9      | 15  | 5     | 10    | 1 0 0            | 0 0 0         | 161   | 0.019            | 0.024             |
| 3315.881               | 3316.0869             |             | 0.799D-21         | 3758.429 | 15   | 5      | 10     | 16  | 5     | 11    | 0 0 1            | 0 0 0         | 161   | 0.032            | 0.038             |
| 3317.279               | 3317.2799             | 13          | C 0.148D-20       | 1255.167 | 7    | 4      | 3      | 8   | 5     | 4     | 1 0 0            | 0 0 0         | 161   | 0.059            | 0.062             |
| 3317.280               |                       | D 0.267D-22 | 4613.574          | 5        | 3    | 2      | 6      | 5   | 1     | 0 0 2 | 0 0 1            | 161           |       | 0.001            |                   |
| 3318.510               | 3318.5088             | -11         | C 0.689D-22       | 648.979  | 7    | 2      | 5      | 6   | 3     | 4     | 0 2 0            | 0 0 0         | 161   | 0.006            | 0.006             |
| 3320.010               | 3320.0140             | 24          | H 0.202D-21       | 4980.227 | 13   | 7      | 7      | 14  | 7     | 8     | 0 1 1            | 0 1 0         | 161   | 0.009            | 0.012             |
| 3320.484               | 3320.4849             | 8           | H 0.167D-20       | 3629.095 | 14   | 7      | 7      | 15  | 7     | 8     | 0 0 1            | 0 0 0         | 161   | 0.063            | 0.077             |
| 3320.820               |                       | D 0.296D-21 | 3685.414          | 13       | 9    | 4      | 14     | 9   | 5     | 0 0 1 | 0 0 0            | 161           |       | 0.014            |                   |
| 3320.824               | 3320.8207             | 5           | H 0.888D-21       | 3685.403 | 13   | 9      | 5      | 14  | 9     | 6     | 0 0 1            | 0 0 0         | 161   | 0.044            | 0.041             |
| 3322.124               |                       | D 0.497D-21 | 4021.219          | 18       | 2    | 17     | 19     | 2   | 18    | 0 0 1 | 0 0 0            | 161           |       | 0.025            |                   |
| 3322.125               | 3322.1233             | -37         | H 0.149D-20       | 4021.218 | 18   | 1      | 17     | 19  | 1     | 18    | 0 0 1            | 0 0 0         | 161   | 0.088            | 0.074             |
| 3322.191               | 3322.1908             | -1          | H 0.164D-20       | 3940.590 | 17   | 3      | 15     | 18  | 3     | 16    | 0 0 1            | 0 0 0         | 161   | 0.068            | 0.080             |
| 3322.255               | 3322.2528             | 28          | H 0.547D-21       | 3940.544 | 17   | 2      | 15     | 18  | 2     | 16    | 0 0 1            | 0 0 0         | 161   | 0.020            | 0.027             |
| 3322.299               | 3322.2828             |             | 0.541D-21         | 3624.163 | 14   | 7      | 8      | 15  | 7     | 9     | 0 0 1            | 0 0 0         | 161   | 0.017            | 0.025             |
| 3323.019               | 3323.0197             | 15          | C 0.767D-22       | 275.497  | 5    | 2      | 4      | 4   | 1     | 3     | 0 2 0            | 0 0 0         | 161   | 0.010            | 0.015             |
| 3323.0932              |                       |             |                   |          |      |        |        |     |       |       |                  |               | 0.007 |                  |                   |
| 3323.150               |                       | D 0.760D-22 | 1742.307          | 3        | 3    | 0      | 2      | 2   | 1     | 0 3 0 | 0 1 0            | 161           |       | 0.003            |                   |
| 3323.152               |                       | D 0.177D-21 | 2764.699          | 7        | 3    | 4      | 8      | 4   | 5     | 1 1 0 | 0 1 0            | 161           |       | 0.007            |                   |
| 3323.159               | 3323.1581             | -30         | H 0.280D-21       | 5094.086 | 15   | 4      | 12     | 16  | 4     | 13    | 0 1 1            | 0 1 0         | 161   | 0.019            | 0.017             |
| 3323.343               | 3323.3406             |             | 0.273D-21         | 1616.452 | 9    | 2      | 7      | 10  | 4     | 6     | 0 0 1            | 0 0 0         | 161   | 0.010            | 0.010             |
| 3324.007               | 3324.0061             | -5          | C 0.537D-22       | 709.609  | 7    | 3      | 5      | 7   | 2     | 6     | 0 2 0            | 0 0 0         | 161   | 0.007            | 0.004             |
| 3324.312               | 3324.3037             |             | 0.237D-21         | 5258.633 | 17   | 2      | 16     | 18  | 2     | 17    | 0 1 1            | 0 1 0         | 161   | 0.015            | 0.015             |
| 3324.321               | 3324.3388             | 18          | H 0.635D-21       | 3812.051 | 16   | 4      | 13     | 17  | 4     | 14    | 0 0 1            | 0 0 0         | 161   | 0.028            | 0.030             |
| 3324.380               | 3324.3844             | 73          | H 0.194D-20       | 3810.940 | 16   | 3      | 13     | 17  | 3     | 14    | 0 0 1            | 0 0 0         | 161   | 0.081            | 0.092             |
| 3324.535               |                       | D 0.272D-21 | 2552.858          | 5        | 4    | 1      | 6      | 5   | 2     | 1 1 0 | 0 1 0            | 161           |       | 0.011            |                   |
| 3324.541               | 3324.5395             | -17         | C 0.381D-21       | 744.163  | 9    | 0      | 9      | 8   | 1     | 8     | 0 2 0            | 0 0 0         | 161   | 0.032            | 0.027             |
| 3324.867               | 3324.8659             | -12         | C 0.127D-21       | 744.064  | 9    | 1      | 9      | 8   | 0     | 8     | 0 2 0            | 0 0 0         | 161   | 0.011            | 0.009             |
| 3325.140               | 3325.1386             | -15         | H 0.144D-20       | 4048.252 | 19   | 1      | 19     | 20  | 1     | 20    | 0 0 1            | 0 0 0         | 161   | 0.093            | 0.072             |
| 3325.140               |                       | D 0.479D-21 | 4048.252          | 19       | 0    | 19     | 20     | 0   | 20    | 0     | 0 1 0            | 0 0 0         | 161   |                  | 0.024             |
| 3325.662               | 3325.6637             |             | 0.257D-21         | 2572.140 | 6    | 3      | 4      | 7   | 4     | 3     | 1 1 0            | 0 1 0         | 161   | 0.010            | 0.010             |
| 3325.731               | 3325.7189             |             | 0.100D-21         | 4938.242 | 14   | 5      | 10     | 15  | 5     | 11    | 0 1 1            | 0 1 0         | 161   | 0.006            | 0.006             |
| 3325.838               | 3325.8379             | 33          | H 0.241D-20       | 3472.880 | 14   | 6      | 8      | 15  | 6     | 9     | 0 0 1            | 0 0 0         | 161   | 0.089            | 0.108             |
| 3325.9447              |                       |             |                   |          |      |        |        |     |       |       |                  |               | 0.007 |                  |                   |
| 3326.010               | 3326.0102             | 47          | H 0.398D-21       | 1843.030 | 10   | 3      | 7      | 11  | 4     | 8     | 1 0 0            | 0 0 0         | 161   | 0.016            | 0.015             |
| 3326.043               | 3326.0436             | 11          | C 0.704D-21       | 1131.776 | 7    | 3      | 5      | 8   | 4     | 4     | 1 0 0            | 0 0 0         | 161   | 0.032            | 0.032             |
| 3326.425               | 3326.4248             | 4           | C 0.212D-21       | 552.912  | 7    | 1      | 6      | 6   | 2     | 5     | 0 2 0            | 0 0 0         | 161   | 0.021            | 0.022             |
| 3326.797               | 3326.7963             | 7           | C 0.345D-21       | 1006.116 | 7    | 1      | 7      | 8   | 3     | 6     | 0 0 1            | 0 0 0         | 161   | 0.016            | 0.017             |
| 3327.046               | 3327.0458             | 0           | H 0.218D-20       | 3639.537 | 15   | 5      | 11     | 16  | 5     | 12    | 0 0 1            | 0 0 0         | 161   | 0.085            | 0.101             |
| 3327.329               | 3327.3282             | -16         | C 0.195D-21       | 648.979  | 5    | 0      | 5      | 6   | 3     | 4     | 1 0 0            | 0 0 0         | 161   | 0.017            | 0.016             |
| 3327.588               | 3327.5875             | -8          | C 0.737D-21       | 1059.647 | 6    | 3      | 4      | 7   | 5     | 3     | 0 0 1            | 0 0 0         | 161   | 0.034            | 0.036             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3328.259               | 3328.2553             | -27    | H 0.418D-21       | 4894.582 | 14   | 4      | 10     | 15  | 4     | 11    | 0 1 1          | 0 1 0       | 161 | 0.022            | 0.024             |
| 3328.424               | 3328.4251             | 22     | H 0.885D-21       | 3623.762 | 15   | 4      | 11     | 16  | 4     | 12    | 0 0 1          | 0 0 0       | 161 | 0.033            | 0.041             |
|                        | 3328.7753             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.008             |
| 3329.644               | 3329.6441             | -3     | C 0.966D-21       | 1122.709 | 7    | 2      | 6      | 8   | 4     | 5     | 0 0 1          | 0 0 0       | 161 | 0.041            | 0.044             |
| 3330.985               | 3330.9834             | -13    | H 0.595D-21       | 3583.372 | 12   | 10     | 2      | 13  | 10    | 3     | 0 0 1          | 0 0 0       | 161 | 0.032            | 0.027             |
| 3330.985               |                       |        | D 0.198D-21       | 3583.372 | 12   | 10     | 3      | 13  | 10    | 4     | 0 0 1          | 0 0 0       | 161 |                  | 0.009             |
|                        | 3331.5851             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.007             |
| 3331.736               | 3331.7341             |        | 0.112D-21         | 3592.425 | 11   | 2      | 9      | 12  | 3     | 10    | 1 1 0          | 0 1 0       | 161 | 0.006            | 0.005             |
| 3331.811               |                       |        | D 0.814D-22       | 5241.742 | 18   | 1      | 18     | 19  | 1     | 19    | 0 1 1          | 0 1 0       | 161 |                  | 0.005             |
| 3331.811               | 3331.8128             | -15    | H 0.244D-21       | 5241.742 | 18   | 0      | 18     | 19  | 0     | 19    | 0 1 1          | 0 1 0       | 161 | 0.021            | 0.015             |
| 3332.519               | 3332.5194             |        | 0.420D-21         | 2327.891 | 13   | 2      | 12     | 14  | 1     | 13    | 1 0 0          | 0 0 0       | 161 | 0.015            | 0.016             |
| 3332.574               |                       |        | D 0.511D-21       | 2358.305 | 14   | 0      | 14     | 15  | 1     | 15    | 1 0 0          | 0 0 0       | 161 |                  | 0.019             |
| 3332.578               | 3332.5779             |        | 0.153D-20         | 2358.304 | 14   | 1      | 14     | 15  | 0     | 15    | 1 0 0          | 0 0 0       | 161 | 0.070            | 0.058             |
| 3332.605               | 3332.6044             |        | 0.665D-21         | 2246.888 | 12   | 3      | 10     | 13  | 2     | 11    | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.025             |
| 3333.046               | 3333.0461             | -9     | H 0.345D-21       | 2248.067 | 12   | 2      | 10     | 13  | 3     | 11    | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.013             |
| 3334.329               | 3334.3355             | -26    | H 0.775D-21       | 3443.205 | 14   | 6      | 9      | 15  | 6     | 10    | 0 0 1          | 0 0 0       | 161 | 0.028            | 0.035             |
|                        | 3334.3726             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.007             |
| 3334.445               | 3334.4457             | 20     | H 0.309D-21       | 4774.047 | 13   | 6      | 8      | 14  | 6     | 9     | 0 1 1          | 0 1 0       | 161 | 0.016            | 0.018             |
| 3334.564               | 3334.5613             |        | 0.878D-21         | 2327.914 | 13   | 1      | 12     | 14  | 2     | 13    | 1 0 0          | 0 0 0       | 161 | 0.030            | 0.033             |
| 3334.629               | 3334.6297             | 7      | C 0.374D-20       | 1059.835 | 6    | 4      | 3      | 7   | 5     | 2     | 1 0 0          | 0 0 0       | 161 | 0.168            | 0.180             |
| 3334.993               | 3334.9856             |        | 0.498D-21         | 3465.060 | 13   | 8      | 5      | 14  | 8     | 6     | 0 0 1          | 0 0 0       | 161 | 0.017            | 0.022             |
| 3335.071               | 3335.0691             | -2     | H 0.149D-20       | 3464.885 | 13   | 8      | 6      | 14  | 8     | 7     | 0 0 1          | 0 0 0       | 161 | 0.056            | 0.067             |
| 3336.713               | 3336.7131             | -3     | C 0.243D-21       | 399.457  | 6    | 2      | 5      | 5   | 1     | 4     | 0 2 0          | 0 0 0       | 161 | 0.029            | 0.035             |
| 3336.845               |                       |        | D 0.119D-20       | 1045.059 | 5    | 5      | 1      | 6   | 6     | 0     | 1 0 0          | 0 0 0       | 161 |                  | 0.058             |
| 3336.846               | 3336.8462             | 2      | C 0.358D-20       | 1045.058 | 5    | 5      | 0      | 6   | 6     | 1     | 1 0 0          | 0 0 0       | 161 | 0.222            | 0.174             |
| 3336.899               | 3336.8982             | 8      | C 0.145D-20       | 1581.336 | 9    | 3      | 6      | 10  | 4     | 7     | 1 0 0          | 0 0 0       | 161 | 0.047            | 0.055             |
|                        | 3337.1386             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.010             |
| 3338.986               | 3338.9864             | 6      | C 0.128D-21       | 385.600  | 8    | 3      | 6      | 8   | 2     | 7     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3339.760               | 3339.7615             | -5     | H 0.210D-21       | 3512.401 | 11   | 11     | 1      | 12  | 11    | 2     | 0 0 1          | 0 0 0       | 161 | 0.010            | 0.009             |
| 3339.760               |                       |        | D 0.698D-22       | 3512.401 | 11   | 11     | 0      | 12  | 11    | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.003             |
|                        | 3339.8840             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.010             |
| 3340.141               | 3340.1392             | -13    | C 0.111D-21       | 920.211  | 10   | 0      | 10     | 9   | 1     | 9     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.006             |
| 3340.298               | 3340.2993             | 9      | C 0.333D-21       | 920.169  | 10   | 1      | 10     | 9   | 0     | 9     | 0 2 0          | 0 0 0       | 161 | 0.016            | 0.019             |
| 3340.633               | 3340.6323             |        | 0.323D-21         | 2246.888 | 12   | 5      | 8      | 13  | 2     | 11    | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.012             |
| 3341.384               | 3341.3835             | 6      | C 0.663D-21       | 1282.919 | 8    | 1      | 7      | 9   | 3     | 6     | 0 0 1          | 0 0 0       | 161 | 0.024            | 0.027             |
| 3342.295               | 3342.2940             | -4     | C 0.525D-21       | 1059.647 | 6    | 4      | 2      | 7   | 5     | 3     | 1 0 0          | 0 0 0       | 161 | 0.023            | 0.025             |
|                        | 3342.6067             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.008             |
| 3344.993               | 3344.9935             | -5     | H 0.332D-20       | 3360.598 | 14   | 5      | 9      | 15  | 5     | 10    | 0 0 1          | 0 0 0       | 161 | 0.121            | 0.146             |
| 3345.300               | 3345.3009             | -29    | H 0.239D-20       | 3647.465 | 17   | 2      | 16     | 18  | 2     | 17    | 0 0 1          | 0 0 0       | 161 | 0.136            | 0.110             |
| 3345.302               |                       |        | D 0.797D-21       | 3647.463 | 17   | 1      | 16     | 18  | 1     | 17    | 0 0 1          | 0 0 0       | 161 |                  | 0.037             |
| 3345.340               |                       |        | D 0.590D-22       | 6019.598 | 13   | 4      | 10     | 14  | 4     | 11    | 0 2 1          | 0 2 0       | 161 |                  | 0.004             |
| 3345.348               | 3345.3389             |        | 0.280D-21         | 4643.867 | 12   | 7      | 5      | 13  | 7     | 6     | 0 1 1          | 0 1 0       | 161 | 0.014            | 0.015             |
| 3345.395               | 3345.3944             | 56     | H 0.262D-20       | 3567.180 | 16   | 2      | 14     | 17  | 2     | 15    | 0 0 1          | 0 0 0       | 161 | 0.105            | 0.119             |
| 3345.732               | 3345.7329             | -44    | H 0.388D-21       | 4847.629 | 15   | 3      | 13     | 16  | 3     | 14    | 0 1 1          | 0 1 0       | 161 | 0.020            | 0.022             |
| 3345.828               | 3345.8277             | -7     | H 0.854D-21       | 3567.234 | 16   | 3      | 14     | 17  | 3     | 15    | 0 0 1          | 0 0 0       | 161 | 0.032            | 0.039             |
| 3345.863               | 3345.8623             |        | 0.150D-21         | 5184.738 | 11   | 1      | 11     | 12  | 1     | 12    | 1 0 1          | 1 0 0       | 161 | 0.006            | 0.009             |
| 3345.987               | 3345.9896             | 22     | H 0.457D-21       | 4728.223 | 14   | 3      | 11     | 15  | 3     | 12    | 0 1 1          | 0 1 0       | 161 | 0.024            | 0.026             |
| 3346.037               | 3346.0387             | 17     | C 0.148D-21       | 842.357  | 7    | 4      | 3      | 7   | 3     | 4     | 0 2 0          | 0 0 0       | 161 | 0.007            | 0.009             |
| 3346.800               | 3346.7971             | -42    | H 0.115D-20       | 3347.780 | 12   | 9      | 3      | 13  | 9     | 4     | 0 0 1          | 0 0 0       | 161 | 0.054            | 0.050             |
| 3346.802               |                       |        | D 0.383D-21       | 3347.777 | 12   | 9      | 4      | 13  | 9     | 5     | 0 0 1          | 0 0 0       | 161 |                  | 0.017             |
| 3347.243               | 3347.2400             |        | 0.272D-21         | 2042.312 | 12   | 4      | 9      | 13  | 1     | 12    | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.010             |
| 3347.296               |                       |        | 0.801D-21         | 3266.538 | 13   | 7      | 6      | 14  | 7     | 7     | 0 0 1          | 0 0 0       | 161 |                  | 0.035             |
| 3347.331               | 3347.3218             |        | 0.123D-21         | 4902.621 | 16   | 2      | 15     | 17  | 2     | 16    | 0 1 1          | 0 1 0       | 161 | 0.030            | 0.007             |
| 3347.343               |                       |        | 0.370D-21         | 4902.609 | 16   | 1      | 15     | 17  | 1     | 16    | 0 1 1          | 0 1 0       | 161 |                  | 0.021             |
| 3347.377               | 3347.3812             | 66     | H 0.300D-20       | 3439.308 | 15   | 4      | 12     | 16  | 4     | 13    | 0 0 1          | 0 0 0       | 161 | 0.112            | 0.133             |
| 3347.422               | 3347.4279             |        | 0.102D-20         | 3437.297 | 15   | 3      | 12     | 16  | 3     | 13    | 0 0 1          | 0 0 0       | 161 | 0.038            | 0.045             |
|                        | 3347.9897             |        |                   |          |      |        |        |     |       |       |                |             |     |                  | 0.007             |
| 3348.170               |                       |        | D 0.774D-21       | 3675.116 | 18   | 1      | 18     | 19  | 1     | 19    | 0 0 1          | 0 0 0       | 161 |                  | 0.036             |
| 3348.170               | 3348.1698             | -30    | H 0.232D-20       | 3675.116 | 18   | 0      | 18     | 19  | 0     | 19    | 0 0 1          | 0 0 0       | 161 | 0.141            | 0.107             |
| 3348.213               | 3348.2117             |        | 0.237D-20         | 3264.338 | 13   | 7      | 7      | 14  | 7     | 8     | 0 0 1          | 0 0 0       | 161 | 0.087            | 0.102             |
| 3348.444               | 3348.4443             | 13     | C 0.569D-21       | 1340.886 | 8    | 3      | 5      | 9   | 4     | 6     | 1 0 0          | 0 0 0       | 161 | 0.021            | 0.023             |
| 3349.674               | 3349.6744             | -31    | H 0.443D-21       | 4585.352 | 13   | 5      | 9      | 14  | 5     | 10    | 0 1 1          | 0 1 0       | 161 | 0.021            | 0.024             |
| 3350.253               | 3350.2492             | -2     | H 0.109D-20       | 3269.531 | 14   | 5      | 10     | 15  | 5     | 11    | 0 0 1          | 0 0 0       | 161 | 0.039            | 0.047             |
| 3351.620               | 3351.6217             | -11    | H 0.433D-20       | 3244.601 | 14   | 4      | 10     | 15  | 4     | 11    | 0 0 1          | 0 0 0       | 161 | 0.156            | 0.186             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|-----|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3352.632               | 3352.6397             | -44    | H 0.926D-21       | 2983.414 | 13  | 5      | 8      | 14  | 5     | 9     | 0 0 1            | 0 0 0         | 161 | 0.031            | 0.038             |
| 3352.969               | 3352.9713             | 35     | H 0.215D-21       | 4525.242 | 13  | 4      | 9      | 14  | 4     | 10    | 0 1 1            | 0 1 0         | 161 | 0.009            | 0.012             |
| 3353.228               | 3353.2280             | 0      | C 0.748D-22       | 709.609  | 8   | 1      | 7      | 7   | 2     | 6     | 0 2 0            | 0 0 0         | 161 | 0.006            | 0.006             |
|                        | 3353.2839             |        |                   |          |     |        |        |     |       |       |                  |               |     | 0.007            |                   |
| 3354.294               |                       | D      | 0.132D-20         | 1962.508 | 11  | 2      | 9      | 12  | 3     | 10    | 1 0 0            | 0 0 0         | 161 |                  | 0.048             |
| 3354.300               | 3354.2974             | -31    | H 0.119D-20       | 3101.436 | 13  | 6      | 7      | 14  | 6     | 8     | 0 0 1            | 0 0 0         | 161 | 0.082            | 0.050             |
| 3354.527               | 3354.5258             | -7     | H 0.381D-21       | 4889.492 | 17  | 1      | 17     | 18  | 1     | 18    | 0 1 1            | 0 1 0         | 161 | 0.028            | 0.022             |
| 3354.527               |                       | D      | 0.127D-21         | 4889.492 | 17  | 0      | 17     | 18  | 0     | 18    | 0 1 1            | 0 1 0         | 161 |                  | 0.007             |
| 3355.185               | 3355.1870             | 20     | C 0.280D-21       | 1114.550 | 11  | 0      | 11     | 10  | 1     | 10    | 0 2 0            | 0 0 0         | 161 | 0.011            | 0.013             |
| 3355.599               |                       | D      | 0.673D-21         | 2073.518 | 13  | 1      | 13     | 14  | 0     | 14    | 1 0 0            | 0 0 0         | 161 |                  | 0.025             |
| 3355.607               | 3355.6044             | 15     | H 0.202D-20       | 2073.519 | 13  | 0      | 13     | 14  | 1     | 14    | 1 0 0            | 0 0 0         | 161 | 0.079            | 0.074             |
| 3355.706               | 3355.7059             | -1     | C 0.213D-20       | 888.599  | 5   | 3      | 3      | 6   | 5     | 2     | 0 0 1            | 0 0 0         | 161 | 0.113            | 0.123             |
| 3355.874               | 3355.8779             | 23     | H 0.536D-21       | 2042.374 | 12  | 1      | 11     | 13  | 2     | 12    | 1 0 0            | 0 0 0         | 161 | 0.020            | 0.020             |
| 3356.908               | 3356.9063             | 6      | H 0.627D-21       | 3266.762 | 11  | 10     | 2      | 12  | 10    | 3     | 0 0 1            | 0 0 0         | 161 | 0.033            | 0.027             |
| 3356.908               |                       | D      | 0.209D-21         | 3266.762 | 11  | 10     | 1      | 12  | 10    | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.009             |
| 3357.024               |                       | D      | 0.135D-20         | 2042.312 | 12  | 2      | 11     | 13  | 1     | 12    | 1 0 0            | 0 0 0         | 161 |                  | 0.050             |
| 3357.034               | 3357.0339             | -3     | C 0.121D-20       | 842.357  | 6   | 2      | 5      | 7   | 3     | 4     | 1 0 0            | 0 0 0         | 161 | 0.082            | 0.074             |
| 3357.931               | 3357.9325             | -5     | H 0.443D-21       | 4442.719 | 12  | 6      | 6      | 13  | 6     | 7     | 0 1 1            | 0 1 0         | 161 | 0.020            | 0.023             |
| 3359.520               | 3359.5196             | -1     | C 0.104D-20       | 888.632  | 5   | 3      | 2      | 6   | 5     | 1     | 0 0 1            | 0 0 0         | 161 | 0.056            | 0.060             |
| 3359.800               | 3359.7996             | -26    | H 0.343D-20       | 3084.835 | 13  | 6      | 8      | 14  | 6     | 9     | 0 0 1            | 0 0 0         | 161 | 0.117            | 0.143             |
| 3360.175               | 3360.1748             | 1      | C 0.141D-21       | 508.812  | 5   | 4      | 1      | 5   | 3     | 2     | 0 2 0            | 0 0 0         | 161 | 0.016            | 0.016             |
| 3360.478               | 3360.4805             |        | 0.176D-21         | 3386.382 | 11  | 1      | 10     | 12  | 2     | 11    | 1 1 0            | 0 1 0         | 161 | 0.007            | 0.008             |
| 3361.178               | 3361.1773             |        | 0.201D-20         | 3127.862 | 12  | 8      | 4      | 13  | 8     | 5     | 0 0 1            | 0 0 0         | 161 | 0.071            | 0.084             |
| 3361.211               | 3361.2077             |        | 0.670D-21         | 3127.808 | 12  | 8      | 5      | 13  | 8     | 6     | 0 0 1            | 0 0 0         | 161 | 0.022            | 0.028             |
| 3361.673               | 3361.6725             | 0      | C 0.281D-20       | 931.237  | 6   | 3      | 4      | 7   | 4     | 3     | 1 0 0            | 0 0 0         | 161 | 0.143            | 0.153             |
| 3362.282               | 3362.2827             | -5     | C 0.189D-20       | 1122.709 | 7   | 3      | 4      | 8   | 4     | 5     | 1 0 0            | 0 0 0         | 161 | 0.080            | 0.086             |
| 3362.933-              | 3362.9305-            | -26    | C 0.316D-22       | 383.842  | 4   | 4      | 0      | 4   | 3     | 1     | 0 2 0            | 0 0 0         | 161 | -0.004           | -0.005            |
| 3363.496               | 3363.4902             | -17    | H 0.108D-21       | 4510.895 | 10  | 9      | 1      | 11  | 9     | 2     | 0 1 1            | 0 1 0         | 161 | 0.008            | 0.006             |
| 3363.496               |                       | D      | 0.362D-22         | 4510.895 | 10  | 9      | 2      | 11  | 9     | 3     | 0 1 1            | 0 1 0         | 161 |                  | 0.002             |
| 3364.246               | 3364.2463             | 2      | C 0.953D-22       | 382.317  | 4   | 4      | 1      | 4   | 3     | 2     | 0 2 0            | 0 0 0         | 161 | 0.010            | 0.014             |
| 3364.347               | 3364.3464             | -7     | C 0.921D-22       | 136.164  | 3   | 3      | 1      | 2   | 2     | 0     | 0 2 0            | 0 0 0         | 161 | 0.019            | 0.026             |
| 3364.699               | 3364.7010             | -43    | H 0.654D-21       | 4285.648 | 12  | 5      | 7      | 13  | 5     | 8     | 0 1 1            | 0 1 0         | 161 | 0.030            | 0.034             |
| 3364.706               |                       | D      | 0.302D-22         | 4889.406 | 7   | 5      | 2      | 8   | 5     | 3     | 1 0 1            | 1 0 0         | 161 |                  | 0.002             |
| 3364.746               | 3364.7447             |        | 0.164D-21         | 3072.728 | 9   | 2      | 7      | 10  | 3     | 8     | 1 1 0            | 0 1 0         | 161 | 0.006            | 0.007             |
| 3364.827               | 3364.8272             | -5     | C 0.111D-20       | 1360.236 | 8   | 2      | 6      | 9   | 4     | 5     | 0 0 1            | 0 0 0         | 161 | 0.036            | 0.044             |
| 3364.905               | 3364.9036             | -16    | C 0.477D-22       | 503.968  | 5   | 4      | 2      | 5   | 3     | 3     | 0 2 0            | 0 0 0         | 161 | 0.014            | 0.005             |
| 3365.281               | 3365.2794             | -17    | H 0.178D-21       | 4926.352 | 9   | 2      | 8      | 10  | 2     | 9     | 1 0 1            | 1 0 0         | 161 | 0.009            | 0.010             |
| 3365.737               | 3365.7365             | -7     | C 0.276D-21       | 134.902  | 3   | 3      | 0      | 2   | 2     | 1     | 0 2 0            | 0 0 0         | 161 | 0.056            | 0.077             |
| 3366.381               | 3366.3769             | -74    | H 0.188D-21       | 4958.902 | 10  | 0      | 10     | 11  | 0     | 11    | 1 0 1            | 1 0 0         | 161 | 0.010            | 0.011             |
| 3366.537               | 3366.5357             | -6     | C 0.157D-21       | 648.979  | 6   | 4      | 3      | 6   | 3     | 4     | 0 2 0            | 0 0 0         | 161 | 0.011            | 0.013             |
| 3367.519               | 3367.5194             | 3      | C 0.245D-21       | 704.214  | 8   | 2      | 7      | 7   | 1     | 6     | 0 2 0            | 0 0 0         | 161 | 0.017            | 0.019             |
| 3367.642               | 3367.6430             | 3      | C 0.198D-20       | 888.599  | 5   | 4      | 1      | 6   | 5     | 2     | 1 0 0            | 0 0 0         | 161 | 0.104            | 0.113             |
| 3367.816               | 3367.8145             | -20    | H 0.111D-20       | 3211.056 | 15  | 2      | 13     | 16  | 2     | 14    | 0 0 1            | 0 0 0         | 161 | 0.043            | 0.047             |
| 3368.296               |                       | D      | 0.124D-20         | 3291.152 | 16  | 2      | 15     | 17  | 2     | 16    | 0 0 1            | 0 0 0         | 161 |                  | 0.053             |
| 3368.300               | 3368.2966             | -5     | H 0.373D-20       | 3291.149 | 16  | 1      | 15     | 17  | 1     | 16    | 0 0 1            | 0 0 0         | 161 | 0.170            | 0.161             |
| 3368.469               | 3368.4698             |        | 0.195D-21         | 4507.523 | 14  | 3      | 12     | 15  | 3     | 13    | 0 1 1            | 0 1 0         | 161 | 0.009            | 0.010             |
| 3368.529               | 3368.5267             | -14    | H 0.405D-20       | 3211.214 | 15  | 3      | 13     | 16  | 3     | 14    | 0 0 1            | 0 0 0         | 161 | 0.149            | 0.172             |
| 3368.819               | 3368.8206             | 15     | C 0.688D-21       | 927.744  | 6   | 2      | 5      | 7   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.060            | 0.038             |
| 3368.822               |                       | D      | 0.623D-21         | 4396.055 | 13  | 4      | 10     | 14  | 4     | 11    | 0 1 1            | 0 1 0         | 161 |                  | 0.033             |
| 3369.122               | 3369.1221             | 2      | H 0.573D-21       | 4506.738 | 14  | 2      | 12     | 15  | 2     | 13    | 0 1 1            | 0 1 0         | 161 | 0.028            | 0.031             |
| 3369.155               | 3369.1527             | -16    | C 0.328D-21       | 888.632  | 5   | 4      | 2      | 6   | 5     | 1     | 1 0 0            | 0 0 0         | 161 | 0.014            | 0.019             |
| 3369.751               | 3369.7524             | -43    | B 0.228D-21       | 1327.110 | 12  | 1      | 12     | 11  | 0     | 11    | 0 2 0            | 0 0 0         | 161 | 0.006            | 0.009             |
| 3369.966               | 3369.9544             | -31    | H 0.185D-21       | 4564.086 | 15  | 1      | 14     | 16  | 1     | 15    | 0 1 1            | 0 1 0         | 161 | 0.010            | 0.010             |
| 3370.274               | 3370.2678             | 5      | H 0.152D-20       | 3083.854 | 14  | 4      | 11     | 15  | 4     | 12    | 0 0 1            | 0 0 0         | 161 | 0.053            | 0.063             |
| 3370.902               | 3370.9019             | -1     | H 0.457D-20       | 3080.181 | 14  | 3      | 11     | 15  | 3     | 12    | 0 0 1            | 0 0 0         | 161 | 0.158            | 0.190             |
| 3371.022               |                       | D      | 0.122D-20         | 3319.451 | 17  | 0      | 17     | 18  | 0     | 18    | 0 0 1            | 0 0 0         | 161 |                  | 0.053             |
| 3371.022               | 3371.0213             | -3     | H 0.365D-20       | 3319.451 | 17  | 1      | 17     | 18  | 1     | 18    | 0 0 1            | 0 0 0         | 161 | 0.200            | 0.158             |
| 3371.177               |                       | D      | 0.101D-21         | 5654.777 | 12  | 3      | 9      | 13  | 3     | 10    | 0 2 1            | 0 2 0         | 161 |                  | 0.007             |
| 3371.188               | 3371.1870             | -12    | H 0.363D-21       | 4329.324 | 11  | 7      | 5      | 12  | 7     | 6     | 0 1 1            | 0 1 0         | 161 | 0.019            | 0.019             |
| 3371.700               | 3371.6998             | -2     | H 0.461D-21       | 4564.113 | 15  | 2      | 14     | 16  | 2     | 15    | 0 1 1            | 0 1 0         | 161 | 0.026            | 0.025             |
| 3372.829               | 3372.8267             |        | D 0.453D-21       | 3032.691 | 11  | 9      | 2      | 12  | 9     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 0.019             |
| 3372.829               | 3373.3589             | -6     | H 0.136D-20       | 3032.690 | 11  | 9      | 3      | 12  | 9     | 4     | 0 0 1            | 0 0 0         | 161 | 0.062            | 0.056             |
|                        |                       |        |                   |          |     |        |        |     |       |       |                  |               |     | 0.005            |                   |
| 3373.876               | 3373.8742             | 2      | H 0.472D-20       | 2918.244 | 13  | 5      | 9      | 14  | 5     | 10    | 0 0 1            | 0 0 0         | 161 | 0.159            | 0.191             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3373.933               | 3373.9318             |             | 0.329D-20         | 2927.939 | 12   | 7      | 5      | 13  | 7     | 6     | 0 0 1          | 0 0 0       | 161 | 0.111            | 0.133             |
| 3374.019               | 3374.0200             |             | 0.537D-21         | 1695.071 | 10   | 2      | 8      | 11  | 3     | 9     | 1 0 0          | 0 0 0       | 161 | 0.018            | 0.020             |
| 3374.097               | 3374.0981             | 79          | H 0.210D-21       | 4252.449 | 12   | 5      | 8      | 13  | 5     | 9     | 0 1 1          | 0 1 0       | 161 | 0.009            | 0.011             |
| 3374.332               | 3374.3319             | -21         | H 0.109D-20       | 2927.076 | 12   | 7      | 6      | 13  | 7     | 7     | 0 0 1          | 0 0 0       | 161 | 0.036            | 0.044             |
| 3374.683               | 3374.6832             | 5           | C 0.130D-21       | 602.774  | 5    | 1      | 5      | 6   | 2     | 4     | 1 0 0          | 0 0 0       | 161 | 0.011            | 0.012             |
| 3375.188               | 3375.1862             | -17         | H 0.227D-20       | 2880.833 | 13   | 4      | 9      | 14  | 4     | 10    | 0 0 1          | 0 0 0       | 161 | 0.076            | 0.091             |
| 3375.285               | 3375.2866             |             | 0.101D-21         | 6077.109 | 14   | 1      | 14     | 15  | 1     | 15    | 0 0 2          | 0 0 1       | 161 | 0.006            | 0.007             |
| 3375.415               |                       | D 0.331D-22 | 6077.109          | 14       | 0    | 14     | 15     | 0   | 15    |       | 0 0 2          | 0 0 1       | 161 |                  | 0.002             |
| 3375.415               |                       | D 0.227D-22 | 3722.731          | 4        | 2    | 3      | 5      | 3   | 2     |       | 1 2 0          | 0 2 0       | 161 |                  | 0.001             |
| 3375.432               | 3375.4217             |             | 0.287D-21         | 1806.673 | 12   | 2      | 10     | 13  | 1     | 13    | 0 2 0          | 0 0 0       | 161 | 0.009            | 0.010             |
| 3375.618               | 3375.6194             | -13         | C 0.126D-21       | 1006.116 | 8    | 4      | 5      | 8   | 3     | 6     | 0 2 0          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3377.031               |                       | D 0.193D-21 | 4554.656          | 16       | 1    | 16     | 17     | 1   | 17    |       | 0 1 1          | 0 1 0       | 161 |                  | 0.010             |
| 3377.031               | 3377.0309             |             | 0.579D-21         | 4554.656 | 16   | 0      | 16     | 17  | 0     | 17    | 0 1 1          | 0 1 0       | 161 | 0.040            | 0.031             |
| 3377.550               | 3377.5495             | -1          | C 0.217D-21       | 885.600  | 9    | 1      | 8      | 8   | 2     | 7     | 0 2 0          | 0 0 0       | 161 | 0.013            | 0.012             |
| 3378.066               | 3378.0639             | -2          | C 0.249D-20       | 1806.672 | 12   | 1      | 12     | 13  | 0     | 13    | 1 0 0          | 0 0 0       | 161 | 0.086            | 0.091             |
| 3378.439               | 3378.4373             | -13         | C 0.201D-20       | 1774.752 | 11   | 1      | 10     | 12  | 2     | 11    | 1 0 0          | 0 0 0       | 161 | 0.067            | 0.073             |
| 3378.911               |                       | D 0.442D-22 | 4387.062          | 7        | 0    | 7      | 8      | 1   | 8     |       | 2 0 0          | 1 0 0       | 161 |                  | 0.002             |
| 3378.919               | 3378.9169             |             | 0.659D-21         | 1774.619 | 11   | 2      | 10     | 12  | 1     | 11    | 1 0 0          | 0 0 0       | 161 | 0.025            | 0.024             |
| 3379.124               | 3379.1239             | 6           | C 0.157D-21       | 816.694  | 6    | 1      | 6      | 7   | 3     | 5     | 0 0 1          | 0 0 0       | 161 | 0.010            | 0.010             |
| 3379.666               | 3379.6656             | 45          | H 0.568D-21       | 1806.673 | 12   | 0      | 12     | 13  | 1     | 13    | 1 0 0          | 0 0 0       | 161 | 0.019            | 0.021             |
| 3380.161               | 3380.1707             |             | 0.101D-20         | 2983.414 | 13   | 6      | 8      | 14  | 5     | 9     | 1 0 0          | 0 0 0       | 161 | 0.035            | 0.041             |
| 3380.259               | 3380.2608             | 37          | H 0.846D-21       | 4174.039 | 12   | 4      | 8      | 13  | 4     | 9     | 0 1 1          | 0 1 0       | 161 | 0.037            | 0.042             |
| 3380.467               | 3380.4678             | 7           | C 0.439D-21       | 927.744  | 6    | 3      | 3      | 7   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.022            | 0.024             |
| 3380.914               | 3380.9168             | 18          | H 0.235D-21       | 4265.980 | 10   | 8      | 2      | 11  | 8     | 3     | 0 1 1          | 0 1 0       | 161 | 0.014            | 0.012             |
| 3380.916               |                       | D 0.785D-22 | 4265.977          | 10       | 8    | 3      | 11     | 8   | 4     |       | 0 1 1          | 0 1 0       | 161 |                  | 0.004             |
| 3382.474               | 3382.4746             |             | 0.498D-20         | 2756.418 | 12   | 6      | 6      | 13  | 6     | 7     | 0 0 1          | 0 0 0       | 161 | 0.165            | 0.196             |
| 3382.915               |                       | D 0.161D-21 | 2972.824          | 10       | 10   | 1      | 11     | 10  | 2     |       | 0 0 1          | 0 0 0       | 161 |                  | 0.007             |
| 3382.915               | 3382.9092             |             | 0.482D-21         | 2972.824 | 10   | 10     | 0      | 11  | 10    | 1     | 0 0 1          | 0 0 0       | 161 | 0.020            | 0.020             |
| 3383.076               | 3383.0762             | 6           | C 0.478D-21       | 742.073  | 4    | 3      | 2      | 5   | 5     | 1     | 0 0 1          | 0 0 0       | 161 | 0.030            | 0.034             |
| 3383.151               | 3383.1507             |             | 0.334D-21         | 2251.863 | 4    | 3      | 2      | 5   | 4     | 1     | 1 1 0          | 0 1 0       | 161 | 0.008            | 0.012             |
| 3384.115               | 3384.1135             | 1           | H 0.598D-20       | 2629.337 | 12   | 5      | 7      | 13  | 5     | 8     | 0 0 1          | 0 0 0       | 161 | 0.194            | 0.232             |
| 3384.387               | 3384.3868             | -2          | C 0.169D-20       | 742.076  | 4    | 3      | 1      | 5   | 5     | 0     | 0 0 1          | 0 0 0       | 161 | 0.109            | 0.119             |
| 3384.494               | 3384.4900             | -70         | H 0.195D-21       | 4125.602 | 11   | 6      | 5      | 12  | 6     | 6     | 0 1 1          | 0 1 0       | 161 | 0.008            | 0.010             |
| 3385.463               | 3385.4657             | 3           | H 0.580D-21       | 4123.285 | 11   | 6      | 6      | 12  | 6     | 7     | 0 1 1          | 0 1 0       | 161 | 0.025            | 0.029             |
| 3385.606               | 3385.6015             | -5          | C 0.127D-20       | 1690.665 | 10   | 3      | 8      | 11  | 2     | 9     | 1 0 0          | 0 0 0       | 161 | 0.042            | 0.046             |
| 3385.666               | 3385.6745             | 119         | H 0.161D-20       | 2748.106 | 12   | 6      | 7      | 13  | 6     | 8     | 0 0 1          | 0 0 0       | 161 | 0.053            | 0.063             |
| 3385.710               | 3385.7101             | 3           | C 0.233D-21       | 212.156  | 4    | 3      | 2      | 3   | 2     | 1     | 0 2 0          | 0 0 0       | 161 | 0.042            | 0.053             |
| 3385.994               | 3385.9960             |             | 0.291D-21         | 3144.579 | 11   | 0      | 11     | 12  | 1     | 12    | 1 1 0          | 0 1 0       | 161 | 0.011            | 0.012             |
| 3387.365               |                       | 0.841D-21   | 2813.533          | 11       | 8    | 3      | 12     | 8   | 4     |       | 0 0 1          | 0 0 0       | 161 |                  | 0.033             |
| 3387.378               | 3387.3778             | -2          | H 0.252D-20       | 2813.515 | 11   | 8      | 4      | 12  | 8     | 5     | 0 0 1          | 0 0 0       | 161 | 0.098            | 0.100             |
| 3387.624               | 3387.6205             | 18          | H 0.227D-21       | 4750.387 | 9    | 1      | 9      | 10  | 1     | 10    | 1 0 1          | 1 0 0       | 161 | 0.009            | 0.013             |
| 3390.133               | 3390.1337             | -3          | H 0.389D-20       | 2952.396 | 15   | 2      | 14     | 16  | 2     | 15    | 0 0 1          | 0 0 0       | 161 | 0.145            | 0.158             |
| 3391.055               | 3391.0473             |             | 0.187D-20         | 2952.389 | 15   | 1      | 14     | 16  | 1     | 15    | 0 0 1          | 0 0 0       | 161 | 0.071            | 0.076             |
| 3391.068               | 3391.0742             | 60          | H 0.101D-20       | 4052.813 | 12   | 3      | 9      | 13  | 3     | 10    | 0 1 1          | 0 1 0       | 161 | 0.071            | 0.049             |
| 3391.077               |                       | D 0.850D-21 | 4184.836          | 13       | 3    | 11     | 14     | 3   | 12    |       | 0 1 1          | 0 1 0       | 161 |                  | 0.043             |
| 3391.260               | 3391.2662             | -8          | H 0.287D-21       | 4183.391 | 13   | 2      | 11     | 14  | 2     | 12    | 0 1 1          | 0 1 0       | 161 | 0.014            | 0.014             |
| 3391.353               | 3391.3393             | -106        | H 0.202D-20       | 2872.572 | 14   | 3      | 12     | 15  | 3     | 13    | 0 0 1          | 0 0 0       | 161 | 0.070            | 0.081             |
| 3391.422               | 3391.4243             | 3           | H 0.609D-20       | 2872.278 | 14   | 2      | 12     | 15  | 2     | 13    | 0 0 1          | 0 0 0       | 161 | 0.213            | 0.244             |
| 3391.511               | 3391.5132             |             | 0.496D-21         | 3472.880 | 14   | 7      | 8      | 15  | 6     | 9     | 1 0 0          | 0 0 0       | 161 | 0.014            | 0.022             |
| 3391.571               | 3391.5703             | -11         | C 0.189D-20       | 1446.129 | 9    | 2      | 7      | 10  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.065            | 0.072             |
| 3391.708               | 3391.7127             | -119        | H 0.119D-21       | 5477.008 | 12   | 2      | 10     | 13  | 2     | 11    | 0 2 1          | 0 2 0       | 161 | 0.009            | 0.008             |
| 3391.740               | 3391.7496             |             | 0.292D-21         | 4074.046 | 12   | 4      | 9      | 13  | 4     | 10    | 0 1 1          | 0 1 0       | 161 | 0.014            | 0.017             |
| 3392.425               | 3392.4256             | 5           | C 0.763D-22       | 206.301  | 4    | 3      | 1      | 3   | 2     | 2     | 0 2 0          | 0 0 0       | 161 | 0.014            | 0.017             |
| 3392.507               | 3392.5069             | -1          | C 0.112D-20       | 757.780  | 5    | 3      | 3      | 6   | 4     | 2     | 1 0 0          | 0 0 0       | 161 | 0.069            | 0.077             |
| 3392.676               | 3392.6776             | 111         | H 0.297D-21       | 3959.255 | 11   | 5      | 6      | 12  | 5     | 7     | 0 1 1          | 0 1 0       | 161 | 0.012            | 0.014             |
| 3392.721               |                       | D 0.732D-22 | 2321.814          | 11       | 5    | 6      | 11     | 7   | 5     |       | 0 0 1          | 0 0 0       | 161 |                  | 0.003             |
| 3392.725               | 3392.7258             | 3           | C 0.945D-21       | 742.073  | 4    | 4      | 0      | 5   | 5     | 1     | 1 0 0          | 0 0 0       | 161 | 0.060            | 0.067             |
| 3392.942               | 3392.9415             | -1          | C 0.258D-20       | 742.076  | 4    | 4      | 1      | 5   | 5     | 0     | 1 0 0          | 0 0 0       | 161 | 0.168            | 0.182             |
| 3393.008               | 3393.0065             | -55         | H 0.665D-20       | 2746.024 | 13   | 4      | 10     | 14  | 4     | 11    | 0 0 1          | 0 0 0       | 161 | 0.223            | 0.261             |
| 3393.206               |                       | D 0.274D-21 | 4243.160          | 14       | 2    | 13     | 15     | 2   | 14    |       | 0 1 1          | 0 1 0       | 161 |                  | 0.014             |
| 3393.207               | 3393.2154             | 75          | H 0.243D-20       | 2739.446 | 13   | 3      | 10     | 14  | 3     | 11    | 0 0 1          | 0 0 0       | 161 | 0.084            | 0.095             |
| 3393.471               | 3393.4743             |             | 0.244D-21         | 3843.414 | 11   | 4      | 7      | 12  | 4     | 8     | 0 1 1          | 0 1 0       | 161 | 0.010            | 0.011             |
| 3393.528               | 3393.5281             | -7          | H 0.176D-20       | 2952.396 | 15   | 3      | 12     | 16  | 2     | 15    | 0 2 0          | 0 0 0       | 161 | 0.064            | 0.071             |
| 3393.690               |                       | D 0.790D-21 | 4243.113          | 14       | 1    | 13     | 15     | 1   | 14    |       | 0 1 1          | 0 1 0       | 161 |                  | 0.040             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |   |     |        |        |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|---|-----|--------|--------|
| 3393.695               |                       | D           | 0.186D-20         | 2981.363 | 16   | 1      | 16     | 17  | 1     | 17    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.076  |        |
| 3393.695               | 3393.6894             | -7          | H 0.557D-20       | 2981.363 | 16   | 0      | 16     | 17  | 0     | 17    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.326  | 0.226  |
|                        | 3395.2191             |             |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.011  |        |
|                        | 3395.8575             |             |                   |          |      |        |        |     |       |       |                  |               |     |                  |                   |   |     | 0.010  |        |
| 3396.173               | 3396.1727             | -11         | C 0.395D-21       | 1131.776 | 7    | 2      | 5      | 8   | 4     | 4     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.015  | 0.018  |
| 3396.852               | 3396.8542             | -37         | H 0.441D-21       | 4038.404 | 10   | 7      | 3      | 11  | 7     | 4     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.016  | 0.021  |
| 3397.213               | 3397.2137             | 6           | C 0.380D-20       | 756.725  | 5    | 3      | 2      | 6   | 4     | 3     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.240  | 0.261  |
| 3398.149               | 3398.1450             | 10          | H 0.221D-20       | 2586.529 | 12   | 5      | 8      | 13  | 5     | 9     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.072  | 0.085  |
| 3398.813               | 3398.8129             | -3          | C 0.350D-21       | 1050.158 | 7    | 1      | 6      | 8   | 3     | 5     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.015  | 0.017  |
| 3398.902               | 3398.9029             | -40         | H 0.139D-20       | 2740.420 | 10   | 9      | 1      | 11  | 9     | 2     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | -0.059 | -0.054 |
|                        |                       | D 0.463D-21 | 2740.420          |          | 10   | 9      | 2      | 11  | 9     | 3     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.018  |        |
| 3398.996               | 3398.9973             | 13          | H 0.858D-21       | 3940.521 | 11   | 5      | 7      | 12  | 5     | 8     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.037  | 0.041  |
| 3399.293               | 3399.2919             | -25         | H 0.852D-21       | 4237.324 | 15   | 1      | 15     | 16  | 1     | 16    | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.045  | 0.043  |
| 3399.294               |                       | D 0.284D-21 | 4237.324          |          | 15   | 0      | 15     | 16  | 0     | 16    | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.014  |        |
| 3399.548               | 3399.5470             |             | 0.160D-21         | 4484.992 | 6    | 3      | 3      | 7   | 3     | 4     | 1                | 0             | 1   | 1                | 0                 | 0 | 161 | 0.006  | 0.008  |
| 3399.753               | 3399.7528             | -2          | H 0.101D-19       | 2533.793 | 12   | 4      | 8      | 13  | 4     | 9     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.327  | 0.385  |
| 3400.407               | 3400.4063             | -8          | H 0.142D-20       | 2613.104 | 11   | 7      | 4      | 12  | 7     | 5     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.046  | 0.055  |
| 3400.566               | 3400.5651             | -23         | H 0.426D-20       | 2612.801 | 11   | 7      | 5      | 12  | 7     | 6     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.138  | 0.164  |
| 3400.650               |                       | D 0.222D-21 | 2612.801          |          | 12   | 5      | 7      | 12  | 7     | 6     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.009  |        |
| 3400.652               | 3400.6502             | -13         | C 0.803D-21       | 1525.137 | 10   | 1      | 9      | 11  | 2     | 10    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.035  | 0.030  |
| 3401.054               | 3401.0536             | 2           | C 0.313D-20       | 1557.850 | 11   | 0      | 11     | 12  | 1     | 12    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.112  | 0.116  |
| 3401.092               | 3401.0917             | -8          | C 0.104D-20       | 1557.844 | 11   | 1      | 11     | 12  | 0     | 12    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.038  | 0.039  |
| 3401.501               | 3401.4988             | -10         | C 0.236D-20       | 1524.849 | 10   | 2      | 9      | 11  | 1     | 10    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.084  | 0.088  |
| 3402.084               | 3402.0853             | 16          | C 0.532D-22       | 224.838  | 5    | 2      | 3      | 4   | 1     | 4     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.008  | 0.012  |
| 3403.429               | 3403.4280             |             | 0.244D-21         | 2904.429 | 9    | 1      | 8      | 10  | 2     | 9     | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.008  | 0.010  |
| 3403.583               | 3403.5831             | 1           | C 0.597D-21       | 661.549  | 5    | 2      | 4      | 6   | 3     | 3     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.042  | 0.048  |
| 3403.713               | 3403.7144             | 8           | C 0.658D-22       | 315.779  | 5    | 3      | 3      | 4   | 2     | 2     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.008  | 0.011  |
| 3404.146               | 3404.1483             | -22         | C 0.200D-21       | 1079.080 | 10   | 2      | 9      | 9   | 1     | 8     | 0                | 2             | 0   | 0                | 0                 | 0 | 161 | 0.010  | 0.009  |
| 3404.150               |                       | D 0.447D-22 | 3592.425          |          | 12   | 2      | 11     | 12  | 3     | 10    | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.002  |        |
| 3405.180               | 3405.1826             |             | 0.128D-21         | 5484.000 | 14   | 0      | 14     | 15  | 0     | 15    | 0                | 2             | 1   | 0                | 2                 | 0 | 161 | 0.009  | 0.008  |
| 3405.255               | 3405.2545             |             | 0.133D-21         | 5563.398 | 10   | 4      | 7      | 11  | 4     | 8     | 0                | 0             | 2   | 0                | 0                 | 1 | 161 | 0.008  | 0.009  |
| 3406.527               |                       | D 0.779D-22 | 3997.511          |          | 9    | 8      | 1      | 10  | 8     | 2     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.004  |        |
| 3406.527               | 3406.5297             | 3           | H 0.234D-21       | 3997.511 | 9    | 8      | 2      | 10  | 8     | 3     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.011  | 0.011  |
| 3406.674               | 3406.6750             | 11          | C 0.707D-21       | 1216.232 | 8    | 2      | 6      | 9   | 3     | 7     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.028  | 0.030  |
| 3408.036               | 3408.0379             |             | 0.344D-21         | 2915.876 | 10   | 1      | 10     | 11  | 0     | 11    | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.014  | 0.014  |
| 3408.148               | 3408.1424             |             | 0.265D-21         | 4559.707 | 8    | 0      | 8      | 9   | 0     | 9     | 1                | 0             | 1   | 1                | 0                 | 0 | 161 | 0.014  | 0.014  |
| 3408.151               |                       | D 0.884D-22 | 4559.754          |          | 8    | 1      | 8      | 9   | 1     | 9     | 1                | 0             | 1   | 1                | 0                 | 0 | 161 | 0.005  |        |
| 3408.855               | 3408.8552             | -5          | C 0.826D-22       | 382.517  | 3    | 0      | 3      | 4   | 3     | 2     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.009  | 0.012  |
| 3409.202               | 3409.2013             |             | 0.324D-21         | 2129.600 | 3    | 3      | 0      | 4   | 4     | 1     | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.009  | 0.012  |
| 3410.209               | 3410.2043             | 7           | H 0.220D-20       | 2437.501 | 11   | 6      | 5      | 12  | 6     | 6     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.068  | 0.083  |
| 3410.578               | 3410.5757             | 20          | H 0.262D-21       | 4426.066 | 6    | 2      | 4      | 7   | 2     | 5     | 1                | 0             | 1   | 1                | 0                 | 0 | 161 | 0.011  | 0.014  |
| 3410.809               | 3410.8078             | -9          | H 0.734D-21       | 3833.146 | 10   | 6      | 4      | 11  | 6     | 5     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.032  | 0.034  |
| 3411.852               | 3411.8526             | -12         | H 0.650D-20       | 2433.803 | 11   | 6      | 6      | 12  | 6     | 7     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.209  | 0.244  |
| 3412.468               | 3412.4733             | 33          | B 0.420D-21       | 1437.969 | 9    | 3      | 7      | 10  | 2     | 8     | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.014  | 0.016  |
| 3413.067               | 3413.0675             | 1           | C 0.485D-21       | 782.410  | 6    | 0      | 6      | 7   | 2     | 5     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.030  | 0.032  |
| 3413.538               | 3413.5354             | -127        | H 0.123D-20       | 3877.090 | 12   | 2      | 10     | 13  | 2     | 11    | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.070  | 0.058  |
| 3413.545               |                       | D 0.398D-21 | 3879.720          |          | 12   | 3      | 10     | 13  | 3     | 11    | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.019  |        |
| 3413.566               | 3413.5669             |             | 0.289D-20         | 2522.267 | 10   | 8      | 2      | 11  | 8     | 3     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.120  | 0.109  |
| 3413.569               |                       | D 0.965D-21 | 2522.263          |          | 10   | 8      | 3      | 11  | 8     | 4     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.037  |        |
| 3413.846               | 3413.8518             |             | 0.303D-20         | 2300.689 | 11   | 5      | 6      | 12  | 5     | 7     | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.145  | 0.112  |
| 3413.859               |                       | D 0.277D-20 | 2631.282          |          | 14   | 2      | 13     | 15  | 2     | 14    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.106  |        |
| 3413.903               | 3413.9018             | -18         | H 0.828D-20       | 2631.272 | 14   | 1      | 13     | 15  | 1     | 14    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.311  | 0.318  |
| 3413.908               |                       | D 0.500D-21 | 3738.544          |          | 11   | 3      | 8      | 12  | 3     | 9     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.023  |        |
| 3413.982               |                       | D 0.278D-22 | 5207.805          |          | 9    | 5      | 4      | 10  | 4     | 7     | 2                | 0             | 0   | 1                | 0                 | 0 | 161 | 0.002  |        |
| 3413.993               | 3413.9906             | -15         | H 0.882D-20       | 2551.486 | 13   | 3      | 11     | 14  | 3     | 12    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.299  | 0.335  |
| 3414.031               | 3414.0304             |             | 0.297D-20         | 2550.883 | 13   | 2      | 11     | 14  | 2     | 12    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.102  | 0.113  |
| 3414.468               | 3414.4690             |             | 0.216D-21         | 2271.712 | 5    | 2      | 3      | 6   | 3     | 4     | 1                | 1             | 0   | 0                | 1                 | 0 | 161 | 0.008  | 0.008  |
| 3414.972               | 3414.9725             | 3           | H 0.118D-20       | 3770.880 | 11   | 4      | 8      | 12  | 4     | 9     | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.050  | 0.054  |
| 3415.534               | 3415.5365             | -43         | H 0.108D-19       | 2414.725 | 12   | 3      | 9      | 13  | 3     | 10    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.370  | 0.404  |
| 3415.547               |                       | D 0.117D-20 | 3939.834          |          | 13   | 2      | 12     | 14  | 2     | 13    | 0                | 1             | 1   | 0                | 1                 | 0 | 161 | 0.056  |        |
| 3415.590               | 3415.5897             |             | 0.285D-21         | 2246.888 | 13   | 1      | 12     | 13  | 2     | 11    | 1                | 0             | 0   | 0                | 0                 | 0 | 161 | 0.007  | 0.010  |
| 3415.669               | 3415.6664             |             | 0.309D-20         | 2426.195 | 12   | 4      | 9      | 13  | 4     | 10    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.100  | 0.116  |
| 3416.160               | 3416.1588             | -26         | H 0.824D-20       | 2660.950 | 15   | 1      | 15     | 16  | 1     | 16    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.405  | 0.318  |
| 3416.160               |                       | D 0.275D-20 | 2660.950          |          | 15   | 0      | 15     | 16  | 0     | 16    | 0                | 0             | 1   | 0                | 0                 | 0 | 161 | 0.106  |        |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$     | $J$      | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |   |     |       |       |  |
|------------------------|-----------------------|--------|-------------------|-----------|----------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|---|-----|-------|-------|--|
| 3417.427               | 3417.4263             |        | 0.185D-21         | 5500.859  | 11       | 1      | 10     | 12  | 1     | 11    | 0              | 0           | 2   | 0                | 0                 | 1 | 161 | 0.010 | 0.012 |  |
| 3417.749               | 3417.7497             |        | 0.208D-21         | 5034.391  | 10       | 3      | 7      | 11  | 3     | 8     | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.011 | 0.012 |  |
| 3417.851               | 3417.8553             |        | 0.163D-21         | 5235.562  | 12       | 1      | 11     | 13  | 1     | 12    | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.010 | 0.010 |  |
| 3418.455               | 3418.4557             | 0 C    | 0.170D-21         | 446.511   | 6        | 3      | 4      | 5   | 2     | 3     | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.017 | 0.021 |  |
| 3418.775               | 3418.7762             |        | 0.183D-21         | 5421.270  | 10       | 3      | 8      | 11  | 3     | 9     | 0              | 0           | 2   | 0                | 0                 | 1 | 161 | 0.008 | 0.012 |  |
| 3419.041               |                       | D      | 0.163D-22         | 5507.484  | 8        | 7      | 1      | 9   | 7     | 2     | 0              | 0           | 2   | 0                | 0                 | 1 | 161 | 0.001 |       |  |
| 3419.050               | 3419.0498             |        | D                 | 0.489D-22 | 5507.477 | 8      | 7      | 2   | 9     | 7     | 3              | 0           | 0   | 2                | 0                 | 0 | 1   | 161   | 0.003 |  |
| 3419.050               | 3419.0498             |        | 0.188D-21         | 5534.113  | 12       | 1      | 12     | 13  | 1     | 13    | 0              | 0           | 2   | 0                | 0                 | 1 | 161 | 0.018 | 0.012 |  |
| 3419.132               | 3419.1335             |        | 0.936D-22         | 1774.752  | 12       | 3      | 10     | 12  | 2     | 11    | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.006 | 0.003 |  |
| 3419.172               | 3419.1804             | 54 H   | 0.353D-21         | 3937.576  | 14       | 1      | 14     | 15  | 1     | 15    | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.011 | 0.017 |  |
| 3419.462               | 3419.4618             | -1 C   | 0.980D-21         | 931.237   | 6        | 2      | 4      | 7   | 4     | 3     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.047 | 0.052 |  |
| 3419.951               | 3419.9503             | 0 C    | 0.228D-20         | 1006.116  | 7        | 2      | 5      | 8   | 3     | 6     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.104 | 0.112 |  |
| 3420.498               | 3420.4981             | 0 C    | 0.371D-20         | 610.341   | 4        | 3      | 2      | 5   | 4     | 1     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.317 | 0.328 |  |
| 3420.514               |                       |        | 0.225D-20         | 2629.337  | 12       | 6      | 7      | 13  | 5     | 8     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.086 |       |  |
| 3420.537               | 3420.5387             |        | 0.114D-20         | 3659.906  | 10       | 5      | 5      | 11  | 5     | 6     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.058 | 0.051 |  |
| 3420.954               | 3420.9527             | -4 H   | 0.120D-20         | 3937.575  | 14       | 0      | 14     | 15  | 0     | 15    | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.055 | 0.057 |  |
| 3421.739               | 3421.7394             | 6 C    | 0.129D-20         | 610.114   | 4        | 3      | 1      | 5   | 4     | 2     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.101 | 0.114 |  |
| 3422.333               | 3422.3322             | -5 C   | 0.277D-20         | 1293.634  | 9        | 1      | 8      | 10  | 2     | 9     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.106 | 0.111 |  |
| 3422.369               | 3422.3687             | -2 C   | 0.179D-21         | 300.362   | 5        | 3      | 2      | 4   | 2     | 3     | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.024 | 0.032 |  |
| 3422.607               |                       | D      | 0.163D-21         | 3770.728  | 9        | 7      | 2      | 10  | 7     | 3     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.007 |       |  |
| 3422.613               | 3422.6135             | -19 H  | 0.488D-21         | 3770.713  | 9        | 7      | 3      | 10  | 7     | 4     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.024 | 0.022 |  |
| 3423.116               | 3423.1158             | -9 C   | 0.902D-20         | 2275.373  | 11       | 5      | 7      | 12  | 5     | 8     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.287 | 0.331 |  |
| 3423.118               |                       | D      | 0.249D-22         | 4052.813  | 13       | 2      | 11     | 13  | 3     | 10    | 1              | 1           | 0   | 0                | 1                 | 0 | 161 | 0.001 |       |  |
| 3423.245               | 3423.2446             | -4 C   | 0.124D-20         | 1327.119  | 10       | 0      | 10     | 11  | 1     | 11    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.054 | 0.049 |  |
| 3423.278               | 3423.2784             | 7 C    | 0.371D-20         | 1327.110  | 10       | 1      | 10     | 11  | 0     | 11    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.149 | 0.146 |  |
| 3423.551               | 3423.5548             | 3 H    | 0.144D-20         | 3535.871  | 10       | 4      | 6      | 11  | 4     | 7     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.058 | 0.064 |  |
| 3424.031               | 3424.0323             | -15 H  | 0.532D-22         | 3937.576  | 14       | 2      | 12     | 15  | 1     | 15    | 0              | 3           | 0   | 0                | 1                 | 0 | 161 | 0.010 | 0.003 |  |
| 3424.086               | 3424.0872             | -5 C   | 0.891D-21         | 1293.019  | 9        | 2      | 8      | 10  | 1     | 9     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.034 | 0.036 |  |
| 3424.308               | 3424.3059             | 1 H    | 0.371D-21         | 3650.506  | 10       | 5      | 6      | 11  | 5     | 7     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.014 | 0.017 |  |
| 3424.733               | 3424.7243             |        | 0.123D-21         | 5027.070  | 9        | 5      | 5      | 10  | 5     | 6     | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.009 | 0.007 |  |
| 3425.017               | 3425.0169             | -5 H   | 0.104D-20         | 2471.254  | 9        | 9      | 1      | 10  | 9     | 2     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.044 | 0.039 |  |
| 3425.017               |                       | D      | 0.346D-21         | 2471.254  | 9        | 9      | 0      | 10  | 9     | 1     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.013 |       |  |
| 3426.186               | 3426.1866             | -17 H  | 0.458D-20         | 2205.652  | 11       | 4      | 7      | 12  | 4     | 8     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.145 | 0.167 |  |
| 3426.586               | 3426.5820             | -35 H  | 0.276D-21         | 4348.414  | 6        | 1      | 5      | 7   | 1     | 6     | 1              | 0           | 1   | 1                | 0                 | 0 | 161 | 0.012 | 0.014 |  |
| 3426.794               | 3426.7922             | -38 H  | 0.518D-20         | 2321.905  | 10       | 7      | 3      | 11  | 7     | 4     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.164 | 0.191 |  |
| 3426.848               | 3426.8485             |        | 0.173D-20         | 2321.814  | 10       | 7      | 4      | 11  | 7     | 5     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.054 | 0.064 |  |
| 3427.917               | 3427.9172             | 0 C    | 0.737D-21         | 648.979   | 5        | 1      | 5      | 6   | 3     | 4     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.054 | 0.060 |  |
| 3428.184               | 3428.0792             |        | 0.181D-21         | 5203.914  | 13       | 1      | 13     | 14  | 1     | 14    | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.012 | 0.011 |  |
| 3428.187               |                       | D      | 0.602D-22         | 5203.906  | 13       | 0      | 13     | 14  | 0     | 14    | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.004 |       |  |
| 3428.600               | 3428.5963             | -40 H  | 0.297D-21         | 4387.062  | 7        | 1      | 7      | 8   | 1     | 8     | 1              | 0           | 1   | 1                | 0                 | 0 | 161 | 0.013 | 0.015 |  |
| 3429.582               | 3429.5812             |        | 0.392D-21         | 2705.141  | 9        | 0      | 9      | 10  | 1     | 10    | 1              | 1           | 0   | 0                | 1                 | 0 | 161 | 0.011 | 0.015 |  |
| 3430.231               | 3430.2316             |        | 0.240D-21         | 2688.080  | 8        | 2      | 7      | 9   | 1     | 8     | 1              | 1           | 0   | 0                | 1                 | 0 | 161 | 0.009 | 0.009 |  |
| 3430.709               | 3430.7144             | 50 H   | 0.203D-21         | 3629.095  | 14       | 8      | 7      | 15  | 7     | 8     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.009 | 0.009 |  |
| 3430.842               | 3430.8439             | 16 C   | 0.503D-22         | 602.774   | 7        | 3      | 5      | 6   | 2     | 4     | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.006 | 0.005 |  |
| 3431.065               | 3431.0646             | 0 C    | 0.583D-21         | 446.511   | 4        | 1      | 4      | 5   | 2     | 3     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.063 | 0.073 |  |
| 3431.097               | 3431.0996             |        | 0.149D-21         | 3639.537  | 15       | 6      | 9      | 16  | 5     | 12    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.007 | 0.007 |  |
| 3432.131               | 3432.1302             |        | 0.257D-21         | 2358.304  | 14       | 3      | 12     | 15  | 0     | 15    | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.011 | 0.010 |  |
| 3432.830               | 3432.8306             | 3 C    | 0.786D-21         | 816.694   | 6        | 2      | 4      | 7   | 3     | 5     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.045 | 0.049 |  |
| 3434.055               | 3434.0525             |        | 0.392D-21         | 1524.849  | 11       | 0      | 11     | 11  | 1     | 10    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.015 | 0.014 |  |
| 3435.554               | 3435.5584             | 34 H   | 0.570D-21         | 3587.669  | 11       | 2      | 9      | 12  | 2     | 10    | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.023 | 0.025 |  |
| 3435.693               | 3435.6935             |        | 0.405D-21         | 1631.384  | 9        | 4      | 6      | 9   | 6     | 3     | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.011 | 0.015 |  |
| 3435.762               | 3435.7554             |        | 0.225D-21         | 4905.648  | 10       | 2      | 8      | 11  | 2     | 9     | 0              | 2           | 1   | 0                | 2                 | 0 | 161 | 0.018 | 0.013 |  |
| 3435.781               |                       | D      | 0.136D-21         | 3084.835  | 14       | 5      | 10     | 14  | 6     | 9     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.006 |       |  |
| 3435.871               | 3435.8717             | -6 H   | 0.162D-20         | 3592.425  | 11       | 3      | 9      | 12  | 3     | 10    | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.068 | 0.072 |  |
| 3435.981               | 3435.9793             | -17 C  | 0.462D-20         | 1899.008  | 10       | 5      | 6      | 11  | 4     | 7     | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.144 | 0.165 |  |
| 3436.294               | 3436.2919             | 11 C   | 0.118D-19         | 2327.914  | 13       | 2      | 12     | 14  | 2     | 13    | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.459 | 0.434 |  |
| 3436.297               |                       | D      | 0.394D-20         | 2327.891  | 13       | 1      | 12     | 14  | 1     | 13    | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.145 |       |  |
| 3436.448               | 3436.4483             | 83 B   | 0.126D-19         | 2246.888  | 12       | 2      | 10     | 13  | 2     | 11    | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.428 | 0.460 |  |
| 3436.460               |                       |        | 0.413D-20         | 2248.067  | 12       | 3      | 10     | 13  | 3     | 11    | 0              | 0           | 1   | 0                | 0                 | 0 | 161 | 0.151 |       |  |
| 3436.827               | 3436.8248             |        | 0.425D-21         | 1962.508  | 12       | 2      | 11     | 12  | 3     | 10    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.015 |       |  |
| 3436.946               | 3436.9386             | -123 H | 0.287D-21         | 3565.004  | 9        | 6      | 3      | 10  | 6     | 4     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.009 | 0.013 |  |
| 3437.112               | 3437.1099             | -17 H  | 0.861D-21         | 3564.705  | 9        | 6      | 4      | 10  | 6     | 5     | 0              | 1           | 1   | 0                | 1                 | 0 | 161 | 0.033 | 0.038 |  |
| 3437.400               | 3437.4014             | 4 C    | 0.112D-21         | 931.237   | 7        | 5      | 2      | 7   | 4     | 3     | 0              | 2           | 0   | 0                | 0                 | 0 | 161 | 0.009 | 0.006 |  |
| 3437.404               |                       | D      | 0.116D-21         | 3244.601  | 15       | 3      | 12     | 15  | 4     | 11    | 1              | 0           | 0   | 0                | 0                 | 0 | 161 | 0.005 |       |  |

## HIGH-TEMPERATURE WATER VAPOR SPECTRUM

439

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu'_1 \nu'_2 \nu'_3$ | $\nu_1 \nu_2 \nu_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------------|---------------------|-----|------------------|-------------------|
| 3437.433               | 3437.4370             |        | 0.211D-20         | 3441.040 | 10   | 3      | 7      | 11  | 3     | 8     | 0 1 1                  | 0 1 0               | 161 | 0.087            | 0.091             |
| 3437.442               |                       | D      | 0.533D-22         | 2927.939 | 13   | 6      | 7      | 13  | 7     | 6     | 1 0 0                  | 0 0 0               | 161 |                  | 0.002             |
| 3437.477               | 3437.4789             | 26     | C 0.830D-20       | 2144.047 | 10   | 6      | 4      | 11  | 6     | 5     | 0 0 1                  | 0 0 0               | 161 | 0.263            | 0.300             |
| 3437.738               | 3437.7372             |        | 0.538D-21         | 3654.218 | 12   | 2      | 11     | 13  | 2     | 12    | 0 1 1                  | 0 1 0               | 161 | 0.021            | 0.024             |
| 3437.761               | 3437.7703             | 3      | B 0.521D-20       | 2105.876 | 11   | 3      | 8      | 12  | 3     | 9     | 0 0 1                  | 0 0 0               | 161 | 0.228            | 0.188             |
| 3437.777               |                       | D      | 0.162D-20         | 3654.050 | 12   | 1      | 11     | 13  | 1     | 12    | 0 1 1                  | 0 1 0               | 161 |                  | 0.073             |
| 3438.191               | 3438.1898             | -5     | C 0.218D-21       | 757.780  | 5    | 2      | 3      | 6   | 4     | 2     | 0 0 1                  | 0 0 0               | 161 | 0.014            | 0.015             |
| 3438.225               | 3438.2204             | -46    | H 0.275D-20       | 2142.597 | 10   | 6      | 5      | 11  | 6     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.085            | 0.099             |
| 3438.448               | 3438.4485             | 16     | C 0.123D-19       | 2124.953 | 11   | 4      | 8      | 12  | 4     | 9     | 0 0 1                  | 0 0 0               | 161 | 0.392            | 0.444             |
| 3438.589               | 3438.5837             |        | -0.391D-20        | 2358.305 | 14   | 1      | 14     | 15  | 1     | 15    | 0 0 1                  | 0 0 0               | 161 | 0.136            | 0.144             |
| 3438.638               | 3438.6417             | 9      | C 0.116D-19       | 2358.304 | 14   | 0      | 14     | 15  | 0     | 15    | 0 0 1                  | 0 0 0               | 161 | 0.410            | 0.428             |
| 3438.686               | 3438.6897             |        | 0.514D-21         | 3487.401 | 10   | 4      | 7      | 11  | 4     | 8     | 0 1 1                  | 0 1 0               | 161 | 0.019            | 0.022             |
|                        | 3438.9508             |        |                   |          |      |        |        |     |       |       |                        |                     |     |                  | 0.012             |
| 3438.979               | 3438.9859             |        | 0.228D-21         | 5255.348 | 10   | 2      | 9      | 11  | 2     | 10    | 0 0 2                  | 0 0 1               | 161 | 0.011            | 0.014             |
| 3439.766               |                       | D      | 0.957D-21         | 2254.284 | 9    | 8      | 1      | 10  | 8     | 2     | 0 0 1                  | 0 0 0               | 161 |                  | 0.035             |
| 3439.766               | 3439.7644             | 44     | B 0.287D-20       | 2254.283 | 9    | 8      | 2      | 10  | 8     | 3     | 0 0 1                  | 0 0 0               | 161 | 0.120            | 0.105             |
| 3439.799               | 3439.8020             |        | 0.217D-21         | 4967.496 | 11   | 2      | 10     | 12  | 2     | 11    | 0 2 1                  | 0 2 0               | 161 | 0.019            | 0.012             |
| 3439.800               |                       | D      | 0.279D-22         | 5008.957 | 7    | 7      | 1      | 8   | 7     | 2     | 0 2 1                  | 0 2 0               | 161 |                  | 0.002             |
| 3439.808               |                       | D      | 0.173D-21         | 4842.137 | 9    | 4      | 6      | 10  | 4     | 7     | 0 2 1                  | 0 2 0               | 161 |                  | 0.010             |
| 3440.172               | 3440.1697             | -19    | C 0.780D-22       | 610.341  | 5    | 5      | 0      | 5   | 4     | 1     | 0 2 0                  | 0 0 0               | 161 | 0.006            | 0.007             |
| 3440.523               | 3440.5236             |        | 0.244D-21         | 5289.152 | 11   | 0      | 11     | 12  | 0     | 12    | 0 0 2                  | 0 0 1               | 161 | 0.016            | 0.015             |
| 3441.870               | 3441.8730             |        | 0.283D-21         | 2495.168 | 7    | 1      | 6      | 8   | 2     | 7     | 1 1 0                  | 0 1 0               | 161 | 0.009            | 0.011             |
| 3442.077               | 3442.0781             | 12     | C 0.104D-20       | 1201.922 | 8    | 3      | 6      | 9   | 2     | 7     | 1 0 0                  | 0 0 0               | 161 | 0.044            | 0.044             |
| 3442.173               |                       | D      | 0.266D-22         | 6553.199 | 8    | 3      | 6      | 9   | 3     | 7     | 0 1 2                  | 0 1 1               | 161 |                  | 0.002             |
| 3442.177               | 3442.1752             | -19    | C 0.137D-21       | 782.410  | 8    | 3      | 6      | 7   | 2     | 5     | 0 2 0                  | 0 0 0               | 161 | 0.010            | 0.009             |
| 3442.503               | 3442.5035             | 2      | C 0.236D-20       | 508.812  | 4    | 2      | 3      | 5   | 3     | 2     | 1 0 0                  | 0 0 0               | 161 | 0.221            | 0.255             |
| 3442.632               |                       | D      | 0.123D-21         | 2054.348 | 10   | 6      | 5      | 10  | 7     | 4     | 1 0 0                  | 0 0 0               | 161 |                  | 0.004             |
| 3442.646               | 3442.6408             |        | 0.137D-21         | 1524.849 | 12   | 2      | 11     | 11  | 1     | 10    | 0 2 0                  | 0 0 0               | 161 | 0.008            | 0.005             |
| 3442.781               | 3442.7793             | -31    | C 0.241D-21       | 1216.194 | 7    | 4      | 4      | 7   | 6     | 1     | 0 0 1                  | 0 0 0               | 161 | 0.011            | 0.010             |
| 3443.102               | 3443.1026             | 1      | C 0.121D-19       | 1998.996 | 10   | 5      | 5      | 11  | 5     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.381            | 0.433             |
| 3443.112               |                       | D      | 0.826D-22         | 2005.917 | 3    | 2      | 2      | 4   | 3     | 1     | 1 1 0                  | 0 1 0               | 161 |                  | 0.003             |
| 3443.204               | 3443.2037             | 2      | C 0.101D-20       | 1080.386 | 8    | 1      | 7      | 9   | 2     | 8     | 1 0 0                  | 0 0 0               | 161 | 0.043            | 0.046             |
| 3443.512               | 3443.5096             | -74    | H 0.169D-20       | 3655.487 | 13   | 1      | 13     | 14  | 1     | 14    | 0 1 1                  | 0 1 0               | 161 | 0.076            | 0.076             |
| 3443.540               | 3443.5415             |        | 0.563D-21         | 3655.486 | 13   | 0      | 13     | 14  | 0     | 14    | 0 1 1                  | 0 1 0               | 161 | 0.028            | 0.025             |
| 3445.149               |                       | D      | 0.155D-22         | 6615.973 | 7    | 5      | 2      | 8   | 5     | 3     | 0 1 2                  | 0 1 1               | 161 |                  | 0.001             |
| 3445.158               | 3445.1581             | 4      | C 0.423D-20       | 1114.550 | 9    | 0      | 9      | 10  | 1     | 10    | 1 0 0                  | 0 0 0               | 161 | 0.193            | 0.188             |
| 3445.219               | 3445.2200             | 3      | C 0.141D-20       | 1114.534 | 9    | 1      | 9      | 10  | 0     | 10    | 1 0 0                  | 0 0 0               | 161 | 0.061            | 0.063             |
| 3445.828               |                       | D      | 0.119D-21         | 2631.282 | 15   | 0      | 15     | 15  | 2     | 14    | 0 0 1                  | 0 0 0               | 161 |                  | 0.005             |
| 3445.838               | 3445.8354             |        | 0.357D-21         | 2631.272 | 15   | 1      | 15     | 15  | 1     | 14    | 0 0 1                  | 0 0 0               | 161 | 0.008            | 0.014             |
| 3446.885               | 3446.8847             | 1      | C 0.284D-20       | 1079.080 | 8    | 2      | 7      | 9   | 1     | 8     | 1 0 0                  | 0 0 0               | 161 | 0.126            | 0.130             |
| 3446.942               | 3446.9416             | 2      | C 0.228D-20       | 648.979  | 5    | 2      | 3      | 6   | 3     | 4     | 1 0 0                  | 0 0 0               | 161 | 0.171            | 0.186             |
| 3446.944               |                       | D      | 0.458D-22         | 1808.363 | 10   | 3      | 7      | 11  | 3     | 8     | 0 0 1                  | 0 0 0               | 181 |                  | 0.002             |
| 3447.077               | 3447.0774             | 3      | C 0.128D-20       | 488.134  | 3    | 3      | 1      | 4   | 4     | 0     | 1 0 0                  | 0 0 0               | 161 | 0.129            | 0.145             |
| 3447.137               | 3447.1340             |        | 0.598D-21         | 2918.244 | 13   | 6      | 7      | 14  | 5     | 10    | 1 0 0                  | 0 0 0               | 161 | 0.023            | 0.024             |
| 3447.189               | 3447.1842             |        | 0.465D-21         | 3084.835 | 13   | 7      | 6      | 14  | 6     | 9     | 1 0 0                  | 0 0 0               | 161 | 0.016            | 0.019             |
| 3447.238               | 3447.2361             | -12    | C 0.386D-20       | 488.108  | 3    | 3      | 0      | 4   | 4     | 1     | 1 0 0                  | 0 0 0               | 161 | 0.388            | 0.437             |
| 3447.617               | 3447.6145             |        | 0.283D-21         | 2414.725 | 13   | 2      | 11     | 13  | 3     | 10    | 1 0 0                  | 0 0 0               | 161 | 0.009            | 0.010             |
| 3447.988               | 3447.9878             | 8      | H 0.461D-21       | 3387.402 | 9    | 5      | 4      | 10  | 5     | 5     | 0 1 1                  | 0 1 0               | 161 | 0.016            | 0.020             |
| 3448.234               | 3448.2330             | -37    | H 0.287D-21       | 3211.214 | 16   | 1      | 15     | 16  | 3     | 14    | 0 0 1                  | 0 0 0               | 161 | 0.010            | 0.012             |
| 3448.360               | 3448.3637             | 28     | H 0.467D-21       | 3526.630 | 8    | 7      | 1      | 9   | 7     | 2     | 0 1 1                  | 0 1 0               | 161 | 0.024            | 0.020             |
| 3448.362               |                       | D      | 0.156D-21         | 3526.627 | 8    | 7      | 2      | 9   | 7     | 3     | 0 1 1                  | 0 1 0               | 161 |                  | 0.007             |
| 3448.393               |                       | D      | 0.957D-22         | 3211.056 | 16   | 2      | 15     | 16  | 2     | 14    | 0 0 1                  | 0 0 0               | 161 |                  | 0.004             |
| 3448.401               | 3448.4008             | 4      | C 0.156D-20       | 842.357  | 6    | 1      | 5      | 7   | 3     | 4     | 0 0 1                  | 0 0 0               | 161 | 0.087            | 0.093             |
| 3448.697               | 3448.6989             | 18     | C 0.392D-20       | 1985.788 | 10   | 5      | 6      | 11  | 5     | 7     | 0 0 1                  | 0 0 0               | 161 | 0.122            | 0.140             |
| 3448.746               | 3448.7423             |        | 0.320D-21         | 4232.184 | 6    | 0      | 6      | 7   | 0     | 7     | 1 0 1                  | 1 0 0               | 161 | 0.011            | 0.016             |
| 3448.937               | 3448.9421             |        | 0.168D-21         | 1590.690 | 8    | 6      | 3      | 8   | 7     | 2     | 1 0 0                  | 0 0 0               | 161 | 0.008            | 0.006             |
| 3448.951               |                       | D      | 0.563D-22         | 1590.691 | 8    | 6      | 2      | 8   | 7     | 1     | 1 0 0                  | 0 0 0               | 161 |                  | 0.002             |
| 3449.134               | 3449.1309             |        | 0.143D-21         | 4784.664 | 8    | 5      | 3      | 9   | 5     | 4     | 0 2 1                  | 0 2 0               | 161 | 0.008            | 0.008             |
| 3449.378               | 3449.3773             | 20     | H 0.240D-21       | 4199.391 | 5    | 2      | 4      | 6   | 2     | 5     | 1 0 1                  | 1 0 0               | 161 | 0.009            | 0.012             |
| 3449.581               | 3449.5881             |        | 0.242D-21         | 4941.617 | 12   | 0      | 12     | 13  | 0     | 13    | 0 2 1                  | 0 2 0               | 161 | 0.012            | 0.014             |
| 3449.780               | 3449.7807             |        | 0.263D-21         | 2004.817 | 3    | 2      | 1      | 4   | 3     | 2     | 1 1 0                  | 0 1 0               | 161 | 0.010            | 0.009             |
| 3449.940               | 3449.9395             | -2     | H 0.136D-20       | 3383.266 | 9    | 5      | 5      | 10  | 5     | 6     | 0 1 1                  | 0 1 0               | 161 | 0.052            | 0.058             |
| 3450.191               | 3450.1909             |        | 0.413D-21         | 1411.612 | 8    | 4      | 4      | 8   | 6     | 3     | 0 0 1                  | 0 0 0               | 161 | 0.013            | 0.016             |
| 3450.881               | 3450.8855             |        | 0.142D-21         | 2512.378 | 8    | 0      | 8      | 9   | 1     | 9     | 1 1 0                  | 0 1 0               | 161 | 0.005            | 0.005             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$     | $J'$     | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO   | $I_{\text{obs}}$ | $I_{\text{calc}}$ |       |
|------------------------|-----------------------|--------|-------------------|-----------|----------|--------|--------|-----|-------|-------|------------------|---------------|-------|------------------|-------------------|-------|
| 3451.237               | 3451.2368             |        | 0.424D-21         | 2512.283  | 8        | 1      | 8      | 9   | 0     | 9     | 1 1 0            | 0 1 0         | 161   | 0.012            | 0.016             |       |
| 3451.961               |                       | D      | 0.429D-22         | 1394.814  | 7        | 6      | 2      | 7   | 7     | 1     | 1 0 0            | 0 0 0         | 161   |                  | 0.002             |       |
| 3451.962               | 3451.9627             |        | 0.129D-21         | 1394.814  | 7        | 6      | 1      | 7   | 7     | 0     | 1 0 0            | 0 0 0         | 161   | 0.008            | 0.005             |       |
| 3451.967               |                       | D      | 0.519D-22         | 4184.836  | 14       | 1      | 13     | 14  | 3     | 12    | 0 1 1            | 0 1 0         | 161   |                  | 0.003             |       |
| 3452.359               | 3452.3570             | -29    | H                 | 0.653D-21 | 3253.739 | 9      | 4      | 5   | 10    | 4     | 6                | 0 1 1         | 0 1 0 | 161              | 0.026             | 0.027 |
| 3453.117               |                       |        | 0.192D-20         | 2054.369  | 9        | 7      | 2      | 10  | 7     | 3     | 0 0 1            | 0 0 0         | 161   |                  | 0.069             |       |
| 3453.128               | 3453.1281             | -19    | D                 | 0.574D-20 | 2054.348 | 9      | 7      | 3   | 10    | 7     | 4                | 0 0 1         | 0 0 0 | 161              | 0.185             | 0.206 |
| 3453.883               |                       |        | D                 | 0.292D-22 | 1922.902 | 3      | 1      | 3   | 4     | 2     | 2                | 1 1 0         | 0 1 0 | 161              |                   | 0.001 |
| 3453.892               | 3453.8879             |        | 0.194D-21         | 5067.078  | 8        | 4      | 5      | 9   | 4     | 6     | 0 0 2            | 0 0 1         | 161   | 0.011            |                   |       |
| 3455.696               | 3455.6971             |        | 0.329D-21         | 3535.871  | 10       | 5      | 6      | 11  | 4     | 7     | 1 1 0            | 0 1 0         | 161   | 0.013            | 0.014             |       |
| 3455.782               | 3455.7809             | -2     | C                 | 0.354D-21 | 610.341  | 4      | 2      | 2   | 5     | 4     | 1                | 0 0 1         | 0 0 0 | 161              | 0.029             | 0.031 |
| 3456.255               | 3456.2543             | 0      | C                 | 0.144D-19 | 1899.008 | 10     | 4      | 6   | 11    | 4     | 7                | 0 0 1         | 0 0 0 | 161              | 0.442             | 0.512 |
| 3456.754               | 3456.7533             | 33     | B                 | 0.506D-21 | 1293.634 | 10     | 1      | 10  | 10    | 2     | 9                | 1 0 0         | 0 0 0 | 161              | 0.018             | 0.020 |
| 3457.252               | 3457.2496             | -6     | H                 | 0.231D-20 | 3314.857 | 10     | 2      | 8   | 11    | 2     | 9                | 0 1 1         | 0 1 0 | 161              | 0.090             | 0.097 |
| 3457.368               | 3457.3762             |        | 0.988D-22         | 4644.219  | 9        | 2      | 7      | 10  | 2     | 8     | 0 2 1            | 0 2 0         | 161   | 0.006            | 0.005             |       |
| 3457.382               |                       |        | D                 | 0.353D-22 | 6212.668 | 11     | 1      | 11  | 12    | 1     | 12               | 0 3 1         | 0 3 0 | 161              |                   | 0.003 |
| 3457.500               | 3457.5027             |        | 0.230D-21         | 1360.236  | 9        | 2      | 8      | 9   | 4     | 5     | 0 0 1            | 0 0 0         | 161   | 0.006            | 0.009             |       |
| 3458.138               | 3458.1357             | -21    | H                 | 0.700D-21 | 3323.271 | 10     | 3      | 8   | 11    | 3     | 9                | 0 1 1         | 0 1 0 | 161              | 0.026             | 0.030 |
| 3458.543               |                       |        | D                 | 0.543D-20 | 2042.374 | 12     | 2      | 11  | 13    | 2     | 12               | 0 0 1         | 0 0 0 | 161              |                   | 0.194 |
| 3458.546               | 3458.5443             | -11    | C                 | 0.163D-19 | 2042.312 | 12     | 1      | 11  | 13    | 1     | 12               | 0 0 1         | 0 0 0 | 161              | 0.686             | 0.582 |
| 3458.592               |                       |        | D                 | 0.764D-22 | 4774.816 | 7      | 6      | 2   | 8     | 6     | 3                | 0 2 1         | 0 2 0 | 161              |                   | 0.004 |
| 3458.596               | 3458.5949             | -6     | C                 | 0.580D-20 | 1960.208 | 11     | 2      | 9   | 12    | 2     | 10               | 0 0 1         | 0 0 0 | 161              | 0.185             | 0.206 |
| 3458.760               | 3458.7607             | 2      | C                 | 0.167D-19 | 1962.508 | 11     | 3      | 9   | 12    | 3     | 10               | 0 0 1         | 0 0 0 | 161              | 0.529             | 0.595 |
| 3458.931               | 3458.9314             |        | 0.252D-21         | 4669.738  | 9        | 3      | 7      | 10  | 3     | 8     | 0 2 1            | 0 2 0         | 161   | 0.017            | 0.014             |       |
| 3458.934               |                       |        | D                 | 0.149D-21 | 2142.597 | 11     | 5      | 7   | 11    | 6     | 6                | 1 0 0         | 0 0 0 | 161              |                   | 0.005 |
| 3459.727               | 3459.7269             | -2     | H                 | 0.215D-20 | 3386.382 | 11     | 2      | 10  | 12    | 2     | 11               | 0 1 1         | 0 1 0 | 161              | 0.114             | 0.092 |
| 3459.730               |                       |        | D                 | 0.720D-21 | 3386.053 | 11     | 1      | 10  | 12    | 1     | 11               | 0 1 1         | 0 1 0 | 161              |                   | 0.031 |
| 3460.015               | 3460.0158             |        | 0.609D-21         | 1874.974  | 10       | 5      | 6      | 10  | 6     | 5     | 1 0 0            | 0 0 0         | 161   | 0.018            | 0.022             |       |
| 3460.217               | 3460.2134             |        | 0.203D-21         | 4611.797  | 8        | 4      | 4      | 9   | 4     | 5     | 0 2 1            | 0 2 0         | 161   | 0.011            | 0.011             |       |
| 3460.409               | 3460.4085             | -6     | C                 | 0.217D-19 | 1813.224 | 10     | 3      | 7   | 11    | 3     | 8                | 0 0 1         | 0 0 0 | 161              | 0.676             | 0.772 |
| 3460.594               | 3460.5943             | -3     | C                 | 0.165D-19 | 2073.519 | 13     | 1      | 13  | 14    | 1     | 14               | 0 0 1         | 0 0 0 | 161              | 0.739             | 0.590 |
| 3460.594               |                       |        | D                 | 0.550D-20 | 2073.518 | 13     | 0      | 13  | 14    | 0     | 14               | 0 0 1         | 0 0 0 | 161              |                   | 0.197 |
| 3460.718               | 3460.7169             |        | 0.621D-21         | 2300.689  | 11       | 6      | 6      | 12  | 5     | 7     | 1 0 0            | 0 0 0         | 161   | 0.019            | 0.023             |       |
| 3460.771               | 3460.7731             |        | 0.294D-21         | 5027.258  | 9        | 1      | 8      | 10  | 1     | 9     | 0 0 2            | 0 0 1         | 161   | 0.014            | 0.017             |       |
| 3460.777               |                       |        | D                 | 0.832D-22 | 3266.538 | 13     | 8      | 6   | 14    | 7     | 7                | 1 0 0         | 0 0 0 | 161              |                   | 0.003 |
| 3461.344               | 3461.3431             | -12    | C                 | 0.295D-21 | 285.419  | 4      | 4      | 1   | 3     | 3     | 0                | 0 2 0         | 0 0 0 | 161              | 0.039             | 0.054 |
| 3461.556               | 3461.5556             | -10    | C                 | 0.984D-22 | 285.219  | 4      | 4      | 0   | 3     | 3     | 1                | 0 2 0         | 0 0 0 | 161              | 0.013             | 0.018 |
| 3461.557               |                       |        | D                 | 0.408D-22 | 5943.113 | 8      | 2      | 6   | 9     | 2     | 7                | 0 3 1         | 0 3 0 | 161              |                   | 0.003 |
| 3461.642               | 3461.6473             |        | 0.282D-21         | 4714.828  | 10       | 1      | 9      | 11  | 1     | 10    | 0 2 1            | 0 2 0         | 161   | 0.015            | 0.015             |       |
| 3461.643               |                       |        | D                 | 0.285D-22 | 5122.352 | 7      | 6      | 2   | 8     | 6     | 3                | 0 0 2         | 0 0 1 | 161              |                   | 0.002 |
| 3461.698               | 3461.6983             | -7     | C                 | 0.519D-20 | 1843.030 | 10     | 4      | 7   | 11    | 4     | 8                | 0 0 1         | 0 0 0 | 161              | 0.161             | 0.184 |
| 3461.772               | 3461.7786             |        | 0.307D-21         | 5062.020  | 10       | 1      | 10     | 11  | 1     | 11    | 0 0 2            | 0 0 1         | 161   | 0.017            | 0.018             |       |
| 3462.294               | 3462.2952             | 22     | H                 | 0.914D-21 | 3162.259 | 9      | 3      | 6   | 10    | 3     | 7                | 0 1 1         | 0 1 0 | 161              | 0.035             | 0.037 |
| 3462.522               |                       |        | D                 | 0.554D-22 | 2327.914 | 14     | 3      | 12  | 14    | 2     | 13               | 0 2 0         | 0 0 0 | 161              |                   | 0.002 |
| 3462.526               | 3462.5241             |        | 0.530D-21         | 1690.665  | 11       | 1      | 10     | 11  | 2     | 9     | 1 0 0            | 0 0 0         | 161   | 0.017            | 0.019             |       |
| 3462.591               | 3462.5904             | -9     | C                 | 0.100D-20 | 503.968  | 4      | 2      | 2   | 5     | 3     | 3                | 1 0 0         | 0 0 0 | 161              | 0.094             | 0.109 |
| 3462.814               | 3462.8142             | -6     | C                 | 0.319D-20 | 885.600  | 7      | 1      | 6   | 8     | 2     | 7                | 1 0 0         | 0 0 0 | 161              | 0.167             | 0.178 |
| 3462.935               | 3462.9381             |        | 0.926D-21         | 3321.013  | 8        | 6      | 2      | 9   | 6     | 3     | 0 1 1            | 0 1 0         | 161   | 0.034            | 0.039             |       |
| 3462.985               | 3462.9843             | -15    | H                 | 0.193D-20 | 3224.548 | 9      | 4      | 6   | 10    | 4     | 7                | 0 1 1         | 0 1 0 | 161              | 0.079             | 0.080 |
| 3464.383               | 3464.3807             | 4      | C                 | 0.326D-20 | 1875.464 | 9      | 6      | 3   | 10    | 6     | 4                | 0 0 1         | 0 0 0 | 161              | 0.100             | 0.116 |
| 3464.622               | 3464.6190             |        | 0.342D-21         | 4493.805  | 8        | 3      | 5      | 9   | 3     | 6     | 0 2 1            | 0 2 0         | 161   | 0.014            | 0.018             |       |
| 3464.668               | 3464.6684             | 3      | C                 | 0.975D-20 | 1874.974 | 9      | 6      | 4   | 10    | 6     | 5                | 0 0 1         | 0 0 0 | 161              | 0.297             | 0.346 |
| 3464.748               | 3464.7416             |        | 0.311D-21         | 2586.529  | 12       | 6      | 6      | 13  | 5     | 9     | 1 0 0            | 0 0 0         | 161   | 0.010            | 0.012             |       |
| 3465.017               | 3465.0148             |        | 0.618D-21         | 2756.418  | 12       | 7      | 6      | 13  | 6     | 7     | 1 0 0            | 0 0 0         | 161   | 0.020            | 0.024             |       |
| 3465.144               |                       |        | D                 | 0.758D-21 | 3391.135 | 12     | 1      | 12  | 13    | 1     | 13               | 0 1 1         | 0 1 0 | 161              |                   | 0.032 |
| 3465.149               | 3465.1480             |        | 0.227D-20         | 3391.131  | 12       | 0      | 12     | 13  | 0     | 13    | 0 1 1            | 0 1 0         | 161   | 0.109            | 0.097             |       |
| 3465.952               | 3465.9498             | -31    | H                 | 0.208D-20 | 2009.805 | 8      | 8      | 0   | 9     | 8     | 1                | 0 0 1         | 0 0 0 | 161              | 0.085             | 0.074 |
| 3465.952               |                       |        | D                 | 0.694D-21 | 2009.805 | 8      | 8      | 1   | 9     | 8     | 2                | 0 0 1         | 0 0 0 | 161              |                   | 0.025 |
| 3466.103               | 3466.1033             | 6      | C                 | 0.579D-21 | 920.211  | 8      | 4      | 4   | 9     | 1     | 9                | 0 2 0         | 0 0 0 | 161              | 0.030             | 0.031 |
| 3466.658               | 3466.6632             |        | 0.330D-21         | 2275.373  | 12       | 4      | 9      | 12  | 5     | 8     | 1 0 0            | 0 0 0         | 161   | 0.008            | 0.012             |       |
| 3466.894               | 3466.8951             | 4      | C                 | 0.459D-20 | 920.169  | 8      | 1      | 8   | 9     | 0     | 9                | 1 0 0         | 0 0 0 | 161              | 0.238             | 0.246 |
| 3467.147               | 3467.1450             | -33    | C                 | 0.957D-21 | 920.211  | 8      | 0      | 8   | 9     | 1     | 9                | 1 0 0         | 0 0 0 | 161              | 0.051             | 0.051 |
| 3467.496               | 3467.4969             | 18     | C                 | 0.452D-22 | 508.812  | 5      | 0      | 5   | 5     | 3     | 2                | 1 0 0         | 0 0 0 | 161              | 0.005             | 0.005 |
| 3467.501               |                       |        | D                 | 0.327D-22 | 5554.836 | 4      | 0      | 4   | 5     | 0     | 5                | 1 1 1         | 1 1 0 | 161              |                   | 0.002 |

## HIGH-TEMPERATURE WATER VAPOR SPECTRUM

441

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3467.575               | 3467.5731             |        | 0.248D-21         | 4949.004 | 8    | 3      | 6      | 9   | 3     | 7     | 0 0 2            | 0 0 1         | 161 | 0.009            | 0.014             |
| 3467.680               | 3467.6757             |        | 0.295D-21         | 4049.536 | 4    | 1      | 3      | 5   | 1     | 4     | 1 0 1            | 1 0 0         | 161 | 0.012            | 0.014             |
| 3468.559               | 3468.5581             | -4 C   | 0.954D-22         | 488.108  | 3    | 2      | 2      | 4   | 4     | 1     | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.011             |
| 3468.784               | 3468.7864             |        | 0.323D-21         | 4792.340 | 7    | 3      | 4      | 8   | 3     | 5     | 0 0 2            | 0 0 1         | 161 | 0.015            | 0.018             |
| 3468.873               | 3468.8677             |        | 0.320D-21         | 4095.803 | 5    | 1      | 5      | 6   | 1     | 6     | 1 0 1            | 1 0 0         | 161 | 0.012            | 0.015             |
| 3469.028               | 3469.0290             | 45 H   | 0.490D-21         | 2327.914 | 14   | 0      | 14     | 14  | 2     | 13    | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.018             |
| 3470.252               | 3470.2531             | 6 H    | 0.374D-21         | 2872.278 | 15   | 2      | 14     | 15  | 2     | 13    | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.015             |
| 3470.341               | 3470.3410             | 0 C    | 0.927D-21         | 882.891  | 7    | 2      | 6      | 8   | 1     | 7     | 1 0 0            | 0 0 0         | 161 | 0.049            | 0.052             |
| 3470.565               | 3470.5636             | -9 C   | 0.487D-20         | 1616.452 | 9    | 4      | 5      | 10  | 4     | 6     | 0 0 1            | 0 0 0         | 161 | 0.156            | 0.175             |
| 3470.831               | 3470.8220             |        | 0.314D-21         | 4696.859 | 11   | 1      | 11     | 12  | 1     | 12    | 0 2 1            | 0 2 0         | 161 | -0.016           | -0.017            |
| 3470.844               |                       | D      | 0.105D-21         | 4696.840 | 11   | 0      | 11     | 12  | 0     | 12    | 0 2 1            | 0 2 0         | 161 |                  | 0.006             |
| 3471.706               | 3471.7049             | -8 C   | 0.545D-21         | 1477.297 | 9    | 3      | 7      | 9   | 5     | 4     | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.020             |
| 3471.794               | 3471.7943             | -3 C   | 0.494D-20         | 1724.707 | 9    | 5      | 4      | 10  | 5     | 5     | 0 0 1            | 0 0 0         | 161 | 0.154            | 0.176             |
| 3471.945               | 3471.9469             |        | 0.441D-21         | 2337.669 | 7    | 0      | 7      | 8   | 1     | 8     | 1 1 0            | 0 1 0         | 161 | 0.014            | 0.016             |
| 3473.152               | 3473.1532             |        | 0.220D-21         | 4861.805 | 7    | 4      | 3      | 8   | 4     | 4     | 0 0 2            | 0 0 1         | 161 | 0.007            | 0.012             |
| 3473.267               | 3473.2620             | 0 H    | 0.272D-21         | 3439.308 | 16   | 2      | 14     | 16  | 4     | 13    | 0 0 1            | 0 0 0         | 161 | 0.009            | 0.012             |
| 3473.347               | 3473.3458             |        | 0.399D-21         | 2904.672 | 8    | 4      | 5      | 9   | 3     | 6     | 1 1 0            | 0 1 0         | 161 | 0.015            | 0.016             |
| 3473.370               | 3473.3683             | -11 C  | 0.248D-21         | 602.774  | 5    | 0      | 5      | 6   | 2     | 4     | 0 0 1            | 0 0 0         | 161 | 0.019            | 0.022             |
| 3474.124               |                       | D      | 0.109D-21         | 3306.296 | 7    | 7      | 0      | 8   | 7     | 1     | 0 1 1            | 0 1 0         | 161 |                  | 0.005             |
| 3474.124               | 3474.1256             | 6 H    | 0.328D-21         | 3306.296 | 7    | 7      | 1      | 8   | 7     | 2     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.014             |
| 3474.739               | 3474.7385             | 8 C    | 0.146D-19         | 1718.719 | 9    | 5      | 5      | 10  | 5     | 6     | 0 0 1            | 0 0 0         | 161 | 0.463            | 0.519             |
| 3474.925               | 3474.9224             | 105 H  | 0.157D-20         | 3141.047 | 8    | 5      | 3      | 9   | 5     | 4     | 0 1 1            | 0 1 0         | 161 | 0.060            | 0.064             |
| 3475.033               | 3475.0336             | 6 C    | 0.906D-21         | 383.842  | 3    | 2      | 2      | 4   | 3     | 1     | 1 0 0            | 0 0 0         | 161 | 0.109            | 0.129             |
| 3475.789               | 3475.7886             | -28 H  | 0.519D-21         | 3139.477 | 8    | 5      | 4      | 9   | 5     | 5     | 0 1 1            | 0 1 0         | 161 | 0.018            | 0.021             |
| 3476.346               | 3476.3469             |        | 0.211D-21         | 1631.384 | 9    | 5      | 4      | 9   | 6     | 3     | 1 0 0            | 0 0 0         | 161 | 0.005            | 0.008             |
| 3478.291               | 3478.2936             |        | 0.891D-22         | 3877.090 | 13   | 2      | 12     | 13  | 2     | 11    | 0 1 1            | 0 1 0         | 161 | 0.007            | 0.004             |
| 3478.687               | 3478.6956             |        | 0.101D-20         | 3058.400 | 9    | 2      | 7      | 10  | 2     | 8     | 0 1 1            | 0 1 0         | 161 | 0.038            | 0.041             |
| 3479.367               |                       | D      | 0.212D-21         | 1080.386 | 9    | 1      | 9      | 9   | 2     | 8     | 1 0 0            | 0 0 0         | 161 |                  | 0.010             |
| 3479.373               | 3479.3700             | -6 C   | 0.552D-20         | 1810.589 | 8    | 7      | 1      | 9   | 7     | 2     | 0 0 1            | 0 0 0         | 161 | 0.230            | 0.195             |
| 3479.377               |                       | D      | 0.184D-20         | 1810.584 | 8    | 7      | 2      | 9   | 7     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 0.065             |
| 3479.643               | 3479.6437             | 6 C    | 0.259D-21         | 1216.194 | 7    | 5      | 2      | 7   | 6     | 1     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.011             |
| 3479.648               |                       | D      | 0.817D-22         | 1216.189 | 7    | 5      | 3      | 7   | 6     | 2     | 1 0 0            | 0 0 0         | 161 |                  | 0.003             |
| 3479.713               | 3479.7082             |        | 0.378D-21         | 4399.543 | 8    | 2      | 6      | 9   | 2     | 7     | 0 2 1            | 0 2 0         | 161 | 0.023            | 0.019             |
| 3480.221               | 3480.2191             | -14 C  | 0.705D-21         | 1446.129 | 10   | 2      | 9      | 10  | 3     | 8     | 1 0 0            | 0 0 0         | 161 | 0.022            | 0.026             |
| 3480.228               |                       | D      | 0.448D-22         | 6212.043 | 7    | 1      | 6      | 8   | 1     | 7     | 0 1 2            | 0 1 1         | 161 |                  | 0.003             |
| 3480.395               | 3480.3954             | 1 C    | 0.233D-19         | 1690.665 | 10   | 2      | 8      | 11  | 2     | 9     | 0 0 1            | 0 0 0         | 161 | 0.761            | 0.829             |
| 3480.472               | 3480.4724             | 63 H   | 0.260D-20         | 3072.728 | 9    | 3      | 7      | 10  | 3     | 8     | 0 1 1            | 0 1 0         | 161 | 0.098            | 0.105             |
| 3480.588               |                       | D      | 0.726D-20         | 1774.619 | 11   | 1      | 10     | 12  | 1     | 11    | 0 0 1            | 0 0 0         | 161 |                  | 0.257             |
| 3480.595               | 3480.5937             | -11 C  | 0.217D-19         | 1774.752 | 11   | 2      | 10     | 12  | 2     | 11    | 0 0 1            | 0 0 0         | 161 | 0.890            | 0.768             |
| 3480.628               |                       | D      | 0.631D-21         | 1079.080 | 9    | 0      | 9      | 9   | 1     | 8     | 1 0 0            | 0 0 0         | 161 |                  | 0.029             |
| 3480.654               | 3480.6537             | -4 C   | 0.105D-20         | 709.609  | 6    | 1      | 5      | 7   | 2     | 6     | 1 0 0            | 0 0 0         | 161 | 0.064            | 0.076             |
| 3480.746               |                       | D      | 0.380D-21         | 4725.062 | 7    | 2      | 5      | 8   | 2     | 6     | 0 0 2            | 0 0 1         | 161 |                  | 0.021             |
| 3480.760               | 3480.7588             | -16 C  | 0.289D-21         | 315.779  | 3    | 1      | 3      | 4   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.044            | 0.049             |
| 3480.885               | 3480.8864             | 5 C    | 0.721D-20         | 1695.071 | 10   | 3      | 8      | 11  | 3     | 9     | 0 0 1            | 0 0 0         | 161 | 0.234            | 0.256             |
| 3481.127               | 3481.1259             | 0 H    | 0.235D-20         | 2998.768 | 8    | 4      | 4      | 9   | 4     | 5     | 0 1 1            | 0 1 0         | 161 | 0.086            | 0.093             |
| 3481.445               | 3481.4430             | -39 H  | 0.279D-20         | 3135.766 | 10   | 1      | 9      | 11  | 1     | 10    | 0 1 1            | 0 1 0         | 161 | 0.108            | 0.113             |
| 3481.516               | 3481.5142             |        | 0.923D-21         | 3136.415 | 10   | 2      | 9      | 11  | 2     | 10    | 0 1 1            | 0 1 0         | 161 | 0.033            | 0.038             |
| 3481.662               |                       | D      | 0.669D-22         | 1045.059 | 6    | 5      | 1      | 6   | 6     | 0     | 1 0 0            | 0 0 0         | 161 |                  | 0.003             |
| 3481.662               | 3481.6624             | 10 C   | 0.199D-21         | 1045.058 | 6    | 5      | 2      | 6   | 6     | 1     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.009             |
| 3482.247               | 3482.2463             | -7 C   | 0.287D-20         | 382.517  | 3    | 2      | 1      | 4   | 3     | 2     | 1 0 0            | 0 0 0         | 161 | 0.338            | 0.410             |
| 3482.480               |                       | D      | 0.741D-20         | 1806.673 | 12   | 1      | 12     | 13  | 1     | 13    | 0 0 1            | 0 0 0         | 161 |                  | 0.262             |
| 3482.482               | 3482.4809             | -7 C   | 0.222D-19         | 1806.672 | 12   | 0      | 12     | 13  | 0     | 13    | 0 0 1            | 0 0 0         | 161 | 1.015            | 0.785             |
| 3482.737               | 3482.7385             |        | 0.372D-21         | 4852.750 | 9    | 0      | 9      | 10  | 0     | 10    | 0 0 2            | 0 0 1         | 161 | 0.015            | 0.021             |
| 3483.455               | 3483.4514             |        | 0.348D-21         | 4483.227 | 9    | 2      | 8      | 10  | 2     | 9     | 0 2 1            | 0 2 0         | 161 | 0.018            | 0.018             |
| 3484.013               | 3484.0118             |        | 0.344D-21         | 4817.734 | 8    | 2      | 7      | 9   | 2     | 8     | 0 0 2            | 0 0 1         | 161 | 0.013            | 0.019             |
| 3484.132               | 3484.1319             | 3 C    | 0.952D-20         | 1538.150 | 9    | 3      | 6      | 10  | 3     | 7     | 0 0 1            | 0 0 0         | 161 | 0.314            | 0.346             |
| 3485.031               | 3485.0304             | 7 C    | 0.798D-22         | 383.842  | 5    | 4      | 2      | 4   | 3     | 1     | 0 2 0            | 0 0 0         | 161 | 0.010            | 0.011             |
| 3485.155               | 3485.1574             | -76 H  | 0.230D-21         | 1255.913 | 8    | 3      | 6      | 8   | 5     | 3     | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.009             |
| 3485.162               |                       | D      | 0.140D-22         | 6215.164 | 7    | 2      | 6      | 8   | 2     | 7     | 0 1 2            | 0 1 1         | 161 |                  | 0.001             |
| 3485.164               |                       | D      | 0.136D-21         | 4017.909 | 17   | 4      | 14     | 17  | 4     | 13    | 0 0 1            | 0 0 0         | 161 |                  | 0.006             |
| 3485.741               | 3485.7408             | 0 C    | 0.191D-19         | 1581.336 | 9    | 4      | 6      | 10  | 4     | 7     | 0 0 1            | 0 0 0         | 161 | 0.624            | 0.688             |
| 3486.470               | 3486.4700             | 0 C    | 0.240D-21         | 382.517  | 5    | 4      | 1      | 4   | 3     | 2     | 0 2 0            | 0 0 0         | 161 | 0.025            | 0.034             |
| 3486.596               | 3486.5913             | -41 H  | 0.296D-20         | 3144.579 | 11   | 1      | 11     | 12  | 1     | 12    | 0 1 1            | 0 1 0         | 161 | 0.148            | 0.120             |
| 3486.601               |                       | D      | 0.986D-21         | 3144.573 | 11   | 0      | 11     | 12  | 0     | 12    | 0 1 1            | 0 1 0         | 161 |                  | 0.040             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3486.687               | 3486.6870             |        | 0.123D-20         | 2275.373 | 11   | 6      | 5      | 12  | 5     | 8     | 1 0 0          | 0 0 0       | 161 | 0.036            | 0.044             |
| 3487.841               | 3487.8415             | 54     | H 0.763D-21       | 2983.324 | 8    | 4      | 5      | 9   | 4     | 6     | 0 1 1          | 0 1 0       | 161 | 0.028            | 0.030             |
| 3488.022               | 3488.0210             | -12    | C 0.480D-20       | 744.163  | 7    | 0      | 7      | 8   | 1     | 8     | 1 0 0          | 0 0 0       | 161 | 0.312            | 0.328             |
| 3488.117               |                       |        | D 0.987D-22       | 2630.194 | 8    | 2      | 7      | 8   | 3     | 6     | 1 1 0          | 0 1 0       | 161 |                  | 0.004             |
| 3488.133               | 3488.1268             |        | 0.318D-21         | 3976.308 | 4    | 0      | 4      | 5   | 0     | 5     | 1 0 1          | 1 0 0       | 161 | 0.011            | 0.015             |
| 3488.320               | 3488.3210             | 4      | C 0.159D-20       | 744.064  | 7    | 1      | 7      | 8   | 0     | 8     | 1 0 0          | 0 0 0       | 161 | 0.106            | 0.109             |
| 3488.351               | 3488.3498             | -6     | C 0.621D-21       | 661.549  | 5    | 1      | 4      | 6   | 3     | 3     | 0 0 1          | 0 0 0       | 161 | 0.043            | 0.049             |
| 3488.829               |                       |        | D 0.287D-21       | 3101.144 | 7    | 6      | 1      | 8   | 6     | 2     | 0 1 1          | 0 1 0       | 161 |                  | 0.012             |
| 3488.847               | 3488.8438             | 18     | H 0.862D-21       | 3101.124 | 7    | 6      | 2      | 8   | 6     | 3     | 0 1 1          | 0 1 0       | 161 | 0.033            | 0.035             |
| 3489.084               | 3489.0834             |        | -0.573D-21        | 1718.719 | 10   | 4      | 7      | 10  | 5     | 6     | 1 0 0          | 0 0 0       | 161 | 0.016            | 0.020             |
| 3489.357               | 3489.3535             |        | 0.285D-21         | 2927.939 | 12   | 8      | 5      | 13  | 7     | 6     | 1 0 0          | 0 0 0       | 161 | 0.010            | 0.011             |
| 3489.575               | 3489.5737             | -8     | H 0.300D-20       | 2904.672 | 8    | 3      | 5      | 9   | 3     | 6     | 0 1 1          | 0 1 0       | 161 | 0.109            | 0.117             |
| 3490.029               | 3490.0221             |        | 0.233D-21         | 4381.734 | 7    | 4      | 4      | 8   | 4     | 5     | 0 2 1          | 0 2 0       | 161 | 0.013            | 0.012             |
| 3490.556               | 3490.5549             | -2     | C 0.123D-21       | 842.357  | 7    | 1      | 7      | 7   | 3     | 4     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.007             |
| 3491.009               | 3491.0089             | -9     | C 0.105D-19       | 1631.384 | 8    | 6      | 2      | 9   | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.336            | 0.375             |
| 3491.102               | 3491.1015             | -2     | C 0.350D-20       | 1631.251 | 8    | 6      | 3      | 9   | 6     | 4     | 0 0 1          | 0 0 0       | 161 | 0.108            | 0.125             |
| 3491.738               | 3491.7367             |        | 0.255D-21         | 2042.374 | 13   | 0      | 13     | 13  | 2     | 12    | 0 0 1          | 0 0 0       | 161 | 0.009            | 0.009             |
| 3491.801               | 3491.7994             |        | 0.764D-21         | 2042.312 | 13   | 1      | 13     | 13  | 1     | 12    | 0 0 1          | 0 0 0       | 161 | 0.021            | 0.027             |
| 3491.898               |                       |        | D 0.527D-22       | 1282.919 | 8    | 6      | 3      | 9   | 3     | 6     | 0 2 0          | 0 0 0       | 161 |                  | 0.002             |
| 3491.898               | 3491.8956             | 2      | C 0.300D-20       | 1616.452 | 9    | 5      | 5      | 10  | 4     | 6     | 1 0 0          | 0 0 0       | 161 | 0.093            | 0.107             |
| 3491.934               |                       |        | 0.131D-21         | 4469.797 | 10   | 1      | 10     | 11  | 1     | 11    | 0 2 1          | 0 2 0       | 161 |                  | 0.007             |
| 3491.968               | 3491.9598             |        | 0.394D-21         | 4469.734 | 10   | 0      | 10     | 11  | 0     | 11    | 0 2 1          | 0 2 0       | 161 | 0.020            | 0.020             |
| 3492.669               | 3492.6682             |        | 0.127D-21         | 4259.879 | 7    | 3      | 4      | 8   | 3     | 5     | 0 2 1          | 0 2 0       | 161 | 0.006            | 0.006             |
| 3493.438               | 3493.4378             | -3     | C 0.734D-21       | 1059.835 | 7    | 3      | 5      | 7   | 5     | 2     | 0 0 1          | 0 0 0       | 161 | 0.029            | 0.034             |
| 3493.689               | 3493.6872             |        | 0.661D-21         | 2551.486 | 14   | 1      | 13     | 14  | 3     | 12    | 0 0 1          | 0 0 0       | 161 | 0.020            | 0.025             |
| 3494.161               | 3494.1607             |        | 0.140D-21         | 1131.776 | 8    | 2      | 7      | 8   | 4     | 4     | 0 0 1          | 0 0 0       | 161 | 0.006            | 0.006             |
| 3494.258               |                       |        | D 0.223D-21       | 2550.883 | 14   | 2      | 13     | 14  | 2     | 12    | 0 0 1          | 0 0 0       | 161 |                  | 0.008             |
| 3494.268               | 3494.2625             |        | 0.204D-21         | 3951.315 | 3    | 2      | 2      | 4   | 2     | 3     | 1 0 1          | 1 0 0       | 161 | 0.015            | 0.009             |
| 3494.934               | 3494.9293             |        | 0.733D-21         | 1581.336 | 10   | 3      | 8      | 10  | 4     | 7     | 1 0 0          | 0 0 0       | 161 | 0.021            | 0.026             |
| 3495.177               | 3495.1774             | 2      | C 0.243D-20       | 704.214  | 6    | 2      | 5      | 7   | 1     | 6     | 1 0 0          | 0 0 0       | 161 | 0.163            | 0.177             |
| 3495.783               | 3495.7847             | -5     | H 0.228D-21       | 3639.537 | 16   | 3      | 13     | 16  | 5     | 12    | 0 0 1          | 0 0 0       | 161 | 0.008            | 0.010             |
| 3496.279               | 3496.2792             |        | 0.234D-21         | 1474.981 | 9    | 4      | 6      | 9   | 5     | 5     | 1 0 0          | 0 0 0       | 161 | 0.008            | 0.009             |
| 3496.382               | 3496.3821             |        | 0.121D-20         | 2124.953 | 11   | 5      | 6      | 12  | 4     | 9     | 1 0 0          | 0 0 0       | 161 | 0.039            | 0.043             |
| 3496.625               | 3496.6227             | -21    | C 0.294D-20       | 552.912  | 5    | 1      | 4      | 6   | 2     | 5     | 1 0 0          | 0 0 0       | 161 | 0.251            | 0.285             |
| 3497.984               | 3497.9845             |        | 0.166D-20         | 1998.996 | 10   | 6      | 5      | 11  | 5     | 6     | 1 0 0          | 0 0 0       | 161 | 0.052            | 0.059             |
| 3498.603               | 3498.6013             | -9     | C 0.201D-21       | 888.632  | 6    | 3      | 4      | 6   | 5     | 1     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3499.563               | 3499.5593             | 7      | H 0.421D-21       | 3080.181 | 15   | 3      | 13     | 15  | 3     | 12    | 0 0 1          | 0 0 0       | 161 | 0.012            | 0.017             |
| 3499.743               |                       |        | D 0.233D-21       | 2433.803 | 12   | 4      | 8      | 12  | 6     | 7     | 0 0 1          | 0 0 0       | 161 |                  | 0.009             |
| 3499.747               | 3499.7463             | -5     | C 0.169D-19       | 1477.297 | 8    | 5      | 3      | 9   | 5     | 4     | 0 0 1          | 0 0 0       | 161 | 0.580            | 0.619             |
| 3500.321               | 3500.3197             | 2      | H 0.380D-20       | 2818.398 | 8    | 2      | 6      | 9   | 2     | 7     | 0 1 1          | 0 1 0       | 161 | 0.140            | 0.146             |
| 3500.327               |                       |        | D 0.755D-22       | 4663.152 | 6    | 4      | 2      | 7   | 4     | 3     | 0 0 2          | 0 0 1       | 161 |                  | 0.004             |
| 3500.676               | 3500.6776             |        | 0.639D-21         | 2433.803 | 11   | 7      | 4      | 12  | 6     | 7     | 1 0 0          | 0 0 0       | 161 | 0.018            | 0.023             |
| 3500.863               |                       |        | D 0.153D-21       | 3822.246 | 16   | 4      | 12     | 16  | 6     | 11    | 0 0 1          | 0 0 0       | 161 |                  | 0.007             |
| 3500.874               | 3500.8734             | 7      | C 0.298D-21       | 1216.232 | 9    | 2      | 8      | 9   | 3     | 7     | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.012             |
| 3501.063               | 3501.0626             | -2     | C 0.560D-20       | 1474.981 | 8    | 5      | 4      | 9   | 5     | 5     | 0 0 1          | 0 0 0       | 161 | 0.186            | 0.205             |
| 3501.227               | 3501.2265             | 0      | C 0.818D-21       | 1255.167 | 8    | 4      | 5      | 8   | 5     | 4     | 1 0 0          | 0 0 0       | 161 | 0.028            | 0.033             |
| 3501.406               | 3501.4078             | 68     | H 0.542D-21       | 2920.133 | 7    | 5      | 2      | 8   | 5     | 3     | 0 1 1          | 0 1 0       | 161 | 0.018            | 0.021             |
| 3501.463               | 3501.4629             | 2      | C 0.774D-21       | 885.600  | 8    | 1      | 8      | 8   | 2     | 7     | 1 0 0          | 0 0 0       | 161 | 0.032            | 0.043             |
| 3501.510               | 3501.5141             |        | 0.407D-21         | 4624.305 | 7    | 1      | 6      | 8   | 1     | 7     | 0 0 2          | 0 0 1       | 161 | 0.009            | 0.021             |
| 3501.563               |                       |        | D 0.189D-22       | 4918.234 | 9    | 3      | 7      | 9   | 3     | 6     | 1 0 1          | 1 0 0       | 161 |                  | 0.001             |
| 3501.568               | 3501.5679             | 0      | C 0.221D-19       | 1360.236 | 8    | 4      | 4      | 9   | 4     | 5     | 0 0 1          | 0 0 0       | 161 | 0.774            | 0.840             |
| 3501.727               | 3501.7274             | 1      | H 0.162D-20       | 2919.634 | 7    | 5      | 3      | 8   | 5     | 4     | 0 1 1          | 0 1 0       | 161 | 0.056            | 0.063             |
| 3501.826               | 3501.8250             | -5     | C 0.101D-19       | 1437.969 | 9    | 2      | 7      | 10  | 2     | 8     | 0 0 1          | 0 0 0       | 161 | 0.351            | 0.374             |
| 3502.229               | 3502.2277             | -7     | C 0.313D-21       | 742.076  | 5    | 3      | 3      | 5   | 5     | 0     | 0 0 1          | 0 0 0       | 161 | 0.021            | 0.021             |
| 3502.408               | 3502.4097             | 7      | C 0.281D-19       | 1524.849 | 10   | 1      | 9      | 11  | 1     | 10    | 0 0 1          | 0 0 0       | 161 | 1.039            | 1.018             |
| 3502.424               |                       |        | 0.903D-20         | 1525.137 | 10   | 2      | 9      | 11  | 2     | 10    | 0 0 1          | 0 0 0       | 161 |                  | 0.327             |
| 3502.875               | 3502.8750             | 0      | C 0.263D-19       | 1446.129 | 9    | 3      | 7      | 10  | 3     | 8     | 0 0 1          | 0 0 0       | 161 | 0.940            | 0.971             |
| 3502.879               |                       |        | D 0.116D-20       | 2903.147 | 9    | 1      | 8      | 10  | 1     | 9     | 0 1 1          | 0 1 0       | 161 |                  | 0.045             |
| 3503.076               |                       |        | D 0.153D-21       | 4173.227 | 7    | 2      | 5      | 8   | 2     | 6     | 0 2 1          | 0 2 0       | 161 |                  | 0.007             |
| 3503.077               | 3503.0757             |        | 0.334D-20         | 2904.429 | 9    | 2      | 8      | 10  | 2     | 9     | 0 1 1          | 0 1 0       | 161 | 0.133            | 0.130             |
| 3503.109               | 3503.1082             |        | 0.102D-20         | 2841.432 | 8    | 3      | 6      | 9   | 3     | 7     | 0 1 1          | 0 1 0       | 161 | 0.035            | 0.039             |
| 3503.261               |                       |        | 0.434D-21         | 4661.449 | 8    | 1      | 8      | 9   | 1     | 9     | 0 0 2          | 0 0 1       | 161 |                  | 0.023             |
| 3503.276               | 3503.2764             | 2      | C 0.282D-20       | 285.419  | 2    | 2      | 1      | 3   | 3     | 0     | 1 0 0          | 0 0 0       | 161 | 0.415            | 0.509             |
| 3503.579               | 3503.5809             |        | 0.567D-21         | 1813.224 | 11   | 2      | 9      | 11  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.015            | 0.020             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3503.827               | 3503.8211             |        | 0.145D-21         | 4661.426 | 8    | 0      | 8      | 9   | 0     | 9     | 0 0 2            | 0 0 1         | 161 | 0.007            | 0.008             |
| 3504.170               | 3504.1650             | -8     | C 0.290D-19       | 1557.850 | 11   | 1      | 11     | 12  | 1     | 12    | 0 0 1            | 0 0 0         | 161 | 1.369            | 1.043             |
| 3504.173               |                       |        | D 0.968D-20       | 1557.844 | 11   | 0      | 11     | 12  | 0     | 12    | 0 0 1            | 0 0 0         | 161 |                  | 0.348             |
| 3504.198               |                       |        | 0.428D-21         | 4263.148 | 8    | 1      | 7      | 9   | 1     | 8     | 0 2 1            | 0 2 0         | 161 |                  | 0.021             |
| 3504.343               | 3504.3445             | 17     | C 0.296D-21       | 1059.647 | 7    | 4      | 4      | 7   | 5     | 3     | 1 0 0            | 0 0 0         | 161 | 0.013            | 0.014             |
| 3504.460               |                       |        | D 0.127D-21       | 4625.937 | 7    | 2      | 6      | 8   | 2     | 7     | 0 0 2            | 0 0 1         | 161 |                  | 0.007             |
| 3504.467               | 3504.4658             | -11    | C 0.204D-21       | 882.891  | 8    | 0      | 8      | 8   | 1     | 7     | 1 0 0            | 0 0 0         | 161 | 0.015            | 0.011             |
| 3504.750               | 3504.7497             | -5     | C 0.946D-21       | 285.219  | 2    | 2      | 0      | 3   | 3     | 1     | 1 0 0            | 0 0 0         | 161 | 0.136            | 0.171             |
| 3504.972               |                       |        | D 0.378D-22       | 2439.956 | 7    | 2      | 6      | 7   | 3     | 5     | 1 1 0            | 0 1 0         | 161 |                  | 0.001             |
| 3504.973               | 3504.9767             |        | 0.547D-22         | 6061.922 | 7    | 0      | 7      | 8   | 0     | 8     | 0 1 2            | 0 1 1         | 161 | 0.006            | 0.004             |
| 3505.554               |                       |        | D 0.130D-20       | 1590.691 | 7    | 7      | 0      | 8   | 7     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 0.046             |
| 3505.555               | 3505.5552             | 2      | C 0.389D-20       | 1590.690 | 7    | 7      | 1      | 8   | 7     | 2     | 0 0 1            | 0 0 0         | 161 | 0.165            | 0.139             |
| 3505.601               | 3505.5977             |        | 0.288D-21         | 4224.586 | 7    | 3      | 5      | 8   | 3     | 6     | 0 2 1            | 0 2 0         | 161 | 0.017            | 0.014             |
| 3505.866               | 3505.8662             | 9      | C 0.807D-21       | 888.599  | 6    | 4      | 3      | 6   | 5     | 2     | 1 0 0            | 0 0 0         | 161 | 0.041            | 0.044             |
| 3506.079               | 3506.0790             | 5      | C 0.139D-21       | 742.073  | 5    | 3      | 2      | 5   | 3     | 1     | 0 0 1            | 0 0 0         | 161 | 0.009            | 0.009             |
| 3506.703               | 3506.7028             | 3      | C 0.189D-21       | 508.812  | 6    | 4      | 3      | 5   | 3     | 2     | 0 2 0            | 0 0 0         | 161 | 0.014            | 0.020             |
| 3507.827               |                       |        | D 0.124D-20       | 2915.897 | 10   | 1      | 10     | 11  | 1     | 11    | 0 1 1            | 0 1 0         | 161 |                  | 0.048             |
| 3507.834               | 3507.8322             | -8     | H 0.372D-20       | 2915.876 | 10   | 0      | 10     | 11  | 0     | 11    | 0 1 1            | 0 1 0         | 161 | 0.176            | 0.145             |
| 3508.377               | 3508.3800             |        | 0.708D-21         | 1843.030 | 10   | 5      | 5      | 11  | 4     | 8     | 1 0 0            | 0 0 0         | 161 | 0.021            | 0.025             |
| 3508.677               | 3508.6730             |        | 0.278D-21         | 3877.575 | 3    | 1      | 3      | 4   | 1     | 4     | 1 0 1            | 1 0 0         | 161 | 0.010            | 0.013             |
| 3508.836               | 3508.8355             | -8     | C 0.159D-20       | 586.479  | 6    | 0      | 6      | 7   | 1     | 7     | 1 0 0            | 0 0 0         | 161 | 0.129            | 0.144             |
| 3509.048               | 3509.0461             | -53    | H 0.784D-21       | 2670.792 | 7    | 3      | 4      | 8   | 3     | 5     | 0 1 1            | 0 1 0         | 161 | 0.026            | 0.029             |
| 3509.421               | 3509.4214             | -2     | C 0.351D-19       | 1282.919 | 8    | 3      | 5      | 9   | 3     | 6     | 0 0 1            | 0 0 0         | 161 | 1.291            | 1.377             |
| 3509.545               |                       |        | 0.864D-21         | 2771.691 | 7    | 4      | 3      | 8   | 4     | 4     | 0 1 1            | 0 1 0         | 161 |                  | 0.033             |
| 3509.552               |                       |        | D 0.302D-21       | 1340.886 | 9    | 3      | 7      | 9   | 4     | 6     | 1 0 0            | 0 0 0         | 161 |                  | 0.012             |
| 3509.560               | 3509.5594             | -5     | C 0.469D-20       | 586.243  | 6    | 1      | 6      | 7   | 0     | 7     | 1 0 0            | 0 0 0         | 161 | 0.405            | 0.424             |
| 3510.500               | 3510.5012             | 12     | C 0.289D-21       | 782.410  | 6    | 3      | 4      | 7   | 2     | 5     | 1 0 0            | 0 0 0         | 161 | 0.017            | 0.018             |
| 3510.653               | 3510.6532             | -1     | C 0.760D-20       | 1340.886 | 8    | 4      | 5      | 9   | 4     | 6     | 0 0 1            | 0 0 0         | 161 | -0.273           | 0.290             |
| 3511.386               | 3511.3874             | 67     | H 0.258D-21       | 3084.835 | 14   | 4      | 10     | 14  | 6     | 9     | 0 0 1            | 0 0 0         | 161 | 0.009            | 0.010             |
| 3511.429               | 3511.4293             |        | 0.465D-21         | 1985.788 | 10   | 6      | 4      | 11  | 5     | 7     | 1 0 0            | 0 0 0         | 161 | 0.015            | 0.016             |
| 3511.594               | 3511.5944             | 2      | C 0.881D-21       | 416.209  | 4    | 1      | 3      | 5   | 2     | 4     | 1 0 0            | 0 0 0         | 161 | 0.098            | 0.115             |
| 3511.599               |                       |        | D 0.727D-22       | 4153.937 | 4    | 4      | 1      | 5   | 3     | 2     | 2 0 0            | 1 0 0         | 161 |                  | 0.003             |
| 3512.079               | 3512.0832             | -13    | C 0.408D-21       | 2042.755 | 5    | 0      | 5      | 6   | 1     | 6     | 1 1 0            | 0 1 0         | 161 | 0.017            | 0.014             |
| 3512.084               |                       |        | D 0.635D-22       | 503.968  | 6    | 4      | 2      | 5   | 3     | 3     | 0 2 0            | 0 0 0         | 161 |                  | 0.007             |
| 3512.373               |                       |        | D 0.264D-22       | 1321.463 | 10   | 1      | 10     | 11  | 1     | 11    | 0 0 1            | 0 0 0         | 181 |                  | 0.001             |
| 3512.378               | 3512.3766             |        | 0.791D-22         | 1321.456 | 10   | 0      | 10     | 11  | 0     | 11    | 0 0 1            | 0 0 0         | 181 | 0.005            | 0.003             |
| 3512.470               | 3512.4635             |        | 0.478D-21         | 4260.469 | 9    | 1      | 9      | 10  | 1     | 10    | 0 2 1            | 0 2 0         | 161 | 0.021            | 0.023             |
| 3512.610               |                       |        | D 0.745D-22       | 3623.762 | 16   | 4      | 13     | 16  | 4     | 12    | 0 0 1            | 0 0 0         | 161 |                  | 0.003             |
| 3512.611               | 3512.6112             | 10     | C 0.218D-21       | 1059.835 | 7    | 4      | 3      | 7   | 5     | 2     | 1 0 0            | 0 0 0         | 161 | 0.010            | 0.010             |
| 3513.072               | 3513.0718             | 6      | C 0.323D-21       | 382.517  | 3    | 1      | 3      | 4   | 3     | 2     | 0 0 1            | 0 0 0         | 161 | 0.037            | 0.046             |
| 3513.168               | 3513.1651             | -48    | H 0.255D-20       | 2764.699 | 7    | 4      | 4      | 8   | 4     | 5     | 0 1 1            | 0 1 0         | 161 | 0.091            | 0.097             |
| 3513.536               | 3513.5357             |        | 0.243D-21         | 4553.273 | 6    | 3      | 4      | 7   | 3     | 5     | 0 0 2            | 0 0 1         | 161 | 0.009            | 0.013             |
| 3513.832               | 3513.8325             | 1      | C 0.451D-21       | 1050.158 | 7    | 4      | 4      | 8   | 3     | 5     | 1 0 0            | 0 0 0         | 161 | 0.020            | 0.021             |
| 3514.046               | 3514.0451             | -4     | C 0.903D-21       | 1201.922 | 9    | 1      | 8      | 9   | 2     | 7     | 1 0 0            | 0 0 0         | 161 | 0.035            | 0.037             |
| 3514.165               | 3514.1652             | 2      | C 0.164D-21       | 742.076  | 5    | 4      | 1      | 5   | 5     | 0     | 1 0 0            | 0 0 0         | 161 | 0.008            | 0.011             |
| 3514.321               | 3514.3188             |        | 0.245D-21         | 4188.395 | 6    | 4      | 2      | 7   | 4     | 3     | 0 2 1            | 0 2 0         | 161 | 0.014            | 0.012             |
| 3514.402               | 3514.4022             |        | 0.108D-20         | 1774.752 | 12   | 0      | 12     | 12  | 2     | 11    | 0 0 1            | 0 0 0         | 161 | 0.040            | 0.038             |
| 3514.535               | 3514.5363             |        | 0.361D-21         | 1774.619 | 12   | 1      | 12     | 12  | 1     | 11    | 0 0 1            | 0 0 0         | 161 | 0.012            | 0.013             |
| 3514.625               | 3514.6230             | -14    | H 0.589D-21       | 2905.435 | 6    | 6      | 0      | 7   | 6     | 1     | 0 1 1            | 0 1 0         | 161 | 0.029            | 0.023             |
| 3514.628               |                       |        | D 0.196D-21       | 2905.431 | 6    | 6      | 1      | 7   | 6     | 2     | 0 1 1            | 0 1 0         | 161 |                  | 0.008             |
| 3516.121               | 3516.1238             | -38    | H 0.330D-21       | 2248.067 | 13   | 1      | 12     | 13  | 3     | 11    | 0 0 1            | 0 0 0         | 161 | 0.012            | 0.012             |
| 3516.125               |                       |        | D 0.131D-22       | 6716.168 | 7    | 7      | 1      | 7   | 7     | 0     | 1 1 1            | 1 1 0         | 161 |                  | 0.001             |
| 3517.185               | 3517.1873             |        | 0.296D-21         | 2612.801 | 11   | 8      | 3      | 12  | 7     | 6     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.011             |
| 3517.190               |                       |        | D 0.217D-22       | 5610.766 | 5    | 4      | 2      | 6   | 4     | 3     | 0 3 1            | 0 3 0         | 161 |                  | 0.001             |
| 3517.321               | 3517.3205             |        | 0.992D-21         | 2246.888 | 13   | 2      | 12     | 13  | 2     | 11    | 0 0 1            | 0 0 0         | 161 | 0.031            | 0.035             |
| 3517.426               | 3517.4270             | 5      | C 0.328D-20       | 1411.647 | 7    | 6      | 1      | 8   | 6     | 2     | 0 0 1            | 0 0 0         | 161 | 0.123            | 0.122             |
| 3517.450               | 3517.4496             | -6     | C 0.983D-20       | 1411.612 | 7    | 6      | 2      | 8   | 6     | 3     | 0 0 1            | 0 0 0         | 161 | 0.343            | 0.365             |
| 3517.676               | 3517.6755             | -4     | H 0.639D-21       | 2746.024 | 14   | 2      | 12     | 14  | 4     | 11    | 0 0 1            | 0 0 0         | 161 | 0.019            | 0.024             |
| 3518.992               | 3518.9929             | 8      | C 0.159D-20       | 508.812  | 4    | 1      | 3      | 5   | 3     | 2     | 0 0 1            | 0 0 0         | 161 | 0.145            | 0.168             |
| 3519.035               | 3519.0332             | 10     | C 0.386D-21       | 1477.297 | 9    | 6      | 3      | 9   | 5     | 4     | 0 2 0            | 0 0 0         | 161 | 0.012            | 0.014             |
| 3519.842               |                       |        | D 0.439D-22       | 1474.981 | 9    | 6      | 4      | 9   | 5     | 5     | 0 2 0            | 0 0 0         | 161 |                  | 0.002             |
| 3519.849               | 3519.8478             | -4     | C 0.109D-20       | 1006.116 | 8    | 2      | 7      | 8   | 3     | 6     | 1 0 0            | 0 0 0         | 161 | 0.047            | 0.052             |
| 3520.966               | 3520.9647             |        | 0.308D-21         | 4052.837 | 6    | 3      | 3      | 7   | 3     | 4     | 0 2 1            | 0 2 0         | 161 | 0.020            | 0.014             |
| 3521.116               | 3521.1153             | 0      | C 0.660D-21       | 931.237  | 7    | 2      | 6      | 7   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 0.030            | 0.034             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3521.290               | 3521.2904             | 2      | C 0.106D-20       | 1122.709 | 8    | 3      | 6      | 8   | 4     | 5     | 1 0 0            | 0 0 0         | 161 | 0.038            | 0.046             |
| 3522.226               | 3522.2266             | 5      | C 0.605D-21       | 542.906  | 5    | 2      | 4      | 6   | 1     | 5     | 1 0 0            | 0 0 0         | 161 | 0.050            | 0.060             |
| 3522.570               | 3522.5718             |        | 0.511D-21         | 2670.792 | 7    | 4      | 4      | 8   | 3     | 5     | 1 1 0            | 0 1 0         | 161 | 0.018            | 0.019             |
| 3522.741               | 3522.7413             | 5      | C 0.120D-20       | 212.156  | 2    | 1      | 2      | 3   | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.195            | 0.260             |
| 3522.776               | 3522.7748             | -5     | C 0.304D-21       | 709.609  | 7    | 1      | 7      | 7   | 2     | 6     | 1 0 0            | 0 0 0         | 161 | 0.016            | 0.022             |
| 3522.824               |                       |        | D 0.161D-21       | 4408.027 | 5    | 3      | 2      | 6   | 3     | 3     | 0 0 2            | 2 0 0         | 161 |                  | 0.008             |
| 3522.825               | 3522.8215             |        | 0.152D-20         | 2595.813 | 7    | 2      | 5      | 8   | 2     | 6     | 0 1 1            | 0 1 0         | 161 | 0.062            | 0.056             |
| 3523.141               | 3523.1415             | 6      | C 0.381D-19       | 1201.922 | 8    | 2      | 6      | 9   | 2     | 7     | 0 0 1            | 0 0 0         | 161 | 1.441            | 1.558             |
| 3523.962               |                       |        | D 0.422D-20       | 2688.080 | 8    | 1      | 7      | 9   | 1     | 8     | 0 1 1            | 0 1 0         | 161 |                  | 0.158             |
| 3523.972               | 3523.9720             | -10    | C 0.117D-19       | 1293.019 | -9   | -1     | 8      | 10  | 1     | 9     | 0 0 1            | 0 0 0         | 161 | 0.487            | 0.455             |
| 3524.102               | 3524.1021             | 2      | C 0.347D-19       | 1293.634 | 9    | 2      | 8      | 10  | 2     | 9     | 0 0 1            | 0 0 0         | 161 | 1.278            | 1.349             |
| 3524.123               |                       |        | 0.487D-21         | 4488.090 | 7    | 0      | 7      | 8   | 0     | 8     | 0 0 2            | 0 0 1         | 161 |                  | 0.025             |
| 3524.569               | 3524.5685             | 5      | H 0.136D-20       | 2690.595 | 8    | 2      | 7      | 9   | 2     | 8     | 0 1 1            | 0 1 0         | 161 | 0.047            | 0.051             |
| 3524.835               | 3524.8362             | 4      | C 0.982D-20       | 1216.232 | 8    | 3      | 6      | 9   | 3     | 7     | 0 0 1            | 0 0 0         | 161 | 0.373            | 0.398             |
| 3524.906               | 3524.9006             |        | 0.167D-21         | 4062.837 | 7    | 1      | 6      | 8   | 1     | 7     | 0 2 1            | 0 2 0         | 161 | 0.009            | 0.008             |
| 3525.638               |                       |        | D 0.122D-19       | 1327.119 | 10   | 1      | 10     | 11  | 1     | 11    | 0 0 1            | 0 0 0         | 161 |                  | 0.467             |
| 3525.640               | 3525.6389             | 0      | C 0.366D-19       | 1327.110 | 10   | 0      | 10     | 11  | 0     | 11    | 0 0 1            | 0 0 0         | 161 | 1.854            | 1.401             |
| 3525.844               | 3525.8422             |        | 0.332D-21         | 4452.352 | 6    | 2      | 5      | 7   | 2     | 6     | 0 0 2            | 0 0 1         | 161 | 0.016            | 0.017             |
| 3526.310               | 3526.3096             | 15     | H 0.344D-20       | 2630.194 | 7    | 3      | 5      | 8   | 3     | 6     | 0 1 1            | 0 1 0         | 161 | 0.119            | 0.128             |
| 3526.394               | 3526.3927             | 5      | C 0.295D-20       | 1581.336 | 9    | 5      | 4      | 10  | 4     | 7     | 1 0 0            | 0 0 0         | 161 | 0.096            | 0.105             |
| 3526.572               | 3526.5685             |        | 0.645D-21         | 2144.047 | 10   | 7      | 4      | 11  | 6     | 5     | 1 0 0            | 0 0 0         | 161 | 0.020            | 0.023             |
| 3526.601               |                       |        | 0.202D-21         | 4491.371 | 5    | 4      | 1      | 6   | 4     | 2     | 0 0 2            | 0 0 1         | 161 |                  | 0.010             |
| 3526.623               | 3526.6154             |        | 0.463D-21         | 4071.733 | 7    | 2      | 6      | 8   | 2     | 7     | 0 2 1            | 0 2 0         | 161 | 0.025            | 0.022             |
| 3527.007               | 3527.0081             | -5     | C 0.591D-20       | 1255.913 | 7    | 5      | 2      | 8   | 5     | 3     | 0 0 1            | 0 0 0         | 161 | 0.208            | 0.234             |
| 3527.031               | 3527.0300             | -16    | C 0.230D-20       | 300.362  | 3    | 1      | 2      | 4   | 2     | 3     | 1 0 0            | 0 0 0         | 161 | 0.316            | 0.397             |
| 3527.036               |                       |        | D 0.451D-22       | 1059.647 | 7    | 3      | 4      | 7   | 5     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 0.002             |
| 3527.414               | 3527.4132             |        | 0.448D-21         | 4350.699 | 5    | 2      | 3      | 6   | 2     | 4     | 0 0 2            | 0 0 1         | 161 | 0.016            | 0.022             |
| 3527.496               | 3527.4960             | 5      | C 0.177D-19       | 1255.167 | 7    | 5      | 3      | 8   | 5     | 4     | 0 0 1            | 0 0 0         | 161 | 0.650            | 0.701             |
| 3527.548               | 3527.5475             |        | 0.147D-20         | 2724.168 | 6    | 5      | 1      | 7   | 5     | 2     | 0 1 1            | 0 1 0         | 161 | 0.051            | 0.055             |
| 3527.641               | 3527.6412             |        | 0.489D-21         | 2724.043 | 6    | 5      | 2      | 7   | 5     | 3     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.018             |
| 3527.829               | 3527.8255             |        | 0.525D-21         | 3967.489 | 6    | 2      | 4      | 7   | 2     | 5     | 0 2 1            | 0 2 0         | 161 | 0.026            | 0.024             |
| 3527.971               | 3527.9705             | 0      | C 0.922D-21       | 704.214  | 7    | 0      | 7      | 7   | 1     | 6     | 1 0 0            | 0 0 0         | 161 | 0.057            | 0.067             |
| 3528.121               | 3528.1199             | -6     | C 0.117D-20       | 446.511  | 4    | 0      | 4      | 5   | 2     | 3     | 0 0 1            | 0 0 0         | 161 | 0.120            | 0.142             |
| 3528.853               |                       |        | 0.151D-20         | 2705.097 | 9    | 0      | 9      | 10  | 0     | 10    | 0 1 1            | 0 1 0         | 161 |                  | 0.057             |
| 3528.866               | 3528.8641             |        | 0.452D-20         | 2705.141 | 9    | 1      | 9      | 10  | 1     | 10    | 0 1 1            | 0 1 0         | 161 | 0.184            | 0.170             |
| 3529.056               | 3529.0555             | -9     | C 0.445D-20       | 447.252  | 5    | 0      | 5      | 6   | 1     | 6     | 1 0 0            | 0 0 0         | 161 | 0.470            | 0.539             |
| 3529.222               | 3529.2212             | -7     | C 0.523D-20       | 1360.236 | 8    | 5      | 4      | 9   | 4     | 5     | 1 0 0            | 0 0 0         | 161 | 0.186            | 0.197             |
| 3530.074               | 3530.0744             | 4      | C 0.381D-21       | 927.744  | 7    | 3      | 5      | 7   | 4     | 4     | 1 0 0            | 0 0 0         | 161 | 0.015            | 0.020             |
| 3530.760               | 3530.7595             | -8     | C 0.144D-20       | 446.697  | 5    | 1      | 5      | 6   | 0     | 6     | 1 0 0            | 0 0 0         | 161 | 0.154            | 0.174             |
| 3530.940               | 3530.9365             |        | 0.265D-21         | 1538.150 | 10   | 2      | 8      | 10  | 3     | 7     | 1 0 0            | 0 0 0         | 161 | 0.008            | 0.009             |
| 3531.253               | 3531.2490             |        | 0.179D-21         | 3314.857 | 11   | 2      | 10     | 11  | 2     | 9     | 0 1 1            | 0 1 0         | 161 | 0.008            | 0.007             |
| 3531.375               | 3531.3754             | 0      | C 0.867D-20       | 1131.776 | 7    | 4      | 3      | 8   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.349            | 0.371             |
| 3531.675               | 3531.6770             |        | 0.488D-21         | 1724.707 | 9    | 6      | 4      | 10  | 5     | 5     | 1 0 0            | 0 0 0         | 161 | 0.014            | 0.017             |
| 3532.839               | 3532.8364             |        | 0.454D-21         | 2918.244 | 14   | 3      | 11     | 14  | 5     | 10    | 0 0 1            | 0 0 0         | 161 | 0.013            | 0.018             |
| 3533.463               | 3533.4598             |        | 0.558D-21         | 4068.704 | 8    | 0      | 8      | 9   | 0     | 9     | 0 2 1            | 0 2 0         | 161 | 0.030            | 0.026             |
|                        |                       |        |                   |          |      |        |        |     |       |       |                  |               |     | 0.007            |                   |
| 3536.185               | 3536.1858             | 9      | C 0.112D-20       | 756.725  | 6    | 3      | 4      | 6   | 4     | 3     | 1 0 0            | 0 0 0         | 161 | 0.061            | 0.074             |
| 3536.266               | 3536.2665             | 3      | C 0.257D-19       | 1122.709 | 7    | 4      | 4      | 8   | 4     | 5     | 0 0 1            | 0 0 0         | 161 | 1.034            | 1.106             |
| 3536.526               | 3536.5254             | -5     | C 0.130D-19       | 1050.158 | 7    | 3      | 4      | 8   | 3     | 5     | 0 0 1            | 0 0 0         | 161 | 0.562            | 0.594             |
| 3536.538               |                       |        | 0.421D-21         | 816.694  | 7    | 2      | 6      | 7   | 3     | 5     | 1 0 0            | 0 0 0         | 161 |                  | 0.025             |
| 3536.880               | 3536.8743             | 43     | B 0.497D-21       | 1525.137 | 11   | 0      | 11     | 11  | 2     | 10    | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.018             |
| 3537.171               | 3537.1664             | -45    | C 0.149D-20       | 1524.849 | 11   | 1      | 11     | 11  | 1     | 10    | 0 0 1            | 0 0 0         | 161 | 0.058            | 0.053             |
| 3537.174               |                       |        | 0.376D-21         | 1255.167 | 8    | 3      | 5      | 8   | 5     | 4     | 0 0 1            | 0 0 0         | 161 |                  | 0.015             |
| 3537.197               | 3537.1964             | 0      | H 0.261D-20       | 2572.140 | 6    | 4      | 2      | 7   | 4     | 3     | 0 1 1            | 0 1 0         | 161 | 0.091            | 0.096             |
| 3537.730               | 3537.7292             |        | 0.137D-20         | 1718.719 | 9    | 6      | 3      | 10  | 5     | 6     | 1 0 0            | 0 0 0         | 161 | 0.043            | 0.048             |
| 3538.350               | 3538.3496             |        | 0.142D-20         | 1962.508 | 12   | 1      | 11     | 12  | 3     | 10    | 0 0 1            | 0 0 0         | 161 | 0.043            | 0.049             |
| 3538.719               | 3538.7155             |        | 0.318D-21         | 2426.195 | 13   | 2      | 11     | 13  | 4     | 10    | 0 0 1            | 0 0 0         | 161 | 0.008            | 0.011             |
| 3538.783               | 3538.7830             | -3     | C 0.362D-21       | 757.780  | 6    | 2      | 5      | 6   | 4     | 2     | 0 0 1            | 0 0 0         | 161 | 0.021            | 0.024             |
| 3538.806               |                       |        | 0.385D-22         | 5496.980 | 10   | 6      | 4      | 10  | 6     | 5     | 1 0 1            | 1 0 0         | 161 |                  | 0.002             |
| 3538.808               | 3538.8061             |        | 0.861D-21         | 2569.508 | 6    | 4      | 3      | 7   | 4     | 4     | 0 1 1            | 0 1 0         | 161 | 0.029            | 0.032             |
| 3539.415               |                       |        | D 0.145D-21       | 648.979  | 7    | 4      | 3      | 6   | 3     | 4     | 0 2 0            | 0 0 0         | 161 |                  | 0.012             |
| 3539.418               | 3539.4157             | 3      | C 0.355D-20       | 2462.876 | 6    | 3      | 3      | 7   | 3     | 4     | 0 1 1            | 0 1 0         | 161 | 0.131            | 0.129             |
| 3539.691               | 3539.6909             | 25     | H 0.151D-21       | 5020.027 | 7    | 7      | 1      | 7   | 7     | 0     | 1 0 1            | 1 0 0         | 161 | 0.006            | 0.008             |
| 3539.691               |                       |        | D 0.503D-22       | 5020.027 | 7    | 7      | 0      | 7   | 7     | 1     | 1 0 1            | 1 0 0         | 161 |                  | 0.003             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu'_1 \nu'_2 \nu'_3$ | $\nu_1 \nu_2 \nu_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------------|---------------------|-----|------------------|-------------------|
| 3540.050               | 3540.0489             |             | 0.588D-21         | 1899.008 | 11   | 3      | 8      | 11  | 4     | 7     | 1 0 0                  | 0 0 0               | 161 | 0.016            | 0.020             |
| 3540.173               | 3540.1737             | 10          | C 0.316D-21       | 610.114  | 5    | 3      | 3      | 5   | 4     | 2     | 1 0 0                  | 0 0 0               | 161 | 0.023            | 0.027             |
| 3540.677               | 3540.6778             | 11          | C 0.384D-21       | 982.912  | 8    | 1      | 7      | 8   | 2     | 6     | 1 0 0                  | 0 0 0               | 161 | 0.017            | 0.019             |
| 3540.709               | 3540.7090             |             | 0.474D-21         | 1960.208 | 12   | 2      | 11     | 12  | 2     | 10    | 0 0 1                  | 0 0 0               | 161 | 0.015            | 0.016             |
| 3540.860               | 3540.8635             |             | 0.217D-21         | 4015.515 | 5    | 4      | 2      | 6   | 4     | 3     | 0 2 1                  | 0 2 0               | 161 | 0.011            | 0.010             |
| 3540.871               |                       | D 0.115D-21 | 3072.728          | 9        | 4    | 5      | 10     | 3   | 8     | 1     | 1 0 0                  | 0 1 0               | 161 |                  | 0.005             |
| 3540.956               | 3540.9567             |             | 0.614D-22         | 2398.382 | 6    | 2      | 4      | 6   | 4     | 3     | 0 1 1                  | 0 1 0               | 161 | 0.006            | 0.002             |
| 3542.639               | 3542.6380             |             | 0.481D-21         | 4290.758 | 5    | 1      | 4      | 6   | 1     | 5     | 0 0 2                  | 0 0 1               | 161 | 0.018            | 0.024             |
| 3542.731               | 3542.7308             | -3          | C 0.587D-21       | 488.108  | 4    | 3      | 2      | 4   | 4     | 1     | 1 0 0                  | 0 0 0               | 161 | 0.055            | 0.065             |
| 3542.892               | 3542.8928             | 11          | C 0.104D-20       | 552.912  | 6    | 1      | 6      | 6   | 2     | 5     | 1 0 0                  | 0 0 0               | 161 | 0.087            | 0.100             |
| 3543.020               | 3543.0197             | 2           | C 0.311D-21       | 383.842  | 3    | 1      | 2      | 4   | 3     | 1     | 0 0 1                  | 0 0 0               | 161 | 0.036            | 0.043             |
| 3543.597               | 3543.5957             | -14         | C 0.116D-20       | 610.341  | 5    | 3      | 2      | 5   | 4     | 1     | 1 0 0                  | 0 0 0               | 161 | 0.086            | 0.099             |
| 3543.659               | 3543.6593             | -2          | C 0.673D-20       | 1216.194 | 6    | 6      | 0      | 7   | 6     | 1     | 0 0 1                  | 0 0 0               | 161 | 0.323            | 0.271             |
| 3543.664               |                       | D 0.224D-20 | 1216.189          | 6        | 6    | 1      | 7      | 6   | 2     | 0 0 1 | 0 0 0                  | 161                 |     | 0.090            |                   |
| 3543.701               |                       | D 0.269D-21 | 2321.905          | 10       | 8    | 3      | 11     | 7   | 4     | 1 0 0 | 0 0 0                  | 161                 |     | 0.010            |                   |
| 3543.719               | 3543.7189             | 0           | C 0.209D-21       | 488.134  | 4    | 3      | 1      | 4   | 4     | 0     | 1 0 0                  | 0 0 0               | 161 | 0.016            | 0.023             |
| 3544.163               | 3544.1629             | -2          | C 0.655D-21       | 206.301  | 2    | 1      | 1      | 3   | 2     | 2     | 1 0 0                  | 0 0 0               | 161 | 0.113            | 0.143             |
| 3544.483               | 3544.4831             |             | 0.236D-21         | 3072.728 | 10   | 1      | 9      | 10  | 3     | 8     | 0 1 1                  | 0 1 0               | 161 | 0.009            | 0.009             |
| 3544.637               | 3544.6352             | -13         | H 0.164D-20       | 2490.355 | 7    | 1      | 6      | 8   | 1     | 7     | 0 1 1                  | 0 1 0               | 161 | 0.058            | 0.060             |
| 3544.942               | 3544.9427             |             | 0.521D-21         | 4332.914 | 6    | 1      | 6      | 7   | 1     | 7     | 0 0 2                  | 0 0 1               | 161 | 0.018            | 0.026             |
| 3545.037               | 3545.0376             | -4          | C 0.153D-19       | 982.912  | 7    | 2      | 5      | 8   | 2     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.715            | 0.746             |
| 3545.223               | 3545.2228             | -6          | C 0.423D-19       | 1079.080 | 8    | 1      | 7      | 9   | 1     | 8     | 0 0 1                  | 0 0 0               | 161 | 1.800            | 1.881             |
| 3545.509               | 3545.5055             |             | 0.562D-21         | 3879.336 | 6    | 1      | 5      | 7   | 1     | 6     | 0 2 1                  | 0 2 0               | 161 | 0.024            | 0.025             |
| 3545.552               | 3545.5505             | -12         | C 0.137D-19       | 1080.386 | 8    | 2      | 7      | 9   | 2     | 8     | 0 0 1                  | 0 0 0               | 161 | 0.597            | 0.608             |
| 3545.906               | 3545.9057             | -4          | H 0.460D-20       | 2495.168 | 7    | 2      | 6      | 8   | 2     | 7     | 0 1 1                  | 0 1 0               | 161 | 0.163            | 0.167             |
| 3545.993               | 3545.9929             | -1          | C 0.104D-20       | 1446.129 | 9    | 4      | 5      | 10  | 3     | 8     | 1 0 0                  | 0 0 0               | 161 | 0.036            | 0.038             |
| 3546.124               | 3546.1158             |             | 0.231D-21         | 2586.529 | 13   | 3      | 10     | 13  | 5     | 9     | 0 0 1                  | 0 0 0               | 161 | 0.006            | 0.009             |
| 3546.744               | 3546.7437             |             | 0.514D-20         | 2392.594 | 6    | 2      | 4      | 7   | 2     | 5     | 0 1 1                  | 0 1 0               | 161 | 0.179            | 0.185             |
| 3546.893               |                       | D 0.149D-19 | 1114.534          | 9        | 0    | 9      | 10     | 0   | 10    | 0     | 0 1 0                  | 0 0 0               | 161 |                  | 0.643             |
| 3546.899               | 3546.8979             | 3           | S 0.446D-19       | 1114.550 | 9    | 1      | 9      | 10  | 1     | 10    | 0 0 1                  | 0 0 0               | 161 | 2.362            | 1.926             |
| 3547.158               | 3547.1577             | -1          | C 0.299D-19       | 1006.116 | 7    | 3      | 5      | 8   | 3     | 6     | 0 0 1                  | 0 0 0               | 161 | 1.343            | 1.422             |
|                        | 3547.6167             |             |                   |          |      |        |        |     |       |       |                        |                     |     | 0.006            |                   |
| 3548.357               | 3548.3589             | 16          | C 0.694D-22       | 285.219  | 2    | 1      | 2      | 3   | 3     | 1     | 0 0 1                  | 0 0 0               | 161 | 0.010            | 0.012             |
| 3548.392               | 3548.3917             | 0           | C 0.130D-20       | 326.625  | 4    | 0      | 4      | 5   | 1     | 5     | 1 0 0                  | 0 0 0               | 161 | 0.172            | 0.209             |
| 3548.519               | 3548.5196             | 8           | C 0.107D-20       | 1340.886 | 8    | 3      | 3      | 9   | 4     | 6     | 1 0 0                  | 0 0 0               | 161 | 0.036            | 0.040             |
| 3549.639               | 3549.6366             | -36         | H 0.529D-20       | 2512.283 | 8    | 0      | 8      | 9   | 0     | 9     | 0 1 1                  | 0 1 0               | 161 | 0.191            | 0.193             |
| 3549.665               | 3549.6635             |             | 0.176D-20         | 2512.378 | 8    | 1      | 8      | 9   | 1     | 9     | 0 1 1                  | 0 1 0               | 161 | 0.060            | 0.064             |
| 3550.203               |                       | 0.712D-21   | 1446.129          | 9        | 6    | 3      | 10     | 3   | 8     | 0 2 0 | 0 0 0                  | 161                 |     | 0.026            |                   |
| 3550.226               | 3550.2244             |             | 0.122D-20         | 2439.956 | 6    | 3      | 4      | 7   | 3     | 5     | 0 1 1                  | 0 1 0               | 161 | 0.040            | 0.044             |
| 3550.413               | 3550.4114             | -10         | C 0.137D-20       | 648.979  | 6    | 2      | 5      | 6   | 3     | 4     | 1 0 0                  | 0 0 0               | 161 | 0.092            | 0.108             |
| 3550.755               | 3550.7523             | -40         | H 0.958D-21       | 2414.725 | 13   | 3      | 11     | 13  | 3     | 10    | 0 0 1                  | 0 0 0               | 161 | 0.029            | 0.034             |
| 3551.732               | 3551.7328             |             | 0.206D-21         | 1695.071 | 10   | 4      | 6      | 11  | 3     | 9     | 1 0 0                  | 0 0 0               | 161 | 0.008            | 0.007             |
| 3551.858               | 3551.8579             | 3           | C 0.110D-20       | 399.457  | 4    | 2      | 3      | 5   | 1     | 4     | 1 0 0                  | 0 0 0               | 161 | 0.124            | 0.148             |
| 3552.104               |                       | D 0.667D-22 | 839.550           | 6        | 3    | 3      | 7      | 3   | 4     | 0 0 1 | 0 0 0                  | 181                 |     | 0.004            |                   |
| 3552.108               | 3552.1081             | 2           | C 0.707D-20       | 842.357  | 6    | 4      | 3      | 7   | 3     | 4     | 1 0 0                  | 0 0 0               | 161 | 0.379            | 0.408             |
| 3552.228               | 3552.2269             | -10         | C 0.365D-20       | 325.348  | 4    | 1      | 4      | 5   | 0     | 5     | 1 0 0                  | 0 0 0               | 161 | 0.483            | 0.587             |
| 3552.410               | 3552.4083             | -14         | C 0.356D-21       | 542.906  | 6    | 0      | 6      | 6   | 1     | 5     | 1 0 0                  | 0 0 0               | 161 | 0.029            | 0.035             |
| 3552.418               |                       | D 0.213D-22 | 6569.930          | 14       | 13   | 1      | 14     | 13  | 2     | 0     | 1 1                    | 0 1 0               | 161 |                  | 0.002             |
| 3552.806               | 3552.8060             | -11         | C 0.135D-20       | 1216.232 | 8    | 4      | 4      | 9   | 3     | 7     | 1 0 0                  | 0 0 0               | 161 | 0.055            | 0.054             |
| 3553.420               |                       | D 0.325D-21 | 2552.880          | 5        | 5    | 0      | 6      | 5   | 1     | 0 1 1 | 0 1 0                  | 161                 |     | 0.012            |                   |
| 3553.440               | 3553.4397             | 0           | H 0.975D-21       | 2552.858 | 5    | 5      | 1      | 6   | 5     | 2     | 0 1 1                  | 0 1 0               | 161 | 0.034            | 0.036             |
| 3553.738               | 3553.7378             | -3          | C 0.161D-19       | 1059.835 | 6    | 5      | 1      | 7   | 5     | 2     | 0 0 1                  | 0 0 0               | 161 | 0.696            | 0.726             |
| 3553.755               |                       | 0.868D-21   | 931.237           | 7        | 3    | 4      | 7      | 4   | 3     | 1 0 0 | 0 0 0                  | 161                 |     | 0.045            |                   |
| 3553.825               | 3553.8204             |             | 0.209D-21         | 3894.800 | 7    | 0      | 7      | 8   | 0     | 8     | 0 2 1                  | 0 2 0               | 161 | 0.008            | 0.009             |
| 3553.880               | 3553.8804             | 7           | C 0.536D-20       | 1059.647 | 6    | 5      | 2      | 7   | 5     | 3     | 0 0 1                  | 0 0 0               | 161 | 0.228            | 0.242             |
| 3553.951               | 3553.9473             |             | 0.625D-21         | 3895.253 | 7    | 1      | 7      | 8   | 1     | 8     | 0 2 1                  | 0 2 0               | 161 | 0.028            | 0.028             |
| 3554.068               | 3554.0635             |             | 0.278D-21         | 3864.966 | 5    | 3      | 3      | 6   | 3     | 4     | 0 2 1                  | 0 2 0               | 161 | 0.017            | 0.013             |
| 3554.443               | 3554.4460             | 15          | C 0.113D-21       | 916.260  | 8    | 0      | 8      | 9   | 0     | 9     | 0 0 1                  | 0 0 0               | 181 | 0.008            | 0.006             |
| 3554.721               | 3554.7189             | -83         | H 0.185D-21       | 1875.464 | 9    | 7      | 3      | 10  | 6     | 4     | 1 0 0                  | 0 0 0               | 161 | 0.010            | 0.006             |
| 3554.722               |                       | D 0.408D-22 | 3738.544          | 12       | 3    | 10     | 12     | 3   | 9     | 0     | 1 1                    | 0 1 0               | 161 |                  | 0.002             |
| 3554.781               | 3554.7796             | -2          | C 0.110D-20       | 1282.919 | 9    | 2      | 7      | 9   | 3     | 6     | 1 0 0                  | 0 0 0               | 161 | 0.036            | 0.043             |
| 3554.886               | 3554.8859             |             | 0.864D-21         | 2275.373 | 12   | 3      | 9      | 12  | 5     | 8     | 0 0 1                  | 0 0 0               | 161 | 0.025            | 0.031             |
| 3554.914               | 3554.9147             |             | 0.834D-21         | 1718.719 | 10   | 3      | 7      | 10  | 5     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.024            | 0.029             |
| 3555.214               | 3555.2096             |             | 0.555D-21         | 1874.974 | 9    | 7      | 2      | 10  | 6     | 5     | 1 0 0                  | 0 0 0               | 161 | 0.015            | 0.019             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3557.130               | 3557.1297             | -2          | C 0.481D-21       | 136.164  | 1    | 1      | 1      | 2   | 2     | 0     | 1 0 0          | 0 0 0       | 161 | 0.093            | 0.127             |
| 3557.553               | 3557.5518             | -4          | C 0.326D-21       | 1131.776 | 8    | 3      | 5      | 8   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.014             |
| 3557.850               | 3557.8526             |             | 0.308D-21         | 1985.788 | 11   | 3      | 8      | 11  | 5     | 7     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3557.999               | 3557.9983             | -4          | C 0.937D-21       | 1360.236 | 9    | 3      | 6      | 9   | 4     | 5     | 1 0 0          | 0 0 0       | 161 | 0.029            | 0.035             |
| 3558.383               | 3558.3816             |             | 0.135D-20         | 2124.953 | 12   | 2      | 10     | 12  | 4     | 9     | 0 0 1          | 0 0 0       | 161 | 0.040            | 0.047             |
| 3559.115               | 3559.1150             | 0           | C 0.199D-20       | 1293.634 | 10   | 0      | 10     | 10  | 2     | 9     | 0 0 1          | 0 0 0       | 161 | 0.073            | 0.077             |
| 3559.670               | 3559.6699             |             | 0.550D-21         | 2462.876 | 6    | 4      | 3      | 7   | 3     | 4     | 1 1 0          | 0 1 0       | 161 | 0.018            | 0.020             |
| 3559.737               | 3559.7374             | 3           | C 0.666D-21       | 1293.019 | 10   | 1      | 10     | 10  | 1     | 9     | 0 0 1          | 0 0 0       | 161 | 0.024            | 0.026             |
| 3560.133               | 3560.1327             | -2          | C 0.269D-19       | 931.237  | 6    | 4      | 2      | 7   | 4     | 3     | 0 0 1          | 0 0 0       | 161 | 1.322            | 1.383             |
| 3560.136               |                       | D 0.658D-21 | 1695.071          |          | 11   | 1      | 10     | 11  | 3     | 9     | 0 0 1          | 0 0 0       | 161 |                  | 0.023             |
| 3561.164               | 3561.1638             | 2           | C 0.448D-21       | 503.968  | 5    | 2      | 4      | 5   | 3     | 3     | 1 0 0          | 0 0 0       | 161 | 0.040            | 0.047             |
| 3561.241               |                       | D 0.633D-22 | 4526.719          |          | 6    | 5      | 2      | 6   | 5     | 1     | 1 0 1          | 1 0 0       | 161 |                  | 0.003             |
| 3561.248               | 3561.2485             | 8           | C 0.375D-21       | 416.209  | 5    | 1      | 5      | 5   | 2     | 4     | 1 0 0          | 0 0 0       | 161 | 0.048            | 0.048             |
| 3562.320               | 3562.3203             | 0           | C 0.888D-20       | 927.744  | 6    | 4      | 3      | 7   | 4     | 4     | 0 0 1          | 0 0 0       | 161 | 0.449            | 0.458             |
| 3562.330               |                       | D 0.117D-20 | 1477.297          |          | 8    | 6      | 3      | 9   | 5     | 4     | 1 0 0          | 0 0 0       | 161 |                  | 0.042             |
| 3562.405               | 3562.4036             | -13         | C 0.259D-21       | 488.108  | 5    | 5      | 0      | 4   | 4     | 1     | 0 2 0          | 0 0 0       | 161 | 0.018            | 0.028             |
| 3563.590               | 3563.5891             | -10         | C 0.169D-20       | 134.902  | 1    | 1      | 0      | 2   | 2     | 1     | 1 0 0          | 0 0 0       | 161 | 0.337            | 0.446             |
| 3563.967               | 3563.9668             | 5           | C 0.357D-21       | 285.419  | 2    | 1      | 1      | 3   | 3     | 0     | 0 0 1          | 0 0 0       | 161 | 0.049            | 0.063             |
| 3564.020               | 3564.0178             |             | 0.761D-21         | 2399.166 | 5    | 4      | 1      | 6   | 4     | 2     | 0 1 1          | 0 1 0       | 161 | 0.026            | 0.027             |
| 3564.061               | 3564.0612             | 5           | C 0.110D-20       | 1131.776 | 7    | 5      | 3      | 8   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.056            | 0.047             |
| 3564.067               |                       | D 0.282D-21 | 4381.902          |          | 5    | 5      | 1      | 5   | 5     | 0     | 1 0 1          | 1 0 0       | 161 |                  | 0.014             |
| 3564.068               |                       | D 0.941D-22 | 4381.902          |          | 5    | 5      | 0      | 5   | 5     | 1     | 1 0 1          | 1 0 0       | 161 |                  | 0.005             |
| 3564.583               | 3564.5821             | 61          | H 0.228D-20       | 2398.382 | 5    | 4      | 2      | 6   | 4     | 3     | 0 1 1          | 0 1 0       | 161 | 0.079            | 0.082             |
| 3564.666               |                       | 0.537D-21   | 4195.477          |          | 5    | 0      | 5      | 6   | 0     | 6     | 0 0 2          | 0 0 1       | 161 |                  | 0.026             |
| 3564.682               |                       | D 0.197D-20 | 1690.665          |          | 11   | 2      | 10     | 11  | 2     | 9     | 0 0 1          | 0 0 0       | 161 |                  | 0.068             |
| 3564.690               | 3564.6891             | -9          | C 0.426D-20       | 842.357  | 6    | 6      | 1      | 7   | 3     | 4     | 0 2 0          | 0 0 0       | 161 | 0.220            | 0.245             |
| 3565.017               | 3565.0161             | -14         | H 0.552D-20       | 2309.731 | 6    | 1      | 5      | 7   | 1     | 6     | 0 1 1          | 0 1 0       | 161 | 0.194            | 0.196             |
| 3565.017               |                       | D 0.331D-22 | 6147.078          |          | 17   | 14     | 4      | 17  | 14    | 3     | 0 0 1          | 0 0 0       | 161 |                  | -0.002            |
| 3565.672               | 3565.6715             | -12         | C 0.316D-19       | 842.357  | 6    | 3      | 3      | 7   | 3     | 4     | 0 0 1          | 0 0 0       | 161 | 1.733            | 1.818             |
| 3566.005               | 3566.0061             | 11          | C 0.147D-20       | 782.410  | 7    | 1      | 6      | 7   | 2     | 5     | 1 0 0          | 0 0 0       | 161 | 0.078            | 0.092             |
| 3566.080               | 3566.0805             | 0           | C 0.164D-19       | 882.891  | 7    | 1      | 6      | 8   | 1     | 7     | 0 0 1          | 0 0 0       | 161 | 0.847            | 0.894             |
| 3566.330               | 3566.3306             | 0           | C 0.841D-20       | 1006.116 | 7    | 4      | 3      | 8   | 3     | 6     | 1 0 0          | 0 0 0       | 161 | 0.390            | 0.398             |
| 3566.534               | 3566.5332             | -5          | C 0.315D-20       | 224.838  | 3    | 0      | 3      | 4   | 1     | 4     | 1 0 0          | 0 0 0       | 161 | 0.516            | 0.652             |
| 3566.753               | 3566.7519             | -9          | S 0.459D-19       | 885.600  | 7    | 2      | 6      | 8   | 2     | 7     | 0 0 1          | 0 0 0       | 161 |                  | 2.492             |
| 3566.754               |                       | D 0.302D-21 | 2495.168          |          | 8    | 0      | 8      | 8   | 2     | 7     | 0 1 1          | 0 1 0       | 161 |                  | 0.011             |
| 3567.198               | 3567.1948             | -62         | H 0.161D-20       | 2318.541 | 6    | 2      | 5      | 7   | 2     | 6     | 0 1 1          | 0 1 0       | 161 | 0.064            | 0.057             |
| 3567.922               | 3567.9228             | 4           | S 0.523D-19       | 920.169  | 8    | 0      | 8      | 9   | 0     | 9     | 0 0 1          | 0 0 0       | 161 |                  | 2.719             |
| 3567.935               |                       | 0.174D-19   | 920.211           |          | 8    | 1      | 8      | 9   | 1     | 9     | 0 0 1          | 0 0 0       | 161 |                  | 0.905             |
| 3568.084               | 3568.0841             | 5           | C 0.461D-21       | 508.812  | 5    | 1      | 5      | 5   | 3     | 2     | 0 0 1          | 0 0 0       | 161 | 0.042            | 0.048             |
| 3568.290               | 3568.2899             | 1           | S 0.519D-19       | 782.410  | 6    | 2      | 4      | 7   | 2     | 5     | 0 0 1          | 0 0 0       | 161 |                  | 3.258             |
| 3568.679               | 3568.6781             |             | 0.123D-20         | 2282.591 | 5    | 3      | 2      | 6   | 3     | 3     | 0 1 1          | 0 1 0       | 161 | 0.041            | 0.043             |
| 3568.799               | 3568.7977             | -8          | C 0.113D-20       | 382.517  | 4    | 2      | 3      | 4   | 3     | 2     | 1 0 0          | 0 0 0       | 161 | 0.130            | 0.157             |
| 3569.368               | 3569.3612             |             | 0.935D-22         | 3680.454 | 0    | 0      | 0      | 1   | 0     | 1     | 1 0 1          | 1 0 0       | 161 | 0.007            | 0.004             |
| 3570.172               | 3570.1722             |             | 0.198D-20         | 2337.468 | 7    | 0      | 7      | 8   | 0     | 8     | 0 1 1          | 0 1 0       | 161 | 0.070            | 0.070             |
| 3570.249               | 3570.2486             | 26          | H 0.593D-20       | 2337.669 | 7    | 1      | 7      | 8   | 1     | 8     | 0 1 1          | 0 1 0       | 161 | 0.212            | 0.210             |
| 3570.321               | 3570.3175             |             | 0.484D-21         | 3736.171 | 5    | 2      | 4      | 6   | 2     | 5     | 0 2 1          | 0 2 0       | 161 | 0.024            | 0.021             |
| 3570.541               | 3570.5399             | -5          | C 0.968D-20       | 816.694  | 6    | 3      | 4      | 7   | 3     | 5     | 0 0 1          | 0 0 0       | 161 | 0.539            | 0.577             |
| 3572.213               | 3572.2127             | -12         | H 0.179D-20       | 2211.192 | 5    | 2      | 3      | 6   | 2     | 4     | 0 1 1          | 0 1 0       | 161 | 0.059            | 0.063             |
| 3572.749               | 3572.7480             | -9          | C 0.480D-21       | 1050.158 | 8    | 2      | 6      | 8   | 3     | 5     | 1 0 0          | 0 0 0       | 161 | 0.018            | 0.022             |
| 3572.949               | 3572.9493             | -3          | C 0.117D-21       | 701.696  | 6    | 1      | 5      | 7   | 1     | 6     | 0 0 1          | 0 0 0       | 161 | 0.007            | 0.008             |
| 3573.127               | 3573.1276             | 1           | C 0.277D-20       | 1122.709 | 7    | 5      | 2      | 8   | 4     | 5     | 1 0 0          | 0 0 0       | 161 | 0.116            | 0.118             |
| 3573.656               | 3573.6562             | 0           | C 0.235D-21       | 285.219  | 3    | 2      | 2      | 3   | 3     | 1     | 1 0 0          | 0 0 0       | 161 | 0.035            | 0.042             |
| 3573.886               | 3573.8842             | -46         | H 0.675D-21       | 3738.609 | 6    | 0      | 6      | 7   | 0     | 7     | 0 2 1          | 0 2 0       | 161 | 0.037            | 0.030             |
| 3573.889               |                       | D 0.404D-22 | 5339.676          |          | 15   | 14     | 1      | 15  | 14    | 2     | 0 0 1          | 0 0 0       | 161 |                  | 0.002             |
| 3573.889               |                       | D 0.121D-21 | 5339.676          |          | 15   | 14     | 2      | 15  | 14    | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.007             |
| 3574.487               | 3574.4871             | 0           | C 0.906D-21       | 222.052  | 3    | 1      | 3      | 4   | 0     | 4     | 1 0 0          | 0 0 0       | 161 | 0.153            | 0.189             |
| 3574.801               | 3574.7986             | -18         | H 0.364D-20       | 2271.712 | 5    | 3      | 3      | 6   | 3     | 4     | 0 1 1          | 0 1 0       | 161 | 0.127            | 0.128             |
| 3575.050               | 3575.0495             | -6          | C 0.547D-21       | 315.779  | 3    | 0      | 3      | 4   | 2     | 2     | 0 0 1          | 0 0 0       | 161 | 0.073            | 0.089             |
| 3575.773               | 3575.7729             | -31         | H 0.604D-21       | 1843.030 | 11   | 2      | 9      | 11  | 4     | 8     | 0 0 1          | 0 0 0       | 161 | 0.019            | 0.021             |
| 3576.732               | 3576.7305             |             | 0.255D-21         | 3722.731 | 4    | 3      | 1      | 5   | 3     | 2     | 0 2 1          | 0 2 0       | 161 | 0.013            | 0.011             |
| 3576.851               | 3576.8506             | -3          | C 0.123D-20       | 399.457  | 5    | 0      | 5      | 5   | 1     | 4     | 1 0 0          | 0 0 0       | 161 | 0.141            | 0.164             |
| 3577.213               | 3577.2125             | -6          | C 0.113D-20       | 300.362  | 4    | 1      | 4      | 4   | 2     | 3     | 1 0 0          | 0 0 0       | 161 | 0.155            | 0.192             |
| 3577.901               | 3577.9042             | -10         | H 0.220D-21       | 4967.043 | 14   | 14     | 0      | 14  | 14    | 1     | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.012             |
| 3577.901               |                       | D 0.732D-22 | 4967.043          |          | 14   | 14     | 1      | 14  | 14    | 0     | 0 0 1          | 0 0 0       | 161 |                  | 0.004             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3578.015               | 3578.0149             | 6      | C 0.127D-21       | 488.108  | 4    | 2      | 2      | 4   | 4     | 1     | 0 0 1            | 0 0 0         | 161 | 0.013            | 0.014             |
| 3578.501               | 3578.4976             |        | 0.526D-21         | 3626.922 | 4    | 2      | 2      | 5   | 2     | 3     | 0 2 1            | 0 2 0         | 161 | 0.016            | 0.023             |
| 3578.651               | 3578.6620             |        | 0.458D-21         | 2105.876 | 12   | 3      | 10     | 12  | 3     | 9     | 0 0 1            | 0 0 0         | 161 | 0.016            | 0.016             |
| 3579.345               | 3579.3462             | 11     | C 0.739D-21       | 285.419  | 3    | 2      | 1      | 3   | 3     | 0     | 1 0 0            | 0 0 0         | 161 | 0.147            | 0.130             |
| 3580.066               | 3580.0654             | 0      | C 0.359D-20       | 888.632  | 5    | 5      | 0      | 6   | 5     | 1     | 0 0 1            | 0 0 0         | 161 | 0.197            | 0.193             |
| 3580.094               | 3580.0942             | -5     | C 0.108D-19       | 888.599  | 5    | 5      | 1      | 6   | 5     | 2     | 0 0 1            | 0 0 0         | 161 | 0.562            | 0.582             |
| 3581.041               | 3581.0410             | 4      | C 0.862D-21       | 1080.386 | 9    | 0      | 9      | 9   | 2     | 8     | 0 0 1            | 0 0 0         | 161 | 0.037            | 0.038             |
| 3581.045               |                       |        | D 0.442D-22       | 2053.969 | 4    | 3      | 2      | 5   | 2     | 3     | 1 1 0            | 0 1 0         | 161 |                  | 0.002             |
| 3581.127               |                       |        | D 0.407D-22       | 5866.230 | 17   | 13     | 5      | 17  | 13    | 4     | 0 0 1            | 0 0 0         | 161 |                  | 0.003             |
| 3581.128               | 3581.1285             | -4     | C 0.264D-20       | 1446.129 | 10   | 1      | 9      | 10  | 3     | 8     | 0 0 1            | 0 0 0         | 161 | 0.091            | 0.095             |
| 3581.848               | 3581.8501             | -11    | H 0.351D-21       | 2630.194 | 8    | 1      | 7      | 8   | 3     | 6     | 0 1 1            | 0 1 0         | 161 | 0.011            | 0.013             |
| 3581.884               | 3581.8870             |        | 0.388D-21         | 1631.384 | 8    | 7      | 2      | 9   | 6     | 3     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.014             |
| 3582.156               | 3582.1539             | 6      | H 0.320D-21       | 3935.345 | 3    | 3      | 1      | 3   | 3     | 0     | 1 0 1            | 1 0 0         | 161 | 0.010            | 0.015             |
| 3582.369               | 3582.3692             | 4      | C 0.258D-20       | 1079.080 | 9    | 1      | 9      | 9   | 1     | 8     | 0 0 1            | 0 0 0         | 161 | 0.110            | 0.114             |
| 3582.717               | 3582.7169             | 2      | C 0.462D-21       | 383.842  | 4    | 2      | 2      | 4   | 3     | 1     | 1 0 0            | 0 0 0         | 161 | 0.054            | 0.064             |
| 3583.379               | 3583.3792             | 9      | C 0.172D-21       | 275.497  | 3    | 2      | 2      | 4   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.025            | 0.031             |
| 3583.664               | 3583.6631             | -4     | C 0.776D-21       | 142.278  | 2    | 0      | 2      | 3   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.153            | 0.199             |
| 3583.710               | 3583.7100             | 2      | C 0.170D-20       | 842.357  | 7    | 2      | 5      | 7   | 3     | 4     | 1 0 0            | 0 0 0         | 161 | 0.086            | 0.097             |
| 3585.248               | 3585.2478             | 0      | C 0.393D-20       | 816.694  | 6    | 4      | 2      | 7   | 3     | 5     | 1 0 0            | 0 0 0         | 161 | 0.216            | 0.233             |
| 3585.292               | 3585.2903             |        | 0.501D-21         | 4076.896 | 4    | 1      | 4      | 5   | 1     | 5     | 0 0 2            | 0 0 1         | 161 | 0.018            | 0.023             |
| 3585.619               | 3585.6186             |        | 0.444D-21         | 4027.804 | 3    | 1      | 2      | 4   | 1     | 3     | 0 0 2            | 0 0 1         | 161 | 0.016            | 0.020             |
| 3585.654               | 3585.6530             |        | 0.197D-20         | 2146.265 | 5    | 1      | 4      | 6   | 1     | 5     | 0 1 1            | 0 1 0         | 161 | 0.068            |                   |
| 3586.543               |                       |        | 0.548D-19         | 704.214  | 6    | 1      | 5      | 7   | 1     | 6     | 0 0 1            | 0 0 0         | 161 |                  | 3.888             |
| 3586.604               | 3586.6036             | 0      | C 0.652D-20       | 661.549  | 5    | 3      | 2      | 6   | 3     | 3     | 0 0 1            | 0 0 0         | 161 | 0.431            | 0.499             |
| 3586.955               | 3586.9550             | -1     | C 0.134D-19       | 709.609  | 6    | 2      | 5      | 7   | 2     | 6     | 0 0 1            | 0 0 0         | 161 | 0.861            | 0.942             |
| 3587.108               | 3587.1081             | -1     | C 0.141D-20       | 508.812  | 5    | 2      | 3      | 5   | 3     | 2     | 1 0 0            | 0 0 0         | 161 | 0.119            | 0.146             |
| 3587.249               |                       |        | D 0.680D-22       | 610.114  | 6    | 5      | 1      | 5   | 4     | 2     | 0 2 0            | 0 0 0         | 161 |                  | 0.006             |
| 3587.256               | 3587.2539             | 61     | C 0.177D-21       | 3441.040 | 11   | 3      | 9      | 11  | 3     | 8     | 0 1 1            | 0 1 0         | 161 | 0.010            | 0.007             |
| 3587.489               | 3587.4884             | -1     | C 0.616D-21       | 602.774  | 6    | 1      | 5      | 6   | 2     | 4     | 1 0 0            | 0 0 0         | 161 | 0.044            | 0.053             |
| 3587.779               | 3587.7779             | -13    | C 0.801D-20       | 757.780  | 5    | 4      | 1      | 6   | 4     | 2     | 0 0 1            | 0 0 0         | 161 | 0.480            | 0.520             |
| 3587.975               | 3587.9743             | -12    | C 0.575D-21       | 661.549  | 6    | 2      | 4      | 6   | 3     | 3     | 1 0 0            | 0 0 0         | 161 | 0.037            | 0.044             |
| 3588.379               | 3588.3770             |        | 0.425D-20         | 2161.286 | 5    | 2      | 4      | 6   | 2     | 5     | 0 1 1            | 0 1 0         | 161 | 0.149            | 0.148             |
| 3588.547               | 3588.5471             | -2     | C 0.239D-19       | 756.725  | 5    | 4      | 2      | 6   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 1.458            | 1.553             |
| 3588.704               |                       |        | D 0.399D-22       | 3894.168 | 6    | 3      | 3      | 7   | 2     | 6     | 1 2 0            | 0 2 0         | 161 |                  | 0.002             |
| 3588.711               | 3588.7108             | 2      | C 0.197D-19       | 744.064  | 7    | 0      | 7      | 8   | 0     | 8     | 0 0 1            | 0 0 0         | 161 | 1.333            | 1.307             |
| 3588.750               | 3588.7504             | 3      | S 0.588D-19       | 744.163  | 7    | 1      | 7      | 8   | 1     | 8     | 0 0 1            | 0 0 0         | 161 |                  | 3.899             |
| 3589.026               | 3589.0237             |        | 0.613D-21         | 3565.455 | 4    | 1      | 3      | 5   | 1     | 4     | 0 2 1            | 0 2 0         | 161 | 0.030            | 0.026             |
| 3589.099               |                       |        | D 0.122D-21       | 2318.541 | 7    | 0      | 7      | 7   | 2     | 6     | 0 1 1            | 0 1 0         | 161 |                  | 0.004             |
| 3589.108               | 3589.1049             | -17    | H 0.317D-21       | 2818.398 | 9    | 2      | 8      | 9   | 2     | 7     | 0 1 1            | 0 1 0         | 161 | 0.018            | 0.012             |
| 3589.285               | 3589.2795             |        | 0.250D-21         | 3788.695 | 2    | 2      | 0      | 2   | 2     | 1     | 1 0 1            | 1 0 0         | 161 | 0.009            | 0.011             |
| 3589.592               | 3589.5903             | -15    | C 0.875D-21       | 1437.969 | 10   | 2      | 9      | 10  | 2     | 8     | 0 0 1            | 0 0 0         | 161 | 0.030            | 0.032             |
| 3589.724               | 3589.7241             | -2     | C 0.223D-20       | 1581.336 | 10   | 2      | 8      | 10  | 4     | 7     | 0 0 1            | 0 0 0         | 161 | 0.069            | 0.078             |
| 3590.075               | 3590.0799             | 18     | H 0.168D-21       | 5066.223 | 15   | 13     | 3      | 15  | 13    | 2     | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.009             |
| 3590.075               |                       |        | D 0.561D-22       | 5066.223 | 15   | 13     | 2      | 15  | 13    | 3     | 0 0 1            | 0 0 0         | 161 |                  | 0.003             |
| 3590.167               | 3590.1663             |        | 0.148D-20         | 2251.863 | 4    | 4      | 0      | 5   | 4     | 1     | 0 1 1            | 0 1 0         | 161 | 0.050            | 0.052             |
| 3590.238               | 3590.2368             | -16    | C 0.336D-21       | 206.301  | 3    | 1      | 3      | 3   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.056            | 0.073             |
| 3590.308               | 3590.3057             |        | 0.493D-21         | 2251.696 | 4    | 4      | 1      | 5   | 4     | 2     | 0 1 1            | 0 1 0         | 161 | 0.019            | 0.017             |
| 3590.432               | 3590.4308             | -6     | C 0.642D-20       | 2180.644 | 6    | 0      | 6      | 7   | 0     | 7     | 0 1 1            | 0 1 0         | 161 | 0.224            |                   |
| 3590.627               | 3590.6253             | -27    | H 0.212D-20       | 2181.092 | 6    | 1      | 6      | 7   | 1     | 7     | 0 1 1            | 0 1 0         | 161 | 0.073            | 0.074             |
| 3590.862               | 3590.8617             | -13    | C 0.259D-21       | 1255.913 | 7    | 6      | 2      | 8   | 5     | 3     | 1 0 0            | 0 0 0         | 161 | 0.012            | 0.010             |
| 3591.609               | 3591.6090             | 1      | C 0.773D-21       | 1255.167 | 7    | 6      | 1      | 8   | 5     | 4     | 1 0 0            | 0 0 0         | 161 | 0.033            | 0.030             |
| 3593.197               | 3593.1975             | -3     | C 0.182D-19       | 602.774  | 5    | 2      | 3      | 6   | 2     | 4     | 0 0 1            | 0 0 0         | 161 | 1.387            | 1.554             |
| 3593.975               | 3593.9734             | -10    | C 0.924D-21       | 756.725  | 6    | 2      | 4      | 6   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 0.051            | 0.060             |
| 3594.127               |                       |        | D 0.102D-21       | 4697.656 | 14   | 13     | 2      | 14  | 13    | 1     | 0 0 1            | 0 0 0         | 161 |                  | 0.005             |
| 3594.127               | 3594.1285             | 11     | H 0.307D-21       | 4697.656 | 14   | 13     | 1      | 14  | 13    | 2     | 0 0 1            | 0 0 0         | 161 | 0.016            | 0.016             |
| 3594.282               | 3594.2842             | 41     | H 0.675D-21       | 3601.859 | 5    | 1      | 5      | 6   | 1     | 6     | 0 2 1            | 0 2 0         | 161 | 0.031            | 0.029             |
| 3595.326               | 3595.3261             | -2     | C 0.287D-19       | 648.979  | 5    | 3      | 3      | 6   | 3     | 4     | 0 0 1            | 0 0 0         | 161 |                  | 2.242             |
| 3595.482               | 3595.4818             | -11    | C 0.194D-20       | 931.237  | 6    | 5      | 2      | 7   | 4     | 3     | 1 0 0            | 0 0 0         | 161 | 0.095            | 0.099             |
| 3595.553               | 3595.5519             | -9     | C 0.137D-21       | 583.779  | 6    | 0      | 6      | 7   | 0     | 7     | 0 0 1            | 0 0 0         | 181 | 0.010            | 0.012             |
| 3596.238               | 3596.2378             | -1     | C 0.719D-20       | 661.549  | 5    | 4      | 2      | 6   | 3     | 3     | 1 0 0            | 0 0 0         | 161 | 0.502            | 0.549             |
| 3597.078               | 3597.0758             | -29    | H 0.320D-20       | 2130.495 | 4    | 3      | 1      | 5   | 3     | 2     | 0 1 1            | 0 1 0         | 161 | 0.109            | 0.111             |
| 3597.178               |                       |        | D 0.409D-22       | 2144.047 | 11   | 7      | 4      | 11  | 6     | 5     | 0 2 0            | 0 0 0         | 161 |                  | 0.001             |
| 3597.179               |                       |        | D 0.657D-22       | 5037.332 | 11   | 11     | 0      | 11  | 11    | 1     | 0 1 1            | 0 1 0         | 161 |                  | 0.004             |
| 3597.179               | 3597.1777             | -15    | H 0.197D-21       | 5037.332 | 11   | 11     | 1      | 11  | 11    | 0     | 0 1 1            | 0 1 0         | 161 | 0.014            | 0.011             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued.

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF | C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|------|---|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3597.893               | 3597.9063             |      |   | 0.540D-21         | 4350.602 | 13   | 13     | 1      | 13  | 13    | 0     | 0 0 1            | 0 0 0         | 161 | 0.029            | 0.026             |
| 3597.893               |                       |      | D | 0.180D-21         | 4350.602 | 13   | 13     | 0      | 13  | 13    | 1     | 0 0 1            | 0 0 0         | 161 |                  | 0.009             |
| 3598.136               | 3598.1352             | -4   | C | 0.164D-20         | 136.761  | 2    | 1      | 2      | 3   | 0     | 3     | 1 0 0            | 0 0 0         | 161 | 0.324            | 0.426             |
| 3598.186               | 3598.1834             |      |   | 0.368D-21         | 2309.731 | 7    | 1      | 7      | 7   | 1     | 6     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.013             |
| 3598.603               | 3598.6030             | -5   | C | 0.391D-20         | 709.609  | 6    | 3      | 3      | 7   | 2     | 6     | 1 0 0            | 0 0 0         | 161 | 0.260            | 0.274             |
| 3598.909               | 3598.9093             | -7   | C | 0.801D-21         | 1340.886 | 9    | 2      | 7      | 9   | 4     | 6     | 0 0 1            | 0 0 0         | 161 | 0.028            | 0.030             |
| 3598.976               | 3598.9763             | -3   | C | 0.612D-21         | 927.744  | 6    | 5      | 1      | 7   | 4     | 4     | 1 0 0            | 0 0 0         | 161 | 0.029            | 0.031             |
| 3599.059               | 3599.0571             | -1   | C | 0.502D-20         | 2053.969 | 4    | 2      | 2      | 5   | 2     | 3     | 0 1 1            | 0 1 0         | 161 | 0.172            | 0.173             |
| 3599.392               | 3599.3922             | 2    | C | 0.176D-20         | 885.600  | 7    | 3      | 4      | 8   | 2     | 7     | 1 0 0            | 0 0 0         | 161 | 0.092            | 0.095             |
| 3599.520               | 3599.5202             | 0    | C | 0.478D-21         | 275.497  | 4    | 0      | 4      | 4   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.064            | 0.086             |
| 3599.743               | 3599.7412             |      |   | 0.973D-21         | 2161.286 | 5    | 3      | 2      | 6   | 2     | 5     | 1 1 0            | 0 1 0         | 161 | 0.036            | 0.034             |
| 3599.850               | 3599.8481             |      |   | 0.105D-20         | 2126.407 | 4    | 3      | 2      | 5   | 3     | 3     | 0 1 1            | 0 1 0         | 161 | 0.037            | 0.036             |
| 3599.995               | 3599.9952             | -4   | C | 0.681D-21         | 134.902  | 2    | 1      | 2      | 2   | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.136            | 0.178             |
| 3600.205               | 3600.2051             | 0    | C | 0.526D-21         | 927.744  | 7    | 2      | 5      | 7   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.025            | 0.027             |
| 3600.760               | 3600.7604             | 11   | C | 0.113D-20         | 1216.232 | 9    | 1      | 8      | 9   | 3     | 7     | 0 0 1            | 0 0 0         | 161 | 0.039            | 0.045             |
| 3600.958               | 3600.9580             | 5    | C | 0.158D-20         | 79.496   | 1    | 0      | 1      | 2   | 1     | 2     | 1 0 0            | 0 0 0         | 161 | 0.358            | 0.480             |
| 3601.027               | 3601.0265             | -3   | C | 0.516D-20         | 552.912  | 5    | 3      | 2      | 6   | 2     | 5     | 1 0 0            | 0 0 0         | 161 | 0.424            | 0.486             |
| 3602.354               | 3602.3538             | 3    | C | 0.217D-20         | 1122.709 | 8    | 2      | 6      | 8   | 4     | 5     | 0 0 1            | 0 0 0         | 161 | 0.087            | 0.092             |
| 3602.485               |                       |      | D | 0.220D-22         | 6197.461 | 19   | 11     | 9      | 19  | 11    | 8     | 0 0 1            | 0 0 0         | 161 |                  | 0.002             |
| 3602.490               | 3602.4905             | 2    | C | 0.325D-20         | 885.600  | 8    | 0      | 8      | 8   | 2     | 7     | 0 0 1            | 0 0 0         | 161 | 0.170            | 0.175             |
| 3603.026               | 3603.0248             | -10  | C | 0.214D-20         | 446.511  | 5    | 1      | 4      | 5   | 2     | 3     | 1 0 0            | 0 0 0         | 161 | 0.219            | 0.254             |
| 3603.036               |                       |      | D | 0.318D-21         | 2271.712 | 6    | 1      | 5      | 6   | 3     | 4     | 0 1 1            | 0 1 0         | 161 |                  | 0.011             |
| 3603.342               | 3603.3418             |      |   | 0.475D-21         | 3974.632 | 3    | 0      | 3      | 4   | 0     | 4     | 0 0 2            | 0 0 1         | 161 | 0.017            | 0.022             |
| 3603.930               | 3603.9275             |      |   | 0.205D-21         | 3597.866 | 3    | 3      | 1      | 4   | 3     | 2     | 0 2 1            | 0 2 0         | 161 | 0.011            | 0.009             |
| 3605.239               |                       |      |   | 0.846D-21         | 2533.793 | 13   | 4      | 10     | 13  | 4     | 9     | 0 0 1            | 0 0 0         | 161 |                  | 0.030             |
| 3605.255               | 3605.2549             | -3   | C | 0.108D-20         | 882.891  | 8    | 1      | 8      | 8   | 1     | 7     | 0 0 1            | 0 0 0         | 161 | 0.059            | 0.058             |
| 3605.383               | 3605.3831             | 3    | C | 0.111D-21         | 445.159  | 4    | 2      | 2      | 5   | 2     | 3     | 0 0 1            | 0 0 0         | 181 | 0.011            | 0.013             |
| 3605.679               |                       |      | D | 0.688D-22         | 1006.116 | 9    | 4      | 5      | 8   | 3     | 6     | 0 2 0            | 0 0 0         | 161 |                  | 0.003             |
| 3605.681               | 3605.6798             |      |   | 0.186D-21         | 2271.712 | 5    | 4      | 1      | 6   | 3     | 4     | 1 1 0            | 0 1 0         | 161 | 0.009            | 0.006             |
| 3605.911               |                       |      | D | 0.787D-22         | 4796.961 | 15   | 12     | 3      | 15  | 12    | 4     | 0 0 1            | 0 0 0         | 161 |                  | 0.004             |
| 3605.911               | 3605.9084             | -16  | H | 0.236D-21         | 4796.961 | 15   | 12     | 4      | 15  | 12    | 3     | 0 0 1            | 0 0 0         | 161 | 0.014            | 0.012             |
| 3605.985               | 3605.9847             | 1    | H | 0.317D-21         | 3360.598 | 15   | 5      | 11     | 15  | 5     | 10    | 0 0 1            | 0 0 0         | 161 | 0.016            | 0.013             |
| 3606.994               | 3606.9934             | -2   | C | 0.195D-19         | 542.906  | 5    | 1      | 4      | 6   | 1     | 5     | 0 0 1            | 0 0 0         | 161 | 1.639            | 1.872             |
| 3607.263               | 3607.2623             | -5   | C | 0.111D-19         | 648.979  | 5    | 4      | 1      | 6   | 3     | 4     | 1 0 0            | 0 0 0         | 161 | 0.799            | 0.864             |
| 3607.421               | 3607.4218             | 11   | C | 0.593D-20         | 2000.866 | 4    | 1      | 3      | 5   | 1     | 4     | 0 1 1            | 0 1 0         | 161 | 0.207            | 0.203             |
| 3607.905               | 3607.8971             | 17   | H | 0.104D-21         | 4291.906 | 17   | 6      | 12     | 17  | 6     | 11    | 0 0 1            | 0 0 0         | 161 | 0.009            | 0.005             |
| 3608.045               | 3608.0434             | -13  | C | 0.192D-20         | 1813.224 | 11   | 3      | 9      | 11  | 3     | 8     | 0 0 1            | 0 0 0         | 161 | 0.058            | 0.066             |
| 3608.708               | 3608.7049             |      |   | 0.901D-22         | 5381.543 | 13   | 10     | 4      | 13  | 10    | 3     | 0 1 1            | 0 1 0         | 161 | 0.007            | 0.005             |
| 3608.708               |                       |      | D | 0.300D-22         | 5381.543 | 13   | 10     | 3      | 13  | 10    | 4     | 0 1 1            | 0 1 0         | 161 |                  | 0.002             |
| 3609.234               | 3609.2350             | 15   | S | 0.636D-19         | 586.243  | 6    | 0      | 6      | 7   | 0     | 7     | 0 0 1            | 0 0 0         | 161 |                  | 5.585             |
| 3609.241               |                       |      | D | 0.747D-21         | 2024.150 | 4    | 2      | 3      | 5   | 2     | 4     | 0 1 1            | 0 1 0         | 161 |                  | 0.026             |
| 3609.339               | 3609.3397             | 6    | C | 0.211D-19         | 586.479  | 6    | 1      | 6      | 7   | 1     | 7     | 0 0 1            | 0 0 0         | 161 | 1.653            | 1.852             |
| 3609.790               | 3609.7887             |      |   | 0.418D-21         | 2161.286 | 6    | 0      | 6      | 6   | 2     | 5     | 0 1 1            | 0 1 0         | 161 | 0.013            | 0.014             |
| 3609.969               | 3609.9731             | -13  | H | 0.425D-21         | 4431.637 | 14   | 12     | 2      | 14  | 12    | 3     | 0 0 1            | 0 0 0         | 161 | 0.027            | 0.021             |
| 3609.969               |                       |      | D | 0.142D-21         | 4431.637 | 14   | 12     | 3      | 14  | 12    | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.007             |
| 3610.170               | 3610.1702             | 9    | C | 0.132D-21         | 285.419  | 3    | 1      | 3      | 3   | 3     | 0     | 0 0 1            | 0 0 0         | 161 | 0.019            | 0.023             |
| 3610.355               |                       |      | D | 0.507D-22         | 1693.652 | 2    | 0      | 2      | 2   | 1     | 1     | 1 1 0            | 0 1 0         | 161 |                  | 0.002             |
| 3610.359               | 3610.3597             | -35  | H | 0.220D-20         | 2041.784 | 5    | 0      | 5      | 6   | 0     | 6     | 0 1 1            | 0 1 0         | 161 | 0.076            | 0.075             |
| 3610.811               | 3610.8106             | -4   | H | 0.648D-20         | 2042.755 | 5    | 1      | 5      | 6   | 1     | 6     | 0 1 1            | 0 1 0         | 161 | 0.225            | 0.222             |
| 3612.023               | 3612.0231             | -3   | C | 0.725D-21         | 315.779  | 4    | 1      | 3      | 4   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.093            | 0.117             |
| 3612.563               | 3612.5622             | -4   | S | 0.478D-19         | 552.912  | 5    | 2      | 4      | 6   | 2     | 5     | 0 0 1            | 0 0 0         | 161 |                  | 4.488             |
| 3612.936               | 3612.9320             |      |   | 0.675D-21         | 3478.987 | 4    | 0      | 4      | 5   | 0     | 5     | 0 2 1            | 0 2 0         | 161 | 0.032            | 0.028             |
| 3613.058               | 3613.0568             | -1   | C | 0.156D-20         | 212.156  | 2    | 0      | 2      | 3   | 2     | 1     | 0 0 1            | 0 0 0         | 161 | 0.257            | 0.330             |
| 3613.768               |                       |      | D | 0.247D-21         | 4087.981 | 13   | 12     | 1      | 13  | 12    | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.011             |
| 3613.769               | 3613.7635             | -22  | H | 0.742D-21         | 4087.981 | 13   | 12     | 2      | 13  | 12    | 1     | 0 0 1            | 0 0 0         | 161 | 0.036            | 0.034             |
| 3614.301               | 3614.3013             | 5    | C | 0.320D-21         | 136.164  | 2    | 1      | 1      | 2   | 2     | 0     | 1 0 0            | 0 0 0         | 161 | 0.067            | 0.083             |
| 3614.359               |                       |      |   | 0.255D-21         | 4769.242 | 11   | 10     | 2      | 11  | 10    | 1     | 0 1 1            | 0 1 0         | 161 |                  | 0.013             |
| 3614.359               |                       |      |   | 0.851D-22         | 4769.242 | 11   | 10     | 1      | 11  | 10    | 2     | 0 1 1            | 0 1 0         | 161 |                  | 0.004             |
| 3614.381               | 3614.3789             | -12  | C | 0.126D-21         | 398.361  | 4    | 1      | 3      | 5   | 1     | 4     | 0 0 1            | 0 0 0         | 181 | 0.017            | 0.017             |
| 3614.510               | 3614.5102             | 2    | C | 0.158D-19         | 610.341  | 4    | 4      | 0      | 5   | 4     | 1     | 0 0 1            | 0 0 0         | 161 | 1.180            | 1.321             |
| 3614.702               | 3614.7028             | 5    | C | 0.527D-20         | 610.114  | 4    | 4      | 1      | 5   | 4     | 2     | 0 0 1            | 0 0 0         | 161 | 0.394            | 0.441             |
| 3615.237               | 3615.2363             | -2   | C | 0.173D-20         | 212.156  | 3    | 1      | 2      | 3   | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.286            | 0.365             |
| 3615.329               | 3615.3294             | 6    | C | 0.165D-21         | 173.365  | 2    | 2      | 1      | 3   | 1     | 2     | 1 0 0            | 0 0 0         | 161 | 0.032            | 0.039             |
| 3615.582               | 3615.5777             |      |   | 0.888D-21         | 2024.150 | 4    | 3      | 1      | 5   | 2     | 4     | 1 1 0            | 0 1 0         | 161 | 0.029            | 0.030             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3615.644               | 3615.6443             | -6     | C 0.230D-21       | 416.209  | 4    | 3      | 1      | 5   | 2     | 4     | 1 0 0          | 0 0 0       | 161 | 0.023            | 0.029             |
| 3615.815               | 3615.8147             | 1      | C 0.341D-20       | 1201.922 | 9    | 2      | 8      | 9   | 2     | 7     | 0 0 1          | 0 0 0       | 161 | 0.127            | 0.136             |
| 3615.934               | 3615.9361             | 24     | C 0.138D-21       | 445.346  | 5    | 1      | 5      | 6   | 1     | 6     | 0 0 1          | 0 0 0       | 181 | 0.014            | 0.016             |
| 3616.009               | 3616.0055             |        | 0.415D-21         | 3482.064 | 3    | 2      | 2      | 4   | 2     | 3     | 0 2 1          | 0 2 0       | 161 | 0.018            | 0.017             |
| 3616.833               | 3616.8316             | -19    | H 0.413D-21       | 4497.199 | 10   | 10     | 0      | 10  | 10    | 1     | 0 1 1          | 0 1 0       | 161 | 0.023            | 0.021             |
| 3616.833               |                       |        | D 0.138D-21       | 4497.199 | 10   | 10     | 1      | 10  | 10    | 0     | 0 1 1          | 0 1 0       | 161 |                  | 0.007             |
| 3617.289               |                       |        | D 0.419D-21       | 3766.388 | 12   | 12     | 1      | 12  | 12    | 0     | 0 0 1          | 0 0 0       | 161 |                  | 0.018             |
| 3617.289               | 3617.2943             | 59     | H 0.126D-20       | 3766.388 | 12   | 12     | 0      | 12  | 12    | 1     | 0 0 1          | 0 0 0       | 161 | 0.060            | 0.055             |
| 3617.651               | 3617.6506             | -10    | S 0.263D-19       | 508.812  | 4    | 3      | 1      | 5   | 3     | 2     | 0 0 1          | 0 0 0       | 161 |                  | 2.707             |
| 3618.007               | 3618.0066             | 1      | C 0.164D-20       | 173.365  | 3    | 0      | 3      | 3   | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.293            | 0.384             |
| 3618.187               | 3618.1873             | 3      | C 0.405D-20       | 1006.116 | 8    | 1      | 7      | 8   | 3     | 6     | 0 0 1          | 0 0 0       | 161 | 0.176            | 0.189             |
| 3619.612               | 3619.6176             | 54     | S 0.517D-19       | 446.511  | 4    | 2      | 2      | 5   | 2     | 3     | 0 0 1          | 0 0 0       | 161 |                  | 6.107             |
| 3619.916               | 3619.9159             | -5     | C 0.325D-21       | 37.137   | 0    | 0      | 0      | 1   | 1     | 1     | 1 0 0          | 0 0 0       | 161 | 0.082            | 0.111             |
| 3621.181               | 3621.1810             | 4      | C 0.920D-20       | 503.968  | 4    | 3      | 2      | 5   | 3     | 3     | 0 0 1          | 0 0 0       | 161 | 0.846            | 0.956             |
| 3621.340               | 3621.3457             |        | 0.314D-21         | 4534.961 | 15   | 11     | 5      | 15  | 11    | 4     | 0 0 1          | 0 0 0       | 161 | 0.018            | 0.016             |
| 3621.340               |                       |        | D 0.105D-21       | 4534.961 | 15   | 11     | 4      | 15  | 11    | 5     | 0 0 1          | 0 0 0       | 161 |                  | 0.005             |
| 3623.166               | 3623.1665             | 9      | C 0.131D-20       | 709.609  | 7    | 0      | 7      | 7   | 2     | 6     | 0 0 1          | 0 0 0       | 161 | 0.084            | 0.091             |
| 3623.203               | 3623.2030             | 0      | C 0.225D-21       | 70.091   | 1    | 1      | 1      | 2   | 0     | 2     | 1 0 0          | 0 0 0       | 161 | 0.053            | 0.070             |
| 3624.123               | 3624.1239             | -3     | C 0.260D-21       | 757.780  | 5    | 5      | 1      | 6   | 4     | 2     | 1 0 0          | 0 0 0       | 161 | 0.017            | 0.017             |
| 3624.228               | 3624.2258             | -50    | H 0.681D-21       | 2005.917 | 3    | 3      | 0      | 4   | 3     | 1     | 0 1 1          | 0 1 0       | 161 | 0.027            | 0.023             |
| 3625.128               | 3625.1276             | 2      | C 0.204D-20       | 2004.817 | 3    | 3      | 1      | 4   | 3     | 2     | 0 1 1          | 0 1 0       | 161 | 0.066            | 0.069             |
| 3625.179               | 3625.1802             | 9      | C 0.770D-21       | 756.725  | 5    | 5      | 0      | 6   | 4     | 3     | 1 0 0          | 0 0 0       | 161 | 0.046            | 0.050             |
| 3625.396               |                       |        | D 0.188D-21       | 4172.148 | 14   | 11     | 4      | 14  | 11    | 3     | 0 0 1          | 0 0 0       | 161 |                  | 0.009             |
| 3625.396               | 3625.3940             | -41    | H 0.564D-21       | 4172.148 | 14   | 11     | 3      | 14  | 11    | 4     | 0 0 1          | 0 0 0       | 161 | 0.027            | 0.026             |
| 3626.206               | 3626.2060             | -2     | C 0.791D-20       | 508.812  | 4    | 4      | 1      | 5   | 3     | 2     | 1 0 0          | 0 0 0       | 161 | 0.704            | 0.812             |
| 3626.803               | 3626.8011             | -38    | H 0.135D-20       | 1922.902 | 3    | 2      | 1      | 4   | 2     | 2     | 0 1 1          | 0 1 0       | 161 | 0.052            | 0.046             |
| 3628.347               | 3628.3508             | 32     | S 0.590D-19       | 399.457  | 4    | 1      | 3      | 5   | 1     | 4     | 0 0 1          | 0 0 0       | 161 |                  | 7.755             |
| 3628.699               | 3628.6979             | -3     | C 0.393D-20       | 704.214  | 7    | 1      | 7      | 7   | 1     | 6     | 0 0 1          | 0 0 0       | 161 | 0.281            | 0.276             |
| 3629.177               | 3629.1782             |        | 0.982D-21         | 3831.174 | 13   | 11     | 3      | 13  | 11    | 2     | 0 0 1          | 0 0 0       | 161 | 0.050            | 0.043             |
| 3629.177               |                       |        | D 0.327D-21       | 3831.173 | 13   | 11     | 2      | 13  | 11    | 3     | 0 0 1          | 0 0 0       | 161 |                  | 0.014             |
| 3629.446               | 3629.4473             | 4      | S 0.218D-19       | 446.697  | 5    | 0      | 5      | 6   | 0     | 6     | 0 0 1          | 0 0 0       | 161 |                  | 2.567             |
| 3629.644               | 3629.6383             | -54    | S 0.638D-19       | 447.252  | 5    | 1      | 5      | 6   | 1     | 6     | 0 0 1          | 0 0 0       | 161 |                  | 7.502             |
| 3629.904               | 3629.9044             | 4      | C 0.644D-20       | 1920.769 | 4    | 0      | 4      | 5   | 0     | 5     | 0 1 1          | 0 1 0       | 161 | 0.249            | 0.218             |
| 3630.148               | 3630.1480             | -9     | C 0.161D-20       | 1922.831 | 4    | 1      | 4      | 5   | 1     | 5     | 0 1 1          | 0 1 0       | 161 | 0.062            | 0.055             |
| 3630.208               | 3630.2093             |        | 0.164D-21         | 5475.758 | 8    | 8      | 1      | 8   | 8     | 0     | 0 0 2          | 0 0 1       | 161 | 0.011            | 0.010             |
| 3630.208               |                       |        | D 0.545D-22       | 5475.758 | 8    | 8      | 0      | 8   | 8     | 1     | 0 0 2          | 0 0 1       | 161 |                  | 0.003             |
| 3630.766               | 3630.7666             | 3      | C 0.550D-21       | 95.176   | 2    | 0      | 2      | 2   | 1     | 1     | 1 0 0          | 0 0 0       | 161 | 0.135            | 0.159             |
| 3630.785               |                       |        | D 0.641D-21       | 1908.017 | 3    | 3      | 0      | 4   | 2     | 3     | 1 1 0          | 0 1 0       | 161 |                  | 0.022             |
| 3630.831               | 3630.8309             | 4      | C 0.203D-20       | 503.968  | 4    | 4      | 0      | 5   | 3     | 3     | 1 0 0          | 0 0 0       | 161 | 0.242            | 0.210             |
| 3630.840               |                       |        | D 0.181D-20       | 1875.474 | 3    | 1      | 2      | 4   | 1     | 3     | 0 1 1          | 0 1 0       | 161 |                  | 0.061             |
| 3630.979               | 3630.9729             | -101   | H 0.323D-21       | 4510.895 | 11   | 9      | 3      | 11  | 9     | 2     | 0 1 1          | 0 1 0       | 161 | 0.021            | 0.016             |
| 3630.979               |                       |        | D 0.108D-21       | 4510.895 | 11   | 9      | 2      | 11  | 9     | 3     | 0 1 1          | 0 1 0       | 161 |                  | 0.005             |
| 3632.122               | 3632.1249             | 33     | H 0.215D-21       | 4665.969 | 16   | 10     | 6      | 16  | 10    | 7     | 0 0 1          | 0 0 0       | 161 | 0.016            | 0.011             |
| 3632.134               |                       |        | D 0.206D-21       | 3375.298 | 3    | 0      | 3      | 4   | 0     | 4     | 0 2 1          | 0 2 0       | 161 |                  | 0.008             |
| 3632.277               | 3632.2762             | -5     | C 0.146D-20       | 816.694  | 7    | 1      | 6      | 7   | 3     | 5     | 0 0 1          | 0 0 0       | 161 | 0.089            | 0.086             |
| 3632.703               | 3632.7046             | 14     | H 0.166D-20       | 3512.401 | 12   | 11     | 1      | 12  | 11    | 2     | 0 0 1          | 0 0 0       | 161 | 0.083            | 0.069             |
| 3632.703               |                       |        | D 0.554D-21       | 3512.401 | 12   | 11     | 2      | 12  | 11    | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.023             |
| 3633.448               |                       |        | D 0.173D-21       | 4240.941 | 10   | 9      | 2      | 10  | 9     | 1     | 0 1 1          | 0 1 0       | 161 |                  | 0.008             |
| 3633.448               | 3633.4500             | 29     | H 0.518D-21       | 4240.941 | 10   | 9      | 1      | 10  | 9     | 2     | 0 1 1          | 0 1 0       | 161 | 0.030            | 0.024             |
| 3633.844               | 3633.8434             | -3     | C 0.163D-19       | 416.209  | 4    | 2      | 3      | 5   | 2     | 4     | 0 0 1          | 0 0 0       | 161 |                  | 2.057             |
| 3634.983               | 3634.9828             | 3      | C 0.118D-21       | 300.362  | 3    | 3      | 0      | 4   | 2     | 3     | 1 0 0          | 0 0 0       | 161 | 0.019            | 0.020             |
| 3635.021               |                       |        | D 0.488D-21       | 1922.831 | 4    | 2      | 2      | 5   | 1     | 5     | 1 1 0          | 0 1 0       | 161 |                  | 0.017             |
| 3635.024               | 3635.0222             |        | 0.588D-21         | 3381.704 | 3    | 1      | 3      | 4   | 1     | 4     | 0 2 1          | 0 2 0       | 161 | 0.048            | 0.024             |
| 3635.417               | 3635.4174             | 7      | C 0.136D-21       | 324.047  | 4    | 0      | 4      | 5   | 0     | 5     | 0 0 1          | 0 0 0       | 181 | 0.016            | 0.021             |
| 3635.700               |                       |        | D 0.270D-21       | 3994.259 | 9    | 9      | 0      | 9   | 9     | 1     | 0 1 1          | 0 1 0       | 161 |                  | 0.012             |
| 3635.700               | 3635.6979             | -22    | H 0.810D-21       | 3994.259 | 9    | 9      | 1      | 9   | 9     | 0     | 0 1 1          | 0 1 0       | 161 | 0.049            | 0.037             |
| 3635.976               |                       |        | D 0.911D-21       | 3216.185 | 11   | 11     | 0      | 11  | 11    | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.036             |
| 3635.976               | 3635.9740             | -6     | H 0.273D-20       | 3216.185 | 11   | 11     | 1      | 11  | 11    | 0     | 0 0 1          | 0 0 0       | 161 | 0.128            | 0.108             |
| 3636.234               | 3636.2317             | -25    | C 0.340D-20       | 1908.017 | 3    | 2      | 2      | 4   | 2     | 3     | 0 1 1          | 0 1 0       | 161 | 0.130            | 0.115             |
| 3636.349               | 3636.3524             | 12     | H 0.397D-21       | 4283.305 | 15   | 10     | 6      | 15  | 10    | 5     | 0 0 1          | 0 0 0       | 161 | 0.018            | 0.019             |
| 3636.357               |                       |        | D 0.132D-21       | 4283.301 | 15   | 10     | 5      | 15  | 10    | 6     | 0 0 1          | 0 0 0       | 161 |                  | 0.006             |
| 3636.563               |                       |        | D 0.697D-22       | 4812.191 | 7    | 7      | 0      | 7   | 7     | 1     | 0 2 1          | 0 2 0       | 161 |                  | 0.004             |
| 3636.564               | 3636.5639             |        | 0.209D-21         | 4812.191 | 7    | 7      | 1      | 7   | 7     | 0     | 0 2 1          | 0 2 0       | 161 | 0.020            | 0.011             |
| 3636.565               |                       |        | D 0.170D-21       | 5289.961 | 8    | 7      | 2      | 8   | 7     | 1     | 0 0 2          | 0 0 1       | 161 |                  | 0.010             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$     | $J$      | $K_a$ | $K_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |   |   |     |       |       |       |
|------------------------|-----------------------|--------|-------------------|-----------|----------|-------|-------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|---|---|-----|-------|-------|-------|
| 3636.567               |                       |        | D                 | 0.568D-22 | 5289.961 | 8     | 7     | 1   | 8     | 7     | 2                | 0             | 0   | 2                | 0                 | 0 | 1 | 161 | 0.003 |       |       |
| 3637.806               | 3637.8042             |        |                   | 0.888D-21 | 1538.150 | 10    | 3     | 8   | 10    | 3     | 7                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.030 | 0.031 |       |
| 3638.082               | 3638.0822             | 0      | C                 | 0.125D-20 | 42.372   | 1     | 0     | 1   | 1     | 1     | 0                | 1             | 0   | 0                | 0                 | 0 | 0 | 0   | 161   | 0.343 | 0.417 |
| 3638.116               | 3638.1128             |        |                   | 0.458D-21 | 3334.626 | 2     | 1     | 1   | 3     | 1     | 2                | 0             | 2   | 1                | 0                 | 2 | 0 | 161 | 0.020 | 0.018 |       |
| 3639.926               |                       |        | D                 | 0.665D-23 | 224.838  | 3     | 2     | 1   | 4     | 1     | 4                | 1             | 0   | 0                | 1                 | 0 | 0 | 0   | 161   | 0.001 |       |
| 3639.934               | 3639.9344             | 6      | C                 | 0.493D-21 | 326.625  | 4     | 2     | 2   | 5     | 1     | 5                | 1             | 0   | 0                | 0                 | 0 | 0 | 0   | 161   | 0.074 | 0.077 |
| 3640.351               |                       |        | D                 | 0.238D-21 | 3922.325 | 14    | 10    | 5   | 14    | 10    | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.011 |       |       |
| 3640.351               | 3640.3484             | 0      | H                 | 0.713D-21 | 3922.324 | 14    | 10    | 4   | 14    | 10    | 5                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.038 | 0.032 |       |
| 3641.643               | 3641.6431             | 4      | C                 | 0.137D-21 | 285.219  | 3     | 1     | 2   | 3     | 3     | 1                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.021 | 0.024 |       |
| 3641.779               | 3641.7780             | -4     | C                 | 0.400D-20 | 648.979  | 6     | 1     | 5   | 6     | 3     | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.310 | 0.308 |       |
| 3642.297               | 3642.2980             | 0      | C                 | 0.871D-22 | 298.620  | 3     | 2     | 2   | 4     | 2     | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 181 | 0.010 | 0.015 |       |
| 3642.566               | 3642.5662             | 2      | C                 | 0.455D-20 | 552.912  | 6     | 0     | 6   | 6     | 2     | 5                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.426 | 0.424 |       |
| 3642.655               | 3642.6529             |        |                   | 0.398D-21 | 1908.017 | 4     | 0     | 4   | 4     | 2     | 3                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.013 |       |       |
| 3643.025               | 3643.0251             | -3     | C                 | 0.143D-20 | 982.912  | 8     | 2     | 7   | 8     | 2     | 6                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.072 | 0.068 |       |
| 3643.330               | 3643.3290             | -4     | C                 | 0.242D-21 | 136.164  | 1     | 0     | 1   | 2     | 2     | 0                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.053 | 0.062 |       |
| 3644.093               | 3644.0932             | -13    | H                 | 0.124D-20 | 3583.372 | 13    | 10    | 4   | 13    | 10    | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.061 | 0.052 |       |
| 3644.093               |                       |        | D                 | 0.414D-21 | 3583.372 | 13    | 10    | 3   | 13    | 10    | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.017 |       |       |
| 3645.288               | 3645.2870             | -5     | C                 | 0.139D-20 | 382.517  | 4     | 1     | 3   | 4     | 3     | 2                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.173 | 0.189 |       |
| 3645.931               | 3645.9310             | -3     | C                 | 0.934D-21 | 503.968  | 5     | 1     | 4   | 5     | 3     | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.092 | 0.096 |       |
| 3646.464               | 3646.4637             | -1     | C                 | 0.709D-20 | 383.842  | 3     | 3     | 0   | 4     | 3     | 1                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.906 | 0.962 |       |
| 3646.933               | 3646.9367             |        |                   | 0.384D-21 | 4265.980 | 11    | 8     | 4   | 11    | 8     | 3                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.032 | 0.018 |       |
| 3646.934               |                       |        | D                 | 0.253D-21 | 4427.117 | 16    | 9     | 7   | 16    | 9     | 8                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.012 |       |       |
| 3646.940               |                       |        | D                 | 0.128D-21 | 4265.977 | 11    | 8     | 3   | 11    | 8     | 4                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.006 |       |       |
| 3647.139               | 3647.1381             | -5     | S                 | 0.141D-19 | 315.779  | 3     | 2     | 1   | 4     | 2     | 2                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 2.260 |       |       |
| 3647.553               | 3647.5526             | -5     | S                 | 0.212D-19 | 382.517  | 3     | 3     | 1   | 4     | 3     | 2                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 2.886 |       |       |
| 3647.595               | 3647.5914             |        |                   | 0.210D-20 | 3266.762 | 12    | 10    | 2   | 12    | 10    | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.111 | 0.083 |       |
| 3647.595               |                       |        | D                 | 0.700D-21 | 3266.762 | 12    | 10    | 3   | 12    | 10    | 2                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.028 |       |       |
| 3648.479               | 3648.4788             |        |                   | 0.534D-21 | 2392.594 | 7     | 2     | 6   | 7     | 2     | 5                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.022 | 0.019 |       |
| 3648.529               | 3648.5276             |        |                   | 0.388D-21 | 2904.672 | 9     | 3     | 7   | 9     | 3     | 6                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.014 | 0.015 |       |
| 3648.668               | 3648.6671             | -10    | C                 | 0.124D-20 | 447.252  | 5     | 2     | 3   | 6     | 1     | 6                | 1             | 0   | 0                | 0                 | 0 | 0 | 0   | 161   | 0.147 | 0.145 |
| 3648.879               | 3648.8691             |        |                   | 0.160D-22 | 299.440  | 3     | 2     | 2   | 4     | 2     | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 171 | 0.010 | 0.003 |       |
| 3649.186               | 3649.1893             |        |                   | 0.196D-20 | 1817.451 | 3     | 0     | 3   | 4     | 0     | 4                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.065 | 0.066 |       |
| 3649.284               | 3649.2762             | -65    | S                 | 0.638D-19 | 325.348  | 4     | 0     | 4   | 5     | 0     | 5                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 9.980 |       |       |
| 3649.382               |                       |        |                   | 0.615D-21 | 3997.511 | 10    | 8     | 2   | 10    | 8     | 3                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.028 |       |       |
|                        | 3649.7219             |        |                   |           |          |       |       |     |       |       |                  |               |     |                  |                   |   |   |     | 0.009 |       |       |
| 3650.636               | 3650.6363             | -1     | S                 | 0.204D-19 | 326.625  | 4     | 1     | 4   | 5     | 1     | 5                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 3.180 |       |       |
| 3650.843               |                       |        | D                 | 0.471D-21 | 4045.316 | 15    | 9     | 7   | 15    | 9     | 6                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.021 |       |       |
| 3650.845               | 3650.8434             |        |                   | 0.346D-20 | 2972.824 | 11    | 10    | 2   | 11    | 10    | 1                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.180 | 0.131 |       |
| 3650.845               |                       |        | D                 | 0.115D-20 | 2972.824 | 11    | 10    | 1   | 11    | 10    | 2                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.043 |       |       |
| 3651.365               | 3651.3657             | 2      | C                 | 0.181D-19 | 275.497  | 3     | 1     | 2   | 4     | 1     | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 3.209 |       |       |
| 3651.547               | 3651.5474             | 9      | S                 | 0.558D-20 | 1821.599 | 3     | 1     | 3   | 4     | 1     | 4                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.221 | 0.188 |       |
| 3651.621               | 3651.6208             |        |                   | 0.961D-21 | 3752.417 | 9     | 8     | 2   | 9     | 8     | 1                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.054 | 0.041 |       |
| 3651.621               |                       |        | D                 | 0.320D-21 | 3752.417 | 9     | 8     | 1   | 9     | 8     | 2                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.014 |       |       |
| 3651.922               | 3651.9213             |        |                   | 0.519D-21 | 3289.242 | 2     | 0     | 2   | 3     | 0     | 3                | 0             | 2   | 1                | 0                 | 2 | 0 | 161 | 0.026 | 0.021 |       |
| 3652.692               |                       |        | D                 | 0.485D-22 | 4775.090 | 8     | 6     | 3   | 8     | 6     | 2                | 0             | 2   | 1                | 0                 | 2 | 0 | 161 | 0.003 |       |       |
| 3652.700               | 3652.7015             |        |                   | 0.507D-21 | 2000.866 | 5     | 1     | 5   | 5     | 1     | 4                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.021 | 0.017 |       |
| 3652.912               | 3652.9117             | -9     | C                 | 0.153D-20 | 542.906  | 6     | 1     | 6   | 6     | 1     | 5                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.143 | 0.145 |       |
| 3653.151               | 3653.1553             |        |                   | 0.653D-22 | 5581.523 | 10    | 6     | 5   | 10    | 6     | 4                | 0             | 0   | 2                | 0                 | 0 | 1 | 161 | 0.006 | 0.004 |       |
| 3653.642               |                       |        | D                 | 0.489D-21 | 3530.958 | 8     | 8     | 1   | 8     | 8     | 0                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.020 |       |       |
| 3653.642               | 3653.6449             | -16    | H                 | 0.147D-20 | 3530.958 | 8     | 8     | 0   | 8     | 8     | 1                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.085 | 0.061 |       |
| 3653.652               |                       |        | D                 | 0.138D-21 | 4612.789 | 17    | 8     | 10  | 17    | 8     | 9                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.007 |       |       |
| 3653.849               |                       |        | D                 | 0.185D-20 | 2701.890 | 10    | 10    | 1   | 10    | 10    | 0                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.067 |       |       |
| 3653.849               | 3653.8483             | -10    | H                 | 0.554D-20 | 2701.890 | 10    | 10    | 0   | 10    | 10    | 1                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.254 | 0.201 |       |
| 3653.924               | 3653.9203             |        |                   | 0.366D-21 | 4759.852 | 6     | 6     | 1   | 6     | 6     | 1                | 0             | 0   | 2                | 0                 | 0 | 1 | 161 | 0.021 | 0.019 |       |
| 3653.925               |                       |        | D                 | 0.122D-21 | 4759.852 | 6     | 6     | 0   | 6     | 6     | 1                | 0             | 0   | 2                | 0                 | 0 | 1 | 161 | 0.006 |       |       |
| 3654.321               | 3654.3210             | 17     | C                 | 0.253D-20 | 1819.337 | 2     | 2     | 0   | 3     | 2     | 1                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.099 | 0.085 |       |
| 3654.432               | 3654.4292             |        |                   | 0.222D-21 | 4578.977 | 7     | 6     | 2   | 7     | 6     | 1                | 0             | 2   | 1                | 0                 | 2 | 0 | 161 | 0.012 | 0.011 |       |
| 3654.797               | 3654.8000             | 74     | H                 | 0.849D-21 | 3685.403 | 14    | 9     | 5   | 14    | 9     | 6                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.034 | 0.036 |       |
| 3654.808               |                       |        | D                 | 0.414D-22 | 221.233  | 3     | 0     | 3   | 4     | 0     | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 181 | 0.008 |       |       |
| 3655.761               | 3655.7581             | 0      | C                 | 0.436D-20 | 1772.413 | 2     | 1     | 1   | 3     | 1     | 2                | 0             | 1   | 1                | 0                 | 1 | 0 | 161 | 0.173 | 0.147 |       |
| 3655.969               | 3655.9670             |        |                   | 0.331D-21 | 4407.047 | 6     | 6     | 0   | 6     | 6     | 1                | 0             | 2   | 1                | 0                 | 2 | 0 | 161 | 0.017 | 0.016 |       |
| 3656.304               | 3656.3034             | -6     | C                 | 0.409D-19 | 300.362  | 3     | 2     | 2   | 4     | 2     | 3                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 6.797 |       |       |
| 3656.736               | 3656.7337             | -12    | C                 | 0.119D-21 | 223.828  | 3     | 1     | 3   | 4     | 1     | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.020 | 0.024 |       |
| 3658.448               | 3658.4466             | -7     | H                 | 0.148D-20 | 3347.780 | 13    | 9     | 5   | 13    | 9     | 4                | 0             | 0   | 1                | 0                 | 0 | 0 | 161 | 0.068 | 0.059 |       |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu'_1 \nu'_2 \nu'_3$ | $\nu_1 \nu_2 \nu_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|-----|--------|--------|-----|-------|-------|------------------------|---------------------|-----|------------------|-------------------|
| 3658.565               | 3658.5629             |             | 0.832D-21         | 1813.788 | 2   | 2      | 1      | 3   | 2     | 2     | 0 1 1                  | 0 1 0               | 161 | 0.031            | 0.028             |
| 3658.750               | 3658.7486             | -78         | H 0.402D-21       | 3472.880 | 15  | 6      | 10     | 15  | 6     | 9     | 0 0 1                  | 0 0 0               | 161 | 0.013            | 0.016             |
| 3658.780               | 3658.7868             |             | 0.905D-22         | 4408.027 | 6   | 3      | 4      | 6   | 3     | 3     | 0 0 2                  | 0 0 1               | 161 | 0.006            | 0.004             |
| 3659.935               | 3659.9349             | -2          | C 0.163D-20       | 416.209  | 5   | 0      | 5      | 5   | 2     | 4     | 0 0 1                  | 0 0 0               | 161 | 0.193            | 0.204             |
| 3660.700               | 3660.7003             | -5          | C 0.551D-22       | 210.799  | 2   | 2      | 0      | 3   | 2     | 1     | 0 0 1                  | 0 0 0               | 181 | 0.009            | 0.012             |
| 3661.776               | 3661.7760             | -3          | C 0.932D-22       | 172.882  | 2   | 1      | 1      | 3   | 1     | 2     | 0 0 1                  | 0 0 0               | 181 | 0.017            | 0.022             |
| 3661.888               |                       | D 0.839D-21 | 3032.691          | 12       | 9   | 4      | 12     | 9   | 3     | 0 0 1 | 0 0 0                  | 161                 |     | 0.032            |                   |
| 3661.890               | 3661.8892             | -16         | H 0.252D-20       | 3032.690 | 12  | 9      | 3      | 12  | 9     | 4     | 0 0 1                  | 0 0 0               | 161 | 0.117            | 0.096             |
| 3662.109               | 3662.1087             | -25         | H 0.425D-21       | 4038.404 | 11  | 7      | 5      | 11  | 7     | 4     | 0 1 1                  | 0 1 0               | 161 | 0.019            | 0.019             |
| 3662.239               | 3662.2431             | 51          | H 0.142D-21       | 4038.355 | 11  | 7      | 4      | 11  | 7     | 5     | 0 1 1                  | 0 1 0               | 161 | 0.008            | 0.006             |
| 3662.703               | 3662.7034             | -7          | H 0.266D-21       | 4206.332 | 16  | 8      | 8      | 16  | 8     | 9     | 0 0 1                  | 0 0 0               | 161 | 0.010            | 0.012             |
| 3662.783               | 3662.7847             | 36          | H 0.101D-20       | 2629.337 | 13  | 5      | 9      | 13  | 5     | 8     | 0 0 1                  | 0 0 0               | 161 | 0.035            | 0.036             |
| 3663.045               | 3663.0449             | 4           | C 0.806D-22       | 586.479  | 6   | 2      | 4      | 7   | 1     | 7     | 1 0 0                  | 0 0 0               | 161 | 0.008            | 0.007             |
| 3663.381               | 3663.3882             |             | 0.245D-22         | 5610.766 | 6   | 4      | 2      | 6   | 4     | 3     | 0 3 1                  | 0 3 0               | 161 | 0.006            | 0.001             |
| 3663.749               | 3663.7497             |             | 0.210D-21         | 4782.660 | 7   | 5      | 2      | 7   | 5     | 3     | 0 0 2                  | 0 0 1               | 161 | 0.008            | 0.011             |
| 3663.801               | 3663.8059             |             | 0.318D-21         | 4613.574 | 6   | 5      | 2      | 6   | 5     | 1     | 0 0 2                  | 0 0 1               | 161 | 0.010            | 0.016             |
| 3663.999               |                       | D 0.157D-21 | 4468.699          | 5        | 5   | 1      | 5      | 5   | 0     | 0     | 0 0 2                  | 0 0 1               | 161 |                  | 0.008             |
| 3664.010               | 3664.0086             |             | 0.472D-21         | 4468.691 | 5   | 5      | 0      | 5   | 5     | 1     | 0 0 2                  | 0 0 1               | 161 | 0.026            | 0.023             |
| 3664.306               |                       | D 0.603D-22 | 1774.752          | 11       | 3   | 8      | 12     | 2   | 11    | 1     | 0 0                    | 0 0 0               | 161 |                  | 0.002             |
| 3664.310               | 3664.3069             | -48         | H 0.511D-21       | 3824.994 | 15  | 8      | 8      | 15  | 8     | 7     | 0 0 1                  | 0 0 0               | 161 | 0.023            | 0.022             |
| 3664.389               |                       | D 0.195D-22 | 5342.195          | 4        | 4   | 1      | 4      | 4   | 0     | 0     | 3 1                    | 0 3 0               | 161 |                  | 0.001             |
| 3664.393               | 3664.3913             | -70         | H 0.212D-20       | 1899.008 | 11  | 4      | 8      | 11  | 4     | 7     | 0 0 1                  | 0 0 0               | 161 | 0.073            | 0.071             |
| 3664.543               | 3664.5439             | 32          | H 0.684D-21       | 3770.713 | 10  | 7      | 3      | 10  | 7     | 4     | 0 1 1                  | 0 1 0               | 161 | 0.027            | 0.029             |
| 3665.099               | 3665.0962             | -18         | H 0.415D-20       | 2740.420 | 11  | 9      | 3      | 11  | 9     | 2     | 0 0 1                  | 0 0 0               | 161 | 0.186            | 0.151             |
| 3665.099               |                       | D 0.138D-20 | 2740.420          | 11       | 9   | 2      | 11     | 9   | 3     | 0 0 1 | 0 0 0                  | 161                 |     | 0.050            |                   |
| 3665.419               | 3665.4188             | 0           | C 0.365D-22       | 212.156  | 4   | 1      | 4      | 3   | 2     | 1     | 1 0 0                  | 0 0 0               | 161 | 0.008            | 0.008             |
| 3666.084               | 3666.0836             | -6          | C 0.371D-20       | 1282.919 | 9   | 3      | 7      | 9   | 3     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.146            | 0.139             |
| 3666.697               | 3666.7008             | 2           | H 0.107D-20       | 3526.630 | 9   | 7      | 3      | 9   | 7     | 2     | 0 1 1                  | 0 1 0               | 161 | 0.054            | 0.044             |
| 3666.709               |                       | D 0.357D-21 | 3526.627          | 9        | 7   | 2      | 9      | 7   | 3     | 0 1 1 | 0 1 0                  | 161                 |     | 0.015            |                   |
| 3668.069               | 3668.0698             | 37          | H 0.667D-20       | 2471.254 | 10  | 9      | 1      | 10  | 9     | 2     | 0 0 1                  | 0 0 0               | 161 | 0.292            | 0.234             |
| 3668.069               |                       | D 0.222D-20 | 2471.254          | 10       | 9   | 2      | 10     | 9   | 1     | 0 0 1 | 0 0 0                  | 161                 |     | 0.078            |                   |
| 3668.425               | 3668.4148             |             | 0.311D-21         | 3465.060 | 14  | 8      | 7      | 14  | 8     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.010            | 0.013             |
| 3668.693               |                       | D 0.545D-21 | 3306.296          | 8        | 7   | 2      | 8      | 7   | 1     | 0 1 1 | 0 1 0                  | 161                 |     | 0.022            |                   |
| 3668.694               | 3668.6950             |             | 0.164D-20         | 3306.296 | 8   | 7      | 1      | 8   | 7     | 2     | 0 1 1                  | 0 1 0               | 161 | 0.082            | 0.065             |
| 3668.777               | 3668.7776             | 6           | S 0.194D-19       | 222.052  | 3   | 0      | 3      | 4   | 0     | 4     | 0 0 1                  | 0 0 0               | 161 |                  | 3.931             |
| 3668.841               | 3668.8395             |             | 0.494D-20         | 1731.898 | 2   | 0      | 2      | 3   | 0     | 3     | 0 1 1                  | 0 1 0               | 161 | 0.205            | 0.166             |
| 3668.895               | 3668.8902             |             | 0.930D-21         | 3464.885 | 14  | 8      | 6      | 14  | 8     | 7     | 0 0 1                  | 0 0 0               | 161 | 0.039            | 0.038             |
| 3669.943               | 3669.9432             | -1          | C 0.523D-20       | 782.410  | 7   | 2      | 6      | 7   | 2     | 5     | 0 0 1                  | 0 0 0               | 161 | 0.338            | 0.319             |
| 3670.509               |                       | D 0.815D-21 | 3109.911          | 7        | 7   | 0      | 7      | 7   | 1     | 0 1 1 | 0 1 0                  | 161                 |     | 0.031            |                   |
| 3670.509               | 3670.5094             |             | 0.244D-20         | 3109.911 | 7   | 7      | 1      | 7   | 7     | 0     | 0 1 1                  | 0 1 0               | 161 | 0.129            | 0.094             |
| 3670.517               |                       | D 0.229D-21 | 4491.371          | 6        | 4   | 3      | 6      | 4   | 2     | 0 0 2 | 0 0 1                  | 161                 |     | 0.011            |                   |
| 3670.750               |                       |             | 0.558D-19         | 224.838  | 3   | 1      | 3      | 4   | 1     | 4     | 0 0 1                  | 0 0 0               | 161 |                  | 11.219            |
| 3670.803               | 3670.8025             |             | 0.104D-19         | 2225.468 | 9   | 9      | 1      | 9   | 9     | 0     | 0 0 1                  | 0 0 0               | 161 | 0.482            | 0.355             |
| 3670.803               |                       | D 0.348D-20 | 2225.468          | 9        | 9   | 0      | 9      | 9   | 1     | 0 0 1 | 0 0 0                  | 161                 |     | 0.119            |                   |
| 3671.048               | 3671.0439             |             | 0.208D-21         | 4368.637 | 7   | 5      | 3      | 7   | 5     | 2     | 0 2 1                  | 0 2 0               | 161 | 0.010            | 0.010             |
| 3671.929               | 3671.9276             |             | 0.146D-20         | 1739.485 | 2   | 1      | 2      | 3   | 1     | 3     | 0 1 1                  | 0 1 0               | 161 | 0.059            | 0.049             |
| 3672.094               | 3672.0945             | 5           | H 0.165D-20       | 3127.862 | 13  | 8      | 6      | 13  | 8     | 5     | 0 0 1                  | 0 0 0               | 161 | 0.058            | 0.064             |
| 3672.245               | 3672.2521             | -25         | H 0.549D-21       | 3127.808 | 13  | 8      | 5      | 13  | 8     | 6     | 0 0 1                  | 0 0 0               | 161 | 0.020            | 0.021             |
| 3672.595               | 3672.5942             |             | 0.539D-21         | 4224.852 | 4   | 4      | 1      | 4   | 4     | 0     | 0 0 2                  | 0 0 1               | 161 | 0.021            | 0.025             |
| 3672.698               | 3672.6980             |             | 0.354D-21         | 4345.273 | 5   | 4      | 1      | 5   | 4     | 2     | 0 0 2                  | 0 0 1               | 161 | 0.014            | 0.017             |
| 3673.092               | 3673.0908             |             | 0.469D-21         | 4050.513 | 5   | 5      | 1      | 5   | 5     | 0     | 0 2 1                  | 0 2 0               | 161 | 0.025            | 0.021             |
| 3673.621               | 3673.6217             | 12          | H 0.506D-21       | 3629.095 | 15  | 7      | 9      | 15  | 7     | 8     | 0 0 1                  | 0 0 0               | 161 | 0.018            | 0.021             |
| 3674.269               | 3674.2683             | -11         | C 0.456D-20       | 300.362  | 4   | 0      | 4      | 4   | 2     | 3     | 0 0 1                  | 0 0 0               | 161 | 0.688            | 0.754             |
| 3674.348               | 3674.3471             | -4          | C 0.104D-21       | 136.336  | 2   | 0      | 2      | 3   | 0     | 3     | 0 0 1                  | 0 0 0               | 181 | 0.020            | 0.026             |
| 3674.697               | 3674.6967             | -4          | C 0.108D-20       | 23.794   | 1   | 1      | 0      | 1   | 0     | 1     | 1 0 0                  | 0 0 0               | 161 | 0.311            | 0.376             |
| 3674.959               |                       |             | 0.258D-19         | 212.156  | 2   | 2      | 0      | 3   | 2     | 1     | 0 0 1                  | 0 0 0               | 161 |                  | 5.357             |
| 3675.486               | 3675.4828             |             | 0.939D-21         | 2813.533 | 12  | 8      | 5      | 12  | 8     | 4     | 0 0 1                  | 0 0 0               | 161 | 0.030            | 0.034             |
| 3675.525               | 3675.5266             |             | 0.282D-20         | 2813.515 | 12  | 8      | 4      | 12  | 8     | 5     | 0 0 1                  | 0 0 0               | 161 | 0.095            | 0.103             |
| 3675.605               | 3675.6054             |             | 0.411D-21         | 3833.146 | 11  | 6      | 6      | 11  | 6     | 5     | 0 1 1                  | 0 1 0               | 161 | 0.021            | 0.018             |
| 3676.020               |                       |             | 0.437D-19         | 173.365  | 2   | 1      | 1      | 3   | 1     | 2     | 0 0 1                  | 0 0 0               | 161 |                  | 10.058            |
| 3677.439               | 3677.4376             | -10         | C 0.499D-20       | 399.457  | 5   | 1      | 5      | 5   | 1     | 4     | 0 0 1                  | 0 0 0               | 161 | 0.616            | 0.647             |
| 3678.498               | 3678.4920             |             | 0.224D-21         | 3565.004 | 10  | 6      | 5      | 10  | 6     | 4     | 0 1 1                  | 0 1 0               | 161 | 0.008            | 0.009             |
| 3678.627               | 3678.6287             | 25          | H 0.468D-20       | 2522.267 | 11  | 8      | 4      | 11  | 8     | 3     | 0 0 1                  | 0 0 0               | 161 | 0.187            | 0.165             |
| 3678.634               |                       | D 0.156D-20 | 2522.263          | 11       | 8   | 3      | 11     | 8   | 4     | 0 0 1 | 0 0 0                  | 161                 |     | 0.055            |                   |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3679.249               | 3679.2469             |        | 0.670D-21         | 3564.705 | 10   | 6      | 4      | 10  | 6     | 5     | 0 1 1            | 0 1 0         | 161 | 0.029            | 0.028             |
| 3679.437               | 3679.4364             | -2     | C 0.846D-20       | 206.301  | 2    | 2      | 1      | 3   | 2     | 2     | 0 0 1            | 0 0 0         | 161 | 1.564            | 1.782             |
| 3679.611               | 3679.6096             |        | 0.342D-21         | 3659.906 | 11   | 5      | 7      | 11  | 5     | 6     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.014             |
| 3679.868               | 3679.8679             |        | 0.527D-21         | 4030.070 | 3    | 3      | 0      | 3   | 3     | 1     | 0 0 2            | 0 0 1         | 161 | 0.021            | 0.024             |
| 3680.374               | 3680.3738             | -6     | C 0.451D-21       | 70.091   | 2    | 1      | 1      | 2   | 0     | 2     | 1 0 0            | 0 0 0         | 161 | 0.118            | 0.138             |
| 3680.804               | 3680.8015             | -73    | H 0.107D-20       | 3321.013 | 9    | 6      | 4      | 9   | 6     | 3     | 0 1 1            | 0 1 0         | 161 | 0.046            | 0.042             |
| 3681.017               | 3681.0135             | -60    | H 0.356D-21       | 3320.933 | 9    | 6      | 3      | 9   | 6     | 4     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.014             |
| 3681.069               | 3681.0730             |        | 0.647D-22         | 5065.457 | 3    | 3      | 1      | 3   | 3     | 0     | 0 3 1            | 0 3 0         | 161 | 0.006            | 0.004             |
| 3681.548               |                       |        | D 0.252D-20       | 2254.284 | 10   | 8      | 3      | 10  | 8     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.086             |
| 3681.550               | 3681.5482             | -15    | C 0.755D-20       | 2254.283 | 10   | 8      | 2      | 10  | 8     | 3     | 0 0 1            | 0 0 0         | 161 | -0.329           | -0.258            |
| 3681.713               | 3681.7122             | 0      | C 0.885D-21       | 1693.652 | 1    | 1      | 0      | 2   | 1     | 1     | 0 1 1            | 0 1 0         | 161 | 0.035            | 0.030             |
| 3682.789               |                       |        | 0.551D-21         | 3101.144 | 8    | 6      | 3      | 8   | 6     | 2     | 0 1 1            | 0 1 0         | 161 |                  | 0.021             |
| 3682.824               | 3682.8290             | -3     | H 0.165D-20       | 3101.124 | 8    | 6      | 2      | 8   | 6     | 3     | 0 1 1            | 0 1 0         | 161 | 0.065            | 0.063             |
| 3683.989               | 3683.9903             |        | 0.617D-21         | 2300.689 | 12   | 5      | 8      | 12  | 5     | 7     | 0 0 1            | 0 0 0         | 161 | 0.019            | 0.021             |
| 3684.245               | 3684.2435             | -8     | C 0.119D-19       | 2009.805 | 9    | 8      | 2      | 9   | 8     | 1     | 0 0 1            | 0 0 0         | 161 | 0.520            | 0.399             |
| 3684.245               |                       |        | D 0.395D-20       | 2009.805 | 9    | 8      | 1      | 9   | 8     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.132             |
| 3684.528               | 3684.5291             | 8      | C 0.107D-20       | 206.301  | 3    | 0      | 3      | 3   | 2     | 2     | 0 0 1            | 0 0 0         | 161 | 0.284            | 0.225             |
| 3684.537               |                       |        | D 0.250D-20       | 2905.435 | 7    | 6      | 2      | 7   | 6     | 1     | 0 1 1            | 0 1 0         | 161 |                  | 0.093             |
| 3684.541               |                       |        | 0.832D-21         | 2905.431 | 7    | 6      | 1      | 7   | 6     | 2     | 0 1 1            | 0 1 0         | 161 |                  | 0.031             |
| 3684.612               | 3684.6070             |        | 0.170D-20         | 2927.939 | 13   | 7      | 7      | 13  | 7     | 6     | 0 0 1            | 0 0 0         | 161 | 0.056            | 0.063             |
| 3685.241               | 3685.2430             | -23    | H 0.926D-21       | 3264.338 | 14   | 7      | 7      | 14  | 7     | 8     | 0 0 1            | 0 0 0         | 161 | 0.032            | 0.036             |
| 3686.094               |                       |        | D 0.123D-20       | 2733.965 | 6    | 6      | 1      | 6   | 6     | 0     | 0 1 1            | 0 1 0         | 161 |                  | 0.044             |
| 3686.095               | 3686.0941             | 6      | H 0.370D-20       | 2733.965 | 6    | 6      | 0      | 6   | 6     | 1     | 0 1 1            | 0 1 0         | 161 | 0.190            | 0.134             |
| 3686.199               | 3686.1950             |        | 0.137D-21         | 3885.738 | 2    | 2      | 0      | 2   | 2     | 1     | 0 0 2            | 0 0 1         | 161 | 0.005            | 0.006             |
| 3686.549               | 3686.5494             |        | 0.915D-22         | 4244.305 | 5    | 3      | 2      | 5   | 3     | 3     | 0 0 2            | 0 0 1         | 161 | 0.009            | 0.004             |
| 3686.715               | 3686.7127             | 0      | C 0.182D-19       | 1789.041 | 8    | 8      | 0      | 8   | 8     | 1     | 0 0 1            | 0 0 0         | 161 | 0.918            | 0.608             |
| 3686.715               |                       |        | D 0.606D-20       | 1789.041 | 8    | 8      | 1      | 8   | 8     | 0     | 0 0 1            | 0 0 0         | 161 |                  | 0.203             |
| 3686.758               |                       |        | 0.561D-21         | 2927.076 | 13   | 7      | 6      | 13  | 7     | 7     | 0 0 1            | 0 0 0         | 161 |                  | 0.021             |
| 3687.200               | 3687.1948             |        | 0.245D-21         | 4015.515 | 6    | 4      | 2      | 6   | 4     | 3     | 0 2 1            | 0 2 0         | 161 | 0.014            | 0.011             |
| 3687.389               | 3687.3874             |        | 0.384D-21         | 3868.987 | 5    | 4      | 2      | 5   | 4     | 1     | 0 2 1            | 0 2 0         | 161 | 0.021            | 0.017             |
| 3688.218               | 3688.2210             |        | 0.145D-20         | 2756.418 | 13   | 6      | 8      | 13  | 6     | 7     | 0 0 1            | 0 0 0         | 161 | 0.050            | 0.053             |
| 3688.276               |                       |        | 0.117D-20         | 1616.452 | 10   | 4      | 7      | 10  | 4     | 6     | 0 0 1            | 0 0 0         | 161 |                  | 0.040             |
| 3688.304               |                       |        | 0.979D-21         | 2613.104 | 12   | 7      | 6      | 12  | 7     | 5     | 0 0 1            | 0 0 0         | 161 |                  | 0.035             |
| 3688.412               |                       |        | 0.585D-21         | 3746.763 | 4    | 4      | 0      | 4   | 4     | 1     | 0 2 1            | 0 2 0         | 161 |                  | 0.025             |
| 3688.453               |                       |        | 0.489D-19         | 136.761  | 2    | 0      | 2      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 12.384            |
| 3688.766               | 3688.7627             |        | 0.662D-21         | 2998.768 | 9    | 4      | 6      | 9   | 4     | 5     | 0 1 1            | 0 1 0         | 161 | 0.024            | 0.025             |
| 3688.805               | 3688.8045             | -7     | C 0.143D-21       | 37.137   | 2    | 0      | 2      | 1   | 1     | 1     | 1 0 0            | 0 0 0         | 161 | 0.037            | 0.048             |
| 3689.070               | 3689.0728             |        | 0.292D-20         | 2612.801 | 12   | 7      | 5      | 12  | 7     | 6     | 0 0 1            | 0 0 0         | 161 | 0.100            | 0.104             |
| 3689.903               | 3689.9057             | -23    | C 0.120D-20       | 1664.971 | 1    | 0      | 1      | 2   | 0     | 2     | 0 1 1            | 0 1 0         | 161 | 0.048            | 0.040             |
| 3690.313               | 3690.3116             | -7     | C 0.128D-20       | 134.902  | 2    | 0      | 2      | 2   | 2     | 1     | 0 0 1            | 0 0 0         | 161 | 0.272            | 0.326             |
| 3690.632               | 3690.6314             | -2     | C 0.123D-20       | 136.761  | 3    | 1      | 2      | 3   | 0     | 3     | 1 0 0            | 0 0 0         | 161 | 0.267            | 0.311             |
| 3690.910               | 3690.9094             | -1     | C 0.172D-20       | 1050.158 | 8    | 3      | 6      | 8   | 3     | 5     | 0 0 1            | 0 0 0         | 161 | 0.082            | 0.075             |
| 3691.062               | 3691.0620             | -5     | C 0.202D-21       | 275.497  | 4    | 2      | 2      | 4   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.032            | 0.035             |
| 3691.298               | 3691.2984             | -2     | S 0.146D-19       | 142.278  | 2    | 1      | 2      | 3   | 1     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 3.639             |
| 3691.398               | 3691.3977             | -7     | C 0.999D-21       | 173.365  | 3    | 2      | 1      | 3   | 1     | 2     | 1 0 0            | 0 0 0         | 161 | 0.204            | 0.229             |
| 3691.462               | 3691.4597             |        | 0.490D-20         | 2321.905 | 11   | 7      | 5      | 11  | 7     | 4     | 0 0 1            | 0 0 0         | 161 | 0.158            | 0.168             |
| 3691.697               | 3691.6974             |        | 0.163D-20         | 2321.814 | 11   | 7      | 4      | 11  | 7     | 5     | 0 0 1            | 0 0 0         | 161 | 0.053            | 0.056             |
| 3692.159               | 3692.1608             | -7     | H 0.946D-21       | 3141.047 | 9    | 5      | 5      | 9   | 5     | 4     | 0 1 1            | 0 1 0         | 161 | 0.038            | 0.036             |
| 3692.491               | 3692.4922             | 11     | C 0.112D-21       | 134.902  | 3    | 1      | 2      | 2   | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.029            | 0.028             |
| 3692.701               | 3692.7011             | 11     | C 0.265D-20       | 1677.063 | 1    | 1      | 1      | 2   | 1     | 2     | 0 1 1            | 0 1 0         | 161 | 0.109            | 0.089             |
| 3693.235               | 3693.2364             |        | 0.216D-21         | 3791.702 | 1    | 1      | 0      | 1   | 1     | 1     | 0 0 2            | 0 0 1         | 161 | 0.011            | 0.009             |
| 3693.294               | 3693.2941             | 1      | C 0.221D-21       | 0.0      | 1    | 1      | 1      | 0   | 0     | 0     | 1 0 0            | 0 0 0         | 161 | 0.076            | 0.082             |
| 3693.629               | 3693.6273             |        | 0.968D-21         | 2462.876 | 7    | 3      | 5      | 7   | 3     | 4     | 0 1 1            | 0 1 0         | 161 | 0.040            | 0.034             |
| 3693.790               | 3693.7890             | -13    | C 0.154D-20       | 602.774  | 6    | 2      | 5      | 6   | 2     | 4     | 0 0 1            | 0 0 0         | 161 | 0.127            | 0.128             |
| 3694.294               | 3694.2933             | 33     | B 0.265D-20       | 2054.369 | 10   | 7      | 4      | 10  | 7     | 3     | 0 0 1            | 0 0 0         | 161 | 0.098            | 0.089             |
| 3694.294               |                       |        | D 0.355D-22       | 4409.312 | 17   | 7      | 10     | 17  | 7     | 11    | 0 0 1            | 0 0 0         | 161 |                  | 0.002             |
| 3694.351               | 3694.3528             | 3      | C 0.795D-20       | 2054.348 | 10   | 7      | 3      | 10  | 7     | 4     | 0 0 1            | 0 0 0         | 161 | 0.271            | 0.266             |
| 3694.794               | 3694.7934             | -4     | C 0.193D-21       | 95.176   | 2    | 2      | 0      | 2   | 1     | 1     | 1 0 0            | 0 0 0         | 161 | 0.046            | 0.055             |
| 3695.133               | 3695.1335             | 1      | H 0.497D-21       | 2920.133 | 8    | 5      | 4      | 8   | 5     | 3     | 0 1 1            | 0 1 0         | 161 | 0.016            | 0.018             |
| 3695.696               | 3695.6943             |        | 0.850D-21         | 2053.969 | 5    | 2      | 4      | 5   | 2     | 3     | 0 1 1            | 0 1 0         | 161 | 0.034            | 0.028             |
| 3696.271               | 3696.2727             |        | 0.866D-21         | 2437.501 | 12   | 6      | 7      | 12  | 6     | 6     | 0 0 1            | 0 0 0         | 161 | 0.024            | 0.030             |
| 3696.338               | 3696.3367             |        | 0.148D-20         | 2919.634 | 8    | 5      | 3      | 8   | 5     | 4     | 0 1 1            | 0 1 0         | 161 | 0.054            | 0.055             |
| 3696.463               | 3696.4621             | -9     | C 0.232D-20       | 399.457  | 5    | 2      | 3      | 5   | 1     | 4     | 1 0 0            | 0 0 0         | 161 | 0.284            | 0.299             |
| 3696.887               | 3696.8874             | 0      | C 0.125D-19       | 1810.589 | 9    | 7      | 3      | 9   | 7     | 2     | 0 0 1            | 0 0 0         | 161 | 0.480            | 0.416             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|-----|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3696.902               |                       |        | 0.418D-20         | 1810.584 | 9   | 7      | 2      | 9   | 7     | 3     | 0 0 1          | 0 0 0       | 161 |                  | 0.139             |
| 3697.177               |                       |        | 0.558D-21         | 3383.266 | 10  | 5      | 5      | 10  | 5     | 6     | 0 1 1          | 0 1 0       | 161 |                  | 0.022             |
| 3697.193               | 3697.1915             | -2 H   | 0.228D-20         | 2724.168 | 7   | 5      | 3      | 7   | 5     | 2     | 0 1 1          | 0 1 0       | 161 | 0.096            | 0.082             |
| 3697.496               | 3697.4971             | 99 H   | 0.760D-21         | 2724.043 | 7   | 5      | 2      | 7   | 5     | 3     | 0 1 1          | 0 1 0       | 161 | 0.028            | 0.027             |
| 3698.804               | 3698.8022             |        | 0.114D-20         | 2552.880 | 6   | 5      | 2      | 6   | 5     | 1     | 0 1 1          | 0 1 0       | 161 | 0.048            | 0.040             |
| 3698.857               | 3698.8566             |        | 0.342D-20         | 2552.858 | 6   | 5      | 1      | 6   | 5     | 2     | 0 1 1          | 0 1 0       | 161 | 0.131            | 0.120             |
| 3699.270               |                       | D      | 0.644D-20         | 1590.691 | 8   | 7      | 2      | 8   | 7     | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.218             |
| 3699.271               | 3699.2681             | -4 C   | 0.193D-19         | 1590.690 | 8   | 7      | 1      | 8   | 7     | 2     | 0 0 1          | 0 0 0       | 161 | 0.900            | 0.655             |
| 3699.494               | 3699.4945             | -12 C  | 0.334D-20         | 1998.996 | 11  | 5      | 7      | 11  | 5     | 6     | 0 0 1          | 0 0 0       | 161 | 0.114            | 0.111             |
| 3700.154               | 3700.1543             | -6 H   | 0.504D-20         | 2406.144 | 5   | 5      | 1      | 5   | 5     | 0     | 0 1 1          | 0 1 0       | 161 | 0.248            | 0.174             |
| 3700.159               |                       | D      | 0.168D-20         | 2406.142 | 5   | 5      | 0      | 5   | 5     | 1     | 0 1 1          | 0 1 0       | 161 |                  | 0.058             |
| 3700.733               | 3700.7303             | 9 C    | 0.988D-21         | 1772.413 | 3   | 1      | 3      | 3   | 1     | 2     | 0 1 1          | 0 1 0       | 161 | 0.039            | 0.033             |
| 3701.157               | 3701.1543             |        | 0.618D-21         | 3500.639 | 3   | 3      | 1      | 3   | 3     | 0     | 0 2 1          | 0 2 0       | 161 | 0.031            | 0.025             |
| 3701.425               |                       | D      | 0.105D-21         | 3650.506 | 11  | 5      | 6      | 11  | 5     | 7     | 0 1 1          | 0 1 0       | 161 |                  | 0.004             |
| 3701.431               | 3701.4318             | 3 C    | 0.291D-19         | 1394.814 | 7   | 7      | 1      | 7   | 7     | 0     | 0 0 1          | 0 0 0       | 161 | 1.453            | 1.034             |
| 3701.431               |                       | D      | 0.970D-20         | 1394.814 | 7   | 7      | 0      | 7   | 7     | 1     | 0 0 1          | 0 0 0       | 161 |                  | 0.345             |
| 3701.597               |                       | D      | 0.298D-21         | 3597.866 | 4   | 3      | 1      | 4   | 3     | 2     | 0 2 1          | 0 2 0       | 161 |                  | 0.012             |
| 3701.607               | 3701.6063             | 24 C   | 0.448D-20         | 2144.047 | 11  | 6      | 6      | 11  | 6     | 5     | 0 0 1          | 0 0 0       | 161 | 0.143            | 0.151             |
| 3701.765               | 3701.7652             | -3 C   | 0.271D-20         | 275.497  | 4   | 1      | 4      | 4   | 1     | 3     | 0 0 1          | 0 0 0       | 161 | 0.440            | 0.474             |
| 3701.806               | 3701.8057             | -1 S   | 0.888D-20         | 95.176   | 1   | 1      | 0      | 2   | 1     | 1     | 0 0 1          | 0 0 0       | 161 |                  | 2.511             |
| 3702.583               | 3702.5825             | -2 C   | 0.214D-20         | 782.410  | 7   | 3      | 4      | 7   | 2     | 5     | 1 0 0          | 0 0 0       | 161 | 0.130            | 0.129             |
| 3705.088               |                       | D      | 0.254D-22         | 445.159  | 5   | 2      | 4      | 5   | 2     | 3     | 0 0 1          | 0 0 0       | 181 |                  | 0.003             |
| 3705.089               | 3705.0897             | 10 C   | 0.248D-20         | 2433.803 | 12  | 6      | 6      | 12  | 6     | 7     | 0 0 1          | 0 0 0       | 161 | 0.085            | 0.086             |
| 3705.112               |                       | D      | 0.147D-20         | 2142.597 | 11  | 6      | 5      | 11  | 6     | 6     | 0 0 1          | 0 0 0       | 161 |                  | 0.049             |
| 3705.358               | 3705.3561             | 8 C    | 0.248D-20         | 1875.464 | 10  | 6      | 5      | 10  | 6     | 4     | 0 0 1          | 0 0 0       | 161 | 0.077            | 0.082             |
| 3705.438               | 3705.4390             | 7 C    | 0.172D-20         | 602.774  | 6   | 3      | 3      | 6   | 2     | 4     | 1 0 0          | 0 0 0       | 161 | 0.141            | 0.142             |
| 3705.726               | 3705.7232             | 75 H   | 0.175D-20         | 2572.140 | 7   | 4      | 4      | 7   | 4     | 3     | 0 1 1          | 0 1 0       | 161 | 0.064            | 0.062             |
| 3705.750               | 3705.7501             | 0 C    | 0.310D-21         | 222.052  | 4   | 1      | 3      | 4   | 0     | 4     | 1 0 0          | 0 0 0       | 161 | 0.055            | 0.062             |
| 3706.417               | 3706.4161             | -11 C  | 0.441D-21         | 982.912  | 8   | 3      | 5      | 8   | 2     | 6     | 1 0 0          | 0 0 0       | 161 | 0.019            | 0.021             |
| 3706.551               | 3706.5505             | -12 C  | 0.741D-20         | 1874.974 | 10  | 6      | 4      | 10  | 6     | 5     | 0 0 1          | 0 0 0       | 161 | 0.235            | 0.246             |
| 3706.618               | 3706.6193             | 4 C    | 0.478D-21         | 542.906  | 6   | 2      | 4      | 6   | 1     | 5     | 1 0 0          | 0 0 0       | 161 | 0.039            | 0.045             |
| 3706.841               | 3706.8420             | 7 C    | 0.601D-20         | 1360.236 | 9   | 4      | 6      | 9   | 4     | 5     | 0 0 1          | 0 0 0       | 161 | 0.221            | 0.216             |
| 3706.852               |                       | D      | 0.244D-22         | 5634.121 | 6   | 1      | 5      | 5   | 1     | 4     | 1 1 1          | 1 1 0       | 161 |                  | 0.001             |
| 3707.428               | 3707.4273             | -2 C   | 0.105D-21         | 446.511  | 5   | 3      | 2      | 5   | 2     | 3     | 1 0 0          | 0 0 0       | 161 | 0.010            | 0.012             |
| 3708.258               | 3708.2584             | 2 C    | 0.120D-19         | 1631.384 | 9   | 6      | 4      | 9   | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.399            | 0.404             |
| 3708.597               | 3708.5980             | 4 C    | 0.399D-20         | 1631.251 | 9   | 6      | 3      | 9   | 6     | 4     | 0 0 1          | 0 0 0       | 161 | 0.132            | 0.134             |
| 3708.837               | 3708.8369             |        | 0.131D-21         | 3864.966 | 6   | 3      | 3      | 6   | 3     | 4     | 0 2 1          | 0 2 0       | 161 | 0.008            | 0.006             |
| 3709.151               | 3709.1515             |        | 0.899D-21         | 2399.166 | 6   | 4      | 3      | 6   | 4     | 2     | 0 1 1          | 0 1 0       | 161 | 0.026            | 0.031             |
| 3709.199               | 3709.1996             | 10 C   | 0.369D-21         | 79.496   | 2   | 2      | 1      | 2   | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.109            | 0.109             |
| 3709.203               |                       | D      | 0.892D-21         | 1282.919 | 9   | 4      | 5      | 9   | 3     | 6     | 1 0 0          | 0 0 0       | 161 |                  | 0.033             |
| 3709.403               | 3709.4023             | -4 S   | 0.119D-19         | 70.091   | 1   | 0      | 1      | 2   | 0     | 2     | 0 0 1          | 0 0 0       | 161 |                  | 3.601             |
| 3709.777               | 3709.7781             | 1 C    | 0.195D-20         | 1724.707 | 10  | 5      | 6      | 10  | 5     | 5     | 0 0 1          | 0 0 0       | 161 | 0.062            | 0.065             |
| 3710.704               |                       | D      | 0.701D-22         | 3966.559 | 5   | 2      | 3      | 4   | 2     | 2     | 1 0 1          | 1 0 0       | 161 |                  | 0.003             |
| 3710.706               | 3710.7061             | 5 C    | 0.623D-20         | 1411.647 | 8   | 6      | 3      | 8   | 6     | 2     | 0 0 1          | 0 0 0       | 161 | 0.218            | 0.220             |
| 3710.781               | 3710.7818             | 2 C    | 0.187D-19         | 1411.612 | 8   | 6      | 2      | 8   | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.671            | 0.659             |
| 3710.917               | 3710.9175             | -1 C   | 0.729D-20         | 842.357  | 7   | 3      | 5      | 7   | 3     | 4     | 0 0 1          | 0 0 0       | 161 | 0.416            | 0.403             |
| 3710.955               | 3710.9550             |        | 0.268D-20         | 2398.382 | 6   | 4      | 2      | 6   | 4     | 3     | 0 1 1          | 0 1 0       | 161 | 0.101            | 0.092             |
| 3711.102               |                       | D      | 0.405D-20         | 2251.863 | 5   | 4      | 2      | 5   | 4     | 1     | 0 1 1          | 0 1 0       | 161 |                  | 0.137             |
| 3711.103               | 3711.1026             | -4 C   | 0.843D-21         | 23.794   | 2   | 1      | 2      | 1   | 0     | 1     | 1 0 0          | 0 0 0       | 161 | 0.386            | 0.290             |
| 3711.348               | 3711.3472             |        | 0.497D-21         | 1813.224 | 11  | 4      | 7      | 11  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.015            | 0.016             |
| 3711.490               | 3711.4891             |        | 0.135D-20         | 2251.696 | 5   | 4      | 1      | 5   | 4     | 2     | 0 1 1          | 0 1 0       | 161 | 0.048            | 0.046             |
| 3711.727               | 3711.7280             |        | 0.570D-21         | 2569.508 | 7   | 4      | 3      | 7   | 4     | 4     | 0 1 1          | 0 1 0       | 161 | 0.016            | 0.020             |
| 3711.876               | 3711.8762             | -3 C   | 0.766D-21         | 79.496   | 3   | 0      | 3      | 2   | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.187            | 0.226             |
| 3712.206               |                       |        | 0.265D-19         | 79.496   | 1   | 1      | 1      | 2   | 1     | 2     | 0 0 1          | 0 0 0       | 161 |                  | 7.805             |
| 3712.385               | 3712.3792             |        | 0.201D-20         | 2129.619 | 4   | 4      | 1      | 4   | 4     | 0     | 0 1 1          | 0 1 0       | 161 | 0.064            | 0.067             |
| 3712.407               |                       |        | 0.511D-21         | 3316.145 | 2   | 2      | 0      | 2   | 2     | 1     | 0 2 1          | 0 2 0       | 161 |                  | 0.020             |
| 3712.430               | 3712.4283             | 7 C    | 0.603D-20         | 2129.600 | 4   | 4      | 0      | 4   | 4     | 1     | 0 1 1          | 0 1 0       | 161 | 0.204            | 0.202             |
| 3712.710               | 3712.7099             | 5 C    | 0.189D-20         | 1618.559 | 0   | 0      | 0      | 1   | 0     | 1     | 0 1 1          | 0 1 0       | 161 | 0.071            | 0.064             |
| 3712.869               | 3712.8687             | -28 C  | 0.284D-19         | 1216.194 | 7   | 6      | 2      | 7   | 6     | 1     | 0 0 1          | 0 0 0       | 161 | 1.289            | 1.093             |
| 3712.883               |                       |        | 0.948D-20         | 1216.189 | 7   | 6      | 1      | 7   | 6     | 2     | 0 0 1          | 0 0 0       | 161 |                  | 0.365             |
| 3712.992               | 3712.9919             | -7 C   | 0.117D-21         | 733.683  | 5   | 5      | 1      | 5   | 5     | 0     | 0 0 1          | 0 0 0       | 181 | 0.006            | 0.008             |
| 3712.999               |                       | D      | 0.389D-22         | 733.679  | 5   | 5      | 0      | 5   | 5     | 1     | 0 0 1          | 0 0 0       | 181 |                  | 0.003             |
| 3713.404               |                       | D      | 0.408D-22         | 382.517  | 5   | 2      | 3      | 4   | 3     | 2     | 1 0 0          | 0 0 0       | 161 |                  | 0.005             |
| 3713.413               | 3713.4121             | -5 C   | 0.544D-21         | 1282.919 | 9   | 6      | 3      | 9   | 3     | 6     | 0 2 0          | 0 0 0       | 161 | 0.020            | 0.020             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3713.882               | 3713.8824             | 44     | H 0.629D-21       | 3084.835 | 14   | 6      | 8      | 14  | 6     | 9     | 0 0 1            | 0 0 0         | 161 | 0.021            | 0.024             |
| 3714.794               |                       |        | D 0.141D-19       | 1045.059 | 6    | 6      | 1      | 6   | 6     | 0     | 0 0 1            | 0 0 0         | 161 |                  | 0.617             |
| 3714.795               | 3714.7945             | -11    | S 0.424D-19       | 1045.058 | 6    | 6      | 0      | 6   | 6     | 1     | 0 0 1            | 0 0 0         | 161 | 2.634            | 1.854             |
| 3715.196               | 3715.1948             | -7     | H 0.103D-20       | 2764.699 | 8    | 4      | 4      | 8   | 4     | 5     | 0 1 1            | 0 1 0         | 161 | 0.038            | 0.037             |
| 3715.789               | 3715.7806             |        | 0.747D-22         | 3244.601 | 15   | 5      | 10     | 15  | 4     | 11    | 1 0 0            | 0 0 0         | 161 | 0.010            | 0.003             |
| 3716.019               | 3716.0174             | -8     | H 0.253D-20       | 2130.495 | 5    | 3      | 3      | 5   | 3     | 2     | 0 1 1            | 0 1 0         | 161 | 0.094            | 0.085             |
| 3716.160               | 3716.1601             | -2     | C 0.980D-20       | 1477.297 | 9    | 5      | 5      | 9   | 5     | 4     | 0 0 1            | 0 0 0         | 161 | 0.342            | 0.338             |
| 3716.313               | 3716.3132             | -4     | C 0.817D-21       | 1201.922 | 9    | 3      | 6      | 9   | 2     | 7     | 1 0 0            | 0 0 0         | 161 | 0.030            | 0.032             |
| 3716.597               | 3716.5968             | -6     | C 0.171D-21       | 142.278  | 3    | 2      | 2      | 3   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.036            | 0.042             |
| 3717.762               | 3717.7616             | -44    | H 0.480D-21       | 1693.652 | 2    | 1      | 2      | 2   | 1     | 1     | 0 1 1            | 0 1 0         | 161 | 0.017            | 0.016             |
| 3717.812               | 3717.8112             | -8     | C 0.401D-22       | 23.755   | 0    | 0      | 0      | 1   | 0     | 1     | 0 0 1            | 0 0 0         | 181 | 0.008            | 0.014             |
| 3718.881               |                       |        | 0.774D-21         | 1050.158 | 8    | 4      | 4      | 8   | 3     | 5     | 1 0 0            | 0 0 0         | 161 |                  | 0.034             |
| 3718.964               | 3718.9636             | -4     | C 0.134D-19       | 446.511  | 5    | 2      | 4      | 5   | 2     | 3     | 0 0 1            | 0 0 0         | 161 | 1.471            | 1.540             |
| 3719.466               | 3719.4676             |        | 0.352D-21         | 1819.337 | 3    | 3      | 0      | 3   | 2     | 1     | 1 1 0            | 0 1 0         | 161 | 0.014            | 0.012             |
| 3719.762               | 3719.7628             | 4      | C 0.342D-20       | 1131.776 | 8    | 4      | 5      | 8   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.144            | 0.139             |
| 3719.860               | 3719.8579             |        | 0.279D-21         | 4095.803 | 7    | 1      | 7      | 6   | 1     | 6     | 1 0 1            | 1 0 0         | 161 | 0.011            | 0.013             |
| 3720.131               | 3720.1323             | 6      | C 0.526D-20       | 1255.913 | 8    | 5      | 4      | 8   | 5     | 3     | 0 0 1            | 0 0 0         | 161 | 0.204            | 0.197             |
| 3720.260               | 3720.2688             |        | 0.943D-22         | 2105.876 | 12   | 4      | 8      | 12  | 3     | 9     | 1 0 0            | 0 0 0         | 161 | 0.005            | 0.003             |
| 3720.340               | 3720.3380             | -13    | H 0.132D-20       | 2005.917 | 4    | 3      | 2      | 4   | 3     | 1     | 0 1 1            | 0 1 0         | 161 | 0.048            | 0.044             |
| 3721.164               | 3721.1661             | 18     | C 0.894D-22       | 604.793  | 5    | 4      | 2      | 5   | 4     | 1     | 0 0 1            | 0 0 0         | 181 | 0.010            | 0.007             |
| 3721.168               |                       |        | D 0.572D-22       | 751.033  | 6    | 4      | 2      | 6   | 4     | 3     | 0 0 1            | 0 0 0         | 181 |                  | 0.004             |
| 3721.520               |                       |        | 0.318D-20         | 1474.981 | 9    | 5      | 4      | 9   | 5     | 5     | 0 0 1            | 0 0 0         | 161 |                  | 0.110             |
| 3721.853               |                       |        | 0.925D-21         | 704.214  | 7    | 2      | 5      | 7   | 1     | 6     | 1 0 0            | 0 0 0         | 161 |                  | 0.063             |
| 3721.878               | 3721.8778             | 0      | C 0.157D-19       | 1255.167 | 8    | 5      | 3      | 8   | 5     | 4     | 0 0 1            | 0 0 0         | 161 | 0.614            | 0.589             |
| 3722.223               | 3722.2182             | -47    | C 0.982D-20       | 173.365  | 3    | 1      | 3      | 3   | 1     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 2.232             |
| 3722.327               |                       |        | D 0.740D-21       | 1899.008 | 11   | 5      | 6      | 11  | 4     | 7     | 1 0 0            | 0 0 0         | 161 |                  | 0.024             |
| 3722.328               | 3722.3268             | -4     | C 0.616D-20       | 1907.617 | 3    | 3      | 1      | 3   | 3     | 0     | 0 1 1            | 0 1 0         | 161 | -0.254           | -0.204            |
| 3722.693               | 3722.6914             | -1     | C 0.205D-20       | 1907.452 | 3    | 3      | 0      | 3   | 3     | 1     | 0 1 1            | 0 1 0         | 161 | 0.073            | 0.068             |
| 3722.753               |                       |        | D 0.260D-22       | 4252.449 | 13   | 5      | 8      | 13  | 5     | 9     | 0 1 1            | 0 1 0         | 161 |                  | 0.001             |
| 3722.756               | 3722.7545             | -11    | C 0.392D-20       | 2004.817 | 4    | 3      | 1      | 4   | 3     | 2     | 0 1 1            | 0 1 0         | 161 | 0.141            | 0.130             |
| 3722.827               | 3722.8264             | -8     | C 0.246D-19       | 1059.835 | 7    | 5      | 3      | 7   | 5     | 2     | 0 0 1            | 0 0 0         | 161 | 1.109            | 1.059             |
| 3723.273               | 3723.2736             | -1     | C 0.819D-20       | 1059.647 | 7    | 5      | 2      | 7   | 5     | 3     | 0 0 1            | 0 0 0         | 161 | 0.373            | 0.353             |
| 3723.379               | 3723.3786             | -4     | C 0.542D-20       | 1718.719 | 10   | 5      | 5      | 10  | 5     | 6     | 0 0 1            | 0 0 0         | 161 | 0.174            | 0.180             |
| 3724.189               | 3724.1885             | -3     | C 0.655D-21       | 325.348  | 5    | 1      | 4      | 5   | 0     | 5     | 1 0 0            | 0 0 0         | 161 | 0.092            | 0.100             |
| 3724.863               |                       |        | 0.807D-21         | 2126.407 | 5    | 3      | 2      | 5   | 3     | 3     | 0 1 1            | 0 1 0         | 161 |                  | 0.027             |
| 3724.894               | 3724.8940             | -2     | C 0.124D-19       | 888.632  | 6    | 5      | 2      | 6   | 5     | 1     | 0 0 1            | 0 0 0         | 161 | 0.644            | 0.642             |
| 3724.914               |                       |        | 0.271D-20         | 1819.337 | 3    | 2      | 2      | 3   | 2     | 1     | 0 1 1            | 0 1 0         | 161 |                  | 0.090             |
| 3724.974               | 3724.9753             | 5      | S 0.373D-19       | 888.599  | 6    | 5      | 1      | 6   | 5     | 2     | 0 0 1            | 0 0 0         | 161 | 2.019            | 1.931             |
| 3725.465               | 3725.4656             |        | 0.240D-21         | 4049.536 | 6    | 1      | 5      | 5   | 1     | 4     | 1 0 1            | 1 0 0         | 161 | 0.010            | 0.011             |
| 3725.472               |                       |        | D 0.870D-22       | 1731.898 | 4    | 1      | 4      | 3   | 0     | 3     | 1 1 0            | 0 1 0         | 161 |                  | 0.003             |
| 3725.686               | 3725.6863             | 1      | C 0.366D-20       | 661.549  | 6    | 3      | 4      | 6   | 3     | 3     | 0 0 1            | 0 0 0         | 161 | 0.270            | 0.270             |
| 3726.449               | 3726.4499             | 6      | C 0.322D-21       | 70.091   | 3    | 1      | 3      | 2   | 0     | 2     | 1 0 0            | 0 0 0         | 161 | 0.076            | 0.097             |
| 3726.477               | 3726.4780             | 6      | C 0.529D-21       | 224.838  | 4    | 2      | 3      | 4   | 1     | 4     | 1 0 0            | 0 0 0         | 161 | 0.084            | 0.105             |
| 3726.617               |                       |        | 0.556D-19         | 742.076  | 5    | 5      | 1      | 5   | 5     | 0     | 0 0 1            | 0 0 0         | 161 |                  | 3.561             |
| 3726.625               |                       |        | 0.185D-19         | 742.073  | 5    | 5      | 0      | 5   | 5     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 1.185             |
| 3727.738               | 3727.7375             | -7     | C 0.171D-19       | 931.237  | 7    | 4      | 4      | 7   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 0.880            | 0.840             |
| 3728.747               | 3728.7462             | -63    | H 0.929D-21       | 1985.788 | 11   | 5      | 6      | 11  | 5     | 7     | 0 0 1            | 0 0 0         | 161 | 0.029            | 0.031             |
| 3728.861               | 3728.8651             | 16     | C 0.166D-20       | 1743.492 | 2    | 2      | 1      | 2   | 2     | 0     | 0 1 1            | 0 1 0         | 161 | 0.063            | 0.055             |
| 3728.909               | 3728.9095             | 0      | C 0.221D-22       | 206.301  | 3    | 3      | 1      | 3   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.006            | 0.005             |
| 3729.256               | 3729.2578             | 14     | C 0.269D-20       | 1640.508 | 1    | 1      | 1      | 1   | 1     | 0     | 0 1 1            | 0 1 0         | 161 | 0.107            | 0.090             |
| 3730.089               | 3730.0901             | 0      | C 0.430D-20       | 842.357  | 7    | 4      | 3      | 7   | 3     | 4     | 1 0 0            | 0 0 0         | 161 | 0.243            | 0.236             |
| 3730.477               | 3730.4767             | -1     | C 0.243D-21       | 300.362  | 4    | 3      | 2      | 4   | 2     | 3     | 1 0 0            | 0 0 0         | 161 | 0.038            | 0.040             |
| 3730.558               |                       |        | 0.135D-21         | 282.307  | 3    | 3      | 1      | 3   | 3     | 0     | 0 0 1            | 0 0 0         | 181 |                  | 0.023             |
| 3730.582               | 3730.5786             | -114   | H 0.135D-20       | 2271.712 | 6    | 3      | 3      | 6   | 3     | 4     | 0 1 1            | 0 1 0         | 161 | 0.049            | 0.046             |
| 3730.681               | 3730.6799             | -1     | C 0.762D-22       | 379.292  | 4    | 3      | 1      | 4   | 3     | 2     | 0 0 1            | 0 0 0         | 181 | 0.007            | 0.010             |
| 3731.351               | 3731.3497             | -4     | C 0.496D-20       | 1742.307 | 2    | 2      | 0      | 2   | 2     | 1     | 0 1 1            | 0 1 0         | 161 | 0.189            | 0.164             |
| 3732.135               |                       |        | 0.189D-19         | 23.794   | 0    | 0      | 0      | 1   | 0     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 6.472             |
| 3732.284               | 3732.2840             | 0      | C 0.910D-20       | 757.780  | 6    | 4      | 3      | 6   | 4     | 2     | 0 0 1            | 0 0 0         | 161 | 0.552            | 0.567             |
| 3732.739               | 3732.7380             | -10    | C 0.310D-21       | 142.278  | 4    | 0      | 4      | 3   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.066            | 0.076             |
| 3734.078               | 3734.0813             | 31     | C 0.138D-21       | 416.209  | 5    | 3      | 3      | 5   | 2     | 4     | 1 0 0            | 0 0 0         | 161 | 0.013            | 0.017             |
| 3734.273               | 3734.2732             | -2     | C 0.661D-20       | 315.779  | 4    | 2      | 3      | 4   | 2     | 2     | 0 0 1            | 0 0 0         | 161 | 0.945            | 1.034             |
| 3734.645               | 3734.6454             | -2     | C 0.270D-19       | 756.725  | 6    | 4      | 2      | 6   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 1.724            | 1.685             |
| 3734.931               | 3734.9324             | 11     | S 0.423D-19       | 610.341  | 5    | 4      | 2      | 5   | 4     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 3.422             |
| 3735.407               | 3735.4077             | 5      | C 0.541D-20       | 927.744  | 7    | 4      | 3      | 7   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.276            | 0.266             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO   | $I_{\text{obs}}$ | $I_{\text{calc}}$ |       |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-------|------------------|-------------------|-------|
| 3735.446               | 3735.4453             | -1          | C 0.141D-19       | 610.114  | 5    | 4      | 1      | 5   | 4     | 2     | 0 0 1            | 0 0 0         | 161   | 1.161            | 1.141             |       |
| 3735.493               | 3735.4934             | 6           | C 0.184D-19       | 508.812  | 5    | 3      | 3      | 5   | 3     | 2     | 0 0 1            | 0 0 0         | 161   | 1.796            | 1.833             |       |
| 3735.916               | 3735.9143             | 43          | B 0.985D-21       | 1813.788 | 3    | 2      | 1      | 3   | 2     | 2     | 0 1 1            | 0 1 0         | 161   | 0.033            | 0.032             |       |
|                        |                       |             | 0.215D-19         | 488.134  | 4    | 4      | 1      | 4   | 4     | 0     | 0 0 1            | 0 0 0         | 161   |                  | 2.240             |       |
|                        |                       |             | 0.644D-19         | 488.108  | 4    | 4      | 0      | 4   | 4     | 1     | 0 0 1            | 0 0 0         | 161   |                  | 6.709             |       |
| 3738.025               | 3738.0249             | 8           | C 0.106D-21       | 133.474  | 2    | 2      | 0      | 2   | 2     | 1     | 0 0 1            | 0 0 0         | 181   | 0.019            | 0.027             |       |
| 3738.078               | 3738.0756             |             | 0.121D-20         | 2275.373 | 12   | 5      | 7      | 12  | 5     | 8     | 0 0 1            | 0 0 0         | 161   | 0.037            | 0.041             |       |
| 3738.401               | 3738.4014             | 4           | C 0.480D-20       | 95.176   | 2    | 1      | 2      | 2   | 1     | 1     | 0 0 1            | 0 0 0         | 161   | 1.126            | 1.344             |       |
| 3738.507               | 3738.5046             | -17         | C 0.156D-21       | 326.625  | 5    | 2      | 4      | 5   | 1     | 5     | 1 0 0            | 0 0 0         | 161   | 0.017            | 0.024             |       |
|                        | 3738.8661             |             |                   |          |      |        |        |     |       |       |                  |               |       | 0.008            |                   |       |
| 3739.003               | 3738.9993             |             | 0.317D-22         | 4585.352 | 14   | 5      | 9      | 14  | 5     | 10    | 0 1 1            | 0 1 0         | 161   | 0.006            | 0.002             |       |
| 3739.095               | 3739.0950             | 2           | C 0.866D-20       | 1122.709 | 8    | 4      | 4      | 8   | 4     | 5     | 0 0 1            | 0 0 0         | 161   | 0.369            | 0.352             |       |
| 3739.884               | 3739.8842             |             | 0.165D-21         | 2439.956 | 7    | 3      | 4      | 7   | 3     | 5     | 0 1 1            | 0 1 0         | 161   | 0.007            | 0.006             |       |
| 3739.998               | 3739.9988             | 2           | C 0.480D-21       | 552.912  | 6    | 3      | 4      | 6   | 2     | 5     | 1 0 0            | 0 0 0         | 161   | 0.039            | 0.044             |       |
| 3740.393               | 3740.3933             | -1          | C 0.237D-20       | 661.549  | 6    | 4      | 2      | 6   | 3     | 3     | 1 0 0            | 0 0 0         | 161   | 0.205            | 0.174             |       |
| 3740.396               |                       | D           | 0.883D-21         | 1634.970 | 1    | 1      | 0      | 1   | 1     | 1     | 0 1 1            | 0 1 0         | 161   |                  | 0.029             |       |
| 3740.775               | 3740.7759             | 13          | C 0.729D-22       | 325.348  | 4    | 2      | 2      | 5   | 0     | 5     | 0 0 1            | 0 0 0         | 161   | 0.010            | 0.011             |       |
| 3740.814               | 3740.8132             | -7          | C 0.101D-20       | 136.761  | 4    | 1      | 4      | 3   | 0     | 3     | 1 0 0            | 0 0 0         | 161   | 0.224            | 0.252             |       |
| 3741.306               | 3741.3063             | -6          | C 0.111D-19       | 383.842  | 4    | 3      | 2      | 4   | 3     | 1     | 0 0 1            | 0 0 0         | 161   | 1.361            | 1.468             |       |
| 3742.386               |                       | 0.133D-21   | 285.419           | 4        | 1    | 3      | 3      | 3   | 0     | 0     | 0 0 1            | 0 0 0         | 161   |                  | 0.022             |       |
| 3743.565               | 3743.5639             | -15         | C 0.153D-21       | 446.697  | 6    | 1      | 5      | 6   | 0     | 6     | 1 0 0            | 0 0 0         | 161   | 0.018            | 0.017             |       |
| 3743.947               |                       | 0.308D-19   | 382.517           | 4        | 3    | 1      | 4      | 3   | 2     | 0     | 0 0 1            | 0 0 0         | 161   |                  | 4.083             |       |
| 3744.184               | 3744.1849             | -1          | C 0.366D-20       | 503.968  | 5    | 3      | 2      | 5   | 3     | 3     | 0 0 1            | 0 0 0         | 161   | 0.347            | 0.368             |       |
| 3744.510               |                       | 0.308D-19   | 212.156           | 3        | 2    | 2      | 3      | 2   | 1     | 0     | 0 1              | 0 0 0         | 161   |                  | 6.274             |       |
| 3744.651               |                       | 0.639D-19   | 285.419           | 3        | 3    | 1      | 3      | 3   | 0     | 0     | 0 1              | 0 0 0         | 161   |                  | 10.764            |       |
| 3745.011               |                       | 0.185D-20   | 1908.017          | 4        | 2    | 2      | 4      | 2   | 3     | 0     | 1 1              | 0 1 0         | 161   |                  | 0.061             |       |
| 3745.087               | 3745.0848             | -27         | S 0.213D-19       | 285.219  | 3    | 3      | 0      | 3   | 3     | 1     | 0 0 1            | 0 0 0         | 161   |                  | 3.589             |       |
| 3745.486               | 3745.4857             | 0           | C 0.156D-20       | 648.979  | 6    | 4      | 3      | 6   | 3     | 4     | 1 0 0            | 0 0 0         | 161   | 0.107            | 0.117             |       |
| 3745.553               | 3745.5526             | -9          | C 0.187D-22       | 36.748   | 1    | 1      | 0      | 1   | 1     | 1     | 0 0 1            | 0 0 0         | 181   | 0.007            | 0.006             |       |
| 3745.556               |                       | D 0.174D-22 | 503.968           | 6        | 2    | 4      | 5      | 3   | 3     | 1 0 0 | 0 0 0            | 161           |       | 0.002            |                   |       |
| 3746.132               | 3746.1318             | -2          | C 0.114D-20       | 1340.886 | 9    | 4      | 5      | 9   | 4     | 6     | 0 0 1            | 0 0 0         | 161   | 0.042            | 0.041             |       |
| 3746.323               | 3746.3230             | -3          | C 0.718D-21       | 42.372   | 2    | 2      | 1      | 1   | 0     | 1     | 0 0 0            | 0 0 0         | 161   | 0.196            | 0.232             |       |
| 3747.429               | 3747.4293             | -3          | C 0.955D-20       | 508.812  | 5    | 4      | 1      | 5   | 3     | 2     | 1 0 0            | 0 0 0         | 161   | 0.943            | 0.948             |       |
| 3747.494               | 3747.4931             | -4          | C 0.174D-20       | 1360.236 | 9    | 5      | 4      | 9   | 4     | 5     | 1 0 0            | 0 0 0         | 161   | 0.063            | 0.062             |       |
| 3748.210               | 3748.2126             | 21          | C 0.148D-21       | 709.609  | 7    | 3      | 5      | 7   | 2     | 6     | 1 0 0            | 0 0 0         | 161   | 0.013            | 0.010             |       |
| 3748.216               |                       | D 0.236D-22 | 4695.836          | 8        | 5    | 4      | 7      | 5   | 3     | 1     | 0 1              | 1 0 0         | 161   |                  | 0.001             |       |
| 3748.393               | 3748.3912             |             | 0.266D-21         | 1690.665 | 11   | 3      | 8      | 11  | 2     | 9     | 1 0 0            | 0 0 0         | 161   | 0.010            | 0.009             |       |
| 3748.967               | 3748.9668             | 3           | C 0.213D-21       | 446.511  | 6    | 0      | 6      | 5   | 2     | 3     | 0 0 1            | 0 0 0         | 161   | 0.020            | 0.024             |       |
| 3749.174               |                       | 0.280D-21   | 300.362           | 5        | 1    | 4      | 4      | 2   | 3     | 1     | 0 0              | 0 0 0         | 161   |                  | 0.045             |       |
| 3749.331               |                       | 0.270D-19   | 42.372            | 1        | 1    | 1      | 1      | 1   | 0     | 0     | 0 1              | 0 0 0         | 161   |                  | 8.733             |       |
| 3749.574               |                       | 0.169D-19   | 136.164           | 2        | 2    | 1      | 2      | 2   | 0     | 0     | 0 1              | 0 0 0         | 161   |                  | 4.215             |       |
| 3750.353               | 3750.3536             | 10          | C 0.141D-21       | 136.761  | 2    | 2      | 0      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 161   | 0.031            | 0.035             |       |
| 3750.948               |                       | D 0.224D-21 | 4387.062          | 9        | 1    | 9      | 8      | 1   | 8     | 1     | 0 1              | 1 0 0         | 161   |                  | 0.011             |       |
| 3750.956               | 3750.9564             | 0           | C 0.297D-20       | 383.842  | 4    | 4      | 0      | 4   | 3     | 1     | 1 0 0            | 0 0 0         | 161   | 0.380            | 0.392             |       |
| 3751.112               | 3751.1122             | 28          | C 0.137D-20       | 1677.063 | 2    | 1      | 1      | 2   | 1     | 2     | 0 1 1            | 0 1 0         | 161   | 0.050            | 0.045             |       |
| 3751.470               | 3751.4705             | 4           | C 0.922D-21       | 224.838  | 5    | 0      | 5      | 4   | 1     | 4     | 1 0 0            | 0 0 0         | 161   | 0.167            | 0.181             |       |
| 3752.139               |                       | 0.373D-21   | 447.252           | 6        | 2    | 5      | 6      | 1   | 6     | 1     | 0 0              | 0 0 0         | 161   |                  | 0.042             |       |
| 3752.213               |                       | 0.502D-19   | 134.902           | 2        | 2    | 0      | 2      | 2   | 1     | 0     | 0 1              | 0 0 0         | 161   |                  | 12.556            |       |
| 3752.496               |                       | D 0.502D-22 | 4308.211          | 7        | 3    | 4      | 6      | 3   | 3     | 1     | 0 1              | 1 0 0         | 161   |                  | 0.002             |       |
| 3752.501               | 3752.5011             | 0           | C 0.111D-19       | 382.517  | 4    | 4      | 1      | 4   | 3     | 2     | 1 0 0            | 0 0 0         | 161   | 1.377            | 1.468             |       |
| 3752.833               | 3752.8325             | 0           | C 0.214D-21       | 37.137   | 2    | 2      | 0      | 1   | 1     | 1     | 1 0 0            | 0 0 0         | 161   | 0.057            | 0.070             |       |
| 3753.652               | 3753.6537             | 4           | C 0.476D-21       | 1581.336 | 10   | 5      | 6      | 10  | 4     | 7     | 1 0 0            | 0 0 0         | 161   | 0.015            | 0.016             |       |
| 3753.655               |                       | D 0.466D-22 | 4030.839          | 5        | 4    | 1      | 4      | 3   | 2     | 2     | 0                | 0 1 0         | 0 0 0 | 161              |                   | 0.002 |
| 3753.819               | 3753.8194             | 5           | C 0.538D-20       | 503.968  | 5    | 4      | 2      | 5   | 3     | 3     | 1 0 0            | 0 0 0         | 161   | 0.520            | 0.539             |       |
| 3754.666               | 3754.6655             | -1          | C 0.116D-21       | 136.164  | 3    | 0      | 3      | 2   | 2     | 0     | 0 0 1            | 0 0 0         | 161   | 0.022            | 0.029             |       |
| 3755.404               | 3755.4041             | 3           | C 0.319D-21       | 222.052  | 5    | 1      | 5      | 4   | 0     | 4     | 1 0 0            | 0 0 0         | 161   | 0.056            | 0.063             |       |
| 3755.671               | 3755.6724             | 17          | C 0.289D-22       | 78.988   | 2    | 1      | 1      | 2   | 1     | 2     | 0 0 1            | 0 0 0         | 181   | 0.008            | 0.008             |       |
| 3756.617               | 3756.6167             | -8          | C 0.994D-20       | 206.301  | 3    | 2      | 1      | 3   | 2     | 2     | 0 0 1            | 0 0 0         | 161   |                  | 2.050             |       |
| 3757.629               | 3757.6283             | -4          | C 0.766D-21       | 1131.776 | 8    | 5      | 3      | 8   | 4     | 4     | 1 0 0            | 0 0 0         | 161   | 0.029            | 0.031             |       |
| 3758.068               | 3758.0686             | 7           | C 0.180D-20       | 648.979  | 6    | 6      | 1      | 6   | 3     | 4     | 0 2 0            | 0 0 0         | 161   | 0.101            | 0.134             |       |
| 3758.394               |                       | D 0.471D-22 | 4457.820          | 8        | 3    | 6      | 7      | 3   | 5     | 1     | 0 1              | 1 0 0         | 161   |                  | 0.002             |       |
| 3758.399               | 3758.3984             | 0           | C 0.354D-21       | 885.600  | 8    | 3      | 6      | 8   | 2     | 7     | 1 0 0            | 0 0 0         | 161   | 0.018            | 0.018             |       |
| 3758.620               | 3758.6200             |             | 0.351D-21         | 1079.080 | 9    | 2      | 7      | 9   | 1     | 8     | 1 0 0            | 0 0 0         | 161   | 0.013            | 0.015             |       |
| 3759.050               | 3759.0507             | 1           | C 0.136D-19       | 648.979  | 6    | 3      | 3      | 6   | 3     | 4     | 0 0 1            | 0 0 0         | 161   | 1.029            | 1.016             |       |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3759.255               | 3759.2520             |        | 0.388D-21         | 2024.150 | 5    | 2      | 3      | 5   | 2     | 4     | 0 1 1          | 0 1 0       | 161 | 0.013            | 0.013             |
| 3759.845               | 3759.8449             | -1     | S 0.885D-20       | 37.137   | 1    | 1      | 0      | 1   | 1     | 1     | 0 0 1          | 0 0 0       | 161 |                  | 2.897             |
| 3760.126               | 3760.1238             | -13    | C 0.612D-21       | 1594.748 | 1    | 0      | 1      | 0   | 0     | 0     | 0 1 1          | 0 1 0       | 161 | 0.020            | 0.020             |
| 3760.364               | 3760.3640             | 4      | C 0.130D-21       | 315.779  | 5    | 0      | 5      | 4   | 2     | 2     | 0 0 1          | 0 0 0       | 161 | 0.017            | 0.020             |
| 3761.674               | 3761.6760             |        | 0.181D-21         | 1446.129 | 10   | 4      | 7      | 10  | 3     | 8     | 1 0 0          | 0 0 0       | 161 | 0.005            | 0.006             |
| 3762.172               | 3762.1707             | -6     | C 0.312D-21       | 586.243  | 7    | 1      | 6      | 7   | 0     | 7     | 1 0 0          | 0 0 0       | 161 | 0.024            | 0.026             |
| 3762.475               | 3762.4758             | 8      | C 0.534D-21       | 212.156  | 4    | 0      | 4      | 3   | 2     | 1     | 0 0 1          | 0 0 0       | 161 | 0.092            | 0.108             |
| 3763.065               | 3763.0656             |        | 0.725D-21         | 1998.996 | 11   | 6      | 5      | 11  | 5     | 6     | 1 0 0          | 0 0 0       | 161 | 0.021            | 0.024             |
| 3763.700               | 3763.7003             | 4      | C 0.230D-21       | 95.176   | 3    | 2      | 2      | 2   | 1     | 1     | 1 0 0          | 0 0 0       | 161 | 0.055            | 0.064             |
| 3764.038               |                       |        | D 0.318D-21       | 3849.386 | 3    | 1      | 2      | 2   | 1     | 1     | 0 0 2          | 0 0 1       | 161 |                  | 0.014             |
| 3764.052               | 3764.0474             | 3      | H 0.599D-21       | 2630.194 | 8    | 3      | 5      | 8   | 3     | 6     | 0 1 1          | 0 1 0       | 161 | 0.025            | 0.021             |
| 3764.599               | 3764.5996             | 5      | C 0.262D-20       | 931.237  | 7    | 5      | 2      | 7   | 4     | 3     | 1 0 0          | 0 0 0       | 161 | 0.131            | 0.127             |
| 3765.760               | 3765.7602             | -3     | S 0.182D-19       | 300.362  | 4    | 2      | 2      | 4   | 2     | 3     | 0 0 1          | 0 0 0       | 161 |                  | 2.935             |
| 3766.057               | 3766.0574             | 11     | C 0.148D-21       | 383.842  | 5    | 1      | 4      | 4   | 3     | 1     | 0 0 1          | 0 0 0       | 161 | 0.019            | 0.019             |
| 3766.600               | 3766.5996             |        | 0.399D-21         | 3895.589 | 4    | 1      | 4      | 3   | 1     | 3     | 0 0 2          | 0 0 1       | 161 | 0.014            | 0.017             |
| 3766.749               | 3766.7497             | 6      | C 0.315D-20       | 1122.709 | 8    | 5      | 4      | 8   | 4     | 5     | 1 0 0          | 0 0 0       | 161 | 0.135            | 0.127             |
| 3766.753               |                       |        | D 0.920D-22       | 586.479  | 7    | 2      | 6      | 7   | 1     | 7     | 1 0 0          | 0 0 0       | 161 |                  | 0.008             |
| 3766.829               | 3766.8269             |        | 0.290D-21         | 1739.485 | 3    | 1      | 2      | 3   | 1     | 3     | 0 1 1          | 0 1 0       | 161 | 0.011            | 0.010             |
| 3766.834               |                       |        | D 0.584D-22       | 1050.158 | 9    | 1      | 8      | 8   | 3     | 5     | 0 0 1          | 0 0 0       | 161 |                  | 0.003             |
| 3767.464               | 3767.4651             | 7      | C 0.117D-20       | 1340.886 | 9    | 5      | 5      | 9   | 4     | 6     | 1 0 0          | 0 0 0       | 161 | 0.045            | 0.042             |
| 3768.092               | 3768.0936             | 12     | C 0.984D-21       | 927.744  | 7    | 5      | 3      | 7   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.052            | 0.048             |
| 3768.690               | 3768.6908             | 9      | C 0.265D-21       | 326.625  | 6    | 0      | 6      | 5   | 1     | 5     | 1 0 0          | 0 0 0       | 161 | 0.041            | 0.040             |
| 3768.940               | 3768.9416             | 13     | C 0.834D-21       | 757.780  | 6    | 5      | 1      | 6   | 4     | 2     | 1 0 0          | 0 0 0       | 161 | 0.054            | 0.051             |
| 3769.890               | 3769.8903             | 5      | S 0.137D-19       | 79.496   | 2    | 1      | 1      | 2   | 1     | 2     | 0 0 1          | 0 0 0       | 161 |                  | 3.972             |
| 3769.985               |                       |        | D 0.465D-22       | 1695.071 | 11   | 4      | 8      | 11  | 3     | 9     | 1 0 0          | 0 0 0       | 161 |                  | 0.002             |
| 3769.989               | 3769.9916             | 25     | A 0.341D-20       | 816.694  | 7    | 3      | 4      | 7   | 3     | 5     | 0 0 1          | 0 0 0       | 161 | 0.323            | 0.192             |
| 3769.995               |                       |        | D 0.259D-20       | 756.725  | 6    | 5      | 2      | 6   | 4     | 3     | 1 0 0          | 0 0 0       | 161 |                  | 0.160             |
| 3770.456               | 3770.4556             | -2     | C 0.810D-21       | 325.348  | 6    | 1      | 6      | 5   | 0     | 5     | 1 0 0          | 0 0 0       | 161 | 0.117            | 0.123             |
| 3770.460               |                       |        | D 0.614D-23       | 141.567  | 3    | 1      | 2      | 3   | 1     | 3     | 0 0 1          | 0 0 0       | 181 |                  | 0.002             |
| 3770.829               | 3770.8240             |        | 0.259D-21         | 3201.914 | 2    | 1      | 1      | 1   | 1     | 0     | 0 2 1          | 0 2 0       | 161 | 0.011            | 0.010             |
| 3771.563               | 3771.5632             | -1     | C 0.172D-20       | 610.341  | 5    | 5      | 0      | 5   | 4     | 1     | 1 0 0          | 0 0 0       | 161 | 0.139            | 0.138             |
| 3771.790               | 3771.7895             | -1     | C 0.578D-21       | 610.114  | 5    | 5      | 1      | 5   | 4     | 2     | 1 0 0          | 0 0 0       | 161 | 0.048            | 0.046             |
| 3772.509               | 3772.5094             |        | 0.329D-21         | 1724.707 | 10   | 6      | 4      | 10  | 5     | 5     | 1 0 0          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3773.927               | 3773.9271             | 2      | C 0.345D-20       | 1581.336 | 10   | 4      | 6      | 10  | 4     | 7     | 0 0 1          | 0 0 0       | 161 | 0.114            | 0.115             |
| 3774.053               | 3774.0540             | 9      | C 0.990D-22       | 416.209  | 6    | 1      | 5      | 5   | 2     | 4     | 1 0 0          | 0 0 0       | 161 | 0.012            | 0.012             |
| 3774.477               | 3774.4784             | 11     | H 0.792D-21       | 2275.373 | 12   | 6      | 7      | 12  | 5     | 8     | 1 0 0          | 0 0 0       | 161 | 0.024            | 0.026             |
| 3776.445               | 3776.4442             | -9     | C 0.839D-21       | 1634.970 | 2    | 1      | 2      | 1   | 1     | 1     | 0 1 1          | 0 1 0       | 161 | 0.030            | 0.028             |
| 3777.950               | 3777.9501             | 5      | C 0.631D-21       | 173.365  | 4    | 2      | 3      | 3   | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.125            | 0.141             |
| 3778.053               | 3778.0508             | -18    | H 0.745D-21       | 2161.286 | 6    | 2      | 4      | 6   | 2     | 5     | 0 1 1          | 0 1 0       | 161 | 0.026            | 0.025             |
| 3778.261               | 3778.2634             |        | 0.109D-20         | 1718.719 | 10   | 6      | 5      | 10  | 5     | 6     | 1 0 0          | 0 0 0       | 161 | 0.034            | 0.036             |
| 3778.810               | 3778.8069             |        | 0.430D-21         | 3237.917 | 3    | 1      | 3      | 2   | 1     | 2     | 0 2 1          | 0 2 0       | 161 | 0.019            | 0.016             |
| 3779.151               | 3779.1515             | 10     | C 0.122D-20       | 1477.297 | 9    | 6      | 3      | 9   | 5     | 4     | 1 0 0          | 0 0 0       | 161 | 0.040            | 0.041             |
| 3779.493               | 3779.4935             | -3     | C 0.610D-20       | 0.0      | 1    | 0      | 1      | 0   | 0     | 0     | 0 0 1          | 0 0 0       | 161 |                  | 2.206             |
| 3779.762               | 3779.7625             | -1     | C 0.381D-20       | 416.209  | 5    | 2      | 3      | 5   | 2     | 4     | 0 0 1          | 0 0 0       | 161 | 0.427            | 0.462             |
| 3780.212               | 3780.2058             |        | 0.153D-21         | 4750.387 | 11   | 1      | 11     | 10  | 1     | 10    | 1 0 1          | 1 0 0       | 161 | 0.009            | 0.008             |
| 3781.401               | 3781.3992             |        | 0.422D-21         | 1474.981 | 9    | 6      | 4      | 9   | 5     | 5     | 1 0 0          | 0 0 0       | 161 | 0.014            | 0.014             |
| 3781.802               | 3781.8006             | -8     | C 0.193D-21       | 744.163  | 8    | 2      | 7      | 8   | 1     | 8     | 1 0 0          | 0 0 0       | 161 | 0.009            | 0.012             |
| 3781.945               | 3781.9457             | 4      | C 0.689D-21       | 508.812  | 6    | 1      | 5      | 5   | 3     | 2     | 0 0 1          | 0 0 0       | 161 | 0.078            | 0.068             |
| 3781.946               |                       |        | D 0.361D-21       | 842.357  | 8    | 1      | 7      | 7   | 3     | 4     | 0 0 1          | 0 0 0       | 161 |                  | 0.020             |
| 3782.180               | 3782.1802             | 9      | C 0.339D-20       | 1618.559 | 2    | 0      | 2      | 1   | 0     | 1     | 0 1 1          | 0 1 0       | 161 | 0.129            | 0.112             |
| 3783.730               | 3783.7317             | 12     | C 0.451D-21       | 1255.913 | 8    | 6      | 2      | 8   | 5     | 3     | 1 0 0          | 0 0 0       | 161 | 0.017            | 0.017             |
| 3784.461               | 3784.4609             | 2      | C 0.137D-20       | 1255.167 | 8    | 6      | 3      | 8   | 5     | 4     | 1 0 0          | 0 0 0       | 161 | 0.051            | 0.051             |
| 3784.584               | 3784.5835             | -6     | C 0.292D-20       | 142.278  | 3    | 1      | 2      | 3   | 1     | 3     | 0 0 1          | 0 0 0       | 161 | 0.595            | 0.710             |
| 3784.933               | 3784.9318             | -6     | C 0.616D-21       | 447.252  | 7    | 0      | 7      | 6   | 1     | 6     | 1 0 0          | 0 0 0       | 161 | 0.070            | 0.069             |
| 3785.268               | 3785.2677             | 1      | C 0.643D-21       | 79.496   | 3    | 2      | 1      | 2   | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.152            | 0.186             |
| 3785.512               | 3785.5098             |        | 0.466D-21         | 3974.632 | 5    | 0      | 5      | 4   | 0     | 4     | 0 0 2          | 0 0 1       | 161 | 0.014            | 0.020             |
| 3785.687               | 3785.6877             | 2      | C 0.207D-21       | 446.697  | 7    | 1      | 7      | 6   | 0     | 6     | 1 0 0          | 0 0 0       | 161 | 0.025            | 0.023             |
| 3786.220               |                       |        | D 0.127D-21       | 3926.862 | 4    | 1      | 3      | 3   | 1     | 2     | 0 0 2          | 0 0 1       | 161 |                  | 0.005             |
| 3786.225               | 3786.2245             | -1     | C 0.618D-20       | 1006.116 | 8    | 3      | 5      | 8   | 3     | 6     | 0 0 1          | 0 0 0       | 161 | 0.292            | 0.275             |
| 3786.688               | 3786.6886             | 24     | H 0.610D-21       | 1821.599 | 4    | 1      | 3      | 4   | 1     | 4     | 0 1 2          | 0 1 1       | 161 | 0.026            | 0.020             |
| 3786.930               |                       |        | 0.707D-22         | 23.755   | 2    | 0      | 2      | 1   | 0     | 1     | 0 0 1          | 0 0 0       | 181 |                  | 0.024             |
| 3786.940               | 3786.9406             | 6      | B 0.129D-20       | 1059.835 | 7    | 6      | 1      | 7   | 5     | 2     | 1 0 0          | 0 0 0       | 161 | 0.062            | 0.055             |
| 3787.127               | 3787.1276             | 11     | C 0.432D-21       | 1059.647 | 7    | 6      | 2      | 7   | 5     | 3     | 1 0 0          | 0 0 0       | 161 | 0.020            | 0.018             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF | C | $S_{\text{calc}}$ | $E''$    | J  | $K_a'$ | $K_c'$ | J  | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|------|---|-------------------|----------|----|--------|--------|----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3787.348               | 3787.3490             | 73   | H | 0.519D-21         | 2918.244 | 14 | 5      | 9      | 14 | 5     | 10    | 0 0 1            | 0 0 0         | 161 | 0.018            | 0.019             |
| 3787.422               | 3787.4215             | 2    | C | 0.202D-21         | 661.549  | 7  | 1      | 6      | 6  | 3     | 3     | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.015             |
| 3787.666               | 3787.6631             | -31  | C | 0.246D-20         | 1640.508 | 2  | 1      | 1      | 1  | 1     | 0     | 0 1 1            | 0 1 0         | 161 | 0.091            | 0.081             |
| 3788.808               | 3788.8098             | -2   | B | 0.739D-21         | 1843.030 | 11 | 4      | 7      | 11 | 4     | 8     | 0 0 1            | 0 0 0         | 161 | 0.024            | 0.024             |
| 3789.244               | 3789.2436             | -4   | C | 0.301D-21         | 888.632  | 6  | 6      | 0      | 6  | 5     | 1     | 1 0 0            | 0 0 0         | 161 | 0.015            | 0.015             |
| 3789.277               | 3789.2770             | -6   | C | 0.903D-21         | 888.599  | 6  | 6      | 1      | 6  | 5     | 2     | 1 0 0            | 0 0 0         | 161 | 0.050            | 0.046             |
| 3789.635               | 3789.6343             | -5   | C | 0.181D-21         | 275.497  | 5  | 2      | 4      | 4  | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.029            | 0.031             |
| 3790.431               | 3790.4316             | -2   | H | 0.520D-21         | 2144.047 | 11 | 7      | 4      | 11 | 6     | 5     | 1 0 0            | 0 0 0         | 161 | 0.016            | 0.017             |
| 3792.636               | 3792.6357             | -3   | C | 0.517D-22         | 42.023   | 2  | 1      | 1      | 1  | 0     | 0     | 0 0 1            | 0 0 0         | 181 | 0.013            | 0.017             |
| 3793.825               | 3793.8259             | 9    | C | 0.437D-21         | 931.237  | 8  | 2      | 6      | 7  | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 0.020            | 0.021             |
| 3795.503               | 3795.5038             | 7    | C | 0.260D-21         | 552.912  | 7  | 1      | 6      | 6  | 2     | 5     | 1 0 0            | 0 0 0         | 161 | 0.022            | 0.023             |
| 3795.646               | 3795.6432             | -5   | H | 0.657D-21         | 1874.974 | 10 | 7      | 4      | 10 | 6     | 5     | 1 0 0            | 0 0 0         | 161 | 0.019            | 0.021             |
| 3796.083               | 3796.0829             | -2   | C | 0.405D-20         | 1677.063 | 3  | 1      | 3      | 2  | 1     | 2     | 0 1 1            | 0 1 0         | 161 | 0.151            | 0.132             |
| 3796.440               | 3796.4393             | -7   | S | 0.843D-20         | 37.137   | 2  | 1      | 2      | 1  | 1     | 1     | 0 0 1            | 0 0 0         | 161 | 2.732            |                   |
| 3796.495               |                       |      |   | 0.702D-21         | 1742.307 | 3  | 3      | 0      | 2  | 2     | 1     | 1 1 0            | 0 1 0         | 161 | 0.023            |                   |
| 3797.788               | 3797.7878             | -7   | C | 0.742D-20         | 552.912  | 6  | 2      | 4      | 6  | 2     | 5     | 0 0 1            | 0 0 0         | 161 | 0.632            | 0.662             |
| 3798.803               | 3798.8007             |      |   | 0.747D-21         | 1631.384 | 9  | 7      | 2      | 9  | 6     | 3     | 1 0 0            | 0 0 0         | 161 | 0.024            | 0.025             |
| 3798.934               | 3798.9333             |      |   | 0.249D-21         | 1631.251 | 9  | 7      | 3      | 9  | 6     | 4     | 1 0 0            | 0 0 0         | 161 | 0.007            | 0.008             |
| 3799.047               | 3799.0471             | -4   | C | 0.353D-21         | 136.164  | 3  | 3      | 1      | 2  | 2     | 0     | 1 0 0            | 0 0 0         | 161 | 0.080            | 0.087             |
| 3799.934               | 3799.9333             |      |   | 0.440D-21         | 399.457  | 6  | 2      | 5      | 5  | 1     | 4     | 1 0 0            | 0 0 0         | 161 | 0.052            | 0.055             |
| 3800.443               | 3800.4418             |      |   | 0.134D-20         | 134.902  | 3  | 3      | 0      | 2  | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.281            | 0.331             |
| 3800.820               | 3800.8189             |      |   | 0.432D-21         | 586.243  | 8  | 1      | 8      | 7  | 0     | 7     | 1 0 0            | 0 0 0         | 161 | 0.039            | 0.036             |
| 3800.879               | 3800.8771             |      |   | 0.876D-22         | 586.479  | 8  | 0      | 8      | 7  | 1     | 7     | 1 0 0            | 0 0 0         | 161 | 0.008            | 0.007             |
| 3800.958               | 3800.9598             |      |   | 0.474D-21         | 4076.896 | 6  | 1      | 6      | 5  | 1     | 5     | 0 0 2            | 0 0 1         | 161 | 0.016            | 0.021             |
| 3801.417               |                       |      | D | 0.112D-21         | 4837.699 | 10 | 2      | 8      | 9  | 2     | 7     | 1 0 1            | 1 0 0         | 161 | 0.006            |                   |
| 3801.420               | 3801.4237             | 41   | S | 0.336D-19         | 23.794   | 2  | 0      | 2      | 1  | 0     | 1     | 0 0 1            | 0 0 0         | 161 | 11.292           |                   |
| 3801.576               |                       |      |   | 0.856D-22         | 78.988   | 3  | 1      | 3      | 2  | 1     | 2     | 0 0 1            | 0 0 0         | 181 | 0.025            |                   |
| 3801.656               |                       |      | D | 0.738D-21         | 1411.612 | 8  | 7      | 2      | 8  | 6     | 3     | 1 0 0            | 0 0 0         | 161 | 0.025            |                   |
| 3801.666               | 3801.6644             |      |   | 0.151D-20         | 1664.971 | 3  | 0      | 3      | 2  | 0     | 2     | 0 1 1            | 0 1 0         | 161 | 0.065            | 0.049             |
| 3801.944               | 3801.9427             |      |   | 0.164D-20         | 1742.307 | 3  | 2      | 2      | 2  | 2     | 1     | 0 1 1            | 0 1 0         | 161 | 0.061            | 0.053             |
| 3802.680               | 3802.6757             |      |   | 0.559D-21         | 3289.242 | 4  | 0      | 4      | 3  | 0     | 3     | 0 2 1            | 0 2 0         | 161 | 0.025            | 0.021             |
| 3802.966               | 3802.9659             | -3   | C | 0.621D-20         | 224.838  | 4  | 1      | 3      | 4  | 1     | 4     | 0 0 1            | 0 0 0         | 161 | 1.005            | 1.204             |
| 3803.833               | 3803.8327             | -2   | C | 0.532D-21         | 1216.194 | 7  | 7      | 0      | 7  | 6     | 1     | 1 0 0            | 0 0 0         | 161 | 0.028            | 0.020             |
| 3803.838               |                       |      | D | 0.177D-21         | 1216.189 | 7  | 7      | 1      | 7  | 6     | 2     | 1 0 0            | 0 0 0         | 161 | 0.007            |                   |
| 3804.390               | 3804.3880             |      |   | 0.144D-21         | 4126.465 | 5  | 3      | 2      | 4  | 3     | 1     | 0 0 2            | 0 0 1         | 161 | 0.008            | 0.006             |
| 3805.592               | 3805.5900             |      |   | 0.403D-21         | 4027.804 | 5  | 1      | 4      | 4  | 1     | 3     | 0 0 2            | 0 0 1         | 161 | 0.014            | 0.018             |
| 3806.050               | 3806.0500             | 1    | C | 0.124D-20         | 1216.232 | 9  | 3      | 6      | 9  | 3     | 7     | 0 0 1            | 0 0 0         | 161 | 0.047            | 0.047             |
| 3806.113               | 3806.1118             | -11  | C | 0.313D-22         | 69.927   | 3  | 0      | 3      | 2  | 0     | 2     | 0 0 1            | 0 0 0         | 181 | 0.005            | 0.009             |
| 3806.212               | 3806.2142             | 10   | C | 0.692D-21         | 1743.492 | 3  | 2      | 1      | 2  | 2     | 0     | 0 1 1            | 0 1 0         | 161 | 0.026            | 0.022             |
| 3807.014               | 3807.0160             | 11   | S | 0.246D-19         | 42.372   | 2  | 1      | 1      | 1  | 0     | 0     | 0 0 1            | 0 0 0         | 161 | 7.834            |                   |
| 3807.443               | 3807.4412             | -15  | C | 0.466D-22         | 133.474  | 3  | 2      | 2      | 2  | 2     | 1     | 0 0 1            | 0 0 0         | 181 | 0.008            | 0.012             |
| 3807.603               | 3807.5982             |      |   | 0.857D-22         | 5153.191 | 12 | 1      | 11     | 11 | 1     | 10    | 1 0 1            | 1 0 0         | 161 | 0.007            | 0.005             |
| 3808.019               | 3808.0191             | 13   | C | 0.147D-21         | 1131.776 | 9  | 2      | 7      | 8  | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.005            | 0.006             |
| 3808.082               | 3808.0785             |      |   | 0.336D-21         | 2321.905 | 11 | 8      | 3      | 11 | 7     | 4     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.011             |
| 3808.594               | 3808.5944             | -71  | H | 0.123D-20         | 2124.953 | 12 | 4      | 8      | 12 | 4     | 9     | 0 0 1            | 0 0 0         | 161 | 0.036            | 0.040             |
| 3810.326               | 3810.3248             | -7   | C | 0.110D-21         | 542.906  | 7  | 2      | 6      | 6  | 1     | 5     | 1 0 0            | 0 0 0         | 161 | 0.008            | 0.010             |
| 3810.815               |                       |      | D | 0.710D-22         | 3266.762 | 12 | 11     | 2      | 12 | 10    | 3     | 1 0 0            | 0 0 0         | 161 | 0.003            |                   |
| 3810.825               | 3810.8245             | 10   | C | 0.302D-21         | 1360.236 | 10 | 2      | 8      | 9  | 4     | 5     | 0 0 1            | 0 0 0         | 161 | 0.010            | 0.011             |
| 3811.256               |                       |      | D | 0.275D-22         | 1114.534 | 10 | 1      | 9      | 10 | 0     | 10    | 1 0 0            | 0 0 0         | 161 | 0.001            |                   |
| 3811.258               | 3811.2589             |      |   | 0.401D-21         | 2054.348 | 10 | 8      | 3      | 10 | 7     | 4     | 1 0 0            | 0 0 0         | 161 | 0.011            | 0.013             |
| 3811.990               | 3811.9883             |      |   | 0.345D-21         | 4066.123 | 5  | 2      | 3      | 4  | 2     | 2     | 0 0 2            | 0 0 1         | 161 | 0.014            | 0.015             |
| 3812.353               | 3812.3485             |      |   | 0.158D-21         | 1731.898 | 3  | 2      | 2      | 3  | 0     | 3     | 0 1 1            | 0 1 0         | 161 | 0.006            | 0.005             |
| 3812.662               | 3812.6627             | 16   | C | 0.130D-20         | 1693.652 | 3  | 1      | 2      | 2  | 1     | 1     | 0 1 1            | 0 1 0         | 161 | 0.055            | 0.042             |
| 3812.723               | 3812.7237             |      |   | 0.309D-21         | 4165.473 | 6  | 2      | 5      | 5  | 2     | 4     | 0 0 2            | 0 0 1         | 161 | 0.011            | 0.014             |
| 3813.494               | 3813.4924             | -1   | C | 0.142D-20         | 1739.485 | 4  | 1      | 4      | 3  | 1     | 3     | 0 1 1            | 0 1 0         | 161 | 0.050            | 0.046             |
| 3813.801               | 3813.7995             |      |   | 0.412D-21         | 1810.589 | 9  | 8      | 1      | 9  | 7     | 2     | 1 0 0            | 0 0 0         | 161 | 0.017            | 0.013             |
| 3813.806               |                       |      | D | 0.137D-21         | 1810.584 | 9  | 8      | 2      | 9  | 7     | 3     | 1 0 0            | 0 0 0         | 161 | 0.004            |                   |
| 3814.437               | 3814.4368             |      |   | 0.593D-21         | 3381.704 | 5  | 1      | 5      | 4  | 1     | 4     | 0 2 1            | 0 2 0         | 161 | 0.027            | 0.023             |
| 3815.545               | 3815.5456             | 9    | C | 0.269D-21         | 744.163  | 9  | 0      | 9      | 8  | 1     | 8     | 1 0 0            | 0 0 0         | 161 | 0.020            | 0.017             |
| 3815.647               | 3815.6469             | -3   | C | 0.304D-21         | 70.091   | 2  | 2      | 1      | 2  | 0     | 2     | 0 0 1            | 0 0 0         | 161 | 0.066            | 0.089             |
| 3815.680               |                       |      | D | 0.326D-22         | 3512.401 | 12 | 12     | 1      | 12 | 11    | 2     | 1 0 0            | 0 0 0         | 161 | 0.001            |                   |
| 3815.689               | 3815.6882             | 0    | C | 0.899D-22         | 744.064  | 9  | 1      | 9      | 8  | 0     | 8     | 1 0 0            | 0 0 0         | 161 | 0.005            | 0.006             |
| 3816.093               | 3816.0997             | 78   | S | 0.409D-19         | 79.496   | 3  | 1      | 3      | 2  | 1     | 2     | 0 0 1            | 0 0 0         | 161 | 11.712           |                   |
| 3816.736               |                       |      | D | 0.457D-21         | 4195.477 | 7  | 0      | 7      | 6  | 0     | 6     | 0 0 2            | 0 0 1         | 161 | 0.020            |                   |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3818.333               |                       | D      | 0.152D-21         | 4195.816 | 7    | 1      | 7      | 6   | 1     | 6     | 0 0 2            | 0 0 1         | 161 | 0.007            |                   |
| 3818.341               | 3818.3411             | -3     | C 0.167D-20       | 709.609  | 7    | 2      | 5      | 7   | 2     | 6     | 0 0 1            | 0 0 0         | 161 | 0.121            | 0.110             |
| 3818.349               |                       | D      | 0.202D-21         | 3375.298 | 5    | 0      | 5      | 4   | 0     | 4     | 0 2 1            | 0 2 0         | 161 |                  | 0.008             |
| 3818.683               | 3818.6831             | 2      | C 0.102D-20       | 212.156  | 4    | 3      | 2      | 3   | 2     | 1     | 1 0 0            | 0 0 0         | 161 | 0.176            | 0.204             |
| 3818.775               | 3818.7744             | 1      | C 0.531D-20       | 1731.898 | 4    | 0      | 4      | 3   | 0     | 3     | 0 1 1            | 0 1 0         | 161 | 0.194            | 0.172             |
| 3819.603               | 3819.6031             |        | 0.713D-21         | 1813.788 | 4    | 2      | 3      | 3   | 2     | 2     | 0 1 1            | 0 1 0         | 161 | 0.022            | 0.023             |
| 3819.854               | 3819.8535             |        | 0.491D-21         | 3334.626 | 4    | 1      | 3      | 3   | 1     | 2     | 0 2 1            | 0 2 0         | 161 | 0.021            | 0.019             |
| 3819.905               | 3819.9049             | 2      | C 0.234D-20       | 136.761  | 3    | 2      | 2      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 161 | 0.462            | 0.572             |
| 3819.956               | 3819.9533             |        | 0.183D-20         | 1907.617 | 4    | 3      | 1      | 3   | 3     | 0     | 0 1 1            | 0 1 0         | 161 | 0.064            | 0.059             |
| 3820.739               | 3820.7395             | 3      | S 0.150D-19       | 70.091   | 3    | 0      | 3      | 2   | 0     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 4.404             |
| 3821.764               | 3821.7661             | 13     | S 0.225D-19       | 134.902  | 3    | 2      | 2      | 2   | 2     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 5.523             |
| 3822.505               | 3822.5062             |        | 0.222D-21         | 4244.305 | 6    | 3      | 4      | 5   | 3     | 3     | 0 0 2            | 0 0 1         | 161 | 0.009            | 0.010             |
| 3823.128               | 3823.1267             | 0      | C 0.110D-21       | 136.336  | 4    | 0      | 4      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 181 | 0.020            | 0.027             |
| 3823.274               | 3823.2740             | -4     | C 0.157D-20       | 326.625  | 5    | 1      | 4      | 5   | 1     | 5     | 0 0 1            | 0 0 0         | 161 | 0.212            | 0.233             |
| 3823.551               | 3823.5518             |        | 0.333D-21         | 2495.168 | 8    | 2      | 6      | 8   | 2     | 7     | 0 1 1            | 0 1 0         | 161 | 0.014            | 0.011             |
| 3824.276               |                       | D      | 0.562D-22         | 3598.727 | 5    | 3      | 2      | 4   | 3     | 1     | 0 2 1            | 0 2 0         | 161 |                  | 0.002             |
| 3824.281               | 3824.2809             | -2     | C 0.851D-21       | 142.278  | 4    | 2      | 2      | 3   | 1     | 3     | 1 0 0            | 0 0 0         | 161 | 0.173            | 0.205             |
| 3824.427               | 3824.4240             |        | 0.367D-21         | 3482.064 | 5    | 2      | 4      | 4   | 2     | 3     | 0 2 1            | 0 2 0         | 161 | 0.021            | 0.014             |
| 3825.552               | 3825.5522             | -5     | C 0.814D-21       | 206.301  | 4    | 3      | 1      | 3   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.145            | 0.165             |
| 3825.944               | 3825.9432             |        | 0.501D-21         | 1813.788 | 4    | 3      | 1      | 3   | 2     | 2     | 1 1 0            | 0 1 0         | 161 | 0.020            | 0.016             |
| 3826.754               | 3826.7538             | -8     | C 0.753D-20       | 136.164  | 3    | 2      | 1      | 2   | 2     | 0     | 0 0 1            | 0 0 0         | 161 | 1.497            | 1.840             |
| 3827.504               | 3827.5043             | 1      | C 0.228D-20       | 1446.129 | 10   | 3      | 7      | 10  | 3     | 8     | 0 0 1            | 0 0 0         | 161 | 0.078            | 0.077             |
| 3827.505               |                       | D      | 0.342D-22         | 3478.987 | 5    | 2      | 4      | 5   | 0     | 5     | 0 2 1            | 0 2 0         | 161 |                  | 0.001             |
| 3828.000               | 3827.9997             | -3     | C 0.111D-20       | 222.052  | 4    | 2      | 3      | 4   | 0     | 4     | 0 0 1            | 0 0 0         | 161 | 0.184            | 0.215             |
| 3828.590               | 3828.5906             | -1     | C 0.376D-21       | 325.348  | 5    | 3      | 2      | 5   | 0     | 5     | 1 0 0            | 0 0 0         | 161 | 0.051            | 0.056             |
| 3828.896               | 3828.8945             |        | 0.259D-21         | 1920.769 | 5    | 2      | 4      | 5   | 0     | 5     | 0 1 1            | 0 1 0         | 161 | 0.010            | 0.008             |
| 3830.057               | 3830.0580             | 12     | C 0.202D-22       | 136.539  | 4    | 0      | 4      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 171 | 0.006            | 0.005             |
| 3830.219               | 3830.2179             | -7     | C 0.147D-21       | 920.169  | 10   | 1      | 10     | 9   | 0     | 9     | 1 0 0            | 0 0 0         | 161 | 0.006            | 0.007             |
| 3830.367               | 3830.3667             | 4      | C 0.121D-21       | 885.600  | 9    | 1      | 8      | 8   | 2     | 7     | 1 0 0            | 0 0 0         | 161 | 0.006            | 0.006             |
| 3831.687               | 3831.6855             | -14    | S 0.130D-19       | 95.176   | 3    | 1      | 2      | 2   | 1     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 3.549             |
| 3831.967               | 3831.9671             | 4      | C 0.567D-20       | 1821.599 | 5    | 1      | 5      | 4   | 1     | 4     | 0 1 1            | 0 1 0         | 161 | 0.203            | 0.182             |
| 3833.365               | 3833.3648             | 32     | H 0.129D-20       | 2129.600 | 5    | 4      | 2      | 4   | 4     | 1     | 0 1 1            | 0 1 0         | 161 | 0.040            | 0.042             |
| 3833.509               | 3833.5055             |        | 0.614D-21         | 3478.987 | 6    | 0      | 6      | 5   | 0     | 5     | 0 2 1            | 0 2 0         | 161 | 0.029            | 0.024             |
| 3833.567               | 3833.5656             |        | 0.429D-21         | 2129.619 | 5    | 4      | 1      | 4   | 4     | 0     | 0 1 1            | 0 1 0         | 161 | 0.017            | 0.014             |
| 3833.691               | 3833.6907             | -6     | C 0.339D-20       | 1819.337 | 4    | 2      | 2      | 3   | 2     | 1     | 0 1 1            | 0 1 0         | 161 | 0.122            | 0.109             |
| 3834.508               | 3834.5085             | 7      | C 0.258D-21       | 315.779  | 5    | 3      | 3      | 4   | 2     | 2     | 1 0 0            | 0 0 0         | 161 | 0.033            | 0.039             |
| 3834.692               | 3834.6887             | -18    | C 0.191D-20       | 1817.451 | 5    | 0      | 5      | 4   | 0     | 4     | 0 1 1            | 0 1 0         | 161 | 0.066            | 0.061             |
| 3834.983               | 3834.9833             | 3      | S 0.163D-19       | 142.278  | 4    | 1      | 4      | 3   | 1     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 3.908             |
| 3835.874               | 3835.8708             | -14    | C 0.470D-20       | 1772.413 | 4    | 1      | 3      | 3   | 1     | 2     | 0 1 1            | 0 1 0         | 161 | 0.168            | 0.151             |
| 3837.453               | 3837.4531             | 13     | C 0.118D-21       | 223.828  | 5    | 1      | 5      | 4   | 1     | 4     | 0 0 1            | 0 0 0         | 181 | 0.020            | 0.023             |
| 3837.458               |                       | D      | 0.465D-22         | 5579.492 | 13   | 3      | 11     | 12  | 3     | 10    | 1 0 1            | 1 0 0         | 161 |                  | 0.003             |
| 3837.870               |                       |        | 0.527D-19         | 136.761  | 4    | 0      | 4      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 12.816            |
| 3839.285               | 3839.2865             | 19     | C 0.396D-22       | 221.233  | 5    | 0      | 5      | 4   | 0     | 4     | 0 0 1            | 0 0 0         | 181 | 0.008            | 0.008             |
| 3839.462               | 3839.4623             | 0      | C 0.349D-20       | 885.600  | 8    | 2      | 6      | 8   | 2     | 7     | 0 0 1            | 0 0 0         | 161 | 0.182            | 0.176             |
| 3839.743               | 3839.7438             | 14     | C 0.739D-22       | 210.799  | 4    | 2      | 2      | 3   | 2     | 1     | 0 0 1            | 0 0 0         | 181 | 0.012            | 0.015             |
| 3839.859               |                       |        | 0.971D-22         | 172.882  | 4    | 1      | 3      | 3   | 1     | 2     | 0 0 1            | 0 0 0         | 181 |                  | 0.021             |
| 3839.930               | 3839.9303             | 2      | C 0.589D-20       | 285.219  | 4    | 3      | 2      | 3   | 3     | 1     | 0 0 1            | 0 0 0         | 161 | 0.854            | 0.968             |
| 3840.127               | 3840.1269             | 8      | C 0.321D-20       | 325.348  | 5    | 2      | 4      | 5   | 0     | 5     | 0 0 1            | 0 0 0         | 161 | 0.430            | 0.477             |
| 3841.045               | 3841.0453             | 1      | S 0.169D-19       | 285.419  | 4    | 3      | 1      | 3   | 3     | 0     | 0 0 1            | 0 0 0         | 161 |                  | 2.774             |
| 3841.648               | 3841.6475             | 13     | C 0.381D-20       | 1908.017 | 5    | 2      | 4      | 4   | 2     | 3     | 0 1 1            | 0 1 0         | 161 | 0.128            | 0.122             |
| 3841.697               | 3841.6957             | -2     | C 0.277D-20       | 2004.817 | 5    | 3      | 3      | 4   | 3     | 2     | 0 1 1            | 0 1 0         | 161 | 0.091            | 0.089             |
| 3843.505               | 3843.5049             | -4     | C 0.366D-20       | 447.252  | 6    | 1      | 5      | 6   | 1     | 6     | 0 0 1            | 0 0 0         | 161 | 0.378            | 0.406             |
| 3843.751               | 3843.7507             | -7     | C 0.115D-19       | 206.301  | 4    | 2      | 3      | 3   | 2     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 2.317             |
| 3844.324               |                       | D      | 0.218D-22         | 224.305  | 5    | 1      | 5      | 4   | 1     | 4     | 0 0 1            | 0 0 0         | 171 |                  | 0.004             |
| 3844.329               | 3844.3295             | 7      | C 0.589D-21       | 542.906  | 6    | 3      | 4      | 6   | 1     | 5     | 0 0 1            | 0 0 0         | 161 | 0.053            | 0.053             |
| 3844.847               | 3844.8476             | 1      | C 0.120D-20       | 399.457  | 5    | 3      | 3      | 5   | 1     | 4     | 0 0 1            | 0 0 0         | 161 | 0.133            | 0.149             |
| 3845.354               | 3845.3529             |        | 0.912D-21         | 2005.917 | 5    | 3      | 2      | 4   | 3     | 1     | 0 1 1            | 0 1 0         | 161 | 0.030            | 0.029             |
| 3845.543               | 3845.5412             |        | 0.274D-21         | 2406.142 | 6    | 5      | 2      | 5   | 5     | 1     | 0 1 1            | 0 1 0         | 161 | 0.011            | 0.009             |
| 3845.572               | 3845.5731             | 42     | H 0.821D-21       | 2406.144 | 6    | 5      | 1      | 5   | 5     | 0     | 0 1 1            | 0 1 0         | 161 | 0.029            | 0.027             |
| 3845.648               | 3845.6481             |        | 0.111D-21         | 2000.866 | 5    | 3      | 3      | 5   | 1     | 4     | 0 1 1            | 0 1 0         | 161 | 0.006            | 0.004             |
| 3846.399               | 3846.3998             | 6      | C 0.514D-21       | 446.511  | 6    | 3      | 4      | 5   | 2     | 3     | 1 0 0            | 0 0 0         | 161 | 0.054            | 0.057             |
| 3847.345               | 3847.3416             |        | 0.588D-21         | 3601.859 | 7    | 1      | 7      | 6   | 1     | 6     | 0 2 1            | 0 2 0         | 161 | 0.028            | 0.023             |
| 3847.397               | 3847.3956             |        | 0.366D-21         | 4488.090 | 9    | 0      | 9      | 8   | 0     | 8     | 0 0 2            | 0 0 1         | 161 | 0.018            | 0.017             |
| 3848.566               | 3848.5679             | -71    | H 0.474D-21       | 1695.071 | 11   | 3      | 8      | 11  | 3     | 9     | 0 0 1            | 0 0 0         | 161 | 0.026            | 0.015             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3848.573               |                       | D           | 0.196D-21         | 3600.052 | 7    | 0      | 7      | 6   | 0     | 6     | 0 2 1            | 0 2 0         | 161 | 0.008            |                   |
| 3848.888               | 3848.8877             |             | 0.193D-20         | 1922.831 | 6    | 1      | 6      | 5   | 1     | 5     | 0 1 1            | 0 1 0         | 161 | 0.069            | 0.062             |
| 3849.059               | 3849.0597             | 1           | C 0.219D-20       | 704.214  | 7    | 3      | 5      | 7   | 1     | 6     | 0 0 1            | 0 0 0         | 161 | 0.142            | 0.145             |
| 3849.396               | 3849.3974             |             | 0.321D-21         | 4452.352 | 8    | 2      | 7      | 7   | 2     | 6     | 0 0 2            | 0 0 1         | 161 | 0.012            | 0.015             |
| 3849.579               |                       |             | 0.487D-21         | 285.219  | 4    | 4      | 0      | 3   | 3     | 1     | 1 0 0            | 0 0 0         | 161 |                  | 0.080             |
| 3849.599               | 3849.5994             | 11          | C 0.215D-20       | 285.419  | 4    | 4      | 1      | 3   | 3     | 0     | 1 0 0            | 0 0 0         | 161 | 0.299            | 0.352             |
| 3849.652               | 3849.6519             | 0           | C 0.214D-21       | 275.497  | 4    | 3      | 2      | 4   | 1     | 3     | 0 0 1            | 0 0 0         | 161 | 0.033            | 0.036             |
| 3849.862               |                       | D           | 0.604D-22         | 5256.848 | 8    | 0      | 8      | 7   | 0     | 7     | 0 3 1            | 0 3 0         | 161 |                  | 0.003             |
| 3849.867               | 3849.8672             | 0           | C 0.853D-21       | 446.697  | 6    | 2      | 5      | 6   | 0     | 6     | 0 0 1            | 0 0 0         | 161 | 0.090            | 0.095             |
| 3850.307               | 3850.3085             | 23          | C 0.582D-20       | 1920.769 | 6    | 0      | 6      | 5   | 0     | 5     | 0 1 1            | 0 1 0         | 161 | 0.209            | 0.186             |
| 3851.072               | 3851.0729             |             | 0.210D-21         | 3722.731 | 6    | 3      | 3      | 5   | 3     | 2     | 0 2 1            | 0 2 0         | 161 | 0.014            | 0.009             |
| 3851.626               | 3851.6270             | 16          | C 0.559D-22       | 298.620  | 5    | 2      | 4      | 4   | 2     | 3     | 0 0 1            | 0 0 0         | 181 | 0.007            | 0.009             |
| 3852.058               |                       |             | 0.562D-19         | 224.838  | 5    | 1      | 5      | 4   | 1     | 4     | 0 0 1            | 0 0 0         | 161 |                  | 10.757            |
| 3853.012               | 3853.0132             |             | 0.486D-21         | 1908.017 | 5    | 3      | 2      | 4   | 2     | 3     | 1 1 0            | 0 1 0         | 161 | 0.019            | 0.016             |
| 3853.096               | 3853.0983             |             | 0.247D-21         | 4408.027 | 7    | 3      | 4      | 6   | 3     | 3     | 0 0 2            | 0 0 1         | 161 | 0.009            | 0.011             |
| 3853.576               | 3853.5760             | -2          | C 0.745D-20       | 300.362  | 5    | 3      | 2      | 4   | 2     | 3     | 1 0 0            | 0 0 0         | 161 | 1.047            | 1.174             |
| 3853.966               |                       |             | 0.357D-19         | 212.156  | 4    | 2      | 2      | 3   | 2     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 7.062             |
| 3854.091               | 3854.0895             | -9          | S 0.190D-19       | 222.052  | 5    | 0      | 5      | 4   | 0     | 4     | 0 0 1            | 0 0 0         | 161 |                  | 3.662             |
| 3854.435               |                       | D 0.400D-22 | 325.215           | 6        | 1    | 6      | 5      | 1   | 5     | 0 0 1 | 0 0 0            | 181           |     | 0.006            |                   |
| 3854.439               | 3854.4410             | 18          | C 0.469D-19       | 173.365  | 4    | 1      | 3      | 3   | 1     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 10.285            |
| 3855.285               | 3855.2834             | -7          | C 0.120D-21       | 324.047  | 6    | 0      | 6      | 5   | 0     | 5     | 0 0 1            | 0 0 0         | 181 | 0.017            | 0.018             |
| 3856.007               | 3856.0063             | 13          | H 0.479D-21       | 2733.965 | 7    | 6      | 2      | 6   | 6     | 1     | 0 1 1            | 0 1 0         | 161 | 0.019            | 0.017             |
| 3856.008               |                       | D 0.160D-21 | 2733.965          | 7        | 6    | 1      | 6      | 6   | 0     | 0 1 1 | 0 1 0            | 161           |     | 0.006            |                   |
| 3856.248               | 3856.2440             |             | 0.198D-21         | 4015.515 | 7    | 4      | 4      | 6   | 4     | 3     | 0 2 1            | 0 2 0         | 161 | 0.011            | 0.008             |
| 3856.445               | 3856.4460             | 1           | C 0.165D-20       | 1875.474 | 5    | 1      | 4      | 4   | 1     | 3     | 0 1 1            | 0 1 0         | 161 | 0.056            | 0.053             |
| 3856.621               | 3856.6186             |             | 0.640D-21         | 2251.696 | 6    | 4      | 3      | 5   | 4     | 2     | 0 1 1            | 0 1 0         | 161 | 0.021            |                   |
| 3856.705               | 3856.7042             | -2          | C 0.223D-21       | 173.365  | 3    | 3      | 1      | 3   | 1     | 2     | 0 0 1            | 0 0 0         | 161 | -0.041           | -0.049            |
| 3856.784               | 3856.7856             | 17          | C 0.434D-21       | 399.457  | 5    | 4      | 1      | 5   | 1     | 4     | 1 0 0            | 0 0 0         | 161 | 0.049            | 0.054             |
| 3857.165               | 3857.1639             | -9          | C 0.137D-19       | 488.108  | 5    | 4      | 2      | 4   | 4     | 1     | 0 0 1            | 0 0 0         | 161 | 1.296            | 1.382             |
| 3857.425               | 3857.4242             | -13         | C 0.458D-20       | 488.134  | 5    | 4      | 1      | 4   | 4     | 0     | 0 0 1            | 0 0 0         | 161 | 0.433            | 0.462             |
| 3857.475               | 3857.4741             |             | 0.192D-20         | 2251.863 | 6    | 4      | 2      | 5   | 4     | 1     | 0 1 1            | 0 1 0         | 161 | 0.068            | 0.063             |
| 3858.176               | 3858.1770             | 0           | C 0.759D-21       | 882.891  | 8    | 3      | 6      | 8   | 1     | 7     | 0 0 1            | 0 0 0         | 161 | 0.038            | 0.038             |
| 3859.036               | 3859.0350             | -14         | C 0.223D-21       | 542.906  | 6    | 4      | 2      | 6   | 1     | 5     | 1 0 0            | 0 0 0         | 161 | 0.020            |                   |
| 3859.409               | 3859.4078             | -9          | C 0.817D-21       | 1080.386 | 9    | 2      | 7      | 9   | 2     | 8     | 0 0 1            | 0 0 0         | 161 | 0.035            | 0.033             |
| 3859.611               | 3859.6091             | -16         | C 0.338D-22       | 274.803  | 5    | 1      | 4      | 4   | 1     | 3     | 0 0 1            | 0 0 0         | 181 | 0.005            | 0.006             |
| 3860.503               | 3860.5028             |             | 0.136D-20         | 1922.902 | 5    | 2      | 3      | 4   | 2     | 2     | 0 1 1            | 0 1 0         | 161 | 0.045            | 0.043             |
| 3861.515               | 3861.5159             | 12          | C 0.230D-21       | 446.697  | 6    | 3      | 3      | 6   | 0     | 6     | 1 0 0            | 0 0 0         | 161 | 0.027            | 0.025             |
| 3861.588               | 3861.5848             | -39         | C 0.144D-20       | 2024.150 | 6    | 2      | 5      | 5   | 2     | 4     | 0 1 1            | 0 1 0         | 161 | 0.053            | 0.046             |
| 3861.589               |                       | D 0.176D-21 | 782.410           | 8        | 3    | 6      | 7      | 2   | 5     | 1 0 0 | 0 0 0            | 161           |     | 0.010            |                   |
| 3861.788               | 3861.7874             | -7          | S 0.241D-19       | 382.517  | 5    | 3      | 3      | 4   | 3     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 3.095             |
| 3862.186               | 3862.1795             |             | 0.430D-21         | 3736.171 | 7    | 2      | 6      | 6   | 2     | 5     | 0 2 1            | 0 2 0         | 161 | 0.020            | 0.017             |
| 3862.343               | 3862.3473             |             | 0.308D-21         | 4661.449 | 10   | 1      | 10     | 9   | 1     | 9     | 0 0 2            | 0 0 1         | 161 | 0.014            | 0.015             |
| 3862.492               | 3862.4916             | 0           | C 0.947D-21       | 586.479  | 7    | 1      | 6      | 7   | 1     | 7     | 0 0 1            | 0 0 0         | 161 | 0.077            | 0.078             |
| 3863.321               | 3863.3196             | -4          | C 0.672D-21       | 23.794   | 2    | 2      | 0      | 1   | 0     | 1     | 0 0 1            | 0 0 0         | 161 | 0.175            | 0.222             |
| 3863.557               | 3863.5553             |             | 0.539D-21         | 3738.609 | 8    | 0      | 8      | 7   | 0     | 7     | 0 2 1            | 0 2 0         | 161 | 0.028            | 0.022             |
| 3863.725               | 3863.7292             |             | 0.279D-21         | 4624.305 | 9    | 1      | 8      | 8   | 1     | 7     | 0 0 2            | 0 0 1         | 161 | 0.011            | 0.013             |
| 3863.774               | 3863.7729             |             | 0.104D-20         | 2126.407 | 6    | 3      | 4      | 5   | 3     | 3     | 0 1 1            | 0 1 0         | 161 | 0.036            | 0.033             |
| 3864.310               | 3864.3102             | 0           | C 0.579D-20       | 383.842  | 5    | 3      | 2      | 4   | 3     | 1     | 0 0 1            | 0 0 0         | 161 | 0.677            | 0.741             |
| 3865.112               | 3865.1106             | 22          | S 0.361D-19       | 300.362  | 5    | 2      | 4      | 4   | 2     | 3     | 0 0 1            | 0 0 0         | 161 |                  | 5.670             |
| 3865.120               |                       | D 0.684D-23 | 70.091            | 3        | 3    | 1      | 2      | 0   | 2     | 1     | 0 0 0            | 0 0 0         | 161 |                  | 0.002             |
| 3865.120               |                       | D 0.173D-21 | 2688.080          | 9        | 3    | 7      | 9      | 1   | 8     | 0 1 1 | 0 1 0            | 161           |     | 0.006            |                   |
| 3865.155               |                       | D 0.108D-20 | 1201.922          | 9        | 4    | 6      | 9      | 2   | 7     | 0 0 1 | 0 0 0            | 161           |     | 0.040            |                   |
| 3865.161               |                       | D 0.117D-21 | 4368.637          | 8        | 5    | 3      | 7      | 5   | 2     | 0 2 1 | 0 2 0            | 161           |     | 0.005            |                   |
| 3865.163               | 3865.1395             | 41          | A 0.557D-20       | 2042.735 | 7    | 1      | 7      | 6   | 1     | 6     | 0 1 1            | 0 1 0         | 161 | 0.149            | 0.178             |
| 3865.852               |                       | D 0.288D-22 | 314.458           | 5        | 2    | 3      | 4      | 2   | 2     | 0 0 1 | 0 0 0            | 181           |     | 0.004            |                   |
| 3865.856               | 3865.8549             | -22         | H 0.186D-20       | 2041.784 | 7    | 0      | 7      | 6   | 0     | 6     | 0 1 1            | 0 1 0         | 161 | 0.069            | 0.060             |
| 3866.110               | 3866.1094             | -2          | C 0.261D-20       | 586.243  | 7    | 2      | 6      | 7   | 0     | 7     | 0 0 1            | 0 0 0         | 161 | 0.213            |                   |
| 3866.759               | 3866.7610             | 23          | C 0.356D-21       | 1437.969 | 10   | 4      | 7      | 10  | 2     | 8     | 0 0 1            | 0 0 0         | 161 | 0.012            | 0.012             |
| 3867.680               | 3867.6805             |             | 0.156D-21         | 2904.429 | 10   | 2      | 8      | 10  | 2     | 9     | 0 1 1            | 0 1 0         | 161 | 0.009            | 0.006             |
| 3867.751               | 3867.7530             |             | 0.890D-21         | 1962.508 | 12   | 3      | 9      | 12  | 3     | 10    | 0 0 1            | 0 0 0         | 161 | 0.025            | 0.028             |
| 3868.232               | 3868.2319             | -3          | C 0.559D-21       | 704.214  | 7    | 4      | 3      | 7   | 1     | 6     | 1 0 0            | 0 0 0         | 161 | 0.036            | 0.037             |
| 3868.395               | 3868.3939             |             | 0.437D-21         | 3626.922 | 6    | 2      | 4      | 5   | 2     | 3     | 0 2 1            | 0 2 0         | 161 | 0.020            | 0.017             |
| 3868.503               | 3868.5032             |             | 0.120D-20         | 2552.858 | 7    | 5      | 3      | 6   | 5     | 2     | 0 1 1            | 0 1 0         | 161 | 0.041            | 0.040             |
| 3868.626               | 3868.6265             | 4           | C 0.308D-21       | 982.912  | 8    | 4      | 5      | 8   | 2     | 6     | 0 0 1            | 0 0 0         | 161 | 0.013            | 0.014             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C      | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_{\text{a}}$ | $K'_{\text{c}}$ | $J$ | $K_{\text{a}}$ | $K_{\text{c}}$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|-------------|-------------------|----------|------|-----------------|-----------------|-----|----------------|----------------|------------------|---------------|-----|------------------|-------------------|
| 3868.659               | 3868.6597             | 77          | H 0.398D-21       | 2552.880 | 7    | 5               | 2               | 6   | 5              | 1              | 0 1 1            | 0 1 0         | 161 | 0.012            | 0.013             |
| 3869.193               | 3869.1931             | -1          | S 0.193D-19       | 326.625  | 6    | 1               | 6               | 5   | 1              | 5              | 0 0 1            | 0 0 0         | 161 |                  | 2.835             |
| 3869.923               | 3869.9249             | 16          | S 0.199D-20       | 1079.080 | 9    | 3               | 7               | 9   | 1              | 8              | 0 0 1            | 0 0 0         | 161 | 0.078            | 0.081             |
| 3870.130               | 3870.1356             | 61          | S 0.580D-19       | 325.348  | 6    | 0               | 6               | 5   | 0              | 5              | 0 0 1            | 0 0 0         | 161 |                  | 8.546             |
| 3870.822               | 3870.8210             | -5          | C 0.115D-21       | 445.346  | 7    | 1               | 7               | 6   | 1              | 6              | 0 0 1            | 0 0 0         | 181 | 0.013            | 0.013             |
| 3871.082               | 3871.0825             | 5           | C 0.545D-21       | 224.838  | 5    | 2               | 3               | 4   | 1              | 4              | 1 0 0            | 0 0 0         | 161 | 0.092            | 0.104             |
| 3871.453               | 3871.4529             | -5          | C 0.301D-20       | 742.073  | 6    | 5               | 2               | 5   | 5              | 1              | 0 0 1            | 0 0 0         | 161 | 0.183            | 0.186             |
| 3871.497               | 3871.4968             | -4          | C 0.904D-20       | 742.076  | 6    | 5               | 1               | 5   | 5              | 0              | 0 0 1            | 0 0 0         | 161 | 0.550            | 0.557             |
| 3871.799               | 3871.7979             |             | 0.293D-20         | 2130.495 | 6    | 3               | 3               | 5   | 3              | 2              | 0 1 1            | 0 1 0         | 161 | 0.100            | 0.094             |
| 3872.735               | 3872.7369             |             | 0.912D-21         | 1690.665 | 11   | 4               | 8               | 11  | 2              | 9              | 0 0 1            | 0 0 0         | 161 | 0.027            | 0.029             |
| 3873.725               | 3873.7247             | 1           | C 0.509D-20       | 382.517  | 5    | 4               | 1               | 4   | 3              | 2              | 1 0 0            | 0 0 0         | 161 | 0.580            | 0.652             |
| 3873.882               | 3873.8837             | 21          | C 0.481D-20       | 2000.866 | 6    | 1               | 5               | 5   | 1              | 4              | 0 1 1            | 0 1 0         | 161 | 0.161            | 0.153             |
| 3873.944               | 3873.9451             | 5           | C 0.387D-20       | 383.842  | 5    | 4               | 2               | 4   | 3              | 1              | 1 0 0            | 0 0 0         | 161 | 0.436            | 0.494             |
| 3874.402               | 3874.4026             | 0           | S 0.164D-19       | 275.497  | 5    | 1               | 4               | 4   | 1              | 3              | 0 0 1            | 0 0 0         | 161 |                  | 2.737             |
| 3876.284               | 3876.2840             | 5           | C 0.979D-22       | 398.361  | 6    | 1               | 5               | 5   | 1              | 4              | 0 0 1            | 0 0 0         | 181 | 0.010            | 0.012             |
| 3876.565               | 3876.5646             | -3          | C 0.646D-21       | 782.410  | 7    | 4               | 4               | 7   | 2              | 5              | 0 0 1            | 0 0 0         | 161 | 0.033            | 0.037             |
| 3877.426               | 3877.4257             | 4           | C 0.170D-20       | 1293.634 | 10   | 2               | 8               | 10  | 2              | 9              | 0 0 1            | 0 0 0         | 161 | 0.059            | 0.060             |
| 3877.684               | 3877.6798             |             | 0.471D-21         | 3895.253 | 9    | 1               | 9               | 8   | 1              | 8              | 0 2 1            | 0 2 0         | 161 | 0.021            | 0.020             |
| 3878.513               | 3878.5188             | 152         | H 0.679D-21       | 2905.435 | 8    | 6               | 2               | 7   | 6              | 1              | 0 1 1            | 0 1 0         | 161 | 0.028            | 0.024             |
| 3879.484               | 3879.4821             | -15         | H 0.211D-20       | 2398.382 | 7    | 4               | 4               | 6   | 4              | 3              | 0 1 1            | 0 1 0         | 161 | 0.069            | 0.069             |
| 3879.788               | 3879.7853             | -10         | C 0.423D-20       | 2161.286 | 7    | 2               | 6               | 6   | 2              | 5              | 0 1 1            | 0 1 0         | 161 | 0.145            | 0.136             |
| 3879.950               | 3879.9500             | 0           | C 0.672D-20       | 610.114  | 6    | 4               | 3               | 5   | 4              | 2              | 0 0 1            | 0 0 0         | 161 | 0.503            | 0.523             |
| 3880.140               | 3880.1415             | 13          | C 0.216D-20       | 744.163  | 8    | 1               | 7               | 8   | 1              | 8              | 0 0 1            | 0 0 0         | 161 | 0.121            | 0.132             |
| 3880.192               | 3880.1911             | -10         | C 0.140D-19       | 315.779  | 5    | 2               | 3               | 4   | 2              | 2              | 0 0 1            | 0 0 0         | 161 |                  | 2.107             |
| 3880.355               | 3880.3552             | 5           | C 0.126D-19       | 416.209  | 6    | 2               | 5               | 5   | 2              | 4              | 0 0 1            | 0 0 0         | 161 | 1.347            | 1.487             |
| 3880.952               | 3880.9531             |             | 0.170D-20         | 2181.092 | 8    | 1               | 8               | 7   | 1              | 7              | 0 1 1            | 0 1 0         | 161 | 0.053            | 0.055             |
| 3881.029               | 3881.0285             | -3          | C 0.201D-19       | 610.341  | 6    | 4               | 2               | 5   | 4              | 1              | 0 0 1            | 0 0 0         | 161 | 1.502            | 1.564             |
| 3881.278               | 3881.2762             | 8           | C 0.510D-20       | 2180.644 | 8    | 0               | 8               | 7   | 0              | 7              | 0 1 1            | 0 1 0         | 161 | 0.182            | 0.164             |
| 3881.873               | 3881.8728             | -5          | C 0.697D-21       | 744.064  | 8    | 2               | 7               | 8   | 0              | 8              | 0 0 1            | 0 0 0         | 161 | 0.041            | 0.043             |
| 3882.070               | 3882.0692             |             | 0.699D-21         | 2399.166 | 7    | 4               | 3               | 6   | 4              | 2              | 0 1 1            | 0 1 0         | 161 | 0.023            | 0.023             |
| 3882.937               | 3882.9371             | 12          | C 0.514D-21       | 1293.019 | 10   | 3               | 8               | 10  | 1              | 9              | 0 0 1            | 0 0 0         | 161 | 0.017            | 0.018             |
| 3883.267               | 3883.2662             | -9          | C 0.890D-20       | 503.968  | 6    | 3               | 4               | 5   | 3              | 3              | 0 0 1            | 0 0 0         | 161 | 0.828            | 0.861             |
| 3884.005               | 3884.0048             | -5          | C 0.544D-20       | 1045.058 | 7    | 6               | 2               | 6   | 6              | 1              | 0 0 1            | 0 0 0         | 161 | 0.276            | 0.228             |
| 3884.014               |                       | D 0.181D-20 | 1045.059          | 7        | 6    | 1               | 6               | 6   | 0              | 0 0 1          | 0 0 0            | 161           |     | 0.076            |                   |
| 3884.792               | 3884.7896             | 3           | H 0.309D-20       | 2271.712 | 7    | 3               | 5               | 6   | 3              | 4              | 0 1 1            | 0 1 0         | 161 | 0.102            | 0.100             |
| 3884.876               | 3884.8753             | -3          | C 0.872D-22       | 550.452  | 7    | 2               | 6               | 6   | 2              | 5              | 0 0 1            | 0 0 0         | 181 | 0.009            | 0.008             |
| 3885.266               | 3885.2668             |             | 0.324D-21         | 1813.224 | 11   | 5               | 7               | 11  | 3              | 8              | 0 0 1            | 0 0 0         | 161 | 0.012            | 0.010             |
| 3885.272               |                       | D 0.426D-22 | 2392.594          | 7        | 4    | 4               | 7               | 2   | 5              | 0 1 1          | 0 1 0            | 161           |     | 0.001            |                   |
| 3885.370               | 3885.3669             | 3           | C 0.421D-20       | 2053.969 | 6    | 2               | 4               | 5   | 2              | 3              | 0 1 1            | 0 1 0         | 161 | 0.143            | 0.134             |
| 3885.652               |                       | D 0.842D-20 | 508.812           | 6        | 4    | 3               | 5               | 3   | 2              | 1              | 0 0 1            | 0 0 0         | 161 |                  | 0.806             |
| 3885.660               | 3885.6508             | -15         | C 0.556D-19       | 447.252  | 7    | 1               | 7               | 6   | 1              | 6              | 0 0 1            | 0 0 0         | 161 |                  | 6.101             |
| 3886.078               | 3886.0767             | -10         | C 0.185D-19       | 446.697  | 7    | 0               | 7               | 6   | 0              | 6              | 0 0 1            | 0 0 0         | 161 |                  | 2.032             |
| 3886.924               | 3886.9234             | -1          | C 0.104D-21       | 583.779  | 8    | 0               | 8               | 7   | 0              | 7              | 0 0 1            | 0 0 0         | 181 | 0.007            | 0.009             |
| 3887.028               |                       | D 0.617D-22 | 3244.601          | 15       | 6    | 10              | 15              | 4   | 11             | 0 0 1          | 0 0 0            | 161           |     | 0.002            |                   |
| 3887.031               | 3887.0310             | -2          | H 0.340D-21       | 3306.296 | 9    | 7               | 3               | 8   | 7              | 2              | 0 1 1            | 0 1 0         | 161 | 0.018            | 0.013             |
| 3887.039               |                       | D 0.113D-21 | 3306.296          | 9        | 7    | 2               | 8               | 7   | 1              | 0 1 1          | 0 1 0            | 161           |     | 0.004            |                   |
| 3888.011               | 3888.0066             |             | 0.405D-21         | 3879.336 | 8    | 1               | 7               | 7   | 1              | 6              | 0 2 1            | 0 2 0         | 161 | 0.022            | 0.017             |
| 3888.727               | 3888.7245             | -32         | H 0.148D-20       | 2146.265 | 7    | 1               | 6               | 6   | 1              | 5              | 0 1 1            | 0 1 0         | 161 | 0.054            | 0.047             |
| 3889.645               | 3889.6439             | -2          | C 0.873D-22       | 445.159  | 6    | 2               | 4               | 5   | 2              | 3              | 0 0 1            | 0 0 0         | 181 | 0.008            | 0.010             |
| 3891.300               | 3891.3011             | 9           | S 0.479D-19       | 399.457  | 6    | 1               | 5               | 5   | 1              | 4              | 0 0 1            | 0 0 0         | 161 |                  | 5.864             |
| 3891.804               | 3891.8002             |             | 0.128D-20         | 2724.168 | 8    | 5               | 3               | 7   | 5              | 2              | 0 1 1            | 0 1 0         | 161 | 0.042            | 0.044             |
| 3892.003               | 3892.0015             | -14         | C 0.250D-20       | 416.209  | 6    | 3               | 3               | 5   | 2              | 4              | 1 0 0            | 0 0 0         | 161 | 0.273            | 0.294             |
| 3892.009               |                       | D 0.360D-22 | 5778.039          | 11       | 1    | 11              | 10              | 1   | 10             | 0 3 1          | 0 3 0            | 161           |     | 0.002            |                   |
| 3892.145               | 3892.1435             |             | 0.482D-21         | 2246.888 | 13   | 4               | 10              | 13  | 2              | 11             | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.016             |
| 3892.827               | 3892.8271             | -6          | C 0.526D-21       | 70.091   | 3    | 2               | 1               | 2   | 0              | 2              | 0 0 1            | 0 0 0         | 161 | 0.120            | 0.152             |
| 3892.998               | 3892.9934             |             | 0.396D-21         | 4068.704 | 10   | 0               | 10              | 9   | 0              | 9              | 0 2 1            | 0 2 0         | 161 | 0.019            | 0.017             |
| 3893.667               | 3893.6674             | -16         | C 0.387D-21       | 1525.137 | 11   | 2               | 9               | 11  | 2              | 10             | 0 0 1            | 0 0 0         | 161 | 0.013            | 0.013             |
| 3894.064               | 3894.0622             | -15         | C 0.131D-19       | 888.599  | 7    | 5               | 3               | 6   | 5              | 2              | 0 0 1            | 0 0 0         | 161 | 0.652            | 0.649             |
| 3894.288               | 3894.2874             | -4          | C 0.435D-20       | 888.632  | 7    | 5               | 2               | 6   | 5              | 1              | 0 0 1            | 0 0 0         | 161 | 0.217            | 0.215             |
| 3894.948               | 3894.9470             |             | 0.337D-21         | 4071.733 | 9    | 2               | 8               | 8   | 2              | 7              | 0 2 1            | 0 2 0         | 161 | 0.018            | 0.014             |
| 3895.147               |                       | D 0.100D-20 | 1394.814          | 8        | 7    | 2               | 7               | 7   | 1              | 0 0 1          | 0 0 0            | 161           |     | 0.034            |                   |
| 3895.148               | 3895.1459             | 14          | C 0.301D-20       | 1394.814 | 8    | 7               | 1               | 7   | 7              | 0              | 0 0 1            | 0 0 0         | 161 | 0.130            | 0.102             |
| 3896.334               |                       | D 0.907D-22 | 1538.150          | 10       | 5    | 6               | 10              | 3   | 7              | 0 0 1          | 0 0 0            | 161           |     | 0.003            |                   |
| 3896.338               | 3896.3386             | -8          | H 0.446D-20       | 2337.669 | 9    | 1               | 9               | 8   | 1              | 8              | 0 1 1            | 0 1 0         | 161 | 0.164            | 0.145             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF | C | $S_{\text{calc}}$ | $E''$    | J  | $K_a'$ | $K_c'$ | J  | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |     |       |       |        |
|------------------------|-----------------------|------|---|-------------------|----------|----|--------|--------|----|-------|-------|------------------|---------------|-----|------------------|-------------------|-----|-------|-------|--------|
| 3896.419               | 3896.4205             | 10   | C | 0.111D-20         | 1524.849 | 11 | 3      | 9      | 11 | 1     | 10    | 0                | 0             | 1   | 0                | 0                 | 161 | 0.036 | 0.036 |        |
| 3896.483               | 3896.4849             | 19   | C | 0.149D-20         | 2337.468 | 9  | 0      | 9      | 8  | 0     | 8     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.054 | 0.049  |
| 3896.484               |                       |      | D | 0.163D-22         | 445.794  | 6  | 2      | 4      | 5  | 2     | 3     | 0                | 0             | 1   | 0                | 0                 | 0   | 171   |       | 0.002  |
| 3896.624               | 3896.6231             | -14  | H | 0.128D-20         | 2318.541 | 8  | 2      | 7      | 7  | 2     | 6     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.044 | 0.042  |
| 3896.781               | 3896.7814             | 8    | C | 0.533D-21         | 920.211  | 9  | 1      | 8      | 9  | 1     | 9     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.027 | 0.025  |
| 3897.248               | 3897.2454             | -4   | H | 0.731D-21         | 2282.591 | 7  | 3      | 4      | 6  | 3     | 3     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.022 | 0.024  |
| 3897.567               | 3897.5679             | 7    | C | 0.158D-20         | 920.169  | 9  | 2      | 8      | 9  | 0     | 9     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.081 | 0.075  |
| 3897.974               | 3897.9739             | -2   | C | 0.221D-20         | 503.968  | 6  | 4      | 2      | 5  | 3     | 3     | 1                | 0             | 0   | 0                | 0                 | 0   | 161   | 0.203 | 0.213  |
| 3898.234               | 3898.2341             | -4   | C | 0.294D-20         | 508.812  | 6  | 6      | 1      | 5  | 3     | 2     | 0                | 2             | 0   | 0                | 0                 | 0   | 161   | 0.209 | 0.280  |
| 3898.762               | 3898.7604             | -0   | C | 0.172D-21         | 446.511  | 5  | 4      | 2      | 5  | 2     | 3     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.017 | -0.019 |
| 3899.217               | 3899.2166             | -7   | C | 0.216D-19         | 508.812  | 6  | 3      | 3      | 5  | 3     | 2     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 2.060  |
| 3899.442               | 3899.4424             | 5    | S | 0.424D-19         | 552.912  | 7  | 2      | 6      | 6  | 2     | 5     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 3.684  |
| 3900.210               | 3900.2054             |      |   | 0.162D-21         | 4381.734 | 9  | 4      | 6      | 8  | 4     | 5     | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.010 | 0.007  |
| 3900.693               | 3900.6919             | 79   | H | 0.704D-21         | 3101.124 | 9  | 6      | 4      | 8  | 6     | 3     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.026 | 0.025  |
| 3901.657               |                       |      | D | 0.672D-21         | 2569.508 | 8  | 4      | 5      | 7  | 4     | 4     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   |       | 0.022  |
| 3901.667               | 3901.6653             | -17  | C | 0.169D-19         | 586.479  | 8  | 1      | 8      | 7  | 1     | 7     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 1.381 | 1.371  |
| 3901.847               | 3901.8451             | -23  | S | 0.508D-19         | 586.243  | 8  | 0      | 8      | 7  | 0     | 7     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 4.122  |
| 3902.250               | 3902.2498             | -5   | C | 0.218D-19         | 756.725  | 7  | 4      | 4      | 6  | 4     | 3     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 1.278 | 1.302  |
| 3902.311               | 3902.3086             |      |   | 0.391D-20         | 2309.731 | 8  | 1      | 7      | 7  | 1     | 6     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.120 | 0.127  |
| 3902.441               | 3902.4406             | -3   | C | 0.933D-21         | 661.549  | 7  | 4      | 4      | 6  | 3     | 3     | 1                | 0             | 0   | 0                | 0                 | 0   | 161   | 0.063 | 0.066  |
| 3904.189               | 3904.1879             | -11  | S | 0.429D-19         | 446.511  | 6  | 2      | 4      | 5  | 2     | 3     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 4.693  |
| 3904.295               | 3904.2948             | -1   | C | 0.281D-19         | 648.979  | 7  | 3      | 5      | 6  | 3     | 4     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 2.020  |
| 3904.586               | 3904.5838             |      |   | 0.945D-21         | 2439.956 | 8  | 3      | 6      | 7  | 3     | 5     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.031 | 0.031  |
| 3905.008               | 3905.0059             | 7    | C | 0.154D-20         | 1789.041 | 9  | 8      | 2      | 8  | 8     | 1     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.060 | 0.049  |
| 3905.008               |                       |      | D | 0.513D-21         | 1789.041 | 9  | 8      | 1      | 8  | 8     | 0     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 0.016  |
| 3905.371               | 3905.3705             | -1   | C | 0.711D-20         | 757.780  | 7  | 4      | 3      | 6  | 4     | 2     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.422 | 0.424  |
| 3905.591               | 3905.5844             |      |   | 0.282D-21         | 4052.837 | 8  | 3      | 5      | 7  | 3     | 4     | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.012 | 0.012  |
| 3906.065               | 3906.0643             | -10  | C | 0.148D-19         | 542.906  | 7  | 1      | 6      | 6  | 1     | 5     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 1.271 | 1.311  |
| 3906.164               | 3906.1584             | 7    | C | 0.256D-20         | 1216.189 | 8  | 6      | 3      | 7  | 6     | 2     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.086 | 0.094  |
| 3906.199               | 3906.1985             | 1    | C | 0.767D-20         | 1216.194 | 8  | 6      | 2      | 7  | 6     | 1     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.274 | 0.281  |
| 3907.224               | 3907.2210             |      |   | 0.321D-21         | 4260.469 | 11 | 1      | 11     | 10 | 1     | 10    | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.016 | 0.014  |
| 3907.445               | 3907.4436             |      |   | 0.131D-20         | 2211.192 | 7  | 2      | 5      | 6  | 2     | 4     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.047 | 0.042  |
| 3907.755               | 3907.7526             | -6   | H | 0.198D-20         | 2572.140 | 8  | 4      | 4      | 7  | 4     | 3     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.065 | 0.066  |
| 3908.584               | 3908.5818             |      |   | 0.772D-21         | 1774.752 | 12 | 2      | 10     | 12 | 2     | 11    | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.023 | 0.024  |
| 3908.626               | 3908.6281             | 62   | H | 0.345D-21         | 3526.630 | 10 | 7      | 3      | 9  | 7     | 2     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.013 | 0.013  |
| 3910.538               | 3910.5387             | -16  | C | 0.198D-21         | 1282.919 | 9  | 5      | 5      | 9  | 3     | 6     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.006 | 0.007  |
| 3910.770               | 3910.7732             |      |   | 0.322D-21         | 2282.591 | 7  | 4      | 4      | 6  | 3     | 3     | 1                | 1             | 0   | 0                | 1                 | 0   | 161   | 0.014 | 0.010  |
| 3911.346               | 3911.3442             |      |   | 0.125D-20         | 2512.378 | 10 | 1      | 10     | 9  | 1     | 9     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.044 | 0.041  |
| 3911.427               | 3911.4267             |      |   | 0.374D-20         | 2512.283 | 10 | 0      | 10     | 9  | 0     | 9     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.138 | 0.124  |
| 3911.768               | 3911.7625             |      |   | 0.345D-21         | 3967.489 | 8  | 2      | 6      | 7  | 2     | 5     | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.019 | 0.014  |
| 3911.949               | 3911.9526             |      |   | 0.881D-22         | 4784.664 | 10 | 5      | 5      | 9  | 5     | 4     | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.006 | 0.004  |
| 3912.339               | 3912.3379             | -7   | H | 0.319D-20         | 2495.168 | 9  | 2      | 8      | 8  | 2     | 7     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.115 | 0.105  |
| 3912.707               | 3912.7069             | 5    | C | 0.115D-20         | 1114.550 | 10 | 1      | 9      | 10 | 1     | 10    | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.050 | 0.045  |
| 3912.834               | 3912.8357             |      |   | 0.350D-22         | 2705.097 | 10 | 2      | 9      | 10 | 0     | 10    | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.004 | 0.001  |
| 3913.027               | 3913.0283             | 8    | C | 0.370D-21         | 1114.534 | 10 | 2      | 9      | 10 | 0     | 10    | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.015 | 0.014  |
| 3913.319               | 3913.3166             |      |   | 0.280D-21         | 4263.148 | 10 | 1      | 9      | 9  | 1     | 8     | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.014 | 0.012  |
| 3913.572               | 3913.5736             | 11   | H | 0.119D-20         | 2919.634 | 9  | 5      | 5      | 8  | 5     | 4     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.042 | 0.042  |
| 3913.854               | 3913.8538             | 13   | H | 0.725D-21         | 2225.468 | 10 | 9      | 1      | 9  | 9     | 0     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.027 | 0.023  |
| 3913.854               |                       |      | D | 0.242D-21         | 2225.468 | 10 | 9      | 2      | 9  | 9     | 1     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 0.008  |
| 3914.037               | 3914.0371             | -2   | C | 0.930D-21         | 842.357  | 8  | 4      | 5      | 7  | 3     | 4     | 1                | 0             | 0   | 0                | 0                 | 0   | 161   | 0.047 | 0.049  |
| 3915.142               | 3915.1434             |      |   | 0.543D-21         | 2462.876 | 8  | 4      | 5      | 7  | 3     | 4     | 1                | 1             | 0   | 0                | 1                 | 0   | 161   | 0.017 | 0.018  |
| 3915.256               | 3915.2553             | -7   | H | 0.394D-21         | 2920.133 | 9  | 5      | 4      | 8  | 5     | 3     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.015 | 0.014  |
| 3915.671               | 3915.6687             |      |   | 0.111D-20         | 2490.355 | 9  | 1      | 8      | 8  | 1     | 7     | 0                | 1             | 1   | 0                | 1                 | 0   | 161   | 0.040 | 0.037  |
| 3916.329               | 3916.3279             | -15  | C | 0.129D-19         | 709.609  | 8  | 2      | 7      | 7  | 2     | 6     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.839 | 0.830  |
| 3916.379               |                       |      |   | 0.622D-21         | 610.341  | 6  | 5      | 2      | 5  | 4     | 1     | 1                | 0             | 0   | 0                | 0                 | 161 |       | 0.048 |        |
| 3916.397               | 3916.3961             | -4   | C | 0.461D-20         | 1059.647 | 8  | 5      | 4      | 7  | 5     | 3     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.187 | 0.189  |
| 3916.606               | 3916.6056             | -1   | C | 0.194D-21         | 610.114  | 6  | 5      | 1      | 5  | 4     | 2     | 1                | 0             | 0   | 0                | 0                 | 0   | 161   | 0.014 | 0.015  |
| 3916.786               | 3916.7863             | 2    | C | 0.411D-20         | 1590.690 | 9  | 7      | 3      | 8  | 7     | 2     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.153 | 0.132  |
| 3916.795               |                       |      | D | 0.137D-20         | 1590.691 | 9  | 7      | 2      | 8  | 7     | 1     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 0.044  |
| 3917.209               | 3917.2084             | -6   | C | 0.138D-19         | 1059.835 | 8  | 5      | 3      | 7  | 5     | 2     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.554 | 0.565  |
| 3917.286               | 3917.2847             | -16  | S | 0.443D-19         | 744.163  | 9  | 1      | 9      | 8  | 1     | 8     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 2.689  |
| 3917.363               | 3917.3633             | 1    | C | 0.148D-19         | 744.064  | 9  | 0      | 9      | 8  | 0     | 8     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   | 0.922 | 0.899  |
| 3920.089               | 3920.0884             | -7   | S | 0.394D-19         | 704.214  | 8  | 1      | 7      | 7  | 1     | 6     | 0                | 0             | 1   | 0                | 0                 | 0   | 161   |       | 2.555  |
| 3921.462               | 3921.4560             |      |   | 0.250D-21         | 4469.734 | 12 | 0      | 12     | 11 | 0     | 11    | 0                | 2             | 1   | 0                | 2                 | 0   | 161   | 0.015 | 0.011  |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v'_1 v'_2 v'_3$ | $v_1 v_2 v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|------------------|---------------|-----|------------------|-------------------|
| 3922.835               | 3922.8331             | -21    | H 0.176D-20       | 2764.699 | 9    | 4      | 6      | 8   | 4     | 5     | 0 1 1            | 0 1 0         | 161 | 0.060            | 0.060             |
| 3922.941               | 3922.9387             |        | 0.632D-21         | 3321.013 | 10   | 6      | 4      | 9   | 6     | 3     | 0 1 1            | 0 1 0         | 161 | 0.020            | 0.024             |
| 3923.006               | 3923.0058             |        | 0.245D-20         | 2630.194 | 9    | 3      | 7      | 8   | 3     | 6     | 0 1 1            | 0 1 0         | 161 | 0.085            | 0.082             |
| 3923.168               | 3923.1632             |        | 0.494D-21         | 2042.312 | 13   | 3      | 11     | 13  | 1     | 12    | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.016             |
| 3923.467               | 3923.4675             | -6     | C 0.507D-20       | 648.979  | 7    | 4      | 3      | 6   | 3     | 4     | 1 0 0            | 0 0 0         | 161 | 0.364            | 0.363             |
| 3923.794               | 3923.7944             | 1      | C 0.682D-20       | 927.744  | 8    | 4      | 5      | 7   | 4     | 4     | 0 0 1            | 0 0 0         | 161 | 0.319            | 0.319             |
| 3924.068               | 3924.0608             |        | 0.219D-21         | 4483.227 | 11   | 2      | 10     | 10  | 2     | 9     | 0 2 1            | 0 2 0         | 161 | 0.010            | 0.010             |
| 3924.373               | 3924.3735             | 4      | C 0.927D-20       | 816.694  | 8    | 3      | 6      | 7   | 3     | 5     | 0 0 1            | 0 0 0         | 161 | 0.508            | 0.502             |
| 3925.135               | 3925.1340             | -5     | C 0.998D-20       | 661.549  | 7    | 3      | 4      | 6   | 3     | 3     | 0 0 1            | 0 0 0         | 161 | 0.719            | 0.697             |
| 3925.176               | 3925.1765             | -4     | C 0.132D-19       | 602.774  | 7    | 2      | 5      | 6   | 2     | 4     | 0 0 1            | 0 0 0         | 161 | 1.017            | 1.031             |
| 3926.027               |                       |        | D 0.681D-21       | 2009.805 | 10   | 8      | 3      | 9   | 8     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.021             |
| 3926.028               |                       |        | D 0.204D-20       | 2009.805 | 10   | 8      | 2      | 9   | 8     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 0.064             |
| 3926.035               | 3926.0289             | 30     | C 0.303D-20       | 2705.141 | 11   | 1      | 11     | 10  | 1     | 10    | 0 1 1            | 0 1 0         | 161 | 0.184            | 0.103             |
| 3926.077               | 3926.0683             |        | 0.101D-20         | 2705.097 | 11   | 0      | 11     | 10  | 0     | 10    | 0 1 1            | 0 1 0         | 161 | 0.034            | 0.034             |
| 3926.115               |                       |        | D 0.256D-22       | 5064.137 | 13   | 10     | 4      | 12  | 10    | 3     | 0 1 1            | 0 1 0         | 161 |                  | 0.001             |
| 3926.125               | 3926.1240             |        | 0.338D-20         | 2392.594 | 8    | 2      | 6      | 7   | 2     | 5     | 0 1 1            | 0 1 0         | 161 | 0.115            | 0.110             |
| 3927.336               | 3927.3339             | -18    | H 0.902D-21       | 2690.595 | 10   | 2      | 9      | 9   | 2     | 8     | 0 1 1            | 0 1 0         | 161 | 0.034            | 0.030             |
| 3928.030               | 3928.0302             | 4      | C 0.791D-20       | 1411.612 | 9    | 6      | 4      | 8   | 6     | 3     | 0 0 1            | 0 0 0         | 161 | 0.252            | 0.264             |
| 3928.088               | 3928.0871             | -16    | C 0.268D-21       | 1327.119 | 11   | 1      | 10     | 11  | 1     | 11    | 0 0 1            | 0 0 0         | 161 | 0.009            | 0.009             |
| 3928.201               | 3928.2009             | -1     | C 0.263D-20       | 1411.647 | 9    | 6      | 3      | 8   | 6     | 2     | 0 0 1            | 0 0 0         | 161 | 0.083            | 0.088             |
| 3928.235               |                       |        | D 0.182D-22       | 222.052  | 5    | 3      | 3      | 4   | 0     | 4     | 1 0 0            | 0 0 0         | 161 |                  | 0.003             |
| 3928.238               | 3928.2372             | 18     | C 0.802D-21       | 1327.110 | 11   | 2      | 10     | 11  | 0     | 11    | 0 0 1            | 0 0 0         | 161 | 0.031            | 0.028             |
| 3929.131               | 3929.1287             |        | 0.272D-20         | 2688.080 | 10   | 1      | 9      | 9   | 1     | 8     | 0 1 1            | 0 1 0         | 161 | 0.098            | 0.092             |
| 3929.351               |                       |        | D 0.267D-22       | 416.209  | 5    | 4      | 1      | 5   | 2     | 4     | 0 0 1            | 0 0 0         | 161 |                  | 0.003             |
| 3929.361               | 3929.3609             | -4     | C 0.175D-20       | 136.761  | 4    | 2      | 2      | 3   | 0     | 3     | 0 0 1            | 0 0 0         | 161 | 0.341            | 0.415             |
| 3929.800               | 3929.7994             | -40    | H 0.303D-21       | 3770.713 | 11   | 7      | 5      | 10  | 7     | 4     | 0 1 1            | 0 1 0         | 161 | 0.010            | 0.012             |
| 3930.566               | 3930.5667             | 4      | C 0.190D-19       | 931.237  | 8    | 4      | 4      | 7   | 4     | 3     | 0 0 1            | 0 0 0         | 161 | 0.887            | 0.885             |
| 3931.370               | 3931.3697             |        | 0.233D-20         | 2462.876 | 8    | 3      | 5      | 7   | 3     | 4     | 0 1 1            | 0 1 0         | 161 | 0.084            | 0.076             |
| 3932.081               | 3932.0808             | -3     | C 0.929D-21       | 552.912  | 7    | 3      | 4      | 6   | 2     | 5     | 1 0 0            | 0 0 0         | 161 | 0.094            | 0.080             |
| 3932.136               | 3932.1352             | -5     | C 0.334D-19       | 885.600  | 9    | 2      | 8      | 8   | 2     | 7     | 0 0 1            | 0 0 0         | 161 | 1.757            | 1.644             |
| 3932.546               | 3932.5460             | 1      | C 0.124D-19       | 920.211  | 10   | 1      | 10     | 9   | 1     | 9     | 0 0 1            | 0 0 0         | 161 | 0.770            | 0.585             |
| 3932.581               | 3932.5820             | 8      | C 0.371D-19       | 920.169  | 10   | 0      | 10     | 9   | 0     | 9     | 0 0 1            | 0 0 0         | 161 | 1.991            | 1.749             |
| 3934.101               | 3934.1008             | 0      | C 0.112D-19       | 882.891  | 9    | 1      | 8      | 8   | 1     | 7     | 0 0 1            | 0 0 0         | 161 | 0.581            | 0.553             |
| 3934.266               |                       |        | D 0.310D-21       | 2471.254 | 11   | 9      | 2      | 10  | 9     | 1     | 0 0 1            | 0 0 0         | 161 |                  | 0.010             |
| 3934.266               | 3934.2628             | -61    | H 0.930D-21       | 2471.254 | 11   | 9      | 3      | 10  | 9     | 2     | 0 0 1            | 0 0 0         | 161 | 0.033            | 0.030             |
| 3934.407               | 3934.4048             | -26    | H 0.563D-21       | 2771.691 | 9    | 4      | 5      | 8   | 4     | 4     | 0 1 1            | 0 1 0         | 161 | 0.019            | 0.019             |
| 3935.130               | 3935.1305             | 2      | C 0.103D-21       | 95.176   | 3    | 3      | 0      | 2   | 1     | 1     | 0 0 1            | 0 0 0         | 161 | 0.021            | 0.027             |
| 3935.861               | 3935.8594             | -48    | H 0.137D-21       | 4265.980 | 12   | 8      | 4      | 11  | 8     | 3     | 0 1 1            | 0 1 0         | 161 | 0.005            | 0.006             |
| 3938.056               | 3938.0564             | -1     | C 0.539D-21       | 757.780  | 7    | 5      | 3      | 6   | 4     | 2     | 1 0 0            | 0 0 0         | 161 | 0.034            | 0.032             |
| 3938.078               | 3938.0793             |        | 0.137D-20         | 1810.584 | 10   | 7      | 4      | 9   | 7     | 3     | 0 0 1            | 0 0 0         | 161 | 0.041            | 0.043             |
| 3938.110               | 3938.1096             | -2     | C 0.411D-20       | 1810.589 | 10   | 7      | 3      | 9   | 7     | 2     | 0 0 1            | 0 0 0         | 161 | 0.118            | 0.129             |
| 3938.290               | 3938.2897             | -13    | C 0.127D-19       | 1255.167 | 9    | 5      | 5      | 8   | 5     | 4     | 0 0 1            | 0 0 0         | 161 | 0.443            | 0.451             |
| 3938.458               | 3938.4592             | 10     | C 0.921D-22       | 552.912  | 6    | 4      | 2      | 6   | 2     | 5     | 0 0 1            | 0 0 0         | 161 | 0.007            | 0.008             |
| 3938.985               | 3938.9927             |        | 0.167D-21         | 4714.828 | 12   | 1      | 11     | 11  | 1     | 10    | 0 2 1            | 0 2 0         | 161 | 0.010            | 0.008             |
| 3939.112               | 3939.1121             | 5      | C 0.132D-20       | 756.725  | 7    | 5      | 2      | 6   | 4     | 3     | 1 0 0            | 0 0 0         | 161 | 0.076            | 0.078             |
| 3939.396               | 3939.3985             | 8      | H 0.995D-21       | 3141.047 | 10   | 5      | 5      | 9   | 5     | 4     | 0 1 1            | 0 1 0         | 161 | 0.034            | 0.036             |
| 3939.977               | 3939.9777             | 23     | H 0.671D-21       | 2841.432 | 10   | 3      | 8      | 9   | 3     | 7     | 0 1 1            | 0 1 0         | 161 | 0.024            | 0.023             |
| 3940.404               | 3940.4023             |        | 0.787D-21         | 2915.897 | 12   | 1      | 12     | 11  | 1     | 11    | 0 1 1            | 0 1 0         | 161 |                  | 0.027             |
| 3940.404               |                       |        | 0.236D-20         | 2915.876 | 12   | 0      | 12     | 11  | 0     | 11    | 0 1 1            | 0 1 0         | 161 | 0.094            | 0.082             |
| 3940.588               |                       |        | D 0.107D-21       | 4842.137 | 11   | 4      | 8      | 10  | 4     | 7     | 0 2 1            | 0 2 0         | 161 |                  | 0.005             |
| 3940.589               | 3940.5899             | 9      | C 0.420D-20       | 1255.913 | 9    | 5      | 4      | 8   | 5     | 3     | 0 0 1            | 0 0 0         | 161 | 0.149            | 0.149             |
| 3941.275               | 3941.2793             | 37     | H 0.920D-21       | 2595.813 | 9    | 2      | 7      | 8   | 2     | 6     | 0 1 1            | 0 1 0         | 161 | 0.032            | 0.031             |
| 3941.532               |                       |        | D 0.130D-21       | 2972.824 | 12   | 10     | 3      | 11  | 10    | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.005             |
| 3941.532               | 3941.5294             | -21    | H 0.390D-21       | 2972.824 | 12   | 10     | 2      | 11  | 10    | 1     | 0 0 1            | 0 0 0         | 161 | 0.014            | 0.014             |
| 3941.680               | 3941.6786             | 0      | H 0.214D-20       | 2904.429 | 11   | 2      | 10     | 10  | 2     | 9     | 0 1 1            | 0 1 0         | 161 | 0.075            | 0.074             |
| 3942.636               |                       |        | 0.716D-21         | 2903.147 | 11   | 1      | 10     | 10  | 1     | 9     | 0 1 1            | 0 1 0         | 161 |                  | 0.025             |
| 3942.653               | 3942.6524             | -8     | C 0.340D-19       | 782.410  | 8    | 2      | 6      | 7   | 2     | 5     | 0 0 1            | 0 0 0         | 161 | 1.951            | 1.930             |
| 3942.762               | 3942.7612             | 75     | H 0.483D-21       | 2983.324 | 10   | 4      | 7      | 9   | 4     | 6     | 0 1 1            | 0 1 0         | 161 | 0.015            | 0.017             |
| 3942.887               | 3942.8860             | -12    | C 0.250D-19       | 1006.116 | 9    | 3      | 7      | 8   | 3     | 6     | 0 0 1            | 0 0 0         | 161 | 1.098            | 1.070             |
| 3943.008               | 3943.0088             | 8      | C 0.545D-21       | 1557.850 | 12   | 1      | 11     | 12  | 1     | 12    | 0 0 1            | 0 0 0         | 161 | 0.015            | 0.017             |
| 3944.045               | 3944.0457             | 4      | H 0.519D-21       | 3564.705 | 11   | 6      | 6      | 10  | 6     | 5     | 0 1 1            | 0 1 0         | 161 | 0.019            | 0.020             |
| 3944.368               | 3944.3685             | 1      | C 0.178D-19       | 1122.709 | 9    | 4      | 6      | 8   | 4     | 5     | 0 0 1            | 0 0 0         | 161 | 0.690            | 0.687             |
| 3946.610               | 3946.6099             | -6     | H 0.198D-20       | 2254.283 | 11   | 8      | 4      | 10  | 8     | 3     | 0 0 1            | 0 0 0         | 161 | 0.070            | 0.063             |
| 3946.613               |                       |        | D 0.660D-21       | 2254.284 | 11   | 8      | 3      | 10  | 8     | 2     | 0 0 1            | 0 0 0         | 161 |                  | 0.021             |

## HIGH-TEMPERATURE WATER VAPOR SPECTRUM

463

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF | C | $S_{\text{calc}}$ | $E''$    | J  | $K_a'$ | $K_c'$ | J  | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|------|---|-------------------|----------|----|--------|--------|----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3947.175               | 3947.1746             | 0    | C | 0.884D-20         | 1080.386 | 10 | 2      | 9      | 9  | 2     | 8     | 0 0 1          | 0 0 0       | 161 | 0.383            | 0.353             |
| 3947.470               | 3947.4648             | -50  | C | 0.299D-19         | 1114.550 | 11 | 1      | 11     | 10 | 1     | 10    | 0 0 1          | 0 0 0       | 161 | 1.471            | 1.160             |
| 3947.483               |                       |      |   | 0.998D-20         | 1114.534 | 11 | 0      | 11     | 10 | 0     | 10    | 0 0 1          | 0 0 0       | 161 |                  | 0.387             |
| 3948.177               | 3948.1771             | -2   | C | 0.276D-19         | 1079.080 | 10 | 1      | 9      | 9  | 1     | 8     | 0 0 1          | 0 0 0       | 161 | 1.180            | 1.102             |
| 3949.572               | 3949.5717             | -5   | C | 0.235D-20         | 1631.251 | 10 | 6      | 5      | 9  | 6     | 4     | 0 0 1          | 0 0 0       | 161 | 0.068            | 0.074             |
| 3949.984               | 3949.9845             | 1    | C | 0.289D-19         | 842.357  | 8  | 3      | 5      | 7  | 3     | 4     | 0 0 1          | 0 0 0       | 161 | 1.490            | 1.500             |
| 3950.140               | 3950.1419             | 5    | C | 0.705D-20         | 1631.384 | 10 | 6      | 4      | 9  | 6     | 3     | 0 0 1          | 0 0 0       | 161 | 0.202            | 0.223             |
| 3950.574               | 3950.5736             | 0    | C | 0.178D-21         | 79.496   | 3  | 3      | 1      | 2  | 1     | 2     | 0 0 1          | 0 0 0       | 161 | 0.042            | 0.049             |
| 3950.810               | 3950.8082             | -24  | H | 0.242D-21         | 4038.404 | 12 | 7      | 5      | 11 | 7     | 4     | 0 1 1          | 0 1 0       | 161 | 0.010            | 0.010             |
| 3952.345               | 3952.3441             | -2   | C | 0.831D-21         | 816.694  | 8  | 4      | 4      | 7  | 3     | 5     | 1 0 0          | 0 0 0       | 161 | 0.045            | 0.045             |
| 3953.098               | 3953.0971             | -5   | C | 0.774D-21         | 173.365  | 4  | 3      | 1      | 3  | 1     | 2     | 0 0 1          | 0 0 0       | 161 | 0.133            | 0.165             |
| 3953.711               | 3953.7062             |      |   | 0.216D-20         | 2818.398 | 10 | 2      | 8      | 9  | 2     | 7     | 0 1 1          | 0 1 0       | 161 | 0.077            | 0.074             |
| 3953.762               | 3953.7638             |      |   | 0.774D-21         | 2670.792 | 9  | 3      | 6      | 8  | 3     | 5     | 0 1 1          | 0 1 0       | 161 | 0.028            | 0.026             |
| 3954.159               |                       |      | D | 0.290D-21         | 2740.420 | 12 | 9      | 4      | 11 | 9     | 3     | 0 0 1          | 0 0 0       | 161 |                  | 0.010             |
| 3954.160               | 3954.1571             | -21  | H | 0.871D-21         | 2740.420 | 12 | 9      | 3      | 11 | 9     | 2     | 0 0 1          | 0 0 0       | 161 | 0.030            | 0.029             |
| 3954.420               | 3954.4165             | -39  | H | 0.178D-20         | 3144.579 | 13 | 1      | 13     | 12 | 1     | 12    | 0 1 1          | 0 1 0       | 161 | 0.069            | 0.064             |
| 3954.452               | 3954.4571             |      |   | 0.592D-21         | 3144.573 | 13 | 0      | 13     | 12 | 0     | 12    | 0 1 1          | 0 1 0       | 161 | 0.024            | 0.021             |
| 3955.241               | 3955.2420             | 4    | C | 0.443D-20         | 1131.776 | 9  | 4      | 5      | 8  | 4     | 4     | 0 0 1          | 0 0 0       | 161 | 0.165            | 0.169             |
| 3955.568               | 3955.5691             | 48   | H | 0.157D-20         | 3072.728 | 11 | 3      | 9      | 10 | 3     | 8     | 0 1 1          | 0 1 0       | 161 | 0.056            | 0.056             |
| 3956.061               | 3956.0588             | -22  | H | 0.163D-20         | 3135.766 | 12 | 1      | 11     | 11 | 1     | 10    | 0 1 1          | 0 1 0       | 161 | 0.059            | 0.058             |
| 3956.251               | 3956.2520             | 3    | H | 0.793D-21         | 3383.266 | 11 | 5      | 7      | 10 | 5     | 6     | 0 1 1          | 0 1 0       | 161 | 0.029            | 0.030             |
| 3956.883               | 3956.8824             | -1   | C | 0.925D-20         | 982.912  | 9  | 2      | 7      | 8  | 2     | 6     | 0 0 1          | 0 0 0       | 161 | 0.413            | 0.404             |
| 3957.536               | 3957.5340             |      |   | 0.358D-21         | 1806.672 | 13 | 2      | 12     | 13 | 0     | 13    | 0 0 1          | 0 0 0       | 161 | 0.011            | 0.011             |
| 3958.177               | 3958.1781             | 13   | C | 0.361D-21         | 888.599  | 7  | 6      | 1      | 6  | 5     | 2     | 1 0 0          | 0 0 0       | 161 | 0.013            | 0.018             |
| 3958.220               | 3958.2200             | -1   | C | 0.317D-20         | 931.237  | 8  | 5      | 4      | 7  | 4     | 3     | 1 0 0          | 0 0 0       | 161 | 0.147            | 0.147             |
| 3958.333               | 3958.3345             |      |   | 0.190D-21         | 4493.805 | 10 | 3      | 7      | 9  | 3     | 6     | 0 2 1          | 0 2 0       | 161 | 0.009            | 0.009             |
| 3959.019               | 3959.0199             | -10  | H | 0.355D-20         | 2054.348 | 11 | 7      | 5      | 10 | 7     | 4     | 0 0 1          | 0 0 0       | 161 | 0.096            | 0.111             |
| 3959.142               | 3959.1419             | -9   | H | 0.118D-20         | 2054.369 | 11 | 7      | 4      | 10 | 7     | 3     | 0 0 1          | 0 0 0       | 161 | 0.032            | 0.037             |
| 3959.503               | 3959.5027             | -2   | C | 0.355D-20         | 1474.981 | 10 | 5      | 6      | 9  | 5     | 5     | 0 0 1          | 0 0 0       | 161 | 0.109            | 0.115             |
| 3959.724               | 3959.7235             | -3   | C | 0.692D-20         | 1216.232 | 10 | 3      | 8      | 9  | 3     | 7     | 0 0 1          | 0 0 0       | 161 | 0.256            | 0.250             |
| 3960.654               | 3960.6577             | -27  | A | 0.128D-20         | 2998.768 | 10 | 4      | 6      | 9  | 4     | 5     | 0 1 1          | 0 1 0       | 161 | 0.041            | 0.045             |
| 3961.121               | 3961.1237             |      |   | 0.950D-22         | 2572.140 | 8  | 5      | 4      | 7  | 4     | 3     | 1 1 0          | 0 1 0       | 161 | 0.009            | 0.003             |
| 3961.304               | 3961.3056             | 0    | H | 0.113D-20         | 3224.548 | 11 | 4      | 8      | 10 | 4     | 7     | 0 1 1          | 0 1 0       | 161 | 0.039            | 0.041             |
| 3961.653               | 3961.6565             |      |   | 0.157D-21         | 173.365  | 4  | 4      | 1      | 3  | 1     | 2     | 1 0 0          | 0 0 0       | 161 | 0.046            | 0.033             |
| 3961.661               |                       |      | D | 0.626D-21         | 927.744  | 8  | 5      | 3      | 7  | 4     | 4     | 1 0 0          | 0 0 0       | 161 |                  | 0.029             |
| 3961.713               | 3961.7115             | -16  | C | 0.217D-19         | 1293.634 | 11 | 2      | 10     | 10 | 2     | 9     | 0 0 1          | 0 0 0       | 161 | 0.800            | 0.751             |
| 3962.035               |                       |      | D | 0.776D-20         | 1327.119 | 12 | 1      | 12     | 11 | 1     | 11    | 0 0 1          | 0 0 0       | 161 |                  | 0.265             |
| 3962.044               | 3962.0392             | -14  | C | 0.233D-19         | 1327.110 | 12 | 0      | 12     | 11 | 0     | 11    | 0 0 1          | 0 0 0       | 161 | 1.116            | 0.794             |
| 3962.187               | 3962.1873             | 1    | C | 0.725D-20         | 1293.019 | 11 | 1      | 10     | 10 | 1     | 9     | 0 0 1          | 0 0 0       | 161 | 0.267            | 0.251             |
| 3963.066               | 3963.0610             | -70  | H | 0.121D-21         | 4905.648 | 12 | 2      | 10     | 11 | 2     | 9     | 0 2 1          | 0 2 0       | 161 | 0.007            | 0.006             |
| 3963.843               | 3963.8422             | -2   | C | 0.493D-20         | 1340.886 | 10 | 4      | 7      | 9  | 4     | 6     | 0 0 1          | 0 0 0       | 161 | 0.162            | 0.167             |
| 3964.530               | 3964.5295             | -8   | H | 0.260D-21         | 3387.402 | 11 | 5      | 6      | 10 | 5     | 5     | 0 1 1          | 0 1 0       | 161 | 0.009            | 0.010             |
| 3964.800               | 3964.8009             | 5    | C | 0.104D-19         | 1477.297 | 10 | 5      | 5      | 9  | 5     | 4     | 0 0 1          | 0 0 0       | 161 | 0.316            | 0.337             |
| 3965.613               | 3965.6208             | 22   | H | 0.366D-21         | 3391.135 | 14 | 1      | 14     | 13 | 1     | 13    | 0 1 1          | 0 1 0       | 161 | 0.006            | 0.014             |
| 3966.773               | 3966.7720             | 46   | H | 0.166D-20         | 2522.267 | 12 | 8      | 4      | 11 | 8     | 3     | 0 0 1          | 0 0 0       | 161 | 0.045            | 0.054             |
| 3967.399               | 3967.3978             | -3   | H | 0.126D-20         | 3391.131 | 14 | 0      | 14     | 13 | 0     | 13    | 0 1 1          | 0 1 0       | 161 | 0.053            | 0.047             |
| 3967.504               | 3967.5000             |      |   | H 0.396D-21       | 3833.146 | 12 | 6      | 6      | 11 | 6     | 5     | 0 1 1          | 0 1 0       | 161 | 0.015            | 0.016             |
| 3967.562               | 3967.5617             | -5   | C | 0.569D-22         | 325.348  | 6  | 3      | 4      | 5  | 0     | 5     | 1 0 0          | 0 0 0       | 161 | 0.010            | 0.008             |
| 3968.999               | 3969.0014             |      |   | 0.120D-20         | 3386.382 | 13 | 2      | 12     | 12 | 2     | 11    | 0 1 1          | 0 1 0       | 161 | 0.045            | 0.045             |
| 3969.139               | 3969.1385             | -3   | C | 0.219D-19         | 1201.922 | 10 | 2      | 8      | 9  | 2     | 7     | 0 0 1          | 0 0 0       | 161 | 0.799            | 0.795             |
| 3969.331               | 3969.3329             | 6    | H | 0.400D-21         | 3386.053 | 13 | 1      | 12     | 12 | 1     | 11    | 0 1 1          | 0 1 0       | 161 | 0.016            | 0.015             |
| 3969.994               | 3969.9932             | -4   | H | 0.393D-21         | 3323.271 | 12 | 3      | 10     | 11 | 3     | 9     | 0 1 1          | 0 1 0       | 161 | 0.014            | 0.014             |
| 3970.681               | 3970.6805             | 0    | C | 0.575D-20         | 1874.974 | 11 | 6      | 6      | 10 | 6     | 5     | 0 0 1          | 0 0 0       | 161 | 0.156            | 0.178             |
| 3972.124               | 3972.1239             | -1   | C | 0.823D-20         | 1050.158 | 9  | 3      | 6      | 8  | 3     | 5     | 0 0 1          | 0 0 0       | 161 | 0.331            | 0.335             |
| 3972.245               | 3972.2446             | -12  | C | 0.191D-20         | 1875.464 | 11 | 6      | 5      | 10 | 6     | 4     | 0 0 1          | 0 0 0       | 161 | 0.050            | 0.059             |
| 3972.655               | 3972.6567             | 11   | C | 0.362D-21         | 275.497  | 5  | 3      | 2      | 4  | 1     | 3     | 0 0 1          | 0 0 0       | 161 | 0.051            | 0.059             |
| 3973.538               | 3973.5404             | -4   | H | 0.705D-21         | 3032.690 | 13 | 9      | 5      | 12 | 9     | 4     | 0 0 1          | 0 0 0       | 161 | 0.026            | 0.025             |
| 3973.543               |                       |      | D | 0.235D-21         | 3032.691 | 13 | 9      | 4      | 12 | 9     | 3     | 0 0 1          | 0 0 0       | 161 |                  | 0.008             |
| 3973.801               | 3973.8062             | 109  | H | 0.187D-20         | 2904.672 | 10 | 3      | 7      | 9  | 3     | 6     | 0 1 1          | 0 1 0       | 161 | 0.068            | 0.064             |
| 3973.919               | 3973.9188             | 0    | C | 0.425D-21         | 222.052  | 5  | 2      | 3      | 4  | 0     | 4     | 0 0 1          | 0 0 0       | 161 | 0.061            | 0.079             |
| 3974.753               | 3974.7526             | -2   | C | 0.493D-20         | 1360.236 | 10 | 5      | 6      | 9  | 4     | 5     | 1 0 0          | 0 0 0       | 161 | 0.155            | 0.165             |
| 3975.140               | 3975.1389             | -3   | C | 0.163D-19         | 1446.129 | 11 | 3      | 9      | 10 | 3     | 8     | 0 0 1          | 0 0 0       | 161 | 0.523            | 0.531             |
| 3975.771               |                       |      | D | 0.121D-20         | 3314.857 | 12 | 2      | 10     | 11 | 2     | 9     | 0 1 1          | 0 1 0       | 161 |                  | 0.044             |
| 3975.780               | 3975.7780             | -17  | C | 0.552D-20         | 1525.137 | 12 | 2      | 11     | 11 | 2     | 10    | 0 0 1          | 0 0 0       | 161 | 0.203            | 0.176             |

TABLE 2. Observed and calculated hot water vapor lines between 2965 and 4005 cm<sup>-1</sup>—Continued

| $\sigma_{\text{calc}}$ | $\sigma_{\text{obs}}$ | DIFF C | $S_{\text{calc}}$ | $E''$    | $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $v_1'v_2'v_3'$ | $v_1v_2v_3$ | ISO | $I_{\text{obs}}$ | $I_{\text{calc}}$ |
|------------------------|-----------------------|--------|-------------------|----------|------|--------|--------|-----|-------|-------|----------------|-------------|-----|------------------|-------------------|
| 3976.009               | 3976.0087             | 0      | C 0.166D-19       | 1524.849 | 12   | 1      | 11     | 11  | 1     | 10    | 0 0 1          | 0 0 0       | 161 | 0.536            | 0.530             |
| 3976.263               | 3976.2645             | 9      | C 0.175D-19       | 1557.850 | 13   | 1      | 13     | 12  | 1     | 12    | 0 0 1          | 0 0 0       | 161 | 0.772            | 0.556             |
| 3976.268               |                       |        | D 0.583D-20       | 1557.844 | 13   | 0      | 13     | 12  | 0     | 12    | 0 0 1          | 0 0 0       | 161 | 0.185            |                   |
| 3976.574               | 3976.5728             | -7     | C 0.211D-20       | 1131.776 | 9    | 5      | 5      | 8   | 4     | 4     | 1 0 0          | 0 0 0       | 161 | 0.079            | 0.080             |
| 3979.304               | 3979.3051             | 16     | H 0.275D-21       | 3583.372 | 14   | 10     | 4      | 13  | 10    | 3     | 0 0 1          | 0 0 0       | 161 | 0.012            | 0.011             |
| 3979.304               |                       |        | D 0.918D-22       | 3583.372 | 14   | 10     | 5      | 13  | 10    | 4     | 0 0 1          | 0 0 0       | 161 | 0.004            |                   |
| 3979.594               | 3979.5959             | -3     | H 0.930D-21       | 2321.814 | 12   | 7      | 6      | 11  | 7     | 5     | 0 0 1          | 0 0 0       | 161 | 0.023            | 0.030             |
| 3979.771               | 3979.7704             | 4      | C 0.838D-20       | 1718.719 | 11   | 5      | 7      | 10  | 5     | 6     | 0 0 1          | 0 0 0       | 161 | 0.238            | 0.261             |
| 3979.792               |                       |        | 0.724D-21         | 1059.835 | 8    | 6      | 3      | 7   | 5     | 2     | 1 0 0          | 0 0 0       | 161 | 0.029            |                   |
| 3979.967               | 3979.9686             | -13    | H 0.279D-20       | 2321.905 | 12   | 7      | 5      | 11  | 7     | 4     | 0 0 1          | 0 0 0       | 161 | 0.070            | 0.089             |
| 3980.835               | 3980.8347             | 1      | C 0.558D-20       | 1437.969 | 11   | 2      | 9      | 10  | 2     | 8     | 0 0 1          | 0 0 0       | 161 | 0.180            | 0.182             |
| 3981.131               | 3981.1274             | -19    | H 0.908D-21       | 3655.487 | 15   | 1      | 15     | 14  | 1     | 14    | 0 1 1          | 0 1 0       | 161 | 0.043            | 0.035             |
| 3981.132               |                       |        | D 0.303D-21       | 3655.486 | 15   | 0      | 15     | 14  | 0     | 14    | 0 1 1          | 0 1 0       | 161 | 0.012            |                   |
| 3982.064               | 3982.0636             | 2      | C 0.118D-19       | 1581.336 | 11   | 4      | 8      | 10  | 4     | 7     | 0 0 1          | 0 0 0       | 161 | 0.352            | 0.373             |
| 3982.290               | 3982.2894             | -4     | C 0.232D-21       | 275.497  | 5    | 4      | 2      | 4   | 1     | 3     | 1 0 0          | 0 0 0       | 161 | 0.033            | 0.038             |
| 3982.752               | 3982.7515             | 2      | H 0.833D-21       | 3654.050 | 14   | 1      | 13     | 13  | 1     | 12    | 0 1 1          | 0 1 0       | 161 | 0.037            | 0.032             |
| 3982.870               | 3982.8710             | 10     | C 0.989D-22       | 142.278  | 4    | 3      | 2      | 3   | 1     | 3     | 0 0 1          | 0 0 0       | 161 | 0.015            | 0.023             |
| 3983.487               | 3983.4857             | -13    | H 0.851D-21       | 3592.425 | 13   | 3      | 11     | 12  | 3     | 10    | 0 1 1          | 0 1 0       | 161 | 0.029            | 0.033             |
| 3983.764               | 3983.7631             |        | 0.232D-21         | 1806.672 | 14   | 3      | 12     | 13  | 0     | 13    | 0 2 0          | 0 0 0       | 161 | 0.011            | 0.007             |
| 3985.021               | 3985.0206             | 3      | C 0.195D-20       | 1122.709 | 9    | 5      | 4      | 8   | 4     | 5     | 1 0 0          | 0 0 0       | 161 | 0.076            | 0.074             |
| 3985.079               | 3985.0767             |        | 0.321D-21         | 1616.452 | 11   | 5      | 7      | 10  | 4     | 6     | 1 0 0          | 0 0 0       | 161 | 0.012            | 0.010             |
| 3986.006               | 3986.0058             | 2      | C 0.638D-21       | 1006.116 | 9    | 4      | 5      | 8   | 3     | 6     | 1 0 0          | 0 0 0       | 161 | 0.030            | 0.027             |
| 3986.442               | 3986.4449             | 11     | H 0.127D-20       | 2813.515 | 13   | 8      | 6      | 12  | 8     | 5     | 0 0 1          | 0 0 0       | 161 | 0.034            | 0.043             |
| 3986.520               | 3986.5262             | 112    | H 0.422D-21       | 2813.533 | 13   | 8      | 5      | 12  | 8     | 4     | 0 0 1          | 0 0 0       | 161 | 0.009            | 0.014             |
| 3986.983               | 3986.9878             | 64     | H 0.288D-21       | 3587.669 | 13   | 2      | 11     | 12  | 2     | 10    | 0 1 1          | 0 1 0       | 161 | 0.010            | 0.011             |
| 3989.456               |                       |        | D 0.408D-20       | 1695.071 | 12   | 3      | 10     | 11  | 3     | 9     | 0 0 1          | 0 0 0       | 161 | 0.127            |                   |
| 3989.456               | 3989.4538             | -8     | C 0.122D-19       | 1774.752 | 13   | 2      | 12     | 12  | 2     | 11    | 0 0 1          | 0 0 0       | 161 | 0.453            | 0.377             |
| 3989.569               | 3989.5693             | 8      | C 0.406D-20       | 1774.619 | 13   | 1      | 12     | 12  | 1     | 11    | 0 0 1          | 0 0 0       | 161 | 0.122            | 0.126             |
| 3989.828               | 3989.8257             | -4     | C 0.263D-20       | 1724.707 | 11   | 5      | 6      | 10  | 5     | 5     | 0 0 1          | 0 0 0       | 161 | 0.071            | 0.082             |
| 3990.216               |                       |        | D 0.517D-21       | 1006.116 | 9    | 6      | 3      | 8   | 3     | 6     | 0 2 0          | 0 0 0       | 161 | 0.022            |                   |
| 3990.220               | 3990.2147             | -8     | C 0.420D-20       | 1806.673 | 14   | 1      | 14     | 13  | 1     | 13    | 0 0 1          | 0 0 0       | 161 | 0.152            | 0.130             |
| 3990.271               | 3990.2723             | -2     | C 0.125D-19       | 1806.672 | 14   | 0      | 14     | 13  | 0     | 13    | 0 0 1          | 0 0 0       | 161 | 0.397            | 0.386             |
| 3990.443               | 3990.4449             | 34     | H 0.574D-21       | 3659.906 | 12   | 5      | 7      | 11  | 5     | 6     | 0 1 1          | 0 1 0       | 161 | 0.021            | 0.022             |
| 3990.713               | 3990.7125             | -13    | C 0.195D-19       | 1282.919 | 10   | 3      | 7      | 9   | 3     | 6     | 0 0 1          | 0 0 0       | 161 | 0.656            | 0.673             |
| 3991.174               | 3991.1766             | -5     | H 0.146D-20       | 2142.597 | 12   | 6      | 7      | 11  | 6     | 6     | 0 0 1          | 0 0 0       | 161 | 0.039            | 0.046             |
| 3992.420               | 3992.4198             | -2     | H 0.521D-21       | 3347.780 | 14   | 9      | 5      | 13  | 9     | 4     | 0 0 1          | 0 0 0       | 161 | 0.015            | 0.019             |
| 3992.670               | 3992.6686             | 4      | C 0.124D-19       | 1690.665 | 12   | 2      | 10     | 11  | 2     | 9     | 0 0 1          | 0 0 0       | 161 | 0.369            | 0.385             |
| 3993.996               | 3993.9988             | -29    | H 0.613D-21       | 3770.880 | 13   | 4      | 10     | 12  | 4     | 9     | 0 1 1          | 0 1 0       | 161 | 0.027            | 0.024             |
| 3994.110               |                       |        | D 0.207D-21       | 3937.576 | 16   | 1      | 16     | 15  | 1     | 15    | 0 1 1          | 0 1 0       | 161 | 0.008            |                   |
| 3994.111               | 3994.1114             | 8      | H 0.621D-21       | 3937.575 | 16   | 0      | 16     | 15  | 0     | 15    | 0 1 1          | 0 1 0       | 161 | 0.037            | 0.025             |
| 3994.844               | 3994.8423             | 27     | H 0.433D-20       | 2144.047 | 12   | 6      | 6      | 11  | 6     | 5     | 0 0 1          | 0 0 0       | 161 | 0.114            | 0.135             |
| 3995.007               |                       |        | 0.764D-21         | 399.457  | 6    | 4      | 3      | 5   | 1     | 4     | 1 0 0          | 0 0 0       | 161 | 0.091            |                   |
| 3995.027               | 3995.0275             | 3      | C 0.113D-19       | 1360.236 | 10   | 4      | 6      | 9   | 4     | 5     | 0 0 1          | 0 0 0       | 161 | 0.368            | 0.377             |
| 3995.980               | 3995.9756             | -17    | H 0.504D-21       | 3939.834 | 15   | 2      | 14     | 14  | 2     | 13    | 0 1 1          | 0 1 0       | 161 | 0.019            | 0.021             |
| 3998.769               | 3998.7660             | -49    | H 0.591D-21       | 3877.090 | 14   | 2      | 12     | 13  | 2     | 11    | 0 1 1          | 0 1 0       | 161 | 0.021            | 0.024             |
| 3998.833               | 3998.8323             | 1      | C 0.299D-20       | 1843.030 | 12   | 4      | 9      | 11  | 4     | 8     | 0 0 1          | 0 0 0       | 161 | 0.083            | 0.092             |
| 3998.890               | 3998.8898             | 18     | C 0.209D-20       | 1985.788 | 12   | 5      | 8      | 11  | 5     | 7     | 0 0 1          | 0 0 0       | 161 | 0.059            | 0.065             |
| 3999.750               | 3999.7478             | -6     | H 0.204D-20       | 2612.801 | 13   | 7      | 7      | 12  | 7     | 6     | 0 0 1          | 0 0 0       | 161 | 0.056            | 0.067             |
| 4000.730               |                       |        | 0.680D-21         | 2613.104 | 13   | 7      | 6      | 12  | 7     | 5     | 0 0 1          | 0 0 0       | 161 | 0.022            |                   |
| 4001.282               | 4001.2814             | 0      | C 0.981D-21       | 1255.167 | 9    | 6      | 3      | 8   | 5     | 4     | 1 0 0          | 0 0 0       | 161 | 0.033            | 0.034             |
| 4002.767               | 4002.7678             | 27     | C 0.288D-20       | 2042.374 | 14   | 2      | 13     | 13  | 2     | 12    | 0 0 1          | 0 0 0       | 161 | 0.083            | 0.089             |
| 4002.841               |                       |        | 0.933D-21         | 3441.040 | 12   | 3      | 9      | 11  | 3     | 8     | 0 1 1          | 0 1 0       | 161 | 0.035            |                   |
| 4002.863               | 4002.8608             | 4      | C 0.864D-20       | 2042.312 | 14   | 1      | 13     | 13  | 1     | 12    | 0 0 1          | 0 0 0       | 161 | 0.262            | 0.267             |
| 4002.972               | 4002.9667             | -11    | C 0.884D-20       | 1962.508 | 13   | 3      | 11     | 12  | 3     | 10    | 0 0 1          | 0 0 0       | 161 | 0.257            | 0.273             |
| 4003.591               | 4003.5882             | -7     | C 0.889D-20       | 2073.519 | 15   | 1      | 15     | 14  | 1     | 14    | 0 0 1          | 0 0 0       | 161 | 0.374            | 0.275             |
| 4003.592               |                       |        | D 0.296D-20       | 2073.518 | 15   | 0      | 15     | 14  | 0     | 14    | 0 0 1          | 0 0 0       | 161 | 0.092            |                   |
| 4004.705               | 4004.7052             | 28     | C 0.297D-20       | 1960.208 | 13   | 2      | 11     | 12  | 2     | 10    | 0 0 1          | 0 0 0       | 161 | 0.086            | 0.092             |

See footnotes to table 2 on next page.

## Footnotes to table 2:

 $\sigma_{\text{calc}}$ : calculated wavenumber in  $\text{cm}^{-1}$  $\sigma_{\text{obs}}$ : observed wavenumber in  $\text{cm}^{-1}$ DIFF: difference (in  $10^{-4} \text{ cm}^{-1}$ ) between  $\sigma_{\text{obs}}$  and previous measurements coded in the C column

C: code with the signification

C, cold water vapor data [1]

H, hot water vapor data [2]

D, blended line

S, very strong cold water line

A, theoretical wavenumber in [1]

B, hand measured wavenumber in [1]

 $S_{\text{calc}}$ : calculated intensity at 1000 K in  $\text{cm}^{-1}/\text{molecule cm}^{-2}$  $E'$ : lower level energy of the transition in  $\text{cm}^{-1}$  $J, K'_s, K'_c; J, K_s, K_c$ : upper and lower rotational quantum numbers of the transition $v'_1 v'_2 v'_3; v_1 v_2 v_3$ : upper and lower vibrational quantum numbers of the transitionISO: isotopic species; 161, 171, and 181 stand, respectively, for  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$  $I_{\text{obs}}$ : observed peak intensity in  $(\text{Torr m})^{-1}$  $I_{\text{calc}}$ : calculated peak intensity in  $(\text{Torr m})^{-1}$  using the temperature profile of figure 5.