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Product review

Instrumental and spectral parameters: their effect on and measurement by microwave limb sounding of the atmosphere

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Abstract

Microwave limb sounding is an important new technique for measuring the temperature of the middle atmosphere and the concentration of various trace species in it. The spectral resolution of the instruments used is such that the measurements are usually made at a number of frequencies across the width of a single spectral line. It is therefore important to model the line shape and the instrument response accurately as inaccurate modelling will lead to a poor match between the measured radiances and those re-calculated from the retrieved atmosphere. In this paper, we consider the 183.3 GHz rotational transition of the water molecule and the 184.4 GHz transition of ozone. These transitions have been used to measure water vapour and ozone in the middle atmosphere by two orbiting instruments: the Microwave Limb Sounder (MLS) on the Upper Atmosphere Research Satellite (UARS) and the Millimetre-wave Atmospheric Sounder (MAS) which was flown on the ATLAS platform on board the space shuttle. Both instruments have had similar problems matching measured and re-calculated 183 GHz radiances. We show that by allowing the retrieval algorithm to fit certain spectral and instrumental parameters in addition to the mixing ratio profiles, we can improve both the quality of the retrieved profiles and our knowledge of certain spectral parameters, in particular the pressure shift of the line. © 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

Microwave limb sounding is a technique for measuring the temperature and composition of the middle atmosphere. Microwave radiation which is thermally emitted by rotational transitions of various molecules is detected by an instrument whose field of view is scanned vertically across the Earth's limb. The instrument may be mounted on an aeroplane, a balloon or a satellite and

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typically consists of a parabolic dish antenna which is scanned mechanically. The radiation is converted to a much lower frequency by a heterodyne mixer and is then fed to a bank of filters or some other sort of spectrometer. The spectral resolution available is such that the spectrometer will normally have a large number of channels spread across the frequency range of a single emission line. Two such instruments, UARS MLS [1] and ATLAS/MAS [2] have been flown in recent years and others are planned for launch in the near future. In particular, Sub-Millimetre Radiometer (SMR) will be launched on the Swedish/French/Canadian ODIN satellite in the Autumn of 1999, EOS MLS will be launched on the EOS CHEM-1 satellite in December 2002 and Superconducting Submillimeter wave Limb Emission Sounder (SMILES) will be installed on the Japanese Experiment Module of the International Space Station in 2003.

2. Line shapes

Millimetre-wave transitions in the atmosphere have a line shape which is affected by both pressure and Doppler broadening. It is therefore usual to assume that the line shape is a Voigt function, a convolution of the Gaussian line shape of Doppler broadening and the Lorentzian line shape of pressure broadening. The Doppler line width may be calculated theoretically; it depends only on the temperature and the molecule mass. In the stratosphere and lower mesosphere pressure broadening is the dominant effect. The pressure broadened line width is directly proportional to the pressure and since the pressure changes by a factor of ten over a height range of 16 km, so does the line width. Unlike the Doppler width, calculation of the pressure broadening is very involved and has not been carried out for many lines of interest. It is usual to assume that the width has the form

$$\gamma_L = \gamma_0 \left(\frac{p}{p_0} \right) \left(\frac{T_0}{T} \right)^{n_\gamma}, \quad (1)$$

and to measure the two parameters γ_0 and n_γ in the laboratory. The parameter γ_0 is the half-width at pressure p_0 and temperature T_0 and is sometimes called the broadening coefficient; n_γ is called the temperature exponent. Both of these parameters depend not only on the emitting molecule but also on the molecule with which it is colliding. It is therefore important to measure the parameters for the emitting gas mixed with oxygen and nitrogen. If the emitting gas forms a large fraction of the atmosphere (e.g. H₂O in the troposphere) it is also important to measure the broadening caused by collisions of the emitting gas with itself — this is known as self-broadening. In this paper we restrict our attention to the middle atmosphere where self-broadening is not significant for O₃ or H₂O.

Theory [3] restricts n_γ to the range $0.5 \leq n_\gamma \leq 1$ if certain assumptions are made — with some molecule pairs n_γ can lie outside this range.

Pressure broadened lines often show a frequency shift $\Delta\nu$ which is also proportional to the pressure. We may assume that $\Delta\nu$ is given by

$$\Delta\nu = \Delta\nu_0 \left(\frac{p}{p_0} \right) \left(\frac{T_0}{T} \right)^{n_s}. \quad (2)$$

It can be shown theoretically [3] that the temperature exponent for the shift n_s is related to that of the broadening by the formula

$$n_s = \left(\frac{1}{4}\right) + \left(\frac{3}{2}\right)n_\gamma. \tag{3}$$

Calculation of $\Delta\nu_0$ is as involved as that of γ_0 but it is often not possible to measure $\Delta\nu_0$ and it is common to assume that it is zero. It is worth noting that for some lines $\Delta\nu_0$ is positive while for others it is negative.

The broadening coefficient of the 183.3 GHz transition of the water molecule has been measured by several groups [4–7]; typical values are in the region of 2.9 MHz at $p_0 = 1$ mb and $T_0 = 300$ K. The temperature exponent n_γ is approximately 0.75. The pressure shift $\Delta\nu_0$ is usually assumed to be zero. The broadening coefficient of the 184.4 GHz ozone line has been reported in the literature only once to our knowledge [8]; for this line $\gamma_0 = 2.37$ MHz/mb at $T_0 = 300$ K and $n_\gamma = 0.7$. As with the water vapour line, the pressure shift has not been measured and is usually taken to be zero.

3. The MLS instrument

3.1. Introduction

The UARS microwave limb sounder has two banks each of 15 filters, known as bands 5 and 6, centred on the 183.3 and 184.4 GHz lines, respectively. The filter centres and widths are as shown in Table 1.

The instrument is a heterodyne receiver and is sensitive to radiation at two parts of the spectrum known as sidebands, located symmetrically above and below the local oscillator frequency. The lower frequency sidebands for bands 5 and 6 are located at the positions of the 183.3 and 184.4 GHz lines. The response from the upper sideband is not filtered out, instead the local oscillator frequency is chosen to ensure that the upper sideband is located in a part of the spectrum where there are no strong lines. Fig. 1 shows the location of the sidebands with a plot of the absorption coefficient of the atmosphere superimposed.

The MLS antenna scans vertically across the Earth’s limb, beginning at a tangent height of about 90 km and ending at a tangent height close to zero. The results of a calculation of the radiance we would expect to measure in one particular filter is shown in Fig. 2.

Note that this radiance comes partly from one sideband and partly from another; the brightness measured by each sideband individually is also shown in the figure. If the brightness in the lower sideband is I_L and that in the upper sideband is I_U then the overall brightness is given by

$$I = \left(\frac{s}{1+s}\right)I_L + \left(\frac{1}{1+s}\right)I_U, \tag{4}$$

where s is a quantity called the sideband ratio. In an ideal double-sideband receiver, $s = 1$ and $I = (I_L + I_U)/2$ but in practice s varies from channel to channel and has to be measured when the instrument is calibrated. Note that the radiances are most sensitive to the mixing ratio where they are changing rapidly with altitude (45–55 km in the example shown). The vertical part of the curve (20–35 km in Fig. 2) is mainly dependent on the temperature and the sideband ratio.

Table 1

Nominal filter widths and positions for MLS bands 5 and 6. The filter centre frequencies are given with respect to the line frequency. Note that channel 76 is not used due to a technical problem

Band 5 channel	Band 6 channel	Width/MHz	Centre frequency/MHz
61	90	128	– 191
62	89	64	– 95
63	88	32	– 47
64	87	16	– 23
65	86	8	– 11
66	85	4	– 5
67	84	2	– 2
68	83	2	0
69	82	2	2
70	81	4	5
71	80	8	11
72	79	16	23
73	78	32	47
74	77	64	95
75	76	128	191

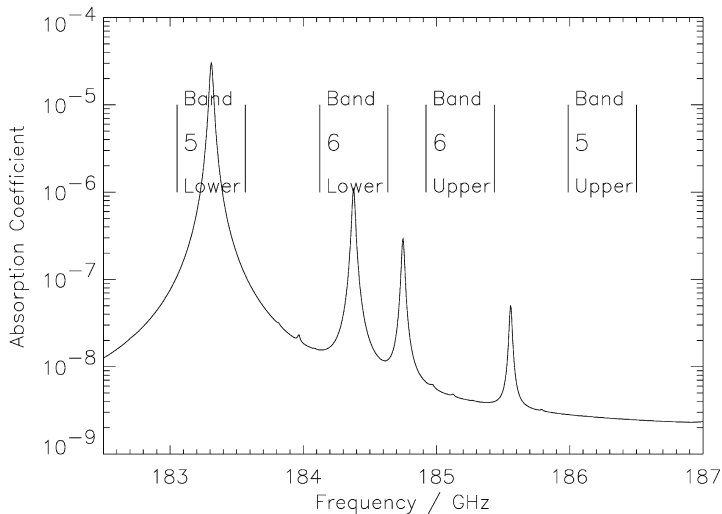


Fig. 1. This shows the positions of the two sidebands of UARS MLS bands 5 and 6, with the absorption coefficient at a mid-stratospheric pressure superimposed.

In use, the instrument makes a complete scan every 65 s. The resulting radiances, known as the ‘measurement vector’, are used as input to the optimal estimation algorithm [9]; the output of this is a vector known as the ‘state vector’ containing an estimate of a water vapour profile. Radiances calculated from this vector using a radiative transfer code or ‘forward model’ should agree with the measured ones to within the known errors. If they do not, then this implies that there are errors in

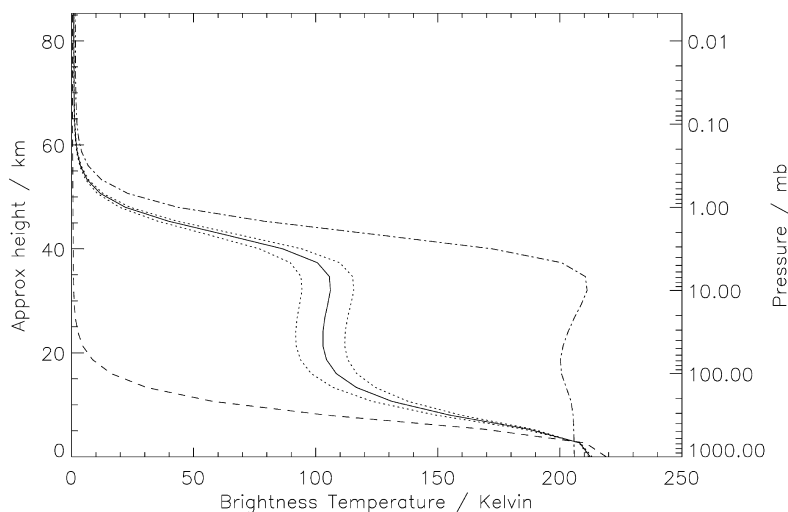


Fig. 2. The solid line shows the brightness temperature calculated at 11 MHz from the centre of MLS band 5, assuming a sideband ratio of 1.0. The dotted lines are the brightness temperatures for sideband ratios of 0.8 and 1.2. The dot-dash line is the brightness temperature for the lower sideband alone, the dashed line for the upper sideband.

the forward model which are not being accounted for. It is important in such cases to increase the size of the errors which are supplied to the optimal estimation equations in order to account for the forward model errors.

3.2. Retrievals of spectral and instrument parameters

The sideband ratios of UARS MLS were calibrated prior to launch. In each band values were obtained for the six ‘line wing’ channels and the values for the remaining channels were obtained by interpolating across the band. This procedure was successful for bands 1–4. The noise characteristics of the 183 GHz radiometer were such that the procedure was less successful for band 5. The measurements on band 6 were affected by the radiometer noise characteristics in the same way and were also compromised by a number of other effects, mostly resulting from the proximity of the two sidebands to the local oscillator frequency. As a result, the sideband ratios for band 6 proved almost impossible to measure and were estimated by fitting a parabola to the measured band 5 values and a value of 1.0 at the frequency of channel 76 (this should really have been the local oscillator frequency but the difference this makes is not large).

After launch, it became clear that the difference between the measured radiances and those recalculated from the retrieved product was in many cases several times larger than the instrument noise. The problem was worst in the region where the lower sideband is saturated, where the radiances depend mainly on the temperature and the sideband ratio. Some typical residuals are shown in Figs. 3 and 4; to reduce the effects of random noise these residuals are the result of retrieving a weekly zonal mean of water vapour from a weekly zonal mean of the radiances. The ‘week’ used is actually the five days centred on UARS day 140 (29 January 1992). Although the random errors are small, there are known forward model errors, so the optimal estimation was

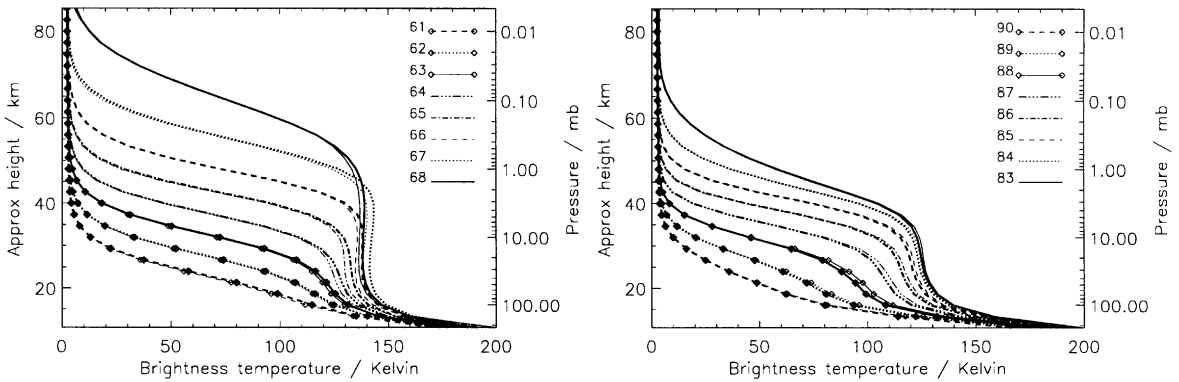


Fig. 3. Measured (thick lines) and re-calculated (thin lines) radiances for channels 61–68 from band 5 (left panel) and 83–90 from band 6 (right panel) of UARS MLS. The calculation assumes version 0003 sideband ratios based on pre-launch calibration. The measured radiances are a weekly zonal mean and the recalculated ones are calculated from the retrieved weekly zonal means of H_2O and O_3 . Both sets have been averaged over all latitude bins before plotting.

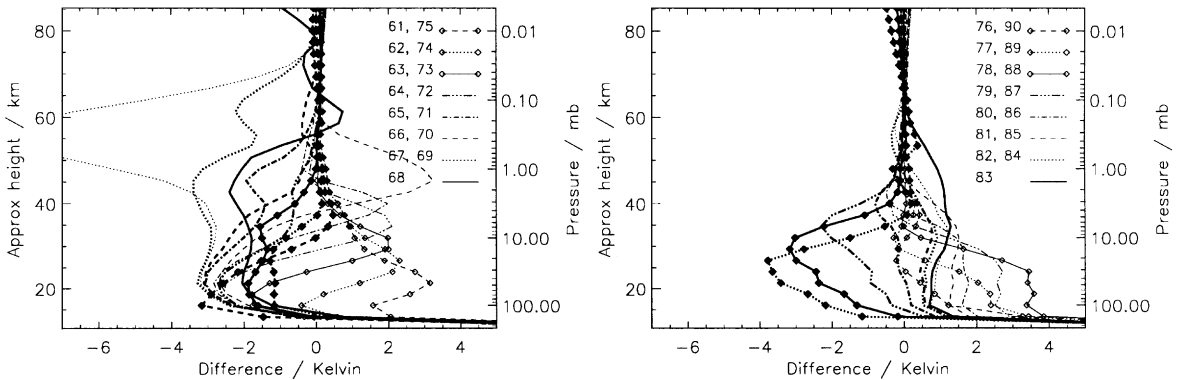


Fig. 4. Residuals (recalculated radiances – measured radiances) assuming version 0003 sideband ratios based on pre-launch calibration. Left panel: channels 61–75, the thin lines are for channels 69–75, the thick lines for channels 61–68. Right panel: channels 77–90, the thin lines are for channels 77–83, the thick lines for channels 84–90.

done on the basis that the radiance errors were about 3 K. Reducing this number does not make the residuals smaller, it just causes the retrieval to be less stable. Note how the residual in most channels of band 5 tends to a value some 2–4 K too small in the portion of the curve where the lower sideband is saturated and there is little signal in the upper sideband. This implies either that the sideband ratios are wrong or that the temperatures are uniformly 4–8 K too cold. Since the temperatures have been validated, we assume that they are correct and that the sideband ratios require some adjustment.

One way to do this is to put the sideband ratios into the state vector and retrieve them along with the state of the atmosphere. As before, we form weekly zonal means of the radiances and retrieve the sideband ratios along with weekly zonal means of the water vapour and ozone. As Fig. 5 shows, the residuals are now much smaller in the saturated portion of the curve.

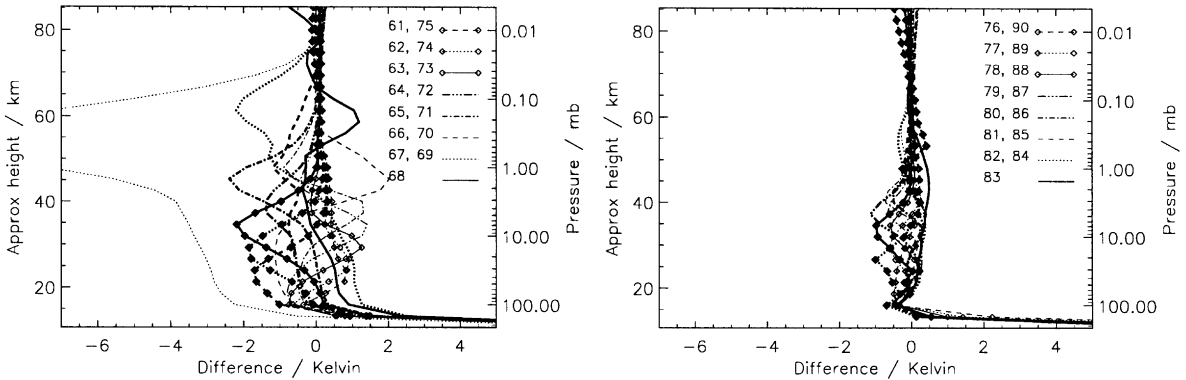


Fig. 5. Residuals (recalculated radiances – measured radiances) for a retrieval in which the sideband ratios are retrieved. Left panel: channels 61–75, the thin lines are for channels 69–75, the thick lines for channels 61–68. Right panel: channels 77–90, the thin lines are for channels 77–83, the thick lines for channels 84–90.

The improvement in band 6 is quite impressive, with the residuals falling from 4 to 1 K. Band 5 is also improved, but not as much. To account for the improvement, the retrieval was actually re-run with errors of 1 K in B6 and 2 K in B5. As before, there is no gain to be had by reducing these values further.

There is clearly some other problem which the retrieval algorithm cannot account for, no matter what values it chooses for the mixing ratios of water vapour and ozone or the sideband ratios. An obvious extension to the approach used with the sideband ratios is to retrieve some of the spectral parameters, such as the pressure broadening parameter γ_0 and/or the pressure shift $\Delta\nu_0$. There is a precedent for this approach: the pressure-broadening parameter for the 204 GHz ClO line has been previously retrieved from MLS data, and the value obtained was subsequently confirmed by laboratory measurements [10]. We try the pressure shift first as (a) the band 5 residuals show clear signs of anti-symmetry and (b) we have no a priori information on this parameter. Residuals from this procedure are shown in Fig. 6.

It is clear that we have an improvement in fitting the band 5 radiances. The band 6 radiances are hardly changed. The reason becomes obvious when we look at the retrieved values of $\Delta\nu_0$: -0.14 ± 0.03 MHz/mb for the H₂O line and 0.002 ± 0.02 MHz/mb (essentially zero) for the O₃ line. The band 5 value compares reasonably well with the value calculated by Gamache of -0.0967 MHz/mb and that determined by Bühler from MAS data of -0.20 ± 0.04 MHz/mb (see Section 4.4).

The residuals are still somewhat larger than the random error and appear to be of the same nature in both bands. Their form suggests that they might be reduced by retrieving either the broadening coefficients or a parameter called the pointing offset. This is the vertical angular difference between the direction in which both the 183 GHz radiometer and the 63 GHz radiometer looks. (The 63 GHz radiometer uses oxygen lines to measure pressure and temperature.) The pointing offset is a very small angle which was measured before launch and which, like the sideband ratios, has been reconsidered since launch. Several post-launch attempts were made to measure the pointing offset by scanning the MLS antenna across the moon [11]. Since changes in the broadening coefficients and the pointing offset would have similar effects, it does not make sense to try to retrieve both things; we try the first one, then the other.

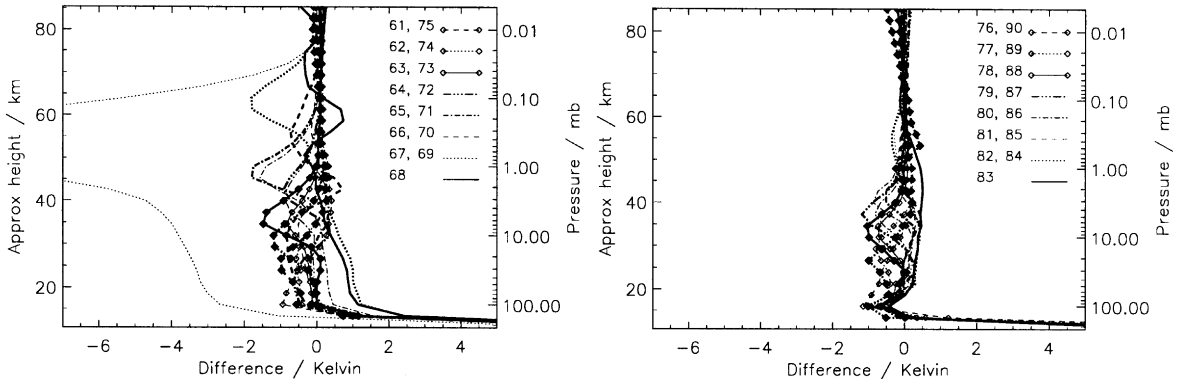


Fig. 6. Residuals (recalculated radiances – measured radiances) for a retrieval in which the sideband ratios and the pressure shift parameters are retrieved. Left panel: channels 61–75, the thin lines are for channels 69–75, the thick lines for channels 61–68. Right panel: channels 77–90, the thin lines are for channels 77–83, the thick lines for channels 84–90.

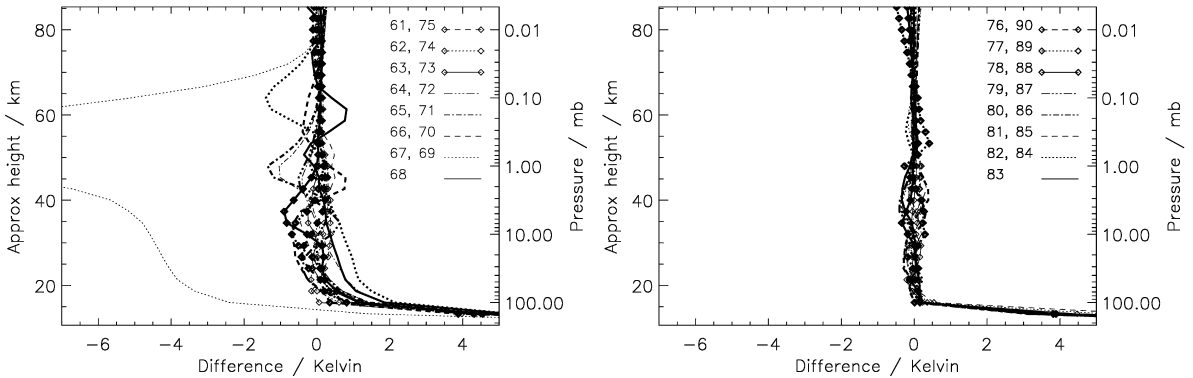


Fig. 7. Residuals (recalculated radiances – measured radiances) for a retrieval in which the sideband ratios, the pointing offset and the pressure shift parameters are retrieved. Left panel: channels 61–75, the thin lines are for channels 69–75, the thick lines for channels 61–68. Right panel: channels 77–90, the thin lines are for channels 77–83, the thick lines for channels 84–90.

Retrieving the pointing offset reduces the residuals further as shown in Fig. 7. However, the retrieved value is $0.008^\circ \pm 0.003^\circ$ while the value obtained from moon scans is a $0.0013^\circ \pm 0.0012^\circ$. The two values are significantly different. Turning to the broadening coefficients, we obtain the residuals shown in Fig. 8. The residuals are improved to a similar extent to those obtained by retrieving the pointing offset. Fig. 9 shows our retrieved value, 3.07 ± 0.07 MHz/mb, with all of the lab measurements of which we are aware and their quoted error bars.

Clearly, our value is higher than most of the laboratory measurements although the value obtained from the MAS instrument (see below) is larger again. The retrieved broadening coefficient for the O_3 line is 2.45 ± 0.03 MHz/mb, again this is larger than the single laboratory value of 2.367 MHz/mb. It is important to note that there are various other effects which could mimic a change in the broadening coefficient. For example, the measured value of the tangent height is

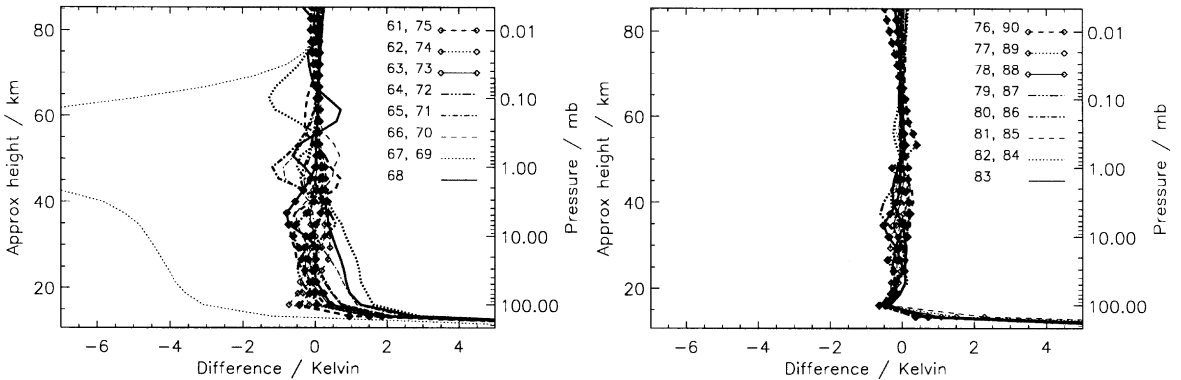


Fig. 8. Residuals (recalculated radiances – measured radiances) for a retrieval in which the sideband ratios and the pressure shift and broadening parameters are retrieved. Left panel: channels 61–75, the thin lines are for channels 69–75, the thick lines for channels 61–68. Right panel: channels 77–90, the thin lines are for channels 77–83, the thick lines for channels 84–90.

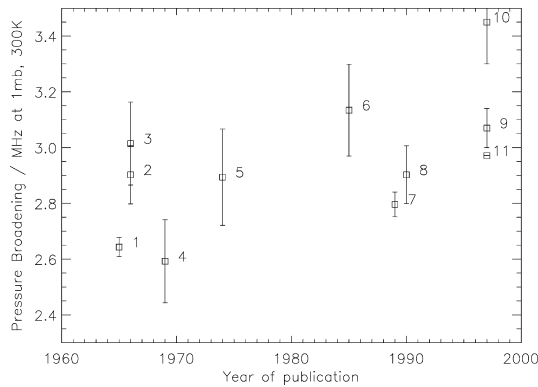


Fig. 9. Measured values of the pressure broadening coefficient γ_0 . The authors responsible are as follows. 1: Rusk [4], 2: Dryagin [5], 3: Frenkel and Woods [5], 4: Hemi and Straiton [5], 5: Ryadov [5], 6: Bauer et al. [5], 7: Bauer et al. [6], 8: Goyette and DeLucia [7], 9: This work — MLS, 10: This work — MAS, 11: Gamache (personal communication, 1997). The bulk of these values were obtained from Bauer et al. [5], not direct from the original references.

dependent on the measured broadening coefficient of the 63 GHz oxygen lines and an error in this would also mimic an error in the water vapour broadening coefficient. Given the quoted accuracies of the pointing offset and the line widths it seems better to keep the pointing offset from the Moon scans and to use the retrieved line widths.

There is, however, no effect we can think of which would mimic a pressure shift so, unlike the retrieved pressure broadening, the retrieved shift is probably a good measurement.

There are still problems in the mesosphere. The fit of channel 69 in particular is very poor — much worse than any of the other channels. We knew about this in advance so this channel was not used to retrieve any of the profiles or spectral parameters. Radiances for this channel were calculated using the parameters retrieved from the other channels. There are still details in other

channels (65, 67 and 70 in particular) which are not being adequately fitted. Various approaches to obtaining a better fit in the mesosphere have been tried but none have so far proved to be effective. They included:

- Dicke narrowing. A Rautian (Dicke-narrowed) line shape was tried but made only a small difference in the centre channel. There is insufficient information in the radiances to determine the size of the Dicke narrowing parameter.
- Retrieving the line centre frequency including channel 69. This was unsuccessful because this frequency, and the local oscillator frequency, which would have a similar effect are accurately known. Retrieving one or the other does not improve the fit much — the fit for channel 69 is slightly improved but the fit for the other line-centre channels becomes worse.
- Retrieving the temperature exponent. The radiances do not contain enough information to separate this parameter from various others. It is better to use the laboratory value which was obtained over a wide temperature range [7].
- Pickett [3] suggests a line shape consisting of a Lorentzian with a small component of its second derivative. This shape does not appear to improve the fit either.

3.3. Discussion of MLS results

3.3.1. Sideband ratios

The sideband ratios were retrieved in four tests described above and the results were different in each case. Fig. 10 shows the results together with the pre-launch measurements and the fit through them.

It is worth noting that retrieving the spectroscopic parameters has quite a large effect on the band 5 sideband ratios. The effect on the band 6 sideband ratios is much less marked — they have

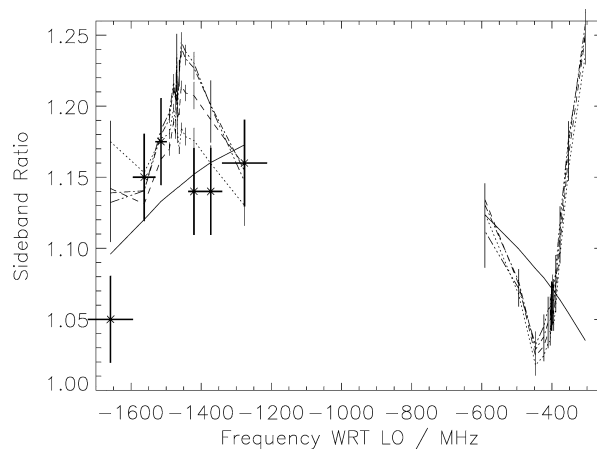


Fig. 10. Sideband ratios for UARS MLS. The band 5 data are grouped to the left of the plot, the band 6 data to the right. The large crosses are the pre-launch measurements, the vertical bar is the estimated error, the horizontal bar is the filter width. The two curved unbroken lines are a quadratic fit to the pre-launch values. The other lines are the results of the retrievals described in this paper. Retrieving sideband ratios only:, retrieving $\Delta\nu$: - - -, retrieving γ_0 and $\Delta\nu$: -.-.-, retrieving $\Delta\nu$ and offset angle: - - - - -

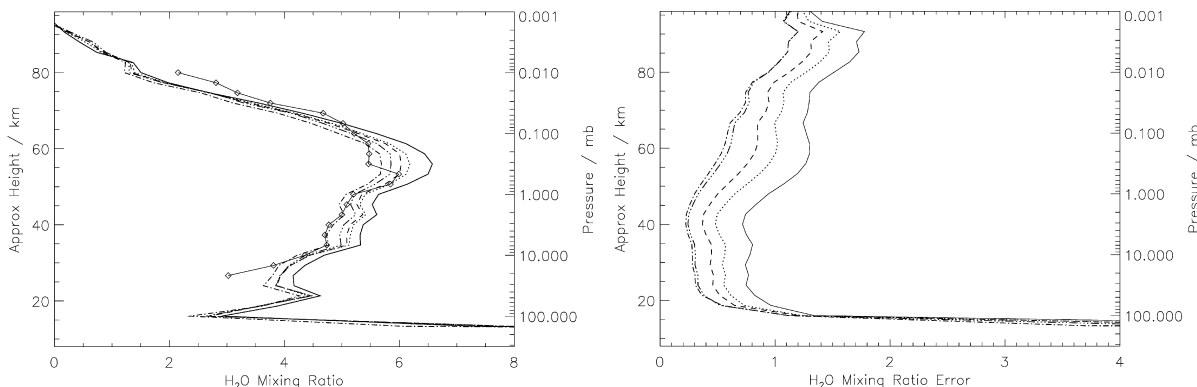


Fig. 11. (left panel) Retrieved H₂O mixing ratio profiles retrieved using the following parameters: solid line: all parameters pre-launch values, dotted line: retrieved sideband ratios used, dashed line: retrieved side band ratios and pressure shift, dot-dash line: retrieved sideband ratios, pressure shift and pointing offset, ...-...: retrieved sideband ratios, pressure shift and broadening coefficient. The thin solid line with diamonds is a coincident measurement from the HALOE instrument. (Right panel) retrieved errors. Line types as top panel.

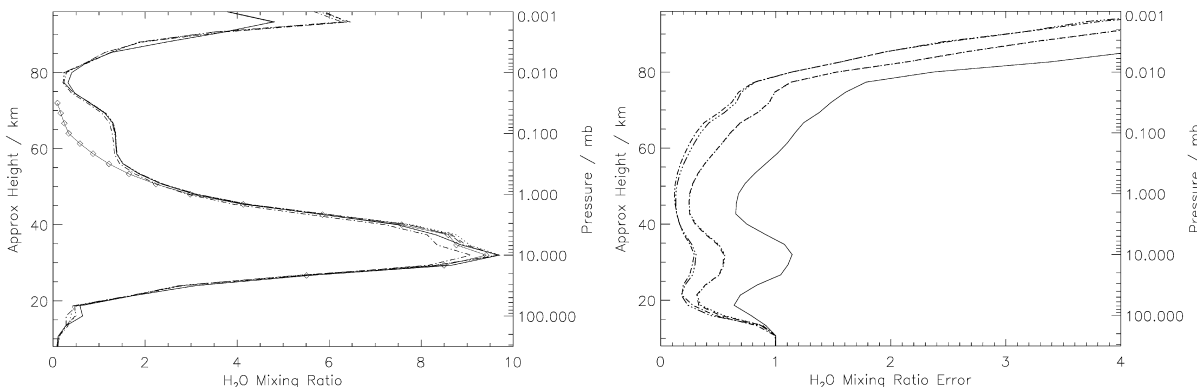


Fig. 12. As Fig. 11, but for ozone. The MLS-HALOE difference above 50 km occurs because ozone has a strong diurnal cycle at this altitude. The MLS measurements were made at night, the HALOE measurements at dawn and dusk.

similar values irrespective of what other parameters you are trying to retrieve and must therefore be regarded as more reliable.

3.3.2. Retrieved water vapour and ozone

To test the effect of the new sideband ratios and spectral parameters on the retrieved mixing ratios, the retrievals were re-run with these parameters constrained to the values obtained in the tests above. In each case the radiance errors were set to a value based on the residuals obtained in the above tests. The resulting profiles are shown in Figs. 11 and 12.

For both species, the retrieved errors get smaller as we use more of the retrieved parameters, this is simply because we know that a better fit is possible and can therefore tell the algorithm that the radiance errors are smaller.

The water vapour results are clearly quite dependent on the values chosen for the sideband ratios and pointing offset in particular and the spectral parameters to a lesser degree. The ozone profiles are all very similar, although the one retrieved using the retrieved pointing offset is noticeably lower than all the others.

4. The MAS instrument

4.1. Instrument description

The Millimetre-wave Atmospheric Sounder, MAS, is an instrument very similar to MLS. It is described by Croskey et al. [2]. The MAS was flown on the Space Shuttle during the Atlas missions Atlas1, Atlas2, and Atlas3 which took place in March 1992, April 1993, and November 1994. The orbit altitude of the shuttle in all three missions was 300 km, the inclination 57° . This paper considers only the first mission, Atlas1.

The instrument observes in six frequency bands, three for oxygen, and then one for ozone, water vapour, and chlorine-monoxide. There are altogether 110 filter bank channels for oxygen, 50 for ozone, 50 for water vapour, and 30 for chlorine-monoxide. We are only concerned with the water vapour band here. There have been several publications about retrievals of water vapour in the stratosphere and the mesosphere. (See, for example, Aellig et al. [12] in the GRL Atlas special issue, which contains a number of MAS publications.)

The structure of the MAS water vapour filter bank is slightly different from that of MLS. It consists of three separate filter banks — broad, medium, and narrow — all centred on the 183.3 GHz water vapour line. A summary is given in Table 2. In contrast to MLS, the line is observed in the *upper* sideband of the receiver. The image sideband is centred around 178.8 GHz. The small ozone line at 178.6 GHz as well as the stronger one at 184.4 GHz are included in the modelling. However, ozone is not retrieved but a climatological ozone profile is used.

As with MLS, the oxygen bands of MAS are used to retrieve the tangent pressure and hence the tangent altitude [13]. Both instruments have a small angular offset between the oxygen bands and the water vapour band; this offset has been estimated by scanning the instrument across the Moon in both cases. For MAS, the angular offset is -0.073° , equivalent to -2.4 km, i.e. the tangent altitude of the water vapour band is 2.4 km lower than that of the oxygen bands.

Table 2
MAS water vapour channels. The frequency ranges are given with respect to the nominal line centre frequency of 183310.22 MHz

Name	Width/MHz	Range/MHz
B1–B10	40	– 200–200
M1–M20	2	– 20–20
N1–N20	0.2	– 2–2

4.2. Retrieval procedure

An optimal estimation method as described for example by Rodgers [9] is used to retrieve water vapour volume mixing ratio profiles from the limb-scan spectra. No linear approximation is made. The iterative solution is found by a Levenberg–Marquardt algorithm, as described for example in Press et al. [14]. Instrumental- or spectroscopic parameters can be introduced as additional retrieval parameters.

For the retrievals presented in this paper, zonal mean spectra of the entire Atlas1 mission were used. The latitude bins were $\pm 1^\circ$ at the equator, $\pm 0.5^\circ$ at mid-latitudes, and $\pm 2^\circ$ at higher latitudes. The size of the bins was chosen such that the number of scans that were integrated for each zonal mean spectrum was between 160 and 270. In total, 12 zonal mean scans were prepared, ranging from -40 to $+70^\circ$ latitude. Different sets of retrieval parameters were tried on these averaged scans.

The scans were truncated to a tangent altitude range of 30–80 km in order to eliminate the influence of the highly variable tropospheric humidity and the influence of cirrus clouds. Maybe truncation below 20 km would have been sufficient, but the antenna pattern is rather wide (FWHM is 0.18° , i.e., approximately 6 km), so 30 km was chosen to be on the safe side.

4.3. Instrumental and spectroscopic parameters

The retrieval of the following parameters was studied:

- pressure shift
- air broadening parameter
- frequency offset
- tangent altitude offset
- sideband ratio.

The initial aim of this study was to retrieve the pressure shift and the air broadening parameter in order to compare them with the values obtained from MLS. It turns out, however, that the other parameters in the list have to be taken into account if one wants to obtain meaningful results for the pressure shift.

The frequency offset was included because the residuals at high tangent altitudes indicate that the line centre frequency is not exactly at its nominal position (Figs. 13 and 14). The two figures show the quality of the fit for a retrieval that did include the pressure shift parameter, but no frequency offset. The small frequency displacement of the water vapour line at high tangent altitudes cannot be explained by any reasonable pressure shift. The most likely cause for the offset is a bias in the MAS Doppler effect correction.

As already mentioned, the pointing information on the Shuttle is very inaccurate, so that the true tangent altitude has to be obtained by a fit to the observed oxygen lines. The fit procedure developed by Berg assumes the atmosphere to be the CIRA [15] reference atmosphere, hence there is still some uncertainty in the true pointing. A tangent altitude offset was included in the retrieval in order to investigate this. The tangent altitude information is obtained from the line width, therefore one can either retrieve a tangent altitude offset or the air broadening parameter, but not both.

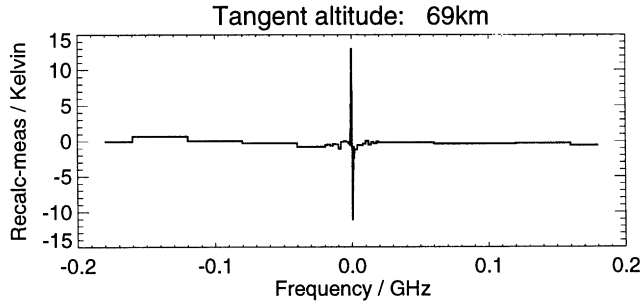


Fig. 13. Recalculated minus measured MAS radiances at a high tangent altitude. The retrieval did include the pressure shift parameter, but no frequency offset.

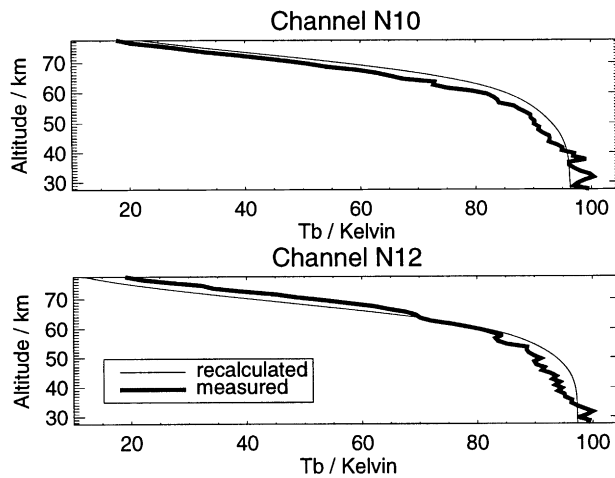


Fig. 14. Measured and recalculated MAS radiances for the filterbank channels N10 and N12. The nominal line centre frequency is between channel N10 and N11. The retrieval did include the pressure shift parameter, but no frequency offset.

The sideband ratio was assumed to be the same for all channels, so that one parameter for the sideband ratio could be retrieved. Retrieving two sideband parameters, corresponding to the response on both edges of the band and assuming linear variation across the band, did not yield useful results, because the two sideband parameters are highly correlated with each other and with the pressure shift parameter.

4.4. Results and discussion

Fig. 15 shows the additional retrieval parameters for a series of retrievals from zonally integrated spectra at different latitudes. Two different cases are displayed, case A where the air broadening parameter is retrieved and case B where a tangent altitude offset is retrieved. The statistical errors in the parameters are small, because the zonally integrated data contains little noise. Therefore,

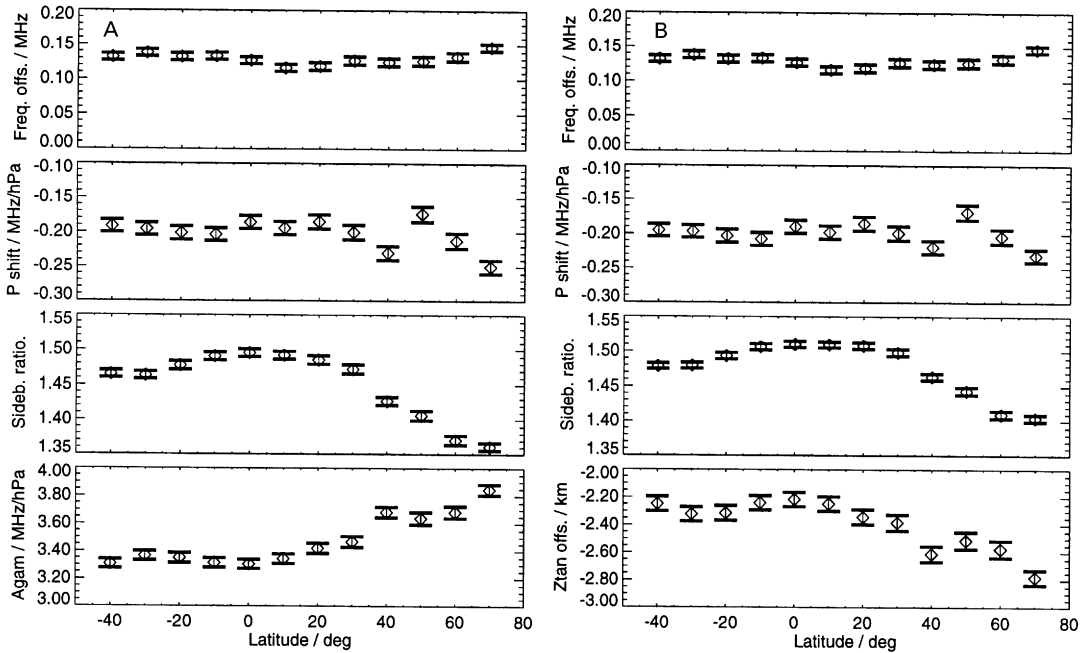


Fig. 15. Additional retrieval parameters for zonal mean retrievals. Displayed are the results for 12 zonal mean spectra with latitudes ranging from 40° south to 70° north. The error bars indicate the total statistical error (measurement error plus null-space error). It is clear that the statistical error underestimates the true error and that there is a bias depending on latitude. Case A (left): Tangent altitude offset fixed at -2.4 km, air broadening parameter retrieved. Case B (right): Air broadening parameter fixed at 3.27 MHz/mb, tangent altitude offset retrieved.

spectra at different latitudes were used in order to get a better idea of the systematic errors. It is clear from the figure that there is a latitude dependent bias in all parameters.

The average of the air broadening parameter in case A is 3.45 MHz/mb, which is significantly higher than all literature values (see Fig. 9) and also higher than the value obtained by MLS. It is therefore likely that there is a systematic error in the tangent altitude offset. Fixing this to a value lower than -2.4 km will result in smaller values for the air broadening parameter.

Neither the sideband ratio nor the air broadening parameter are expected to depend on latitude. The tangent altitude, on the other hand, may well have a latitude-dependent bias if the reference atmosphere has such a bias. A likely explanation comes from the MAS orbit characteristics. The orbit is such that most measurements in the northern hemisphere are taken during local daytime, whereas most measurements in the southern hemisphere are taken during local nighttime. This is illustrated in Fig. 16. Thermal tides are not taken into account by the reference atmosphere but they seem to have an impact on the tangent altitude retrieval. This means that a thorough investigation of the impact of the reference atmosphere on the retrieved tangent altitude will be necessary, before a retrieval of sideband ratio or air broadening parameter is possible.

The average retrieved values for frequency offset and pressure shift are identical for cases A and B up to a reasonable number of digits. Because of the systematic errors, it is not legitimate

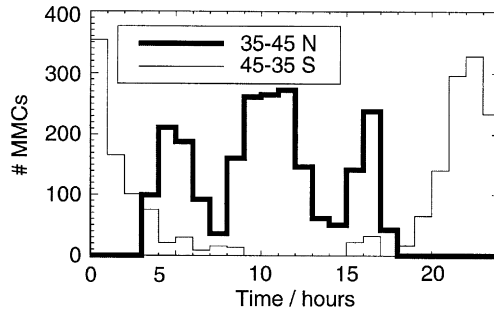


Fig. 16. Local time at tangent point.

to compute the error in these values according to a Gaussian distribution. Instead, one can use the maximum and minimum values to estimate the error. This procedure results in $f_{\text{offs}} = 0.130 \pm 0.015$ MHz and $p_{\text{shift}} = -0.20 \pm .04$ MHz/mb. The value of p_{shift} is slightly higher than the MLS value of -0.14 ± 0.03 MHz/mb. It has to be noted that the retrieval of the frequency offset has a very strong impact on the pressure shift parameter. Fixing the frequency offset to a value of 0 MHz results in a completely different p_{shift} value of $-0.10 \pm .03$ MHz/mb, which is now *lower* than the MLS value. Still, as stated above, the fit residuals indicate that the frequency offset is really there and should be taken into account.

To conclude, the MAS data allows the retrieval of the pressure shift parameter of the water vapour line at 183 GHz. The obtained value is consistent with MLS but somewhat higher. A retrieval of the water vapour air broadening parameter is not possible with the current pointing accuracy.

5. Conclusions

The radiances measured by a microwave limb-sounding instrument often contain enough information for both the desired constituent profile and various spectral and instrument parameters to be retrieved. Of course, it is better if these things are known before launch and efforts are (hopefully) being made to ensure that this is the case for future instruments. However, certain parameters, including the pressure shift, are hard to measure in the laboratory. Microwave limb-sounding instruments appear to be capable of providing a better measurement of the pressure shift of the 183 GHz water vapour line than any laboratory technique of which we are aware.

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References

- [1] Barath FT . *J Geophys Res* 1993;98(D6):10751–62.
- [2] Croskey CL, Kämpfer N, Bevilacqua RM, Hartmann GM, Künzi KF, Schwartz PR, Olivero JJ, Puliafito SE, Aellig C, Umlauf G, Waltmann WB, Degenhardt W. *IEEE Trans Microwave Theory Techn* 1992;40(6):1090–100.
- [3] Pickett HM. *J Chem Phys* 1980;73:6090–4.
- [4] Rusk JR. *J Chem Phys* 1965;42:493–500.
- [5] Bauer A, Godon M, Duterage B. *JQSRT* 1985;33:167–75.
- [6] Bauer A, Godon M, Kheddar M, Hartmann JM. *JQSRT* 1989;41:49–54.
- [7] Goyette TM, De Lucia FC. *J Mol Spec* 1990;143:346–58.
- [8] Oh JJ, Cohen EA. *JQSRT* 1992;48:405–8.
- [9] Rodgers CD. *Rev Geophys Space Phys* 1976;14(4):609–24.
- [10] Waters JW, Read WG, Froidevaux L, Lungu TA, Perun VS, Stachnik RA, Jarnot RF, Cofield RE, Fishbein E, Flower DA, Burke JR, Hardy JC, Nakamura LL, Ridenoure BP, Shippony Z, Thurstans RP, Avallone LM, Toohey DW, DeZafra RL, Shindell DT. *J Geophys Res* 1996;101(D6):10 091–127.
- [11] Jarnot RF, Cofield RE, Waters JE, Peckham GE, Flower DA. *J Geophys Res* 1996;101:9957–82.
- [12] Aellig CP, Bacmeister J, Bevilacqua RM, Daehler M, Kriebel D, Pauls T, Siskind D, Kämpfer N, Langen J, Hartmann G, Berg A, Park JH, Russell III JM. *Geophys Res Lett* 1996;23(17):2325–8.
- [13] Berg, A. Bestimmung des atmosphärischen Druckes mit Hilfe von satellitengetragener passiver Mikrowellenradiometrie. Ph.D. thesis, University of Bremen, Germany, December 1995.
- [14] Press WH et al. *Numerical recipes in fortran*. C. U. P., 1992.
- [15] COSPAR international reference atmosphere. Committee on Space Research (COSPAR), 1986.