

Thermodynamic and Transport Properties of Carbohydrates and their Monophosphates: The Pentoses and Hexoses

Robert N. Goldberg and Yadu B. Tewari

Chemical Thermodynamics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

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This review contains recommended values of the thermodynamic and transport properties of the five and six membered ring carbohydrates and their phosphates in both the condensed and aqueous phases. Equilibrium data, enthalpies, heat capacities, and entropies have been collected from the literature. The accuracy of these data have been assessed, adjusted to 298.15 K and to a common standard state, and entered into a catalog of thermochemical reactions. The solution of this reaction catalog yields a set of recommended values for the formation properties of these substances. The volumetric data have also been critically evaluated. Recommended values are presented for standard state molar volumes and the temperature and pressure derivatives of the molar volume, i. e., the expansivity and the compressibility. The excess property data of aqueous solutions of these substances have been correlated to yield recommended values of the parameters of the virial expansion model used to represent the data. The transport data considered here includes both viscosity and diffusion data of aqueous solutions of the carbohydrates. The available phase diagram data and transition temperatures are summarized.

Key words: carbohydrates; chemical thermodynamics; diffusion; enthalpy; entropy; evaluated data; excess properties; Gibbs energy; heat capacity; phase diagrams; viscosity; volumetric properties.

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1. Introduction

This review emerges from a research effort at the National Institute of Standards and Technology designed to provide fundamental data on processes in which biomass is enzymatically converted to useful chemicals and fuels. Data on the thermodynamic and transport properties of the five and six membered ring carbohydrates and their monophosphates in the condensed and aqueous phases play a key role in the optimization and design of both currently used and proposed industrial processes.

For many years, carbohydrates have been of interest to chemists because of their prominent and significant roles in a variety of areas. These include metabolic reactions, industrial operations yielding chemical feedstocks, and processes encountered by researchers involved in synthesis, structural elucidations, and separations. The stabilities of these compounds and their position in chemical equilibria are dictated largely by thermodynamic considerations. Because of this we have assembled the available thermodynamic data from the literature on the five and six membered ring carbohydrates (see Fig. 1) and their monophosphates.

Earlier reviews in the literature in this area include the thermodynamic tables of Burton¹ and of Wilhoit.² The former pioneering review dealt only with Gibbs energy data while the latter also included enthalpy, entropy, and heat capacity data with some attention being given to partial molar properties of solutions. The extensive review of Atkinson and Morton³ dealt primarily with phosphorylation reactions and contained only Gibbs energy data for biochemical processes. Barman's *Enzyme Handbook*⁴ contains extensive references to equilibrium data for enzyme-catalyzed reactions. Enthalpies of combustion and of formation of condensed phases of organic compounds are dealt with in four excellent reviews.⁵⁻⁸ Domalski, Evans, and Hearing⁹ have compiled the available data on the heat capacities and entropies of organic compounds in the condensed phase. In a comprehensive paper, Angyal¹⁰ has reviewed the available data dealing with the detailed anomeric composition of reducing sugars in solution. Most recently, Cesaro¹¹ has summarized a substantial body of physicochemical data on carbohydrates. His review also contains an extensive discussion of the physical models that have been used to rationalize some features of the data.

Most of the data which have been examined in this review involve equilibrium and calorimetric measurements on the pure compounds and on their aqueous solutions. Insofar as possible, we have recalculated the original data from the experimental measurements to obtain values of the thermochemical parameters which are then entered into a catalog. This catalog serves as the basis for the solution of the thermochemical network for these processes and substances. The least-squares solution^{12,13} of the network leads to a set of recommended values for both formation properties and thermochemical parameters for specific processes.

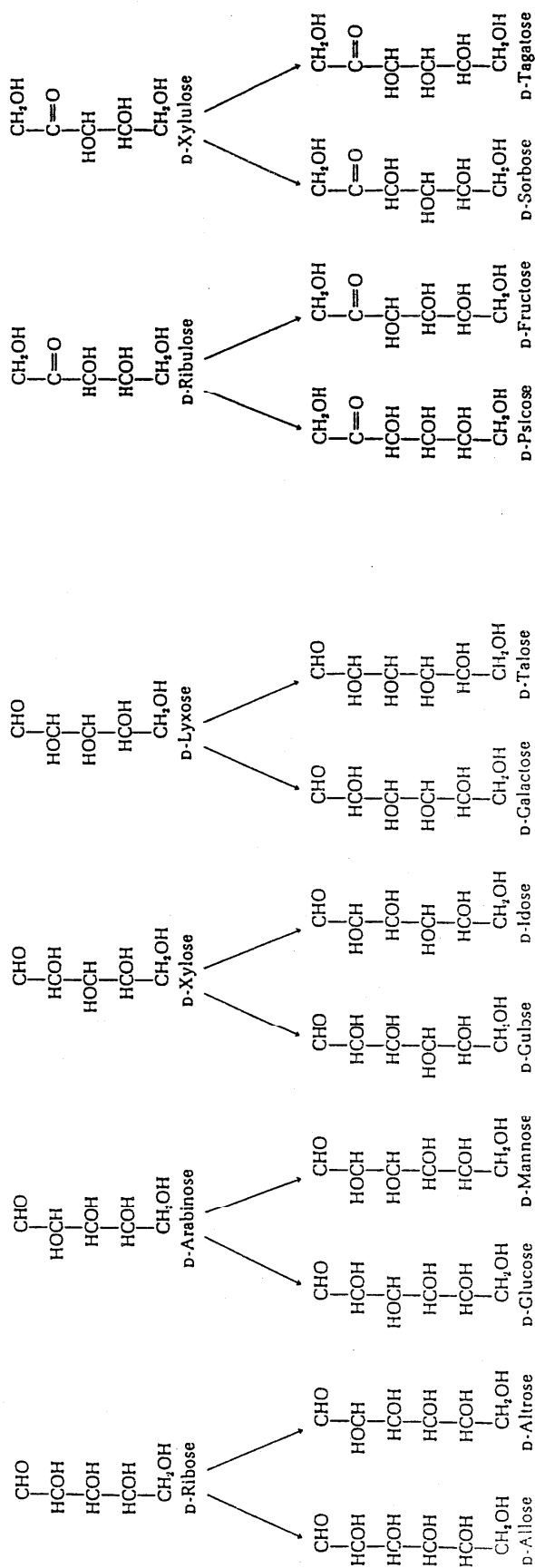
This review also includes the transport property data for these substances and a correlation of the data leading to the excess Gibbs energy of aqueous solutions of these substances and its temperature and pressure derivatives. Information on solubilities, phase diagrams, and the pressure derivative of the Gibbs energy is also considered. The general aim has been to provide an essentially complete coverage of the thermodynamic and transport properties of these substances. The literature is covered through 1987.

This review identifies those areas where measurements are most needed. Also, the structural similarities of the compounds can serve as a guide to estimating property data where measurements do not currently exist.

2. Conventions

2.1. Symbols, Nomenclature, Standard States, and Units

The symbols used in this review are given in the Glossary. With only a few exceptions, we have attempted to adhere to the recommendations of the International Union of Pure and Applied Chemistry (IUPAC) on symbols, nomenclature, and units.¹⁴ The standard states used in the construction of the tables are the same as those used in "The NIST Tables of Chemical Thermodynamic Properties".¹⁵ Thus for a pure solid or liquid the standard state thermodynamic properties pertain to the pure substance at a pressure of 0.1 MPa. For aqueous solutions, the standard state for the solution is the hypothetical ideal solution at unit molality and the standard state for the solvent is the pure solvent. The thermochemical reference temperature is 298.15 K. These standard states and reference temperature were selected prima-



D-ketoses

D-aldoses

Fig. 1. Open chain structural formulas of the D-pentoses and D-hexoses.

ily because of the very large existing body of thermodynamic data which is referred to it.

The notation for physical states follows that used in "The NBS Tables of Chemical Thermodynamic Properties." It is also summarized in the Glossary.

2.2. Conventions Regarding Detailed Structural Forms

The open chain structural formulas of the *D*-pentoses and *D*-hexoses are shown in Fig. 1. The chemistry of the carbohydrates is made both complicated and interesting by the existence of different anomeric forms for each of these compounds. Thus, for each substance there exists a pure *D* and *L* form, an α and a β form, the furanose and pyranose conformers, and the open chain aldehyde and keto forms. Clearly any chemical sample of a carbohydrate may be a mixture of one or more of these forms. It will be necessary in this review to distinguish between these various forms. Also, in many cases, we do not know the specific form of the carbohydrate that was used in particular investigations. Where the investigators have provided detailed structural information for the condensed phase, we shall specify whether the compound is in the α or β form and/or in the furanose or pyranose form. In such cases, the absence of the *D* or *L* specification shall be taken to imply that the compound is the pure *D* or *L* form. The equimolar mixture of the *D* and *L* forms will be specified as "DL". The same conventions will be adhered to for the aqueous solutions of carbohydrates except that the absence of any designation will imply that what is intended is the equilibrium mixture of the various anomers of the pure *D* or *L* form of the carbohydrate in solution.

The thermodynamic properties of the pure *D* and *L* forms are predicted by theory to be identical. The molar entropy of a mixture of *D* and *L* forms is given by:

$$S_{DL} = S_D - R(x_D \log_e x_D + x_L \log_e x_L) \quad (1)$$

Here, x_D and x_L are, respectively, the mole fractions of the *D* and *L* forms in the mixture; S_D is the molar entropy of the pure *D* or *L* form. Since the enthalpy of the DL mixture will be same as the enthalpy of the pure *D* or *L* form, the Gibbs energy of the DL mixture is given by the following:

$$G_{DL} = G_D + T(S_D - S_{DL}) \quad (2)$$

Since the temperature and pressure derivatives of the entropy of mixing term in Eq. (1) are zero, all of the other thermodynamic properties of DL mixtures are predicted to be identical to those of the pure *D* or *L* forms.

2.3. Arrangement of Tables and of Compounds

The tables are arranged in the following general order: melting and transition temperatures, standard state volumetric properties, excess properties, transport properties, and standard state thermochemical properties. The arrangement of the compounds in the thermochemical tables follows the standard order of arrangement used in "The NBS Tables of Chemical Thermodynamic Properties." An effort was made to have the tables reasonably self-documenting. Thus, as a rule, the tables contain references to the sources of

the data, either the original or adjusted values of the data and the recommended property values.

2.4. Treatment of Uncertainties

The uncertainties associated with the recommended values of the physical properties or of the parameters of the correlating equations in Tables 1-7 were obtained in two different ways. The first method is purely statistical and assumes a normal distribution of errors with final error estimates being made at approximately 95% confidence limits. The general procedure followed when fitting data to correlating equations was to include all parameters until the standard deviation of an additional parameter became more than half the absolute value of that parameter. When these statistical methods were used the uncertainty is given to two significant figures. The other method of assignment of uncertainties is based upon the judgment of the reviewers as to the overall reliability of the measurements. This involves both consideration of random and systematic errors. Since it frequently involves subjective judgment, error estimates obtained this way are given to only one significant figure. The reader should draw no conclusion about the relative superiority of either of these two methods of presenting uncertainties.

The uncertainties given in the reaction catalogs are assigned primarily on the basis of the evaluators initial judgment of the reliability of that particular measurement. This initial judgment may later be modified on the basis of how well that measurement fits into the solution for the entire thermochemical network. These modifications are usually kept to a minimum and the overall fit of the network is accomplished primarily by the decision of whether or not to include a particular measurement in the final network solution. When there are cross links in the thermochemical network, the residuals (observed minus calculated values obtained from the fit) are useful in assessing both the accuracy of how well a particular measurement fits into the network and, in part, the accuracy of that particular measurement. This device serves as a good test of the overall accuracy of the thermochemical data and is useful in locating possible errors in existing measurements. In the absence of either these cross links or replicate measurements on a specific process, the user should exercise caution in accepting the assigned uncertainties for an individual processes.

The uncertainties given in the calculated values of thermochemical properties at 298.15 K (Table 15) are standard deviations and are a measure of the overall fit of the network. It is not the uncertainty to be associated with the property and it should not be used to calculate the uncertainty pertinent to a given process.^{13,16}

2.5 References for the Tables

The form of the references in the tables follows that used in the "CODATA Thermodynamic Tables." Thus, the references are ordered chronologically and alphabetically by author(s) within each year using a code consisting of the final two digits of the year and the first three letters of the first two authors' names.

3. Excess and Partial Molar Properties

The excess Gibbs energy of aqueous solutions of the carbohydrates is represented by a virial expansion in the molality of the solute:

$$G^{\text{ex}} = \sum g_i m^{(i+1)}.$$

The index "i" in the above equation and in the ones below runs from unity to the total number of parameters needed to represent the experimental data over the molality range of interest. The symbols are defined in the Glossary. Appropriate derivatives of the excess Gibbs energy lead to the following working equations for the activity and osmotic coefficients, apparent molar, and excess properties:

$$G^{\text{ex}} = \sum g_i m^{(i+1)} = m_1^* G_1^{\text{ex}} + m G_2^{\text{ex}},$$

$$G_2^{\text{ex}} = \left(\frac{\partial G^{\text{ex}}}{\partial m} \right)_{T,p} = \sum (i+1) g_i m^i,$$

$$G_1^{\text{ex}} = (-1/m_1^*) \sum g_i m^{(i+1)},$$

$$G_2^{\text{id}} = G_2^\circ + RT \log_e a_2 = G_2^\circ + RT \log_e (m/m^\circ),$$

$$G_1^{\text{id}} = G_1^\circ + RT \log_e a_1 = G_1^\circ - (RTm/m_1^*),$$

$$\gamma = \exp[(G_2^{\text{ex}}/(RT))],$$

$$\phi = (m_1^*/m) \log_e a_1 = [m_1^* G_1^{\text{ex}}/(mRT)] + 1,$$

$$S^{\text{ex}} = - \left(\frac{\partial G^{\text{ex}}}{\partial T} \right)_p = \sum s_i m^{(i+1)},$$

$$S_2^{\text{id}} = S_2^\circ + R \log_e (m/m^\circ),$$

$$S_1^{\text{id}} = S_1^\circ - (Rm/m_1^*),$$

$$H^{\text{ex}} = G^{\text{ex}} + T \left(\frac{\partial G^{\text{ex}}}{\partial T} \right)_p = \sum h_i m^{(i+1)},$$

$$H_2^{\text{ex}} = \left(\frac{\partial H^{\text{ex}}}{\partial m} \right)_{T,p} = L_2 = \sum (i+1) h_i m^i,$$

$$H_2^{\text{id}} = H_2^\circ = H_2^\infty,$$

$$H_1^{\text{id}} = H_1^\circ = H_1^*,$$

$$L = H - H^\circ = H^{\text{ex}}/m^\circ,$$

$$L_\phi = (L - m_1^* L_1^*)/m = H^{\text{ex}}/m = \sum h_i m^i,$$

$$C_p^{\text{ex}} = \left(\frac{\partial H^{\text{ex}}}{\partial T} \right)_p = \sum c_i m^{(i+1)},$$

$$C_{p,2}^{\text{ex}} = \left(\frac{\partial C_p^{\text{ex}}}{\partial m} \right)_{T,p} = \sum (i+1) c_i m^i,$$

$$C_{p,\phi} = C_{p,2}^\circ + (C_p^{\text{ex}}/m) = C_{p,2}^\circ + \sum c_i m^{(i+1)},$$

$$c_p = (m C_{p,\phi} + c_{p,1}^*) (1 + m M_2)^{-1},$$

$$V^{\text{ex}} = \left(\frac{\partial G^{\text{ex}}}{\partial p} \right)_T = \sum v_i m^{(i+1)},$$

$$V_2^{\text{ex}} = \left(\frac{\partial V^{\text{ex}}}{\partial m} \right)_{T,p} = \sum (i+1) v_i m^i,$$

$$V_1^{\text{id}} = V_1^\circ = V_1^*,$$

$$V_2^{\text{id}} = V_2^\circ = V_2^\infty,$$

$$V_\phi = V_2^\circ + (V^{\text{ex}}/m) = V_2^\circ + \sum v_i m^i,$$

$$\rho = (1 + m M_2) [(1/\rho^*) + \sum v_i m^{(i+1)} + m V_2^\circ]^{-1},$$

$$E^{\text{ex}} = \left(\frac{\partial V^{\text{ex}}}{\partial T} \right)_p = \sum e_i m^{(i+1)},$$

$$E_2^{\text{ex}} = \left(\frac{\partial E^{\text{ex}}}{\partial m} \right)_{T,p} = \sum (i+1) e_i m^i,$$

$$K_S^{\text{ex}} = \left(\frac{\partial V^{\text{ex}}}{\partial p} \right)_S = \sum k_{S,i} m^{(i+1)},$$

$$K_T^{\text{ex}} = \left(\frac{\partial V^{\text{ex}}}{\partial p} \right)_T = \sum k_{T,i} m^{(i+1)},$$

$$K_{S,\phi} = (K_S - m_1^* K_{S,1}^*)/m = K_{S,2}^\circ + (K_S^{\text{ex}}/m) \\ = K_{S,2}^\circ + \sum k_{S,i} m^i,$$

$$K_{S,\phi}^\circ = K_{S,2}^\circ.$$

The above equations also include expressions for the ideal Gibbs energy, entropy, enthalpy, and volume. The quantities m° and m_1^* , respectively, are equal to 1 and 55.5084 mol kg⁻¹. The former quantity is introduced to preserve the dimensionality of units, and the latter is the amount of water in a kilogram of water. The use of excess and apparent molar properties offers a concise and convenient way of representing the results of a large variety of physical property data. Note that the excess Gibbs energy is not a molar Gibbs energy; it has units of J kg⁻¹. The excess Gibbs energy is obtained primarily from both direct and relative (isopiestic) vapor pressure measurements, the excess enthalpy from heats of dilution, and the excess heat capacity from direct heat capacity measurements on aqueous solutions. The excess volume and expansivity are obtained from precise density measurements, the latter quantity requiring that the densities be determined as a function of temperature. The isothermal compressibility is rarely measured. However, the isentropic compressibility is conveniently determined from measurements of the speed of sound (u) and a knowledge of the density (ρ):

$$\kappa_S = V^{-1} \left(\frac{\partial V}{\partial p} \right)_S = K_S/V = 1/(\rho u^2).$$

The isothermal compressibility is then calculated using the following relationship¹⁷:

$$K_{T,2}^\circ = K_{S,2}^\circ + 2(\kappa_{T,1}^* - \kappa_{S,1}^*) \\ \times \left[\left\{ \left(\frac{\partial V_2^\circ}{\partial T} \right)_p / E_1^* \right\} - \left(\frac{C_{p,2}^\circ V_1^*}{C_{p,1}^*} \right) \right].$$

4. Sources of Auxiliary Data

The sources for the values of the fundamental physical constants and atomic masses used in this review are, respectively, the 1986 Committee on Data for Science and Technology (CODATA)¹⁸ and the 1981 IUPAC recommendations.¹⁹ Auxiliary thermochemical data (see Table I) were taken primarily from the most recent set of CODATA recommended values.²¹ The properties of Ni²⁺(aq) are those given in "The NBS Tables of Chemical Thermodynamic Properties".¹⁵ The partial molar heat capacities of HPO₄²⁻(aq) and of H₂PO₄⁻(aq) are from Larson, Zeeb, and Hepler.²² The partial molar heat capacities of Mg²⁺(aq) and Ca²⁺(aq) are from Spitzer, Olofsson, Singh, and

Hepler.²³ Except for the entropy and the Gibbs energy and enthalpy of formation, the properties of pure water were taken from the "NBS/NRC Steam Tables".²⁴

5. Contents and Descriptions of the Tables

Tables 1–3 contain data on the transition temperatures and volumetric properties of the pure carbohydrates in condensed phases. Note that many of the densities were calculated using the results of crystallographic studies.²⁵ All of the crystalline carbohydrates considered in this review are orthorhombic with four molecules per unit cell and fall into space group $2_12_12_1$. There is a very limited amount of data available on the cubic expansion coefficients of these carbohydrates in condensed phases and no information on their compressibilities.

The available phase diagram data are shown in Figs. 2 and 3 and are based primarily upon careful work done at the National Bureau of Standards over 60 years ago.^{26,27} Glucose exists as both a monohydrate and in the anhydrous form with the transition occurring at 323.15 K. The phase diagram for fructose is more complex and shows the existence of a gel, the anhydrous compound, a metastable crystalline phase, a dihydrate, and a hemihydrate.

The standard state volumetric data from the literature on aqueous carbohydrates are given in Table 4. The recommended values of the standard state partial molar volumes, expansivity, isentropic and isothermal compressibility, and the temperature derivative of the isentropic compressibility are given in Table 5. In computing isothermal compressibili-

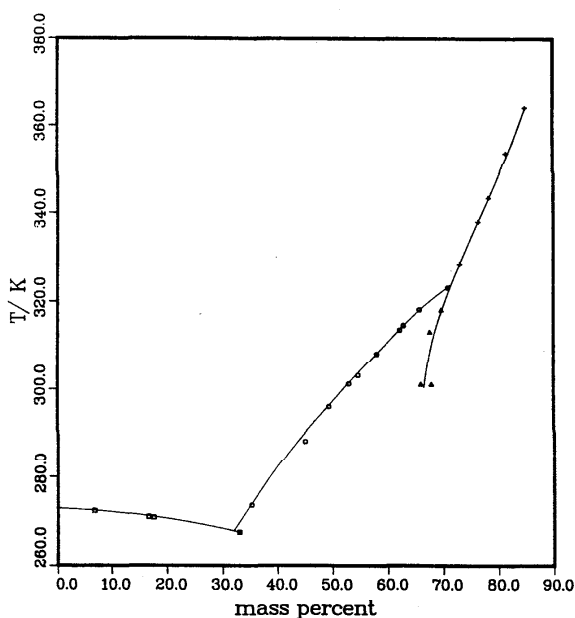


FIG. 2. Phase diagram for the system *D*-glucose + water. The curves refer to the following solid phases in equilibrium with aqueous *D*-glucose solutions: (□) ice; (○) *D*-glucose monohydrate; (+) anhydrous *D*-glucose; and (Δ) the metastable anhydrous form. The transition of *D*-glucose monohydrate to the anhydrous form and water occurs at 30 °C (323.15 K). The data are from Jackson and Silsbee.²⁶

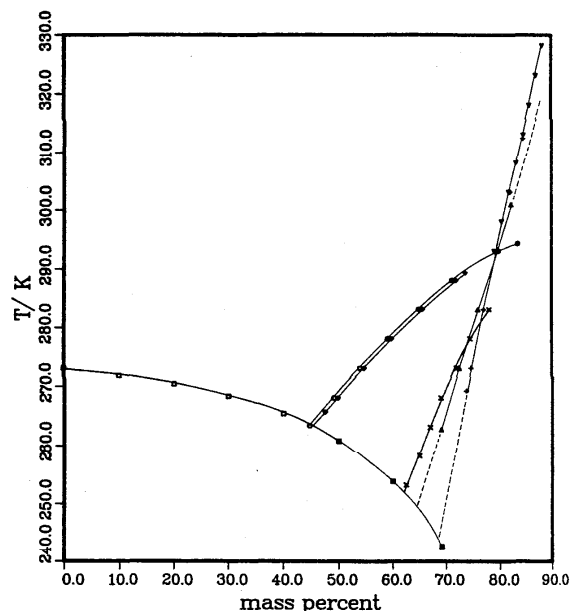


FIG. 3. Phase diagram for the system *D*-fructose + water. The solid curves refer to the following solid phases in equilibrium with aqueous *D*-fructose solutions: (□) ice; (○) *D*-fructose dihydrate; (◇) a metastable crystalline phase; (x) gel; (Δ) hemihydrate; and {(▽) and (+)} anhydrous *D*-fructose. All of the data are from Young and Johnson (Ref. 28) with the exception of the points (▽) of Jackson and Silsbee (Ref. 27) Jackson and Silsbee (Ref. 27) for the solubility of anhydrous fructose. The broken lines were extrapolated from the experimental data. The transition of *D*-fructose dihydrate to the anhydrous form and water occurs at 20 °C (293.15 K).

ties from the isentropic compressibilities, the needed values of $C_{p,2}^{\circ}$ were taken from Table 15 of this paper. The extremely precise and careful measurements of Bernal and van Hook⁴⁵ on aqueous glucose and fructose are preferred over the earlier data.

Table 6 contains values of the parameters of the correlating equations (see Sec. 3 above) of the excess Gibbs energy, enthalpy, heat capacity, volume, expansivity, and the isentropic compressibility and its temperature derivative. In nearly all cases the correlations are based upon the results of a single investigation, the exceptions being the data leading to the excess Gibbs energy and enthalpy of aqueous glucose solutions. For the excess Gibbs energy the most weight has been given to the isopiestic data of Stokes and Robinson²⁹ and of Miyajima, Sawada, and Nakagi.³⁰ The results of Taylor and Rowlinson³¹ are based upon direct vapor pressure measurements. This method of measurement is more difficult than the isopiestic approach, and typically yields results that are less accurate. A deviation plot of observed minus calculated values of the osmotic coefficient of aqueous glucose solutions as a function of the molality is shown in Fig. 4. The heat of dilution data of aqueous glucose solutions determined by Lange and Markgraf³² and by Savage and Wood^{33,34} are in excellent agreement with each other. Plots of the excess Gibbs energy, enthalpy, and entropy are shown in Figs. 5–7. Note that in all cases the excess Gibbs energies, entropies, and enthalpies are positive and that the entropic contributions (TS^{ex}) to the excess Gibbs energies serve to

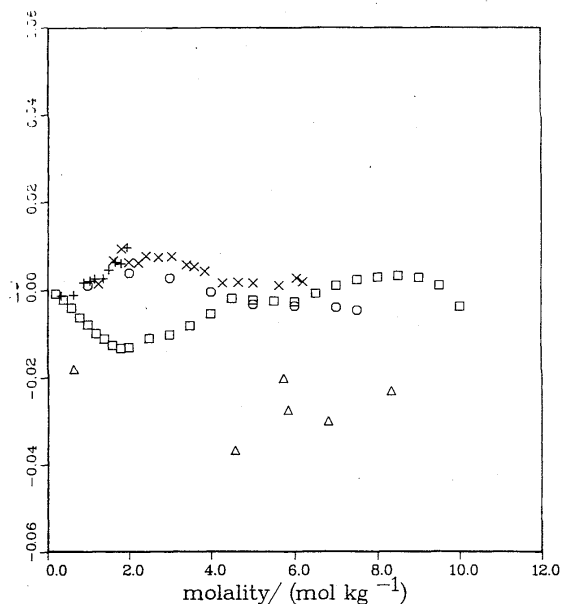


Fig. 4. Deviation plot (observed minus calculated values) of the osmotic coefficient of aqueous glucose solutions as a function of the molality. The data sets are from the following sources: (Δ) Taylor and Rowlinson (Ref. 31), (\square) Bonner and Breazeale (Ref. 29a), (\circ) Stokes and Robinson (Ref. 29), ($+$) Miyajima *et al.* (Ref. 30), NaCl reference solution and (\times) Miyajima *et al.* (Ref. 30), CaCl_2 reference solution.

offset a substantial proportion (30%–70%) of the enthalpic contributions.

There is a very limited amount of transport property data available on aqueous carbohydrate solutions. It is summarized in Table 7.

Table 8 contains the percent composition of the anomeric forms of the hexoses and pentoses taken from the thor-

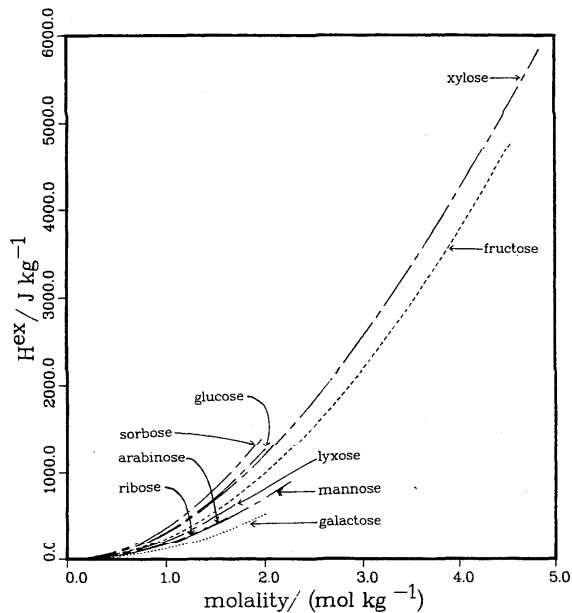


Fig. 6. The excess enthalpy of aqueous carbohydrate solutions as a function of molality.

ough review of Angyal.¹⁰ Using these data and the few estimates given in Table 9, the Gibbs energy changes at 298.15 K for the conversion of the various anomeric forms to the equilibrium mixture have been calculated. The results of these calculations are given in Table 9. In the main body of the thermochemical tables (Tables 11–15) only the equilibrium mixture of the anomeric forms of the carbohydrates is considered. Thus, Gibbs energy changes for processes involving specific anomeric forms of the carbohydrates can be calculated using an appropriate combination of the Gibbs energy

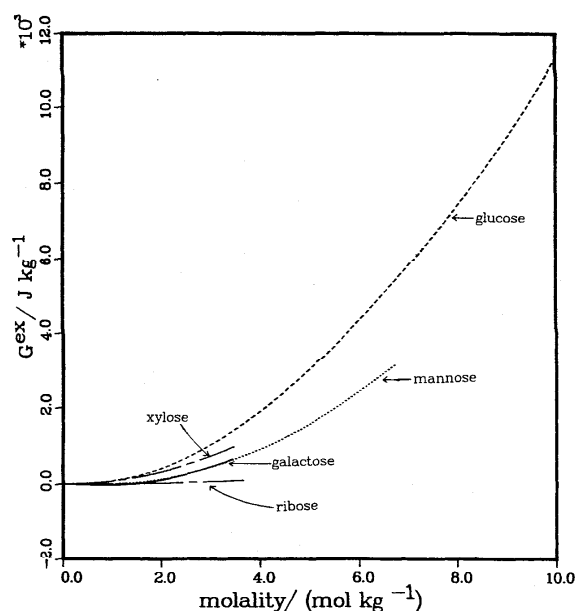


Fig. 5. The excess Gibbs energy of aqueous carbohydrate solutions as a function of molality.

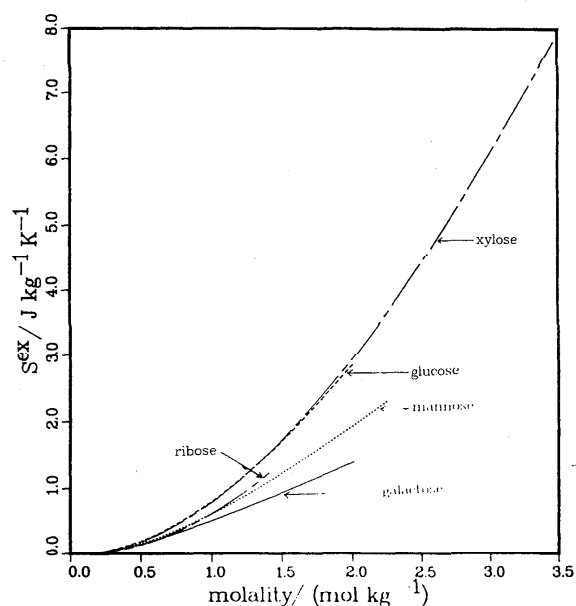


Fig. 7. The excess entropy of aqueous carbohydrate solutions as a function of molality.

changes in Table 9 with the Gibbs energy data contained in Tables 11–15. There is also a limited amount of information available on enthalpy, heat capacity, and volume changes involving specific anomeric forms of the carbohydrates. It is summarized in Table 10. Note that there is a large enthalpy difference between the pyranose and furanose forms of fructose. However, the enthalpy differences between the α and β forms of the carbohydrates are relatively small and the entropy differences between these forms are close to zero.

Table 11 contains the reaction catalog of Gibbs energy, enthalpy, and entropy data pertinent to these carbohydrates and their monophosphates; the heat capacity catalog is given in Table 12. The indexes of compounds and their reactions in reference to these two catalogs are given in Tables 13 and 14, respectively. These indexes are useful in examining cross links between the data for specific compounds and reactions. Table 15 contains the calculated values of the thermochemical properties at 298.15 K with the auxiliary thermochemical data used being given at the end of the table. The reaction catalogs are similar in format to those given¹⁶ in the "CODATA Thermodynamic Tables" and in the review by Parker, Evans, and Nuttall¹³ on rubidium compounds. Note that compounds having the same empirical formula are distinguished in the Tables 12–15 by the addition of a number to the abbreviation designating the physical state of the substance. The molar masses used in these tables are based upon the 1981 Atomic Weights¹⁹; the mass of the electron is considered when calculating molar masses of charged species.

The thermochemical tables have been prepared by editing the computer output of the "CATCH" system^{12,20} presently in use at the National Institute of Standards and Technology. A principal advantage of this system is that once a reaction catalog is established it can be updated to include the new and/or revised data. Also, the effects on the solution of the thermochemical network due to changes in the relative weights given to individual results can be conveniently investigated.

In the thermochemical catalogs, the experimental data reported in individual papers have been adjusted, insofar as possible, to 298.15 K and to the thermochemical standard state (see Sec. 2.1). These adjustments have frequently required the use of estimated enthalpies and/or heat capacities, activity coefficients, and equilibrium modeling calculations^{35,36} to obtain the thermochemical parameters for appropriate reference reactions at 298.15 K and at the standard state. In the absence of direct measurements, it has frequently been necessary to estimate activity coefficients. This has usually been done using an extended Debye-Hückel expression with the B or "ion size" parameter set equal³⁷ to $1.6 \text{ mol}^{-1/2} \text{ kg}^{1/2}$.

In constructing the thermochemical tables it was necessary to make estimates of two entropies, specifically the partial molar entropies of aqueous ribose and ribose 5-phosphate. The estimated entropy of $204 \pm 20 \text{ J mol}^{-1} \text{ K}^{-1}$ for aqueous ribose is based upon the partial molar entropy of aqueous xylose. In this respect, note that the values of the partial molar entropies of the aqueous hexoses are reasonably close to each other. The estimated entropy of $69 \text{ J mol}^{-1} \text{ K}^{-1}$ for aqueous ribose 5-phosphate is based upon

an experimental determination of the enthalpy change ($-5.69 \text{ kJ mol}^{-1}$) and an estimated equilibrium constant of 420 for the hydrolysis of ribose 5-phosphate.³⁶ Since these two estimates substantially extend the thermochemical network, we believe that they are useful. Clearly, measurements which would eliminate the need for these estimates are desirable.

6. Trends and Physical Interpretation of the Data

6.1. Ranges of Property Values

Table 16 contains the range of values for many of the properties considered in this review. Among the more useful of these are the values found for the quantities $\{C_{p,2}^{\circ} [\text{sugar}(\text{ao})] - C_{p,2}^{\circ} [\text{sugar-phosphate}(\text{ao})]\}$ and $\{S_2^{\circ} [\text{sugar}(\text{ao})] - S_2^{\circ} [\text{sugar-phosphate}(\text{ao})]\}$. Thus, if either Δ or $C_{p,2}^{\circ}$ is known for the sugar or its phosphate, the corresponding quantity can be estimated. In this regard, the recommended values to be used for the differences in these heat capacities and entropies are, respectively, 280 and $13 \text{ J mol}^{-1} \text{ K}^{-1}$. Generally, the entropies and the heat capacities have proven to be the most useful thermodynamic functions for estimation purposes. While in several cases it is difficult to state whether the observed ranges of values are real or attributable to measurement errors, an understanding of the detailed differences within a given range of values will require a better knowledge of the variations in thermodynamic property values between the various anomeric forms of the carbohydrates than is now available.

6.2. Physical Interpretation of the Data

The molecular interpretation of the physical property data is a difficult problem which is presently unresolved. While attempts at molecular calculations have been attempted (see, for example, the review of Cesaro¹¹) the results that have been obtained are far from satisfactory. Therefore, the current rationalization of the properties of carbohydrates have relied principally upon either hydration or group contribution effects. Some of the significant efforts in this direction will be summarized briefly.

Kabayama and Patterson³⁸ have attempted to rationalize the enthalpy and entropy changes for the mutarotation data of aqueous carbohydrates in terms of changes in the hydration of the reducing hydroxyl groups. Later, Stokes and Robinson²⁹ used a successive hydration model to represent the osmotic coefficients of aqueous carbohydrate solutions to $\approx 7 \text{ mol kg}^{-1}$. Franks, Ravenhill, and Reid³⁹ have argued for the absence of solute-solute interactions in aqueous solutions of carbohydrates and for specific hydration models as applied to understanding the aqueous volumetric properties. Hydration effects have been extensively invoked by Angyal¹⁰ in rationalizing the relative stabilities of aqueous carbohydrates. Closely related to rationalizations involving hydration are those involving the number of equatorial hydroxyl groups on the carbohydrates. Uedair and Uedaira^{40,41} have used this approach to understand the diffusion and partial molar heat capacity data. Most recent

Wilk and Somsen^{42,43} used both preferential solvation and hydrophobic hydration arguments to account for enthalpies of transfer of carbohydrates from water to *N,N*-dimethylformamide solutions.

An alternative approach for the representation of the excess properties has been proposed by Savage and Wood.³³ They assumed that each functional group in a molecule interacts with every functional group in the other molecule and that this interaction is independent of the positions of the functional groups in the two molecules. Each interaction has a characteristic effect on the excess property. These interaction energies are regressed from a body of experimental data and can be used to predict properties of additional systems which have not yet been measured. Barone and co-workers⁴⁴ have applied this approach to the excess properties of aqueous carbohydrate solutions. They have also attempted to correlate the property differences between the isomers with differences in stereochemistry.

Bernal and van Hook⁴⁵ have summarized several attempts at property data rationalization which involved structure making and breaking effects. They concluded that arguments along this line had not been successful. They also made the useful observation that the "volumetric properties of carbohydrates are similar in sign if not in magnitude to those commonly associated with strong electrolytes."

The problem of the rationalization of properties of systems of the type considered here is a particularly difficult and, presently, unresolved issue. The systematic collection and evaluation of additional property data would significantly aid progress in this area. This data can then be carefully examined either to suggest or substantiate improved physical models for these systems.

7. Needed Measurements

Examination of the data in the tables can also serve to guide in the selection of new measurements. In certain areas, the data is particularly sparse, e.g., transport properties and phase diagrams. Additional data in these areas should prove useful. While the equilibrium or Gibbs energy data relating different anomeric forms of the carbohydrates is reasonably good, there is relatively little information available on enthalpy, heat capacity, or volume changes in this field. In the area of excess property data the enthalpies are the most complete in terms of available data. Thus, we would like to see additional isopiestic measurements performed on other aqueous sugar and sugar phosphate solutions. There is a real need for the measurements of heat capacities of solutions as a function of molality. This would permit the accurate calculation of the virial parameters of the excess heat capacity. Examination of the heat capacity catalog (Table 12) shows several discrepancies which need to be resolved. Here, the data for aqueous fructose is the prime example. Also, there are no direct heat capacity measurements on aqueous solutions of the sugar phosphates.

All of the third law entropies contained in the thermochemical tables involved long extrapolations to the absolute zero of temperature and, therefore, have larger uncertainties than can be obtained using modern methods. In particular, we would welcome third law entropies determined on ana-

merically well characterized samples of crystalline glucose, fructose, ribose, and xylose. An understanding of how the various anomeric forms differ in their third law entropies would be extremely interesting. Similarly, the discrepancies in several of the enthalpies of combustion, mannose and fructose in particular, need to be resolved. In constructing the thermochemical catalog we were able to obtain a very tight and consistent solution of the network involving the aqueous solute species by giving zero weight to those reactions involving ATP (adenosine *s'*-triphosphate) coupled processes. Therefore, the residuals in these latter processes are larger than their assigned uncertainties. We suspect that these discrepancies are due either to (i) unsuspected side reactions or (ii) to the proton and metal-ion binding corrections, or (iii) to the adjustment to the thermochemical standard state. In any case the uncertainties in the Gibbs energies and enthalpies of ATP coupled processes (reactions 105–110) are larger than initially believed. Further attention in this area is needed. The thermochemical network also used two estimated entropies, specifically for aqueous ribose and ribose 5-phosphate (see Sec. 5 above). The former estimate could be made redundant if a third law entropy were determined for ribose(cr). The preferred pathway for eliminating the second estimate involves a determination of the equilibrium constant for the hydrolysis of ribose 5-phosphate to ribose and inorganic phosphate. This data could then be combined with the enthalpy change for this reaction and the partial molar entropy of aqueous ribose determined from a third law entropy of the crystal. Examination of the thermochemical network also indicates the need for additional measurements on other enzyme-catalyzed reactions. Specifically, we would like to see equilibrium data determined for the hydrolyses of ribulose 5-phosphate and ribose 1-phosphate and direct calorimetric measurements performed on the isomerizations of glucose 1-phosphate to glucose 6-phosphate, of galactose 1-phosphate to glucose 1-phosphate, and of aqueous mannose to fructose. An error in the enthalpy change for this latter process could help to explain the discrepancies in the enthalpies of combustion of crystalline mannose and fructose.

The thermodynamic data contained in these tables is useful both for examining efficiencies and for optimizing the reaction conditions for industrially useful processes. For example, the data contained in these tables can be used to calculate the temperature dependency of the conversion of glucose to fructose.⁴⁶ Similarly, there is substantial interest in the production of ethanol from biomass.^{47,48} The formation properties given in Table 15 together with those for ethanol¹⁵ can be used to examine the efficiencies of proposed processes in this area. In summary, the thermochemical catalog approach is useful for examining the consistency of thermodynamic data and in expanding its predictions. We would like to see it extended to other networks involving enzyme-catalyzed reactions and to biochemical processes in general.

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10 Tables

TABLE 1. Melting and transition temperatures of the pure carbohydrates.
Unless indicated otherwise, the data were taken from [42BAT]

Carbohydrate	Melting or transition temperature
	°C
β -arabinose	160
lyxose:	
α form	106-107
β form	117-118
ribose	87
ribulose	syrup
α -xylose	145
xylulose	syrup
β -allose	128
β -altrose	\approx 106
β -fructose:	
dihydrate	20.0 ^a
anhydrous	102-104
α -galactose:	
anhydrous	167
hydrate	118-120 ^b
glucose:	
α form	146
α monohydrate	50 ^c
β form	148-150
gulose	syrup
idose	
mannose:	
α form	133
β form	132
psicose	syrup
sorbose	159-161
tagatose	134-135 ^b
talose:	
α form	133-134
β form	120-121

^aTransition temperature of dihydrate to anhydrous [52YOU/JON].

^bData from compilation of [82BAI].

^cTransition temperature of monohydrate to anhydrous [22JAC/SIL].

TABLE 2. Densities and cubic expansion coefficients of the pure carbohydrates near 298 K obtained from the literature

Carbohydrate	ρ^* g cm ⁻³	Reference
β -D-allose(cr)	1.593 ^c	[84KRO/SLU]
β -arabinose(cr)	1.619 ^c	[61HOR]
β -L-arabinose(cr)	1.626 ^{b,c}	[77TAK/JEF]
β -DL-arabinose(cr)	1.636 ^{b,c}	[67KIM/JEF]
	1.640 ^{b,c}	[79TAK/NOR]
β -D-fructose(cr)	1.601 ^{b,c}	[77KAN/ROE]
β -D-fructopyranose(cr)	1.599 ^{b,c}	[77TAK/JEF ²]
α -D-galactose(cr)	1.619 ^c	[76OHA/GIL] ^d
	1.61 ^c	[76SHE]
β -D-galactose(cr)	1.579 ^c	[75LON/OHA] ^d
	1.595 ^c	[76SHE]
glucose(glass)	1.523 ^b	[28PAR/HUF]
glucose(cr)	1.540 ^b	[65RAM/GOR]
α -D-glucose(cr)	1.566 ^c	[65BRO/LEV]
	1.560 ^c	[74SWA/MUR]
	1.562 ^c	[79BRO/LEV]
β -D-glucose(cr)	1.528 ^{b,c}	[63FER]
	1.552 ^{b,c}	[68CHU/JEF]
lyxose(cr)	1.544 ^c	[66HOR]
β -L-xylopyranose(cr)	1.536 ^c	[78NOR/TAK]
mannose(cr)	1.501 ^b	[31MAR]
α -D-mannopyranose(cr)	1.564 ^c	[76LON/AVE]
D-ribose(cr)	1.59 ^{b,c}	[56FUR/HOR]
α -L-sorbopyranose(cr)	1.607 ^{b,c}	[67KIM/ROS]
	1.605 ^{b,c}	[79NOR/TAK]
α -D-tagatose(cr)	1.655 ^c	[69TAK/ROS]
α -D-talose(cr)	1.591 ^{b,c}	[77HAN/HOR]
α -D-talopyranose(cr)	1.602 ^c	[77OHA/AVE]
D-xylose(cr)	1.617 ^c	[58WOO]
α -xylose(cr)	1.511 ^c	[71HOR]
α -L-xylopyranose(cr)	1.663 ^{ab}	[80JEF/ROB]
	1.524 ^c	[79TAK/JEF]

Cubic expansion coefficients at 298.15 K

Compound	$\frac{\alpha^* \times 10^4}{K^{-1}}$	Reference
glucose(cr)	3.1	[28PAR/HUF]
glucose(glass)	2.4	[65RAM/GOR] ^d

^aOne set of x-ray data for α -L-xylopyranose was determined at 123 K by [80JEF/ROB].

^bDetermined by flotation method.

^cCalculated from x-ray data.

^d[65RAM/GOR] report the existence of a second order phase transition at ≈ 296.2 K. Below this temperature, the cubic expansion coefficient is equal to $5.1 \times 10^{-4} K^{-1}$.

Table 1. Recommended values of the densities, molar volumes, cubic expansion coefficients, and expansivities of the pure carbohydrates at 298.15 K. Unless indicated otherwise, the values pertain to the pure D or L form of the compound

Carbohydrate	ρ^* g cm ⁻³	$V^* \times 10^6$ m ³ mol ⁻¹	$\alpha^* \times 10^4$ K ⁻¹	$E^* \times 10^8$ m ³ mol ⁻¹ K ⁻¹
D-glucose(cr)	1.593±0.005	113.1±0.4		
D-arabinose(cr)	1.624±0.01	92.44±0.6		
D-xylose(cr)	1.638±0.005	91.65±0.3		
D-fructose(cr)	1.600±0.005	112.6±0.4		
D-fructopyranose(cr)	1.599±0.005	112.7±0.4		
D-galactose(cr)	1.619±0.005	111.3±0.4		
L-galactose(cr)	1.587±0.01	113.5±0.7		
D-glucose(glass)	1.523±0.005	118.3±0.4	3.1±0.2	3.7±0.2
D-glucose(cr)	1.562±0.003	115.3±0.2	2.4±0.1	2.8±0.1
D-glucose(cr)	1.552±0.005	116.1±0.4		
D-fructose(cr)	1.544±0.01	97.23±0.6		
D-fructopyranose(cr)	1.536±0.005	97.74±0.3		
D-mannose(cr)	1.501±0.01	120.0±0.8		
D-mannopyranose(cr)	1.564±0.01	115.2±0.8		
D-xylose(cr)	1.59±0.02	94.4±1.		
D-sorbose(cr)	1.606±0.005	112.2±0.3		
D-tagatose(cr)	1.655±0.01	108.9±0.7		
D-talose(cr)	1.591±0.005	113.2±0.4		
D-talopyranose(cr)	1.602±0.005	112.5±0.4		
D-xylose(cr)	1.511±0.01	99.36±0.7		
D-xylopyranose(cr)	1.524±0.01	98.51±0.7		

TABLE 4. Values of standard state volumetric properties of aqueous carbohydrates at 298.15 K from the literature

Compound	"Best" value	Worker(s)														
		25RIB/ESP	26RIB/MIN	58SHI	69UED/UED	70NEA/GOR	72FRA/RAV	76SHA/FAR	77SAV	78HOI/HOL	78LOS/SHI	82JAS/AHL	83MIY/SAW2	84JAS/AHL	85UED/UED	86BER/HOO
arabinose	93.7±0.3			94.0			91.9		93.2			94.0				
fructose	110.7±0.1	110.7 ^a	110.5			110.4						110.9				110.69
galactose	110.5±0.3	110.2 ^a				110.7		111.9	110.2			110.6				
glucose	112.0±0.1	111.5 ^a	112.2		111.9		112.2	111.9	111.7	112.04		111.7	111.3		111.9	111.99
lyxose	95.7±0.3											95.7				
mannose	111.5±0.3					111.2 ^b			111.3			112.0				
ribose	95.2±0.1					95.3			95.2		95.21	95.6		95.2		95.2
sorbose	111.0±0.3							110.6								
xylose	95.4±0.3		95.9	95.1		95.4		94.8	95.4						95.6	

^aAdjusted from 293.15 K using values of E_2^0 given in Table 4.^bData determined at 278.15 K and adjusted to 298.15 K using estimated value of E_2^0 .

TABLE 4. Values of standard state volumetric properties of aqueous carbohydrates at 298.15 K from the literature — Continued

Standard state partial molar expansivities $\{E_2^\circ = E_\phi^\circ = (\partial V_2^\circ/\partial T)_p\}$. The units are $10^{-6} \text{ m}^3 \text{ mol}^{-1} \text{ K}^{-1}$.

Compound	"Best" value	Worker(s)				
		70NEA/GOR	72FRA/RAV	77SAV	83MIY/SAW2	86BER/HOO
fructose	0.136 ± 0.01					0.136
glucose	0.15 ± 0.03		0.15			
fructose	0.091 ± 0.01	0.10	0.12	0.11	0.11	0.091
glucose	0.12 ± 0.03		0.15			

Standard state partial molar isentropic compressibilities $\{K_{S,2}^\circ = K_{S,\phi}^\circ = (\partial V_2^\circ/\partial T)_S\}$. The units are $10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1}$.

Compound	"Best" value	Worker(s)				
		58SHI	72FRA/RAV	78HOL/HOL	78LOS/SHI	86BER/HOO
fructose	-19.3 ± 0.1	-14.5		-19.3		
glucose	-21.37 ± 0.02	-16.5				-21.37
fructose	-20.8 ± 0.1			-20.8		
glucose	-17.80 ± 0.02	-13.8	-16.0	-17.8	-17.50	-17.80
fructose	-16.0 ± 0.1			-16.0		
glucose	-12.5 ± 0.1		-13.0	-12.5	-12.46	
fructose	-12.9 ± 0.1	-9.4		-12.9		

Values of the temperature derivative of the standard state partial molar isentropic compressibilities $\{(\partial K_{S,2}^\circ/\partial T)_p\}$. The units are $10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1} \text{ K}^{-1}$.

Compound	"Best" value	Worker(s)	
		72FRA/RAV	86BER/HOO
fructose	0.80 ± 0.1	1.03	0.80
glucose	0.64 ± 0.1	1.14	0.64

TABLE 5. Recommended values of the standard state volumetric properties of aqueous carbohydrates at 298.15 K

Compound	$V_2^s \times 10^6$ $\text{m}^3 \text{mol}^{-1}$	$E_2^s \times 10^6$ $\text{m}^3 \text{mol}^{-1} \text{K}^{-1}$	$K_{S_2}^s \times 10^{15}$ $\text{m}^3 \text{mol}^{-1} \text{Pa}^{-1}$	$K_{T_2}^s \times 10^{15}$ $\text{m}^3 \text{mol}^{-1} \text{Pa}^{-1}$	$(\partial K_{S_2}^s / \partial T)_P \times 10^4$ $\text{m}^3 \text{mol}^{-1} \text{Pa}^{-1} \text{K}^{-1}$
arabinose	93.7±0.3		-19.3±0.1	-15.2±0.2	
fructose	110.7±0.1	0.136±0.01	-21.37±0.02	-16.7±0.1	0.80±0.1
galactose	110.5±0.3	0.15±0.03	-20.8±0.1	-15.6±0.2	
glucose	112.0±0.1	0.091±0.01	-17.80±0.02	-14.8±0.1	0.64±0.1
lyxose	95.7±0.3				
mannose	111.5±0.3		-16.0±0.1	-12.7±0.2	
ribose	95.2±0.1	0.12±0.03	-12.5±0.1	-8.4±0.2	
sorbose	111.0±0.3				
xylose	95.4±0.3		-12.9±0.1	-8.8±0.2	

TABLE 6. Recommended values of the parameters of the correlating equations of the excess properties of aqueous carbohydrate solutions at 298.15 K. In each case the maximum molalities to which the parameters are valid are given in the next to last column.

Parameters of the excess Gibbs energy. The units of the parameters are $\text{J kg}^i \text{mol}^{-(i+1)}$							
Compound	g_1	g_2	g_3	g_4	g_5	m_{max} mol kg^{-1}	Workers
galactose	-129.678 ± 42.0	140.352 ± 47.0	-37.884 ± 21.0	3.693 ± 2.0		3.45	[83MIY/SAW]
glucose	63.102 ± 21.0	27.543 ± 9.5	-4.084 ± 1.5	0.183 ± 0.081		10.00	[55TAY/ROW], [65BON/BRE], [66STO/ROB], [83MIY/SAW]
mannose	-46.678 ± 20.0	68.112 ± 19.0	-18.062 ± 7.3	2.369 ± 1.2	-0.120 ± 0.069	6.74	[83MIY/SAW]
ribose	7.501 ± 1.6					3.66	[85UED/UED]
xylose	81.523 ± 3.6					3.47	[69UED/UED]
Parameters of the excess enthalpy. The units of the parameters are $\text{J kg}^i \text{mol}^{-(i+1)}$							
Compound	h_1	h_2	$m_{\text{max}}/\text{mol kg}^{-1}$	Worker(s)			
arabinose	177.8±20.	7.42±5.3	1.61	[82BAR/CAC]			
fructose	264.2±19.	-7.15±4.2	4.54	[81BAR/CAS]			
galactose	133.3±8.0		2.01	[81BAR/CAC]			
glucose	342.±10.	-12.4±4.0	2.00	[50LAN/MAR], [76SAV/WOO], [77SAV]			
lyxose	242.7±7.5	-10.7±3.9	1.69	[83BAR/CAS]			
mannose	207.2±17.	-14.0±5.2	2.26	[81BAR/CAC]			
ribose	201.7±9.1	-5.5±5.7	1.41	[83BAR/CAS]			
sorbose	394.9±12.	-16.2±6.0	1.96	[82BAR/CAC]			
xylose	339.3±17.	-18.6±3.1	4.84	[81BAR/CAC]			

Table 6. Recommended values of the parameters of the correlating equations of the excess properties of aqueous carbohydrate solutions at 298.15 K. In each case the maximum molalities to which the parameters are valid are given in the next to last column — Continued

Parameters of the excess heat capacity. The units of the parameters are $\text{J K}^{-1} \text{kg}^i \text{mol}^{-(i+1)}$.

Compound	c_1	$m_{\text{max}}/\text{mol kg}^{-1}$	Workers
Fructose	7.70 ± 0.15	4.07	[76BON/CER]

Parameters of the excess volume. The units of the parameters are $10^{-6} \text{m}^3 \text{kg}^i \text{mol}^{-(i+1)}$.

Compound	v_1	v_2	$m_{\text{max}}/\text{mol kg}^{-1}$	Workers
Fructose	0.534 ± 0.03		2.08	[86BER/HOO]
Glucose	0.511 ± 0.03		1.99	[86BER/HOO]
Sucrose	0.37 ± 0.1		0.44	[85UED/UED]
Galactose	0.782 ± 0.23	-0.101 ± 0.056	3.00	[69UED/UED]

Parameters of the excess expansivity. The units of the parameters are $10^{-8} \text{m}^3 \text{K}^{-1} \text{kg}^i \text{mol}^{-(i+1)}$.

Compound	e_1	$m_{\text{max}}/\text{mol kg}^{-1}$	Workers
Fructose	-1.2 ± 0.3	2.08	[86BER/HOO]
Glucose	-0.9 ± 0.5	1.99	[86BER/HOO]

Parameters of the excess isentropic compressibility. The units of the parameters are $10^{-15} \text{m}^3 \text{Pa}^{-1} \text{kg}^i \text{mol}^{-(i+1)}$.

Compound	k_{S1}	$m_{\text{max}}/\text{mol kg}^{-1}$	Workers
Fructose	4.01 ± 0.01	1.2	[86BER/HOO]
Glucose	2.73 ± 0.01	0.4	[86BER/HOO]

Parameters of the temperature derivative of the excess isentropic compressibility. The units of the parameters are $10^{-15} \text{m}^3 \text{Pa}^{-1} \text{K}^{-1} \text{kg}^i \text{mol}^{-(i+1)}$.

Compound	$(\partial k_{S1} / \partial T)_p$	$m_{\text{max}}/\text{mol kg}^{-1}$	Workers
Fructose	-0.165 ± 0.02	1.2	[86BER/HOO]
Glucose	-0.081 ± 0.02	0.4	[86BER/HOO]

TABLE 7. Diffusion and viscosity data for aqueous carbohydrate solutions

Limiting values of the diffusion coefficients				
Carbohydrate	<i>T</i> /K	$D^\infty \times 10^{10}/\text{m}^2 \text{ s}^{-1}$	Workers	
fructose	298.15	7.001±0.01	[70UED/UED]	
glucose	298.15	6.735±0.05	[53GLA/DOL]; also see [55LON]	
	308.15	8.401±0.05	[53GLA/DOL]	
ribose	298.15	7.795±0.01	[85UED/UED]	
xylose	298.15	7.480±0.02	[69UED/UED]	

Expressions for the diffusion coefficients of aqueous carbohydrates as a function of concentration				
Carbohydrate	<i>T</i> /K	Expression (<i>D</i> has units of $10^{10} \text{ m}^2 \text{ s}^{-1}$)	$m_{\text{max}}/\text{mol kg}^{-1}$ or $c_{\text{max}}/\text{mol L}^{-1}$	Workers
fructose	298.15	$D = 7.00149 - 1.42416m$	0.14	[70UED/UEI]
glucose	298.15	$D = 67.3865 - 16.8107m + 2.60593m^2 - 0.250149m^3 + 0.0122802m^4 - 0.000226402m^5$	22.43	[53GLA/DOL]
	308.15	$D = 84.0051 - 13.9645m + 0.897491m^2 - 0.0193112m^3$	23.08	[53GLA/DOL]
ribose	298.15	$D = 7.79508 - 0.553466c$	0.16	[85UED/UEI]
xylose	298.15	$D = 7.48034 - 0.984835c$	0.45	[69UED/UEI]

Expressions for the reduced viscosities of aqueous carbohydrate solutions				
Carbohydrate	<i>T</i> /K	Expression	$c_{\text{max}}/\text{mol L}^{-1}$	Workers
glucose	288.15	$(\eta/\eta^*) = 1.0 + 0.49c$	0.12	[83MIY/SAW]
	298.15	$(\eta/\eta^*) = 1.0 + 0.45c$	0.12	[83MIY/SAW]
	308.15	$(\eta/\eta^*) = 1.0 + 0.43c$	0.12	[83MIY/SAW]
xylose	298.15	$(\eta/\eta^*) = (1.0 - 0.337c)^{-1}$	0.5	[69UED/UEI]

TABLE 8. Percent compositions of the anomeric forms of the hexoses and pentoses in D₂O. The data are taken from the review of [84ANG]

A. Aldo-hexoses and pentoses							
Compound	T/K	pyranose		furanose		aldehyde	
		α	β	α	β		
arabinose	304.15	60.	35.5	2.5	2.	0.03	
lyxose	304.15	70.	28.	1.5	0.5	0.03	
ribose	304.15	21.5	58.5	6.5	13.5	0.05	
xylose	304.15	36.5	63.		<1	0.02	
allose	304.15	14.	77.5	3.5	5.	0.01	
altrose	295.15	27.	43.	17.	13.	0.04	
galactose	304.15	30.	64.	2.5	3.5	0.02	
glucose	304.15	38.	62.	—	0.14	0.002	
gulose	295.15	16.	81.	—	3.	—	
idose	304.15	38.5	36.	11.5	14.	0.2	
mannose	317.15	65.5	34.5	0.6	0.3	0.005	
talose	295.15	42.	29.	16.	13.	0.03	

B. Keto-hexoses							
Compound	T/K	pyranose		furanose		keto form	
		α	β	α	β		
fructose	303.15	2.	70.	5.	23.	0.7	
psicose	300.15	22.	24.	39.	15.	0.2	
sorbose	300.15	98.	—	2.	—	0.2	
tagatose	300.15	79.	16.	1.	4.	0.6	

TABLE 9. Gibbs energy changes at 298.15 K for the conversion of the various forms of the carbohydrates to the equilibrium mixture. The units are kJ mol⁻¹.

Carbohydrate	α -pyranose	β -pyranose	α -furanose	β -furanose	aldehyde ^a
arabinose	+0.84	-0.44	-7.34	-7.87	-18
lyxose	+0.85	-1.40	-8.98	-11.7	-19
ribose ^a	-1.05	+1.45	-4.32	-2.48	-16
xylose	-0.77	+0.63			-20
allose	-3.03	+1.23	-6.78	-5.86	-21
altrose	-0.10	+1.04	-1.09	-1.77	-16
galactose	-0.86	+1.05	-7.32	-6.46	-19
glucose ^a	-0.74	+0.49		-14.9	-26
gulose ^a	-3.12	+0.89		-7.1	
idose	+0.85	+0.70	-2.45	-1.94	-13
mannose	+0.71	-0.99	-11.8	-13.7	-24
talose	+0.99	+0.06	-1.25	-1.77	-17

Carbohydrate	α -pyranose	β -pyranose	α -furanose	β -furanose	ketone
fructose	-7.61	+1.23	-5.58	-1.78	-10
psicose	-0.38	-0.16	+0.94	-1.42	-11
sorbose ^a	+0.23		-9.52		-15
tagatose	+1.11	-2.84	-9.82	-6.38	-11

^aIn calculating these Gibbs energy changes it was necessary to estimate the percent compositions of a few isomers. These estimates were: 0.5% for both the α and β furanose forms of xylose; 0.01% for the α -furanose form of glucose; 0.01% for the α -furanose and 0.005% for the aldehyde form of gulose; and 0.01% for the β -furanose form of sorbose. Where necessary estimated enthalpies were used to adjust the data in Table 8 at 298.15 K.

TABLE 10. Additional thermodynamic data for anomeric conversions at 298.15 K

Process	ΔG° kJ mol ⁻¹	ΔH° kJ mol ⁻¹	ΔS° J mol ⁻¹ K ⁻¹	ΔC_p° J mol ⁻¹ K ⁻¹	$\frac{\Delta V^\circ \times 10^6}{\text{m}^3 \text{mol}^{-1}}$
α -xylose = β -xylose	-1.40 ± 0.2 ^a	-2.24 ± 0.1 ^b	-2.8 ± 0.8		
α -galactose = β -galactose	-1.90 ± 0.2 ^a	-1.30 ± 0.1 ^c	2.0 ± 0.8		
α -glucose = β -glucose	-1.24 ± 0.1 ^a	-1.15 ± 0.05 ^d	0.30 ± 0.4	-9. ± 3. ^f	0.31 ± 0.02 ^e
α -mannose = β -mannose	1.70 ± 0.2 ^a	1.85 ± 0.1 ^c	0.50 ± 0.8		
β -fructopyranose = β -fructofuranose	3.01 ± 0.2 ^a	15.2 ± 0.5 ^e	41. ± 2.		

^aCalculated from data in Table 8; adjustments to 298.15 K were done using the enthalpies given in this table.

^bBased on data given in [58KAB/PAT].

^cBased on data given in [73TAK/ONO].

^dBased on data given in [41STU] and [58KAB/PAT].

^eBased on data given in [88BAL/SOM]; also see [65AND/GRO] and [66GRO/AND].

^fBased on data given in [41STU].

^gBased on data given in [86BER/HOO]; also see [25RIB].

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
1	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Calorimetric measurement using alkaline phosphatase Enthalpy of hydrolysis of glucose-6P	ΔH	0.91	0.35	-0.162	88TEW/STE
2	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of glucose-6P Adj. to 298.15 K using $\Delta H = 0.9$ kJ mol ⁻¹ and $\Delta C_p = -48$ J mol ⁻¹ K ⁻¹ ; adj. from pH 7 Listed for information only	ΔG	-10.3	0.7	0.571	49MEY/GRE
3	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of glucose-6P Adjusted from pH 7 Listed for information only	ΔG	-9.84	0.50	1.031	54GIN
4	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of glucose-6P Adjusted from pH 7 Listed for information only	ΔG	-11.0	0.5	-2.129	61ATK/JOH
5	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of glucose-6P Adj. to 298.15 K using $\Delta H = 0.9$ kJ mol ⁻¹ and $\Delta C_p = -48$ J mol ⁻¹ K ⁻¹ ; adj. from pH 7	ΔG	-10.80	0.10	0.071	79LAW/VEE
6	$C_6H_{11}O_9P_2^-(ao3) + H_2O(l) = C_6H_{12}O_6(ao2) + HPO_4^{2-}(ao)$ Calorimetric measurement using alkaline phosphatase Enthalpy of hydrolysis of mannose-6P	ΔH	1.4	0.3	0.000	88TEW/STE
7	$C_6H_{11}O_9P_2^-(ao3) + H_2O(l) = C_6H_{12}O_6(ao2) + HPO_4^{2-}(ao)$ Equilibrium measurement using alkaline phosphatase Equilibrium constant for the hydrolysis of mannose-6P	ΔG	-9.08	0.70	0.000	49MEY/GRE
8	$C_6H_{11}O_9P_2^-(ao4) + H_2O(l) = C_6H_{12}O_6(ao3) + HPO_4^{2-}(ao)$ Calorimetric measurement using alkaline phosphatase Enthalpy of hydrolysis of fructose-6P	ΔH	-7.61	0.70	0.175	88TEW/STE
9	$C_6H_{11}O_9P_2^-(ao4) + H_2O(l) = C_6H_{12}O_6(ao3) + HPO_4^{2-}(ao)$ Equilibrium measurement using alkaline phosphatase Equilibrium constant for the hydrolysis of fructose-6P Adj. from 38 °C using $\Delta H = -7.6$ kJ mol ⁻¹ , $\Delta C_p = -28$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-12.3	0.5	1.327	49MEY/GRE

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
10	$C_6H_{11}O_9P_2^{2-}(ao4) + H_2O(l) = C_6H_{12}O_8(ao3) + HPO_4^{2-}(ao)$ Equilibrium measurement using alkaline phosphatase Equilibrium constant for the hydrolysis of fructose-6P	ΔG	-13.70	0.30	-0.073	88TEW/STE
11	$C_3H_5O_8P_2^{2-}(ao) + H_2O(l) = C_3H_{10}O_8(ao) + HPO_4^{2-}(ao)$ Calorimetric measurement using alkaline phosphatase Enthalpy of hydrolysis of ribulose-5P	ΔH	-5.69	0.50	0.000	88TEW/STE
12	$C_3H_5O_8P_2^{2-}(ao2) + H_2O(l) = C_3H_{10}O_8(ao2) + HPO_4^{2-}(ao)$ Calorimetric measurement using alkaline phosphatase Enthalpy of hydrolysis of ribulose-5P	ΔH	-12.43	0.50	0.000	88TEW/STE
13	$C_6H_{11}O_9P_2^{2-}(ao5) + H_2O(l) = C_6H_{12}O_8(ao4) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of galactose-6P Adj. from 38 °C using $\Delta H = 1.5$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹	ΔG	-11.15	0.70	0.000	49MEY/GRE
14	$C_6H_{11}O_9P_2^{2-}(ao7) + H_2O(l) = C_6H_{12}O_8(ao3) + HPO_4^{2-}(ao)$ Equilibrium constant for the hydrolysis of fructose-1P Adj. from 38 °C using $\Delta H = -7.6$ kJ mol ⁻¹ and $\Delta C_p = -28$ J mol ⁻¹ K ⁻¹	ΔG	-10.23	0.70	0.000	49MEY/GRE
15	$C_3H_5O_8P_2^{2-}(ao5) + H_2O(l) = C_3H_{10}O_8(ao) + HPO_4^{2-}(ao)$ From cycle calc. (two steps) Equil. constant for the hydrolysis of ribose-1P	ΔG	-22.0	0.5	0.000	80CAM/GIR
16	$C_6H_{11}O_9P_2^{2-}(ao) = C_6H_{11}O_9P_2^{2-}(ao4)$ Enthalpy of isomerization of glucose-6P to fructose-6P Second law treatment Listed for information only	ΔH	9.5	0.8	-2.168	60KAH/LOW
17	$C_6H_{11}O_9P_2^{2-}(ao) = C_6H_{11}O_9P_2^{2-}(ao4)$ Calorimetric measurement using phosphoglucose isomerase Enthalpy of isomerization of glucose-6P to fructose-6P	ΔH	11.7	0.2	0.032	88TEW/STE
18	$C_6H_{11}O_9P_2^{2-}(ao) = C_6H_{11}O_9P_2^{2-}(ao4)$ Equil. constant for the isomerization of glucose-6P to fructose-6P Adj. from 30 °C using $\Delta H = 11.7$ kJ mol ⁻¹ and $\Delta C_p = 44$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	2.21	0.20	-0.937	50SLE
19	$C_6H_{11}O_9P_2^{2-}(ao) = C_6H_{11}O_9P_2^{2-}(ao4)$ Equil. constant for the isomerization of glucose-6P to fructose-6P Adj. from 40 °C using $\Delta H = 11.7$ kJ mol ⁻¹ and $\Delta C_p = 44$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	1.48	0.20	-0.667	56GRAM/IR

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
20	$C_6H_{11}O_9P^{2-}(ao) = C_6H_{11}O_9P^{2-}(ao4)$ Equil. constant for the isomerization of glucose-6P to fructose-6P Adj. from 37 °C using $\Delta H = 11.7$ kJ mol ⁻¹ and $\Delta C_p = 44$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	1.44	0.20	-1.707	58NOL/BRU
21	$C_6H_{11}O_9P^{2-}(ao) = C_6H_{11}O_9P^{2-}(ao4)$ Equil. constant for the isomerization of glucose-6P to fructose-6P	ΔG	3.17	0.05	0.023	60KAH/LOW
22	$C_6H_{11}O_9P^{2-}(ao) = C_6H_{11}O_9P^{2-}(ao4)$ Equilibrium measurement using calorimetric data Equil. constant for the isomerization of glucose-6P to fructose-6P	ΔG	3.11	0.05	-0.037	88TEW/STE
23	$C_6H_{11}O_9P^{2-}(ao3) = C_6H_{11}O_9P^{2-}(ao4)$ Calorimetric measurement using phosphomannose isomerase Enthalpy of isomerization of mannose-6P to fructose-6P	ΔH	8.46	0.20	0.000	88TEW/STE
24	$C_6H_{11}O_9P^{2-}(ao3) = C_6H_{11}O_9P^{2-}(ao4)$ Equil. constant for the isomerization of mannose-6P to fructose-6P Adj. from 30 °C using $\Delta H = 8.4$ kJ mol ⁻¹ and $\Delta C_p = 38$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-0.85	0.20	-0.875	50SLE
25	$C_6H_{11}O_9P^{2-}(ao3) = C_6H_{11}O_9P^{2-}(ao4)$ Equil. constant for the isomerization of mannose-6P to fructose-6P Adj. from 37 °C using $\Delta H = 8.4$ kJ mol ⁻¹ and $\Delta C_p = 38$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-1.18	0.30	-1.205	58NOL/BRU
25	$C_6H_{11}O_9P^{2-}(ao3) = C_6H_{11}O_9P^{2-}(ao4)$ Equil. constant for the isomerization of mannose-6P to fructose-6P	ΔG	0.025	0.100	0.000	88TEW/STE
27	$C_5H_9O_8P^{2-}(ao2) = C_5H_9O_8P^{2-}(ao)$ Enthalpy of isomerization of ribulose-5P to ribose-5P Second law treatment Listed for information only	ΔH	-13.2	1.0	4.529	54AXE/JAN
28	$C_5H_9O_8P^{2-}(ao2) = C_5H_9O_8P^{2-}(ao)$ Enthalpy of isomerization of ribulose-5P to ribose-5P Second law treatment Listed for information only	ΔH	-17.	12.	0.729	60AGO/ARA

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
29	$C_5H_8O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Enthalpy of isomerization of ribulose-5P to ribose-5P Calorimetric measurement using phosphoribose isomerase Listed for information only	ΔH	-14.1	5.0	3.629	88TEW/STE
30	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Listed for information only	ΔG	-3.3	0.5	-2.100	54AXE/JAN
31	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Adj. from 37 °C using $\Delta H = -16.1$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-1.69	0.50	-0.490	56DIC/WIL
32	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Adj. from 37 °C using $\Delta H = -16.1$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-1.26	0.50	-0.060	57ASH/HIC
33	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Temperature not given Listed for information only	ΔG	-2.7	0.5	-1.500	57DIS/SHI
34	$C_5H_8O_8P_2^-(ao2) = C_5H_8O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Adj. from 37 °C using $\Delta H = -16.1$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-3.57	0.50	-2.370	58TAB/SRE
35	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Listed for information only	ΔG	-4.3	0.5	-3.100	60AGO/ARA
36	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Adj. from 37 °C using $\Delta H = -16.1$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	>3.6	0.5	-2.400	63DOB/DEM
37	$C_5H_9O_8P_2^-(ao2) = C_5H_9O_8P_2^-(ao)$ Equil. constant for the isomerization of ribulose-5P to ribose-5P Adj. from 38 °C using $\Delta H = -16.1$ kJ mol ⁻¹ and $\Delta C_p = -40$ J mol ⁻¹ K ⁻¹	ΔG	-1.20	0.10	0.000	86CAS/VEE

TABLE 1. CALCULATION OF THERMODYNAMIC PROPERTIES OF CARBOHYDRATES FROM THERMODYNAMIC DATA

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
38	C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 24 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-0.19	0.50	1.020	56DIC/WIL
39	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 37 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-0.19	0.50	1.020	56STU/HOR
40	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 37 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-0.51	0.50	0.700	57ASH/HIC
41	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 37 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-0.19	0.50	1.020	58BUR/HOR
42	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 37 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-2.5	0.5	-1.290	58TAB/SRE
43	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 24 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	-1.6	0.5	-0.390	58WOL
44	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Temperature not stated Listed for information only	ΔG	-1.0	0.5	0.210	62HUR
45	C ₃ H ₅ O ₈ P ²⁻ (ao2) = C ₃ H ₅ O ₈ P ²⁻ (ao3) Equil. constant for the isomerization of ribulose-5P to xylulose-5P Adj. from 35 °C using $\Delta H = +10.7$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹	ΔG	-1.21	0.10	0.000	86CAS/VEE
46	C ₃ H ₅ O ₈ P ²⁻ (ao4) = C ₃ H ₅ O ₈ P ²⁻ (ao2) Equil. constant for the isomerization of arabinose-5P to ribulose-5P Adj. from 38 °C using $\Delta H = 25.0$ kJ mol ⁻¹ and $\Delta C_p = 0$ J mol ⁻¹ K ⁻¹	ΔG	3.8	1.0	0.000	66VOL

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
47	$C_6H_{11}O_9P^2-(ao2) = C_6H_{11}O_9P^2-(ao)$ Equil. constant for the isomerization of glucose-1P to glucose-6P	ΔG	-7.13	0.20	-0.055	42COL/SUT
48	$C_6H_{11}O_9P^2-(ao2) = C_6H_{11}O_9P^2-(ao)$ Equilibrium measurement Equil. constant for the isomerization of glucose-1P to glucose-6P Equilibrium constant determined at 310.15 K. adjusted to 298.15 K using $\Delta H = 0$ kJ mol ⁻¹ Listed for information only	ΔG	-7.9	0.5	-0.825	61BEN/SCH
49	$C_6H_{11}O_9P^2-(ao2) = C_6H_{11}O_9P^2-(ao)$ Equilibrium measurement Equil. constant for the isomerization of glucose-1P to glucose-6P	ΔG	-7.02	0.20	0.055	61ATK/JOH
50	$C_6H_{11}O_9P^2-(ao6) = C_6H_{11}O_9P^2-(ao2)$ Equil. constant for the isomerization of galactose-1P to glucose-1P Equil. measurement at 37 °C. value uncorrected.	ΔG	-2.8	0.5	0.000	52LEL/CAR
51	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	8.9	2.0	6.088	67TAK
52	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	0.4	3.0	-2.412	73HAV/PIT
53	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	6.0	2.0	3.188	74LAN
54	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	1.5	4.0	-1.312	74SCA/SHI
55	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	3.1	2.0	0.288	76LLO/KHA

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
56	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	7.1	1.0	4.288	76SPR/LIM
57	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	2.9	15.0	0.088	79CLI
58	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	6.3	20.0	3.488	79MCK/TAV
59	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	2.6	0.6	-0.212	83TIL
60	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Listed for information only	ΔH	2.7	0.7	-0.112	84LLO/CHA
61	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Enthalpy of isomerization of glucose to fructose Second law treatment Listed for information only	ΔH	2.6	0.3	-0.212	84TEW/GOL
62	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Calorimetric measurement Enthalpy of isomerization of glucose to fructose	ΔH	2.78	0.20	-0.032	84TEW/GOL
63	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of glucose to fructose Adjusted to 298.15 K using $\Delta C_p = 76 \text{ J mol}^{-1} \text{ K}^{-1}$ Listed for information only	ΔH	3.7	0.8	0.888	86OLI/TOI

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
64	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Adjusted to 298 K using $\Delta H = 2.78$ kJ mol ⁻¹ and $\Delta C_p = 76$ J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	0.50	0.30	0.110	67DAN/YOS
65	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.71	0.20	0.320	67TAK
66	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.14	0.60	-0.250	73HAV/PIT
67	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.55	3.00	0.160	74LAN
68	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.32	0.70	-0.070	74SCA/SHI
69	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.41	0.20	0.020	76LLO/KHA
70	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.58	0.10	0.190	76SPR/LIM
71	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.37	2.00	-0.020	79CLI
72	C ₆ H ₁₂ O ₆ (ao) = C ₆ H ₁₂ O ₆ (ao3) Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.97	3.00	0.580	79MCK/TAY

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
73	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Listed for information only	ΔG	0.30	0.10	-0.090	83TIL
74	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of glucose to fructose	ΔG	0.41	0.20	0.020	84LLO/CHA
75	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of glucose to fructose	ΔG	0.349	0.050	-0.041	84TEW/GOL
76	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of glucose to fructose Adjusted to 298.15 K using $\Delta C_p = 76 \text{ J mol}^{-1} \text{ K}^{-1}$	ΔG	0.44	0.08	0.050	86OLI/TOI
77	$C_6H_{12}O_6(ao2) = C_6H_{12}O_6(ao3)$ Second law treatment Enthalpy of isomerization of mannose to fructose Listed for information only	ΔH	0.0	2.0	0.725	67TAK
78	$C_6H_{12}O_6(ao2) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of mannose to fructose Adj. from 30 °C using $\Delta H = 0.0 \text{ kJ mol}^{-1}$ Listed for information only	ΔG	-2.22	0.50	2.302	86PAL/DOU
79	$C_6H_{12}O_6(ao2) = C_6H_{12}O_6(ao3)$ Equilibrium measurement Equil. constant for the isomerization of mannose to fructose Listed for information only	ΔG	-2.72	0.20	1.802	67TAK
80	$C_3H_{10}O_5(ao) = C_3H_{10}O_5(ao5)$ Second law treatment Enthalpy of isomerization of ribose to arabinose	ΔH	-9.8	3.0	-0.017	85TEW/GOL
81	$C_3H_{10}O_5(ao) = C_3H_{10}O_5(ao5)$ Equilibrium measurement Equil. constant for the isomerization of ribose to arabinose Listed for information only	ΔG	-3.44	0.30	0.000	85TEW/GOL

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
82	C ₃ H ₁₀ O ₅ (ao) = C ₃ H ₁₀ O ₅ (ao2) Calorimetric measurement Enthalpy of isomerization of ribose to ribulose	ΔH	11.0	2.0	0.011	85TEW/GOL
83	C ₃ H ₁₀ O ₅ (ao) = C ₃ H ₁₀ O ₅ (ao2) Equilibrium measurement Equil. constant for the isomerization of ribose to ribulose	ΔG	2.85	0.20	0.000	85TEW/GOL
84	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Second law treatment Enthalpy for the isomerization of xylose to xylulose Listed for information only	ΔH	22.3	4.0	6.210	82HSI/CHI
85	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Calorimetric measurement Enthalpy of isomerization of xylose to xylulose	ΔH	16.09	0.70	0.000	85TEW/STE
86	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Second law treatment Enthalpy of isomerization of xylose to xylulose Listed for information only	ΔH	18.8	6.0	2.710	86OLI/TOI
87	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Equilibrium measurement Equil. constant for the isomerization of xylose to xylulose Adj. from 27 °C using ΔH = 16.09 kJ mol ⁻¹	ΔG	4.22	0.50	-0.113	54HOC/WAT
88	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Equilibrium measurement Equil. constant for the isomerization of xylose to xylulose Adj. from 30 °C using ΔH = 16.09 kJ mol ⁻¹ Listed for information only	ΔG	4.38	0.50	0.047	55SLE
89	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Equilibrium measurement Equil. constant for the isomerization of xylose to xylulose Listed for information only	ΔG	5.37	0.50	1.037	82HSI/CHI
90	C ₃ H ₁₀ O ₅ (ao3) = C ₃ H ₁₀ O ₅ (ao4) Equilibrium measurement Equil. constant for the isomerization of xylose to xylulose	ΔG	4.389	0.030	0.056	85TEW/STE

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
91	C ₅ H ₁₀ O ₅ (ao3) = C ₅ H ₁₀ O ₅ (ao4) Equilibrium measurement Equil. constant for the isomerization of xylose to xylulose Adjusted to 298.15 K using ΔC _p = 40 J mol ⁻¹ K ⁻¹ Listed for information only	ΔG	4.99	0.55	0.657	86OLI/TOI
92	C ₅ H ₁₀ O ₅ (ao5) = C ₅ H ₁₀ O ₅ (ao2) Second law treatment Enthalpy of isomerization of arabinose to ribulose	ΔH	20.75	4.00	-0.022	86TEW/GOL
93	C ₅ H ₁₀ O ₅ (ao5) = C ₅ H ₁₀ O ₅ (ao2) Equilibrium measurement Equil. constant for the isomerization of arabinose to ribulose Adj. from 37 °C using ΔH = -20.75 kJ mol ⁻¹ Listed for information only	ΔG	5.10	0.50	-1.190	53COH
94	C ₃ H ₁₀ O ₅ (ao5) = C ₃ H ₁₀ O ₅ (ao2) Equilibrium measurement Equil. constant for the isomerization of arabinose to ribulose	ΔG	6.29	0.40	0.000	86TEW/STE
95	C ₃ H ₁₀ O ₅ (ao6) = C ₃ H ₁₀ O ₅ (ao7) Second law treatment Enthalpy of isomerization of allose to psicose No solution for variable or data missing	ΔH	7.42	2.00		86TEW/STE
96	C ₃ H ₁₀ O ₅ (ao6) = C ₃ H ₁₀ O ₅ (ao7) Equilibrium measurement Equil. constant for the isomerization of allose to psicose No solution for variable or data missing	ΔG	-1.41	0.10		86TEW/GOL
97	C ₅ H ₁₀ O ₅ (ao7) = C ₅ H ₁₀ O ₅ (ao9) Equilibrium measurement Equil. constant for the isomerization of psicose to altrose No solution for variable or data missing	ΔG	3.4	0.1		86TEW/GOL
98	C ₃ H ₁₀ O ₅ (ao4) = C ₃ H ₁₀ O ₅ (ao8) Equilibrium measurement Equil. constant for the isomerization of xylose to lyxose Assume K(298.15 K) = K(303.15 K)	ΔG	-2.33	0.50	0.655	56PAL/DOU

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
99	$C_3H_{10}O_5(ao4) = C_3H_{10}O_5(ao8)$ Equilibrium measurement Equil. constant for the isomerization of xylose to lyxose	ΔG	-3.64	0.50	-0.655	65AND/ALL
100	$C_3H_{12}N_5O_{13}P_3^{3-}(ao) + H_2O(l) = C_3H_{12}N_5O_{13}P_2^{2-}(ao) + HPO_4^{2-}(ao) + H^+(ao)$ Calorimetric measurement Enthalpy of hydrolysis of ATP Adj. to 298.15 K with $\Delta H = -21.5$ kJ mol ⁻¹ and $\Delta C_p = -237$ J mol ⁻¹ K ⁻¹ . Corr. to std. state is uncertain Listed for information only	ΔH	-22.3	3.0	-1.800	55KIT/BEN
101	$C_3H_{12}N_5O_{13}P_3^{3-}(ao) + H_2O(l) = C_3H_{12}N_5O_{13}P_2^{2-}(ao) + HPO_4^{2-}(ao) + H^+(ao)$ Calorimetric measurement Enthalpy of hydrolysis of ATP Adj. to 298.15 K with $\Delta H = -21.5$ kJ mol ⁻¹ and $\Delta C_p = -237$ J mol ⁻¹ K ⁻¹ . Corr. to std. state is uncertain Listed for information only	ΔH	-22.3	3.0	-1.800	5FOD/MOR
102	$C_3H_{12}N_5O_{13}P_3^{3-}(ao) + H_2O(l) = C_3H_{12}N_5O_{13}P_2^{2-}(ao) + HPO_4^{2-}(ao) + H^+(ao)$ Calorimetric measurement Enthalpy of hydrolysis of ATP Adj. to 298.15 K with $\Delta H = -21.5$ kJ mol ⁻¹ and $\Delta C_p = -237$ J mol ⁻¹ K ⁻¹ . Corr. to std. state is uncertain Listed for information only	ΔH	-19.0	3.0	1.500	55POD/STU
103	$C_3H_{12}N_5O_{13}P_3^{3-}(ao) + H_2O(l) = C_3H_{12}N_5O_{13}P_2^{2-}(ao) + HPO_4^{2-}(ao) + H^+(ao)$ Calorimetric measurement Enthalpy of hydrolysis of ATP Adj. to 298.15 K with $\Delta H = -21.5$ kJ mol ⁻¹ and $\Delta C_p = -237$ J mol ⁻¹ K ⁻¹ . Corr. to std. state is uncertain Listed for information only	ΔH	-20.5	0.4	0.000	86GAJ/STE
104	$C_3H_{12}N_5O_{13}P_3^{3-}(ao) + H_2O(l) = C_3H_{12}N_5O_{13}P_2^{2-}(ao) + HPO_4^{2-}(ao) + H^+(ao)$ Equilibrium Measurement Equil. constant for the hydrolysis of ATP	ΔG	3.03	0.50	0.000	73GUY/VEE
105	$C_6H_{12}O_6(ao) + C_3H_{12}N_5O_{13}P_3^{3-}(ao) = C_6H_{11}O_9P^-(ao) + C_9H_{12}N_5O_{10}P_2^3(ao) + H^+(ao)$ Calorimetric measurement Enthalpy of phosphorylation (ATP) of glucose Listed for information only	ΔH	-23.8	0.7	-2.228	75GOL

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. J mol ⁻¹ K ⁻¹	Residual	Reference
106	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Enthalpy of phosphorylation (ATP) of glucose Calorimetric measurement Data adjusted using information on the magnesium dependency of the measured enthalpy (see 76GOL) Listed for information only	ΔH	-234	2.0	-1.828	75MCG/JOR
107	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Equilibrium constant for the phosphorylation (ATP) of glucose Listed for information only	ΔG	19.0	0.5	5.099	57ROB/BOY
108	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Equilibrium constant for the phosphorylation (ATP) of glucose Approx. ΔG since metal conc and ion. strength not given Listed for information only	ΔG	21.0	4.0	7.099	57VLA
109	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Calorimetric measurement Enthalpy of phosphorylation (ATP) of mannose Listed for information only	ΔH	-219	0.7	0.000	75GOL
110	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Calorimetric measurement Enthalpy of phosphorylation (ATP) of fructose Listed for information only	ΔH	-150	0.9	-2.285	75GOL
111	$C_6H_{12}O_6(aq) + C_3H_{12}N_3O_{13}P_3^-(aq) =$ $C_6H_{11}O_9P_2^-(aq) + C_3H_{12}N_3O_{10}P_2^-(aq) + H^+(aq)$ Equil. const. for the phosphorylation (ATP) of galactose to galactose-1P Listed for information only	ΔG	25.8	2.0	8.993	61ATK/BUR
112	$C_3H_{10}O_5(cr)$ 3rd law entropy of xylose(cr)	S	143.5	10.0	0.000	35MIL
113	$C_3H_{10}O_5(cr)$ 3rd law entropy of glucose(cr). Based on data of Simon (1922) Assumed to be α form	S	211.3	10.0	0.000	29PAR/KEL

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
114	C ₆ H ₁₂ O ₆ (cr5) 3rd law entropy of galactose	S	205.4	10.0	0.000	4IJAC/STE
115	C ₆ H ₁₂ O ₆ (cr7) 3rd law entropy of sorbose	S	220.9	10.0	0.000	4IJAC/STE
116	C ₃ H ₁₀ O ₅ (ao) Estimated entropy for aqueous ribose	S	204.	20.	0.000	88GOL/TEW
117	C ₃ H ₉ O ₅ P ²⁻ (ao) Estimated entropy for aqueous ribose-3P	S	69.	20.	0.000	88GOL/TEW
118	C ₃ H ₁₀ O ₅ (cr) + 5 O ₂ (g) = 5 CO ₂ (g) + 5 H ₂ O(l) Enthalpy of combustion of ribose(cr) Listed for information only	ΔH	-2345.84	1.00	3.630	70DES/WIL
119	C ₃ H ₁₀ O ₅ (cr) + 5 O ₂ (g) = 5 CO ₂ (g) + 5 H ₂ O(l) Enthalpy of combustion of ribose(cr) Sample was approximately 65/35 ratio of α/β pyranose	ΔH	-2349.47	1.00	0.000	87COL/DOM
120	C ₃ H ₁₀ O ₅ (cr2) + 5 O ₂ (g) = 5 CO ₂ (g) + 5 H ₂ O(l) Enthalpy of combustion of β-arabinose(cr) Review article, recommended value is adopted for reaction catalog Listed for information only	ΔH	-2338.8	1.0	0.873	72DOM
121	C ₃ H ₁₀ O ₅ (cr3) + 5 O ₂ (g) = 5 CO ₂ (g) + 5 H ₂ O(l) Enthalpy of combustion of α-xylose(cr) Review article, recommended value is adopted for reaction catalog	ΔH	-2338.86	2.00	0.000	72DOM
122	C ₆ H ₁₂ O ₆ (cr) + 6 O ₂ (g) = 6 CO ₂ (g) + 6 H ₂ O(l) Enthalpy of combustion of α-glucose(cr) Review article, recommended value is adopted for reaction catalog	ΔH	-2803.0	0.5	0.000	72DOM
123	C ₆ H ₁₂ O ₆ (cr2) + 6 O ₂ (g) = 6 CO ₂ (g) + 6 H ₂ O(l) Enthalpy of combustion of β-glucose(cr) Review article, recommended value is adopted for reaction catalog Listed for information only	ΔH	-2809.3	0.5	-0.102	72DOM
124	C ₆ H ₁₄ O ₇ (cr) + 6 O ₂ (g) = 6 CO ₂ (g) + 7 H ₂ O(l) Enthalpy of combustion of α-glucose monohydrate(cr) Review article, recommended value is adopted for reaction catalog Listed for information only	ΔH	-2793.0	0.5	-0.027	72DOM

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
125	$C_6H_{12}O_6(\text{cr4}) + 6 O_2(\text{g}) = 6 CO_2(\text{g}) + 6 H_2O(\text{l})$ Enthalpy of combustion of mannose(cr) Review article, recommended value is adopted for reaction catalog Listed for information only	ΔH	-2812.9	2.0	-3.387	72DOM
126	$C_6H_{12}O_6(\text{cr5}) + 6 O_2(\text{g}) = 6 CO_2(\text{g}) + 6 H_2O(\text{l})$ Enthalpy of combustion of α -galactose(cr) Review article, recommended value is adopted for reaction catalog	ΔH	-2803.7	2.0	0.000	72DOM
127	$C_6H_{12}O_6(\text{cr6}) + 6 O_2(\text{g}) = 6 CO_2(\text{g}) + 6 H_2O(\text{l})$ Enthalpy of combustion of β -fructose(cr) Review article, recommended value is adopted for reaction catalog Listed for information only	ΔH	-2811.6	2.0	-5.022	72DOM
128	$C_6H_{12}O_6(\text{cr7}) + 6 O_2(\text{g}) = 6 CO_2(\text{g}) + 6 H_2O(\text{l})$ Enthalpy of combustion of sorbose(cr) Review article, recommended value is adopted for reaction catalog	ΔH	-2805.8	2.0	0.000	72DOM
129	$C_3H_{10}O_5(\text{cr}) = C_3H_{10}O_5(\text{ao})$ Enthalpy of solution of ribose	ΔH	13.04	0.50	-0.187	82JAS/AHL
130	$C_3H_{10}O_5(\text{cr}) = C_3H_{10}O_5(\text{ao})$ Enthalpy of solution of ribose	ΔH	13.32	0.20	0.093	84STE/HUB
131	$C_3H_{10}O_5(\text{cr2}) = C_3H_{10}O_5(\text{ao5})$ Enthalpy of solution of arabinose	ΔH	13.24	0.50	0.000	82JAS/AHL
132	$C_3H_{10}O_5(\text{cr3}) = C_3H_{10}O_5(\text{ao3})$ Enthalpy of solution of xylose	ΔH	12.1	0.5	0.000	82JAS/AHL
133	$C_3H_{10}O_5(\text{cr4}) = C_3H_{10}O_5(\text{ao8})$ Enthalpy of solution of lyxose No solution for variable or data missing	ΔH	10.10	0.50		82JAS/AHL
134	$C_6H_{12}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao})$ Enthalpy of solution of α -glucose Listed for information only	ΔH	8.9	1.0	-1.946	96BER
135	$C_6H_{12}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao})$ Enthalpy of solution of α -glucose	ΔH	11.1	0.3	0.254	20BAR
136	$C_6H_{12}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao})$ Enthalpy of solution of α -glucose	ΔH	10.95	0.40	0.104	30HEN/DOR

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
137	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.93	0.30	0.084	34HEN/STE
138	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.72	0.20	-0.126	41STU
139	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.63	0.20	-0.216	46ROW/PAR
140	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	11.00	0.20	0.154	55TAY/ROW
141	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.7	0.2	-0.146	82JAS/AHL
142	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.88	0.20	0.034	82LIA/CHE
143	$C_6H_{12}O_6(cr) = C_6H_{12}O_6(ao)$ Enthalpy of solution of α -glucose	ΔH	10.73	0.20	-0.116	86BAL/SOM
144	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose Listed for information only	ΔH	5.0	1.0	0.352	96BER
145	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose	ΔH	4.66	0.30	0.012	34HEN/STE
146	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose	ΔH	4.68	0.20	0.032	41STU
147	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose	ΔH	4.52	0.20	-0.128	55TAY/ROW
148	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose	ΔH	4.42	0.20	-0.228	82JAS/AHL
149	$C_6H_{12}O_6(cr2) = C_6H_{12}O_6(ao)$ Enthalpy of solution of β -glucose	ΔH	4.96	0.20	0.312	86BAL/SOM
150	$C_6H_{14}O_7(cr) = C_6H_{12}O_6(ao) + H_2O(l)$ Enthalpy of solution of glucose monohydrate	ΔH	20.9	1.0	0.027	97BRO/PIC

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
151	$C_6H_{12}O_7(cr) = C_6H_{12}O_6(ao) + H_2O(l)$ Enthalpy of solution of glucose monohydrate	ΔH	20.9	0.5	0.027	34HEN/STE
152	$C_6H_{12}O_7(cr) = C_6H_{12}O_6(ao) + H_2O(l)$ Enthalpy of solution of glucose monohydrate	ΔH	20.84	0.40	-0.033	55TAY/ROW
153	$C_6H_{12}O_6(cr8) = C_6H_{12}O_6(ao)$ Enthalpy of solution of glucose(vit)	ΔH	4.4	0.5	0.000	46ROW/PAR
154	$C_6H_{12}O_6(cr4) = C_6H_{12}O_6(ao2)$ Enthalpy of solution of mannose Listed for information only	ΔH	6.86	0.50	-1.010	82JAS/AHL
155	$C_6H_{12}O_6(cr4) = C_6H_{12}O_6(ao2)$ Enthalpy of solution of mannose	ΔH	7.87	0.30	0.000	86BAL/SOM
156	$C_6H_{12}O_6(cr5) = C_6H_{12}O_6(ao4)$ Enthalpy of solution of galactose Listed for information only	ΔH	16.45	0.50	-0.687	34HEN/STE
157	$C_6H_{12}O_6(cr5) = C_6H_{12}O_6(ao4)$ Enthalpy of solution of galactose	ΔH	17.20	0.50	0.063	82JAS/AHL
158	$C_6H_{12}O_6(cr5) = C_6H_{12}O_6(ao4)$ Enthalpy of solution of galactose	ΔH	17.10	0.30	-0.037	86BAL/SOM
159	$C_6H_{12}O_6(cr6) = C_6H_{12}O_6(ao3)$ Enthalpy of solution of fructose Listed for information only	ΔH	9.4	2.0	-0.680	97BRO/PIC
160	$C_6H_{12}O_6(cr6) = C_6H_{12}O_6(ao3)$ Enthalpy of solution of fructose Listed for information only	ΔH	9.05	1.00	-1.030	34HEN/STE
161	$C_6H_{12}O_6(cr6) = C_6H_{12}O_6(ao3)$ Enthalpy of solution of fructose Listed for information only	ΔH	8.80	1.00	-1.280	82JAS/AHL
162	$C_6H_{12}O_6(cr6) = C_6H_{12}O_6(ao3)$ Enthalpy of solution of fructose	ΔH	10.08	0.20	0.000	88BAL/SOM

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K	Residual	Reference
163	$C_6H_{12}O_6(\text{cr7}) = C_6H_{12}O_6(\text{ao5})$ Enthalpy of solution of sorbose	ΔH	6.94	0.50	0.000	82JAS/AHL
164	$C_6H_{14}O_7(\text{cr}) = C_6H_{12}O_6(\text{ao}) + H_2O(\text{l})$ Gibbs energy of solution of α -glucose monohydrate Use solubility of 4.55 mol kg ⁻¹ , γ of 1.22, $a(\text{H}_2\text{O})=0.889$ Listed for information only	ΔG	-4.0	0.5	0.741	17DEH
165	$C_6H_{12}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao}) + H_2O(\text{l})$ Gibbs energy of solution of α -glucose monohydrate Use solubility of 5.89 mol kg ⁻¹ , γ of 1.295, $a(\text{H}_2\text{O})=0.889$	ΔG	-4.74	0.20	0.001	22JAC/SIL
166	$C_6H_{14}O_7(\text{cr}) = C_6H_{12}O_6(\text{ao}) + H_2O(\text{l})$ Gibbs energy of solution of α -glucose monohydrate Use solubility of 5.75 mol kg ⁻¹ , γ of 1.29, $a(\text{H}_2\text{O})=0.889$	ΔG	-4.68	0.50	0.061	23GIL
167	$C_6H_{14}O_7(\text{cr}) = C_6H_{12}O_6(\text{ao}) + H_2O(\text{l})$ Gibbs energy of solution of α -glucose monohydrate Use solubility of 5.63 mol kg ⁻¹ , γ of 1.28, $a(\text{H}_2\text{O})=0.889$	ΔG	-4.79	0.40	-0.049	52TAL/HUN
168	$C_6H_{12}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao})$ Gibbs energy of solution of glucose (anhydrous) Assumed to be α form Uses solubility of 11.27 and γ of 1.56	ΔG	-7.11	0.50	0.000	22JAC/SIL
169	$C_6H_{12}O_6(\text{cr5}) = C_6H_{12}O_6(\text{ao4})$ Gibbs energy of solution of galactose Use solubility of 3.79 mol kg ⁻¹ and γ of 1.17 Listed for information only	ΔG	-3.69	0.50	-1.090	17DEH
170	$C_6H_{12}O_6(\text{cr5}) = C_6H_{12}O_6(\text{ao4})$ Gibbs energy of solution of galactose Use solubility of 2.62 mol kg ⁻¹ and γ of 1.10 Assumes that solid phase is anhydrous	ΔG	-2.60	0.50	0.000	40GOU
171	$C_6H_{12}O_6(\text{cr5}) = C_6H_{12}O_6(\text{ao4})$ Gibbs energy of solution of galactose Use solubility of 2.62 mol kg ⁻¹ and γ of 1.10 Assumes that solid phase is anhydrous	ΔG	-2.6	0.5	0.000	52TAL/HUN
172	$C_6H_{12}O_6(\text{cr6}) = C_6H_{12}O_6(\text{ao3})$ Gibbs energy of solution of fructose Use solubility of 22.59 mol kg ⁻¹ and γ of 2.3	ΔG	-9.8	0.5	0.067	26JAC/SIL

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
173	$C_6H_{12}O_6(\text{cr6}) = C_6H_{12}O_6(\text{ao3})$ Gibbs energy of solution of fructose Use solubility of 23.26 mol kg ⁻¹ and γ of 2.4	ΔG	-10.0	1.0	-0.133	52YOU/JOH
174	$C_6H_{11}O_6(\text{cr}) = C_6H_{12}O_6(\text{ao3}) + 0.5 H_2O(l)$ Gibbs energy of solution of fructose hemihydrate Use sol. of 23.91 mol kg ⁻¹ , $a(H_2O)=1.0$, and γ of 2.4	ΔG	-10.0	1.0	0.000	52YOU/JOH
175	$C_6H_{12}O_6(\text{cr7}) = C_6H_{12}O_6(\text{ao5})$ Gibbs energy of solution of sorbose Uses solubility of 3.08 mol kg ⁻¹ and γ of 1.13 Assumes that solid phase is anhydrous	ΔG	-3.1	0.5	0.000	00LOB/EKE
176	$C_6H_{12}O_6(\text{cr4}) = C_6H_{12}O_6(\text{ao2})$ Gibbs energy of solution of mannose Use solubility of 17.3 mol kg ⁻¹ and γ of 2.0 Unpublished data Assumes that solid phase is anhydrous	ΔG	-8.8	0.5	0.000	88TEW/GOL
177	$C_5H_{10}O_5(\text{cr}) = C_5H_{10}O_5(\text{ao})$ Gibbs energy of solution of ribose Use solubility of 20.0 mol kg ⁻¹ and γ of 1.7 Unpublished data Assumes that solid phase is anhydrous	ΔG	-8.7	0.5	0.000	88TEW/GOL
178	$C_5H_{10}O_5(\text{cr3}) = C_5H_{10}O_5(\text{ao3})$ Gibbs energy of solution of xylose Use solubility of 8.3 mol kg ⁻¹ and γ of 1.28 Unpublished data Assumes that solid phase is anhydrous	ΔG	-5.9	0.5	0.000	88TEW/GOL
179	$C_5H_{10}O_5(\text{cr2}) = C_5H_{10}O_5(\text{ao5})$ Gibbs energy of solution of arabinose Use solubility of 5.17 mol kg ⁻¹ and γ of 1.18 Unpublished data Assumes that solid phase is anhydrous	ΔG	-4.5	0.5	0.000	88TEW/GOL
180	$C_5H_{10}O_5(\text{cr4}) = C_5H_{10}O_5(\text{ao8})$ Gibbs energy of solution of lyxose Use solubility of 17.84 mol kg ⁻¹ and γ of 1.6 Unpublished data Assumes that solid phase is anhydrous	ΔG	-8.3	0.5	0.000	88TEW/GOL

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
181	$C_3H_{10}O_5(ao) = C_3H_9O_5^-(ao) + H^+(ao)$ 1st ionization of ribose Listed for information only	ΔG	69.75	0.50	0.630	66IZA/RYT
182	$C_3H_{10}O_5(ao) = C_3H_9O_5^-(ao) + H^+(ao)$ 1st ionization of ribose	ΔG	69.12	0.20	0.000	70CHR/RYT
183	$C_3H_{10}O_5(ao) = C_3H_9O_5^-(ao) + H^+(ao)$ 1st ionization of ribose Listed for information only	ΔH	33.89	1.00	-2.210	66IZA/RYT
184	$C_3H_{10}O_5(ao) = C_3H_9O_5^-(ao) + H^+(ao)$ 1st ionization of ribose	ΔH	36.1	0.5	0.000	70CHR/RYT
185	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose Adjusted to 298.15 K using $\Delta H = 37.7$ kJ mol ⁻¹ The ionic strength was not specified by the authors Listed for information only	ΔG	69.2	0.5	-0.200	00OSA
186	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose Adjusted to 298.15 K using $\Delta H = 37.7$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	69.2	0.5	-0.200	13MIC
187	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	67.8	0.5	-1.600	55SCH
188	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose Listed for information only	ΔG	70.2	0.5	0.800	66IZA/RYT
189	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose	ΔG	69.4	0.2	0.000	70CHR/RYT
190	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose Listed for information only	ΔH	34.31	1.00	-3.390	66IZA/RYT
191	$C_3H_{10}O_5(ao3) = C_3H_9O_5^-(ao3) + H^+(ao)$ 1st ionization of xylose	ΔH	37.7	0.5	0.000	70CHR/RYT

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
192	$C_3H_6O_5(ao3) = C_3H_4O_3^-(ao3) + H^+(ao)$ 2nd ionization of xylose The temperature and ionic strength were not specified by the authors	ΔG	81.63	1.00	0.000	55SCH
193	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose Adjusted to 298.15 K using $\Delta H = 40.0$ kJ mol ⁻¹ The ionic strength was not specified by the authors Listed for information only	ΔG	69.98	0.50	-0.460	00OSA
194	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose Adjusted to 298.15 K using $\Delta H = 40.0$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	71.20	0.50	0.760	13MIC
195	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose Adjusted to 298.15 K using $\Delta H = 40.0$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	71.2	0.5	0.760	13MIC/RON
196	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	68.5	0.5	-1.940	55SCH
197	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose Listed for information only	ΔG	71.58	0.50	1.140	66IZA/RYT
198	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose	ΔG	70.44	0.20	0.000	70CHR/RYT
199	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose Listed for information only	ΔH	34.73	1.00	-5.270	66IZA/RYT
200	$C_3H_{10}O_5(ao5) = C_3H_9O_5^-(ao5) + H^+(ao)$ 1st ionization of arabinose	ΔH	40.0	0.5	0.000	70CHR/RYT

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
201	$C_3H_9O_7(ao5) = C_3H_6O_5^-(ao5) + H^+(ao)$ 2nd ionization of arabinose The temperature and ionic strength were not specified by the authors	ΔG	84.02	1.00	0.000	55SCH
202	$C_3H_{10}O_5(ao8) = C_3H_9O_5^-(ao8) + H^+(ao)$ 1st ionization of lyxose Listed for information only	ΔG	69.12	0.50	0.000	66IZA/RYT
203	$C_3H_{10}O_5(ao8) = C_3H_9O_5^-(ao8) + H^+(ao)$ 1st ionization of lyxose	ΔG	69.12	0.20	0.000	70CHR/RYT
204	$C_4H_{10}O_4(ao8) = C_4H_6O_5^-(ao8) + H^+(ao)$ 1st ionization of lyxose For information only, also, variable not solved or data missing	ΔH	33.47	1.00		66IZA/RYT
205	$C_4H_{10}O_4(ao8) = C_4H_9O_5^-(ao8) + H^+(ao)$ 1st ionization of lyxose No solution for variable or data missing	ΔH	33.5	0.5		70CHR/RYT
206	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol ⁻¹ The ionic strength was not specified by the authors Listed for information only	ΔG	69.18	0.50	-0.920	00OSA
207	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to 298.15 K using $\Delta H = +36.7$ kJ mol ⁻¹ Listed for information only	ΔG	70.39	0.50	0.290	01MAD
208	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	69.85	0.50	-0.250	13MIC
209	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to 298.15 K using $\Delta G = 36.7$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	69.85	0.50	-0.250	13MIC/RON

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
210	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted from 18 C using $\Delta H = 36.7$ kJ mol ⁻¹ No correction made for ionic strength Listed for information only	ΔG	68.98	0.50	-1.120	25BRI
211	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	70.75	0.50	0.650	29HIR/SCH
212	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol ⁻¹ Listed for information only	ΔG	70.72	0.50	0.620	31STE
213	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	70.7	0.5	0.600	32URB/SHA
214	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	68.3	0.5	-1.800	50SOU/SCH
215	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to 298.15 K using $\Delta H = 36.7$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	71.3	0.5	1.200	52THA
216	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	71.40	0.50	1.300	53KIL/WYN
217	$C_6H_{12}O_6(ao) = C_6H_{11}O_6^-(ao) + H^+(ao)$ 1st ionization of glucose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	68.3	0.5	-1.800	55SCH

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
218	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Listed for information only	ΔG	70.3	0.5	0.200	57LOS/SIM
219	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^{\frac{1}{2}} \text{ mol}^{-\frac{1}{2}}$ The temperature was not specified by the authors Listed for information only	ΔG	74.7	0.5	4.600	61RAM/KAT
220	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Assumed to be at zero ionic strength Listed for information only	ΔG	70.5	0.5	0.400	66BUN/CHA
221	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Listed for information only	ΔG	71.2	0.5	1.100	66IZA/RYT
222	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose	ΔG	70.1	0.2	0.000	70CHR/RYT
223	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Second law treatment Listed for information only	ΔH	30.5	3.0	-6.200	53KIL/WYN
224	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Second law treatment Listed for information only	ΔH	41.8	3.0	5.100	57LOS/SIM
225	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose Listed for information only	ΔH	32.2	1.0	-4.500	66IZA/RYT
226	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of glucose	ΔH	36.7	0.5	0.000	70CHR/RYT
227	$C_6H_{11}O_6^-(aq) = C_6H_{10}O_6^{2-}(aq) + H^+(aq)$ 2nd ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^{\frac{1}{2}} \text{ mol}^{-\frac{1}{2}}$ Listed for information only	ΔG	77.2	1.0	-3.850	29HIR/SCH

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
228	$C_6H_{11}O_7^-(ao) = C_6H_{10}O_6^2-(ao) + H^+(ao)$ 2nd ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 36.7 \text{ kJ mol}^{-1}$	ΔG	81.3	1.0	0.250	31STE
229	$C_6H_{11}O_7^-(ao) = C_6H_{10}O_6^2-(ao) + H^+(ao)$ 2nd ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$	ΔG	82.5	1.0	1.450	32URB/SHA
230	$C_6H_{11}O_7^-(ao) = C_6H_{10}O_6^2-(ao) + H^+(ao)$ 2nd ionization of glucose The temperature and ionic strength were not specified by the authors	ΔG	80.2	1.0	-0.850	50SOU/SCH
231	$C_6H_{11}O_7^-(ao) = C_6H_{10}O_6^2-(ao) + H^+(ao)$ 2nd ionization of glucose The temperature and ionic strength were not specified by the authors	ΔG	80.2	1.0	-0.850	55SCH
232	$C_6H_{10}O_6^2-(ao) = C_6H_9O_5^-(ao) + H^+(ao)$ 3rd ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 36.7 \text{ kJ mol}^{-1}$	ΔG	85.3	1.0	0.000	31STE
233	$C_6H_9O_5^-(ao) = C_6H_8O_4^2-(ao) + H^+(ao)$ 4th ionization of glucose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 36.7 \text{ kJ mol}^{-1}$	ΔG	86.5	1.0	0.000	31STE
234	$C_6H_{12}O_8(ao2) = C_6H_{11}O_7^-(ao2) + H^+(ao)$ 1st ionization of mannose Adjusted to 298.15 K using $\Delta H = 33.1 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	74.4	0.5	3.450	13MIC
235	$C_6H_{12}O_8(ao2) = C_6H_{11}O_7^-(ao2) + H^+(ao)$ 1st ionization of mannose Adjusted to 298.15 K using $\Delta H = 33.1 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	74.39	0.50	3.440	13MIC/RON
236	$C_6H_{12}O_8(ao2) = C_6H_{11}O_7^-(ao2) + H^+(ao)$ 1st ionization of mannose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	67.47	0.50	-1.480	55SCH

TABLE 1.1. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
237	$C_6H_{12}O_6(ao2) = C_6H_{11}O_6^-(ao2) + H^+(ao)$ 1st ionization of mannose	ΔG	68.95	0.20	0.000	66IZA/RYT
238	$C_6H_{12}O_6(ao2) = C_6H_{11}O_6^-(ao2) + H^+(ao)$ 1st ionization of mannose	ΔG	68.95	0.20	0.000	70CHR/RYT
239	$C_6H_{12}O_6(ao2) = C_6H_{11}O_6^-(ao2) + H^+(ao)$ 1st ionization of mannose	ΔH	33.05	0.50	-0.025	66IZA/RYT
240	$C_6H_{12}O_6(ao2) = C_6H_{11}O_6^-(ao2) + H^+(ao)$ 1st ionization of mannose	ΔH	33.1	0.5	0.025	70CHR/RYT
241	$C_6H_{11}O_6^-(ao2) = C_6H_{10}O_6^{2-}(ao2) + H^+(ao)$ 2nd ionization of mannose The temperature and ionic strength were not specified by the authors	ΔG	80.8	1.0	0.000	55SCH
242	$C_6H_{12}O_6(ao3) = C_6H_{11}O_6^-(ao3) + H^+(ao)$ 1st ionization of fructose Adjusted to 298.15 K using $\Delta H = 39.2$ kJ mol ⁻¹ The ionic strength was not specified by the authors Listed for information only	ΔG	72.8	0.5	4.100	00OSA
243	$C_6H_{12}O_6(ao3) = C_6H_{11}O_6^-(ao3) + H^+(ao)$ 1st ionization of fructose Adjusted to 298.15 K using $\Delta H = +35.7$ kJ mol ⁻¹ Listed for information only	ΔG	69.2	0.5	0.500	01MAD
244	$C_6H_{12}O_6(ao3) = C_6H_{11}O_6^-(ao3) + H^+(ao)$ 1st ionization of fructose Adjusted to 298.15 K using $\Delta H = 39.2$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	69.1	0.5	0.400	13MIC
245	$C_6H_{12}O_6(ao3) = C_6H_{11}O_6^-(ao3) + H^+(ao)$ 1st ionization of fructose Adjusted to 298.15 K using $\Delta H = 39.2$ kJ mol ⁻¹ Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	69.1	0.5	0.400	13MIC/RON
246	$C_6H_{12}O_6(ao3) = C_6H_{11}O_6^-(ao3) + H^+(ao)$ 1st ionization of fructose Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Listed for information only	ΔG	68.35	0.50	-0.350	29HIR/SCH

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
247	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Adjusted to zero ionic strength using B = 1.6 kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = 39.2$ kJ mol ⁻¹ Listed for information only	ΔG	69.85	0.50	1.150	31STE
248	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Adjusted to zero ionic strength using B = 1.6 kg ¹ mol ⁻¹ Listed for information only	ΔG	68.4	0.5	-0.300	32URB/SHA
249	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose The temperature and ionic strength were not specified by the authors Listed for information only	ΔG	67.7	0.5	-1.000	55SCH
250	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Adjusted to zero ionic strength using B = 1.6 kg ¹ mol ⁻¹ The temperature was not specified by the authors Listed for information only	ΔG	73.5	0.5	4.800	61RAM/KAT
251	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Listed for information only	ΔG	70.0	0.5	1.300	66IZA/RYT
252	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Listed for information only	ΔG	68.7	0.2	0.000	70CHR/RYT
253	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose Listed for information only	ΔH	34.3	5.0	-4.900	66IZA/RYT
254	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 1st ionization of fructose	ΔH	39.2	0.5	0.000	70CHR/RYT
255	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 2nd ionization of fructose Adjusted to zero ionic strength using B = 1.6 kg ¹ mol ⁻¹	ΔG	77.2	1.0	-2.175	29HIR/SCH
256	$C_6H_{12}O_6(aq) = C_6H_{11}O_6^-(aq) + H^+(aq)$ 2nd ionization of fructose Adjusted to zero ionic strength using B = 1.6 kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = 39.2$ kJ mol ⁻¹	ΔG	81.7	1.0	2.325	31STE

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
257	$C_6H_{10}O_6(ao3) = C_6H_{10}O_6^-(ao3) + H^+(ao)$ 2nd ionization of fructose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$	ΔG	79.0	1.0	-0.375	32URB/SHA
258	$C_6H_{10}O_6(ao3) = C_6H_{10}O_6^-(ao3) + H^+(ao)$ 2nd ionization of fructose The temperature and ionic strength were not specified by the authors	ΔG	79.6	1.0	0.225	55SCH
259	$C_6H_{10}O_6^-(ao3) = C_6H_9O_6^-(ao3) + H^+(ao)$ 3rd ionization of fructose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 39.2 \text{ kJ mol}^{-1}$	ΔG	83.0	1.0	0.000	31STE
260	$C_6H_9O_6^-(ao3) = C_6H_8O_6^-(ao3) + H^+(ao)$ 4th ionization of fructose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 39.2 \text{ kJ mol}^{-1}$	ΔG	90.2	1.0	0.000	31STE
261	$C_6H_{12}O_6(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$ The ionic strength was not specified by the authors Listed for information only	ΔG	67.2	0.5	-3.300	00OSA
262	$C_6H_{12}O_6(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	70.3	0.5	-0.200	13MIC
263	$C_6H_{12}O_6(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	70.3	0.5	-0.200	13MIC/RON
264	$C_6H_{12}O_6(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$ Listed for information only	ΔG	71.55	0.50	1.050	31STE

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
265	$C_6H_{12}O_4(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Listed for information only	ΔG	71.24	0.50	0.740	66ZA/RYT
266	$C_6H_{12}O_4(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose	ΔG	70.5	0.2	0.000	70CHR/RYT
267	$C_6H_{12}O_4(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose Listed for information only	ΔH	37.7	1.0	-3.000	66ZA/RYT
268	$C_6H_{12}O_4(ao4) = C_6H_{11}O_6^-(ao4) + H^+(ao)$ 1st ionization of galactose	ΔH	40.7	0.5	0.000	70CHR/RYT
269	$C_6H_{11}O_7^-(ao4) = C_6H_{10}O_8^{2-}(ac4) + H^+(eo)$ 2nd ionization of galactose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$	ΔG	82.4	1.0	0.000	31STE
270	$C_6H_{10}O_7^-(ao4) = C_6H_9O_8^-(ac4) + H^+(eo)$ 3rd ionization of galactose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$	ΔG	85.0	1.0	0.000	31STE
271	$C_6H_9O_8^{2-}(ao4) = C_6H_8O_9^-(ao4) + H^+(ao)$ 4th ionization of galactose Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = 40.7 \text{ kJ mol}^{-1}$	ΔG	86.2	1.0	0.000	31STE
272	$C_6H_{12}O_4(ao5) = C_6H_{11}O_6^-(ao5) + H^+(ao)$ 1st ionization of sorbose Adjusted to 298.15 K using $\Delta H = 40.0 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$	ΔG	66.2	0.5	-1.300	13MIC
273	$C_6H_{12}O_4(ao5) = C_6H_{11}O_6^-(ao5) + H^+(ao)$ 1st ionization of sorbose The temperature and ionic strength were not specified by the authors	ΔG	68.8	0.5	1.300	55SCH
274	$C_6H_{11}O_7^-(ao5) = C_6H_{10}O_8^-(ac5) + H^+(eo)$ 2nd ionization of sorbose The temperature and ionic strength were not specified by the authors	ΔG	81.2	1.0	0.000	55SCH
275	$C_5H_{10}O_5P^{1-}(ao) = C_5H_9O_5P^{2-}(ao) + H^+(ao)$ 2nd ionization of ribose-5P	ΔG	38.1	0.2	-0.080	62CHR/IZA

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
276	$C_3H_{10}O_8P^1-(ao) = C_3H_9O_8P^2-(ao) + H^+(ao)$ 2nd ionization of ribose-5P	ΔG	38.2	0.2	0.020	62IZA/CHR
277	$C_3H_{10}O_8P^1-(ao) = C_3H_9O_8P^2-(ao) + H^+(ao)$ 2nd ionization of ribose-5P Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = -11.3 \text{ kJ mol}^{-1}$	ΔG	38.3	0.5	0.120	72FRE/STU
278	$C_3H_{10}O_8P^1-(ao) = C_3H_9O_8P^2-(ao) + H^+(ao)$ 2nd ionization of ribose-5P	ΔH	-11.3	0.5	0.000	62CHR/IZA
279	$C_3H_9O_8P^2-(ao) = C_3H_8O_8P^3-(ao) + H^+(ao)$ 3rd ionization of ribose-5P	ΔG	74.5	0.2	0.000	66IZA/RYT
280	$C_3H_9O_8P^2-(ao) = C_3H_8O_8P^3-(ao) + H^+(ao)$ 3rd ionization of ribose-5P	ΔH	25.5	0.5	0.000	66IZA/RYT
281	$NiC_3H_9O_8P(ao) = Ni^{2+}(ao) + C_3H_9O_8P^2-(ao2)$ Dissociation of Ni-ribose-5P Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = -11.0 \text{ kJ mol}^{-1}$	ΔG	16.1	0.2	0.000	72FRE/STU
282	$MgC_3H_9O_8P(ao) = Mg^{2+}(ao) + C_3H_9O_8P^2-(ao2)$ Dissociation of Mg-ribose-5P Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = -11.0 \text{ kJ mol}^{-1}$	ΔG	14.9	0.2	0.000	72FRE/STU
283	$C_6H_{13}O_9P(ao2) = C_6H_{12}O_9P^1-(ao2) + H^+(ao)$ 1st ionization of glucose-1P Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = -1.3 \text{ kJ mol}^{-1}$	ΔG	7.48	0.50	0.750	37COR/COL
284	$C_6H_{13}O_9P(ao2) = C_6H_{12}O_9P^1-(ao2) + H^+(ao)$ 1st ionization of glucose-1P Adjusted to 298.15 K using $\Delta H = -1.3 \text{ kJ mol}^{-1}$	ΔG	6.28	0.30	-0.450	55SNE
285	$C_6H_{12}O_9P^1-(ao2) = C_6H_{11}O_9P^2-(ao2) + H^+(ao)$ 2nd ionization of glucose-1P Adjusted to 298.15 K using $\Delta H = -1.3 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	38.7	0.5	1.590	52TRE/MAN

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
286	$C_6H_{12}O_9P^{1-}(ao2) = C_6H_{11}O_9P^{2-}(ao2) + H^+(ao)$ 2nd ionization of glucose-1P Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Adjusted to 298.15 K using $\Delta H = -1.8 \text{ kJ mol}^{-1}$ Listed for information only	ΔG	37.43	0.30	0.320	37COR/COIL
287	$C_6H_{12}O_9P^{1-}(ao2) = C_6H_{11}O_9P^{2-}(ao2) + H^+(ao)$ 2nd ionization of glucose-1P	ΔG	37.11	0.10	0.000	55ASH/CLA
288	$C_6H_{12}O_9P^{1-}(ao2) = C_6H_{11}O_9P^{2-}(ao2) + H^+(ao)$ 2nd ionization of glucose-1P Adjusted to 298.15 K using $\Delta H = -1.8 \text{ kJ mol}^{-1}$ Listed for information only	ΔG	35.39	0.50	-1.720	55SNE
289	$C_6H_{12}O_9P^{1-}(ao2) = C_6H_{11}O_9P^{2-}(ao2) + H^+(ao)$ 2nd ionization of glucose-1P Second law treatment No solution for variable or data missing	ΔH	-1.80	0.50		55ASH/CLA
290	$CaC_4H_{11}O_9P(ao2) = Ca^{2+}(ao) + C_6H_{11}O_9P^{2-}(ao2)$ Dissociation of Ca-glucose-1P	ΔG	14.24	0.10	0.000	56CLA/DAT
291	$CaC_4H_{11}O_9P(ao2) = Ca^{2+}(ao) + C_6H_{11}O_9P^{2-}(ao2)$ Dissociation of Ca-glucose-1P Second law treatment No solution for variable or data missing	ΔH	-10.05	0.50		56CLA/DAT
292	$MgC_4H_{11}O_9P(ao2) = Mg^{2+}(ao) + C_6H_{11}O_9P^{2-}(ao2)$ Dissociation of Mg-glucose-1P Adjusted to 298.15 K using $\Delta H = -122 \text{ kJ mol}^{-1}$ Adjusted to zero ionic strength using $B = 1.6 \text{ kg}^1 \text{ mol}^{-1}$ Listed for information only	ΔG	13.36	0.50	-0.790	52TRE/MAN2
293	$MgC_4H_{11}O_9P(ao2) = Mg^{2+}(ao) + C_6H_{11}O_9P^{2-}(ao)$ Dissociation of Mg-glucose-1P	ΔG	14.15	0.10	0.000	54CLA/CUS
294	$MgC_4H_{11}O_9P(ao2) = Mg^{2+}(ao) + C_6H_{11}O_9P^{2-}(ao)$ Dissociation of Mg-glucose-1P Second law treatment No solution for variable or data missing	ΔH	-12.2	0.5		54CLA/CUS
295	$C_6H_{13}O_9P(ao) = C_6H_{12}O_9P^{1-}(ao) + H^+(ao)$ 1st ionization of glucose-6P Temperature and ionic strength not given by authors Listed for information only	ΔG	5.4	0.5	-3.383	26MEY/LOH

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. K ⁻¹	Residual	Reference
296	$C_6H_{12}O_9P(aq) = C_6H_{12}O_9P^{1-}(aq) + H^+(aq)$ 1st ionization of glucose-6P Adjusted to 298.15 K using $\Delta H = -1.8$ kJ mol ⁻¹	ΔG	6.85	0.50	-1.933	55SNE
297	$C_6H_{12}O_9P(aq) = C_6H_{12}O_9P^{1-}(aq) + H^+(aq)$ 1st ionization of glucose-6P Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹	ΔG	10.4	0.5	1.617	66BUN/CHA
298	$C_6H_{12}O_9P(aq) = C_6H_{12}O_9P^{1-}(aq) + H^+(aq)$ 1st ionization of glucose-6P Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = -1.8$ kJ mol ⁻¹	ΔG	9.1	0.5	0.317	66DEG/HAL
299	$C_6H_{12}O_9P^{1-}(aq) = C_6H_{11}O_9P^{2-}(aq) + H^+(aq)$ 2nd ionization of glucose-6P Temperature and ionic strength not given by authors Listed for information only	ΔG	34.88	0.50	-1.770	26MEY/LOH
300	$C_6H_{12}O_9P^{1-}(aq) = C_6H_{11}O_9P^{2-}(aq) + H^+(aq)$ 2nd ionization of glucose-6P Adjusted to 298.15 K using $\Delta H = -1.8$ kJ mol ⁻¹ Listed for information only	ΔG	35.4	0.5	-1.250	55SNE
301	$C_6H_{12}O_9P^{1-}(aq) = C_6H_{11}O_9P^{2-}(aq) + H^+(aq)$ 2nd ionization of glucose-6P Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹	ΔG	36.8	0.2	0.150	66BUN/CHA
302	$C_6H_{12}O_9P^{1-}(aq) = C_6H_{11}O_9P^{2-}(aq) + H^+(aq)$ 2nd ionization of glucose-6P Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = -1.8$ kJ mol ⁻¹	ΔG	36.5	0.2	-0.150	66DEG/HAL
303	$C_6H_{11}O_9P^{2-}(aq) = C_6H_{10}O_9P^{3-}(aq) + H^+(aq)$ 3rd ionization of glucose-6P	ΔG	66.8	0.2	0.000	66IZA/RYT
304	$C_6H_{11}O_9P^{2-}(aq) = C_6H_{10}O_9P^{3-}(aq) + H^+(aq)$ 3rd ionization of glucose-6P	ΔH	35.2	0.5	0.000	66IZA/RYT
305	$C_6H_{12}O_9P^{1-}(aq) = C_6H_{11}O_9P^{2-}(aq) + H^+(aq)$ 2nd ionization of fructose-6P Adjusted to zero ionic strength using $B = 1.6$ kg ¹ mol ⁻¹ Adjusted to 298.15 K using $\Delta H = -1.8$ kJ mol ⁻¹	ΔG	35.8	0.3	0.000	57SCH/AND

TABLE 11. Catalog of thermochemical measurements at 298.15 K: equilibrium, enthalpy, and entropy data — Continued

No.	Reaction	Property	Observed kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual	Reference
306	CaC ₆ H ₁₁ O ₉ P(ao4) = C ₆ H ₁₁ O ₉ P ²⁻ (ao4) + Ca ²⁺ (ao) Dissociation of Ca-fructose-6P Adjusted to zero ionic strength using B = 1.6 kg ^l mol ⁻¹ Adjusted to 298.15 K using ΔH = -10.0 kJ mol ⁻¹	ΔG	13.4	0.3	0.000	57SCH/AND
307	MgC ₆ H ₁₁ O ₉ P(ao4) = C ₆ H ₁₁ O ₉ P ²⁻ (ao4) + Mg ²⁺ (ao) Dissociation of Mg-fructose-6P Adjusted to zero ionic strength using B = 1.6 kg ^l mol ⁻¹ Adjusted to 298.15 K using ΔH = -10.0 kJ mol ⁻¹	ΔG	14.1	0.3	0.000	57SCH/AND
308	C ₆ H ₁₃ O ₉ P(ao6) = C ₆ H ₁₂ O ₉ P ⁻ (ao6) + H ⁺ (ao) 1st ionization of galactose-1P Adjusted to zero ionic strength using B = 1.6 kg ^l mol ⁻¹ Adjusted to 298.15 K using ΔH = -1.8 kJ mol ⁻¹	ΔG	6.96	0.50	0.000	43KOS
309	C ₆ H ₁₂ O ₉ P ¹⁻ (ao6) = C ₆ H ₁₁ O ₉ P ²⁻ (ao6) + H ⁺ (ao) 2nd ionization of galactose-1P Adjusted to zero ionic strength using B = 1.6 kg ^l mol ⁻¹ Adjusted to 298.15 K using ΔH = -1.8 kJ mol ⁻¹	ΔG	37.7	0.3	0.000	43KOS
310	5C ₆ H ₁₁ O ₉ P(ao) - 5.5H ₂ (g) + 4.5O ₂ (g) = C ₆ H ₁₁ O ₉ P ²⁻ (ao) Constraint - solved exactly	HGS	0.000	0.000	0.000	

310-333 These reactions, with the property type "HGS", represent the constraint $\Delta_f G^\circ - \Delta_f H^\circ + T\Delta_f S^\circ = 0$ for the formation of individual substances. As an example, reaction 310 is given below. [87GAR/PAR]

TABLE 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data

No.	Reaction	Property Measured	Observed	Unc.	Residual Obs.-calc.	Reference
				kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹		
1	$C_6H_{11}O_9P_2^-(ao) + H_2O(l) = C_6H_{12}O_6(ao) + HPO_4^{2-}(ao)$ Calorimetric measurement ΔC_p of hydrolysis of glucose-6P	ΔC_p	-48.	20.	-6.681	88TEW/STE
2	$C_6H_{11}O_9P_2^-(ao3) + H_2O(l) = C_6H_{12}O_6(ao2) + HPO_4^{2-}(ao)$ Calorimetric measurement ΔC_p of hydrolysis of mannose-6P	ΔC_p	-46.	10.	-2.089	88TEW/STE
3	$C_6H_{11}O_9P_2^-(ao4) + H_2O(l) = C_6H_{12}O_6(ao3) + HPO_4^{2-}(ao)$ Calorimetric measurement ΔC_p of hydrolysis of fructose-6P	ΔC_p	-28.	40.	21.299	88TEW/STE
4	$C_3H_5O_8P_2^-(ao) + H_2O(l) = C_3H_6O_5(ao) + HPO_4^{2-}(ao)$ Calorimetric measurement ΔC_p of hydrolysis of ribose-5P	ΔC_p	-63.	40.	0.000	88TEW/STE
5	$C_3H_5O_8P_2^-(ao2) + H_2O(l) = C_3H_6O_5(ao2) + HPO_4^{2-}(ao)$ Calorimetric measurement ΔC_p of hydrolysis of ribulose-5P No solution for variable or data missing.	ΔC_p	-84.	30.		88TEW/STE
6	$C_6H_{11}O_9P_2^-(ao) = C_6H_{11}O_9P_2^-(ao4)$ Calorimetric measurement ΔC_p of isomerization of glucose-6P to fructose-6P	ΔC_p	44.	10.	3.341	88TEW/STE
7	$C_6H_{11}O_9P_2^-(ao3) = C_6H_{11}O_9P_2^-(ao4)$ Calorimetric measurement ΔC_p of isomerization of mannose-6P to fructose-6P	ΔC_p	38.	30.	5.669	88TEW/STE
8	$C_6H_{12}O_6(ao) = C_6H_{12}O_6(ao3)$ Calorimetric measurement ΔC_p of isomerization of glucose to fructose	ΔC_p	76.	30.	43.321	84TEW/GOL
9	$C_3H_{10}O_5(ao3) = C_3H_{10}O_5(ao4)$ Calorimetric measurement ΔC_p of isomerization of xylose to xylulose	ΔC_p	40.	20.	0.000	85TEW/STE
10	$C_3H_{10}O_5(ao6) = C_3H_{10}O_5(ao7)$ Obtained from temp. dependency of equilibrium constants. ΔC_p of isomerization of allulose to psicose No solution for variable or data missing.	ΔC_p	59.	90.		86TEW/STE

TABLE 12. Catalog of thermochemical measurements at 298.15 K. Heat capacity data

No.	Reaction	Property Measured	Observed	Unc. $\text{kJ mol}^{-1} \text{K}^{-1}$	Residual Obs-calc.	Reference
11	$\text{C}_6\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_3^-(\text{ao}) + \text{H}_2\text{O}(\text{l}) = \text{C}_6\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_2^-(\text{ao}) + \text{HPO}_4^{2-}(\text{ao}) + \text{H}^+(\text{ao})$ Calorimetric measurement ΔC_p of hydrolysis of ATP	ΔC_p	-237.	30.	0.000	86GAJ/STE
12	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}) + \text{C}_9\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_3^-(\text{ao}) = \text{C}_6\text{H}_{11}\text{O}_9\text{P}_2^-(\text{ao}) + \text{C}_3\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_2^-(\text{ao}) + \text{H}^+(\text{ao})$ Calorimetric measurement ΔC_p of phosphorylation (ATP) of glucose Listed for information only.	ΔC_p	-156.	300.	39.681	75GOL
13	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}2) + \text{C}_9\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_3^-(\text{ao}) = \text{C}_6\text{H}_{11}\text{O}_9\text{P}_2^-(\text{ao}3) + \text{C}_9\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_2^-(\text{ao}) + \text{H}^+(\text{ao})$ Calorimetric measurement ΔC_p of phosphorylation (ATP) of mannose Listed for information only.	ΔC_p	10.	200.	203.089	75GOL
14	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}3) + \text{C}_9\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_3^-(\text{ao}) = \text{C}_6\text{H}_{11}\text{O}_9\text{P}_2^-(\text{ao}4) + \text{C}_9\text{H}_{12}\text{N}_5\text{O}_{10}\text{P}_2^-(\text{ao}) + \text{H}^+(\text{ao})$ Calorimetric measurement ΔC_p of phosphorylation (ATP) of fructose Listed for information only.	ΔC_p	-41.	200.	146.701	75GOL
15	$\text{HPO}_4^{2-}(\text{ao})$ C_p of $\text{HPO}_4^{2-}(\text{ao})$	C_p	-254.	4.	0.000	82LAR/ZEE
16	$\text{C}_3\text{H}_{10}\text{O}_5(\text{cr}3)$ C_p of xylose(cr)	C_p	184.	2.	0.000	81KAW/KUS
17	$\text{C}_3\text{H}_{10}\text{O}_5(\text{cr}5)$ C_p of xylose(cr)	C_p	184.	2.	0.000	82JAS/AHL
18	$\text{C}_6\text{H}_{12}\text{O}_6(\text{cr}5)$ C_p of galactose(cr)	C_p	222.1	1.0	1.280	41JAC/STE
19	$\text{C}_6\text{H}_{12}\text{O}_6(\text{cr}5)$ C_p of galactose(cr). Also see 81KAW/NIS.	C_p	217.	3.	-3.820	81KAW/KUS
20	$\text{C}_6\text{H}_{12}\text{O}_6(\text{cr}7)$ C_p of sorbose(cr)	C_p	231.4	1.0	0.000	41JAC/STE
21	$\text{C}_6\text{H}_{12}\text{O}_6(\text{cr})$ C_p of α -D-glucose(cr)	C_p	229.3	5.0	10.155	22SIM

TABLE 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data — Continued

No.	Reaction	Property Measured	Observed	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual Obs.-calc.	Reference
22	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr)	C _p	220.8	2.0	1.655	34PAR/THO
23	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr)	C _p	218.1	2.0	-1.045	41NEL/NEW
24	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr)	C _p	218.9	0.5	-0.245	51DOU/BAL
25	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr)	C _p	218.4	1.0	-0.745	55TAY/ROW
26	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr)	C _p	219.79	0.40	0.645	82LIA/CHE
27	C ₆ H ₁₂ O ₆ (cr) C _p of α-D-glucose(cr). Also see 81KAW/NIS.	C _p	224.	3.	4.855	81KAW/KUS
28	C ₆ H ₁₂ O ₆ (vit) C _p of glucose(vit)	C _p	381.9	10.0	9.467	28PAR/HUF
29	C ₆ H ₁₂ O ₆ (vit) C _p of glucose(vit)	C _p	367.7	5.0	-4.733	41NEL/NEW
30	C ₆ H ₁₂ O ₆ (cr4) C _p of mannose(cr). Also see 81KAW/NIS.	C _p	216.	3.	0.000	81KAW/KUS
31	C ₆ H ₁₂ O ₆ (cr6) C _p of fructose(cr). Also see 81KAW/NIS.	C _p	232.	3.	0.000	81KAW/KUS
32	C ₅ H ₁₀ O ₅ (cr) C _p of ribose(cr)	C _p	187.	2.	1.500	81KAW/KUS
33	C ₅ H ₁₀ O ₅ (cr) C _p of ribose(cr)	C _p	184.	2.	-1.500	82JAS/AHL
34	C ₅ H ₁₀ O ₅ (cr2) C _p of arabinose(cr)	C _p	184.	2.	0.000	81KAW/KUS
35	C ₅ H ₁₀ O ₅ (cr4) C _p of lyxose(cr)	C _p	184.	2.	0.000	82JAS/AHL

TABLE 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data — Continued

No.	Reaction	Property Measured	Observed	Unc.	Residual Obs.-calc.	Reference
				kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹		
36	C ₆ H ₁₂ O ₆ (cr) = C ₆ H ₁₂ O ₆ (ao) ΔC _p of solution of α-D-glucose(cr)	ΔC _p	151.	20.	33.849	41STU
37	C ₆ H ₁₂ O ₆ (cr) = C ₆ H ₁₂ O ₆ (ao) ΔC _p of solution of α-D-glucose(cr)	ΔC _p	134.	20.	16.849	82JAS/AHL
38	C ₆ H ₁₂ O ₆ (cr) = C ₆ H ₁₂ O ₆ (ao) ΔC _p of solution of α-D-glucose(cr)	ΔC _p	128.	10.	10.849	82LIA/CHE
39	C ₆ H ₁₂ O ₆ (cr2) = C ₆ H ₁₂ O ₆ (ao) ΔC _p of solution of β-D-glucose(cr)	ΔC _p	134.	20.	3.000	41STU
40	C ₆ H ₁₂ O ₆ (cr2) = C ₆ H ₁₂ O ₆ (ao) ΔC _p of solution of β-D-glucose(cr)	ΔC _p	128.	20.	-3.000	82JAS/AHL
41	C ₆ H ₁₂ O ₆ (cr4) = C ₆ H ₁₂ O ₆ (ao2) ΔC _p of solution of mannose(cr) Listed for information only.	ΔC _p	148.	20.	21.968	82JAS/AHL
42	C ₆ H ₁₂ O ₆ (cr5) = C ₆ H ₁₂ O ₆ (ao4) ΔC _p of solution of galactose(cr) Listed for information only.	ΔC _p	139.	20.	40.820	82JAS/AHL
43	C ₆ H ₁₂ O ₆ (cr6) = C ₆ H ₁₂ O ₆ (ao3) ΔC _p of solution of fructose(cr) Listed for information only.	ΔC _p	242.	20.	105.025	82JAS/AHL
44	C ₆ H ₁₂ O ₆ (cr7) = C ₆ H ₁₂ O ₆ (ao5) ΔC _p of solution of sorbose(cr) Can be used to calculate C _p = 448 J mol ⁻¹ K ⁻¹ for sorbose(ao). This value seems low. For information only. Also, variable not solved or data missing.	ΔC _p	217.	20.		82JAS/AHL
45	C ₅ H ₁₀ O ₅ (cr) = C ₅ H ₁₀ O ₅ (ao) ΔC _p of solution of ribose(cr) Listed for information only.	ΔC _p	110.	20.	19.500	82JAS/AHL
46	C ₅ H ₁₀ O ₅ (cr3) = C ₅ H ₁₀ O ₅ (ao3) ΔC _p of solution of xylose(cr) Listed for information only.	ΔC _p	102.	20.	7.000	82JAS/AHL
47	C ₅ H ₁₀ O ₅ (cr2) = C ₅ H ₁₀ O ₅ (ao5) ΔC _p of solution of arabinose(cr) Listed for information only.	ΔC _p	134.	20.	39.000	82JAS/AHL

TABLE 12. Catalog of thermochemical measurements at 298.15 K: heat capacity data — Continued

No.	Reaction	Property Measured	Observed	Unc.	Residual Obs.-calc.	Reference
				kJ mol^{-1} or $\text{J mol}^{-1} \text{K}^{-1}$		
48	$\text{C}_3\text{H}_{10}\text{O}_4(\text{cr4}) = \text{C}_3\text{H}_{10}\text{O}_4(\text{ao8})$ ΔC_p of solution of lyxose(cr)	ΔC_p	101.	20.	0.000	82JAS/AHL
49	$\text{C}_3\text{H}_{10}\text{O}_4(\text{ao3})$ C_p of xylose(ao)	C_p	279	20.	0.000	81KAW/KUS
50	$\text{C}_3\text{H}_{10}\text{O}_4(\text{ao})$ C_p of ribose(ao)	C_p	276	20.	0.000	81KAW/KUS
51	$\text{C}_3\text{H}_{10}\text{O}_4(\text{ao5})$ C_p of arabinose(ao)	C_p	279	20.	0.000	81KAW/KUS
52	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao3})$ C_p of fructose(ao). Also see 81KAW/NIS.	C_p	328.	20.	-40.975	81KAW/KUS
53	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao4})$ C_p of galactose(ao). Also see 81KAW/NIS.	C_p	319.	20.	0.000	81KAW/KUS
54	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao). Listed for information only.	C_p	346.	50.	9.704	33FRE/BUR
55	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao). Also see 81KAW/NIS.	C_p	336.	30.	-0.296	36BEN/KRA
56	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao).	C_p	318.	20.	-18.296	55TAY/ROW
57	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao).	C_p	323.	20.	-13.296	76BON/CER
58	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao). Also see 81KAW/NIS.	C_p	318.	20.	-18.296	81KAW/KUS
59	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao})$ C_p of glucose(ao).	C_p	351.	20.	14.704	84JAS/AHL
60	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao2})$ C_p of mannose(ao). Also see 81KAW/NIS.	C_p	346.	20.	3.968	81KAW/KUS
61	$\text{C}_6\text{H}_{12}\text{O}_6\text{P}^-(\text{ao2}) = \text{C}_6\text{H}_{11}\text{O}_6\text{P}^{2-}(\text{ao2}) + \text{H}^+(\text{ao})$ 2nd ionization of glucose-1P Based on 2nd derivative of equilibrium data No solution for variable or data missing	ΔC_p	-196.	40.		55ASH/CLA

TABLE 12. Catalog of thermochemical measurements at 298.15 K. heat capacity data — Continued

No.	Reaction	Property Measured	Observed	Unc. kJ mol ⁻¹ or J mol ⁻¹ K ⁻¹	Residual Obs.-calc.	Reference
62	$\text{MgC}_6\text{H}_{11}\text{O}_9\text{P}(\text{ao}2) = \text{Mg}^{2+}(\text{ao}) + \text{C}_6\text{H}_{11}\text{O}_9\text{P}^{2-}(\text{ao}2)$ Dissociation of Mg-glucose-1P Based on 2nd derivative of equilibrium data No solution for variable or data missing.	ΔC_p	-247.	70.		54CLA/CUS
63	$\text{Ca}_3\text{C}_6\text{H}_{11}\text{O}_9\text{P}(\text{ao}2) = \text{Ca}^{2+}(\text{ao}) + \text{C}_6\text{H}_{11}\text{O}_9\text{P}^{2-}(\text{ao}2)$ Dissociation of Ca-glucose-1P Based on 2nd derivative of equilibrium data No solution for variable or data missing.	ΔC_p	-262.	50.		56CLA/CUS
64	$\text{C}_5\text{H}_{10}\text{O}_4(\text{ao}) = \text{C}_5\text{H}_9\text{O}_4^-(\text{ao}) + \text{H}^+(\text{ao})$ 1st ionization of ribose Based on enthalpies at two temperatures	ΔC_p	-112.	40.	0.000	70CHR/RYT
65	$\text{C}_5\text{H}_{10}\text{O}_4(\text{ao}3) = \text{C}_5\text{H}_9\text{O}_4^-(\text{ao}3) + \text{H}^+(\text{ao})$ 1st ionization of xylose Based on enthalpies at two temperatures	ΔC_p	-103.	40.	0.000	70CHR/RYT
66	$\text{C}_5\text{H}_{10}\text{O}_4(\text{ao}5) = \text{C}_5\text{H}_9\text{O}_4^-(\text{ao}5) + \text{H}^+(\text{ao})$ 1st ionization of arabinose Based on enthalpies at two temperatures	ΔC_p	-114.	40.	0.000	70CHR/RYT
67	$\text{C}_5\text{H}_{10}\text{O}_4(\text{ao}8) = \text{C}_5\text{H}_9\text{O}_4^-(\text{ao}8) + \text{H}^+(\text{ao})$ 1st ionization of lyxose Based on enthalpies at two temperatures	ΔC_p	-117.	40.	0.000	70CHR/RYT
68	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}) = \text{C}_6\text{H}_{11}\text{O}_6^-(\text{ao}) + \text{H}^+(\text{ao})$ 1st ionization of glucose Based on enthalpies at two temperatures	ΔC_p	-120.	40.	0.000	70CHR/RYT
69	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}2) = \text{C}_6\text{H}_{11}\text{O}_6^-(\text{ao}2) + \text{H}^+(\text{ao})$ 1st ionization of mannose Based on enthalpies at three temperatures	ΔC_p	-121.	40.	0.000	70CHR/RYT
70	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}3) = \text{C}_6\text{H}_{11}\text{O}_6^-(\text{ao}3) + \text{H}^+(\text{ao})$ 1st ionization of fructose Based on enthalpies at two temperatures	ΔC_p	-3.	40.	0.000	70CHR/RYT
71	$\text{C}_6\text{H}_{12}\text{O}_6(\text{ao}4) = \text{C}_6\text{H}_{11}\text{O}_6^-(\text{ao}4) + \text{H}^+(\text{ao})$ 1st ionization of galactose Based on enthalpies at two temperatures	ΔC_p	-131.	40.	0.000	70CHR/RYT

Table 13. Index to the compounds and their reactions in reference to Tables 11 and 15

Compound	Reactions
$C_5H_8O_5^{2-}$ (ao3) xylose ²⁻ (ao)	192
$C_5H_8O_5^{2-}$ (ao5) arabinose ²⁻ (ao)	201
$C_5H_9O_5$ (ao) ribose ⁻ (ao)	340, 340, 340, 182, 184
$C_5H_9O_5$ (ao3) xylose ⁻ (ao)	341, 341, 341, 189, 191
$C_5H_9O_5$ (ao5) arabinose ⁻ (ao)	342, 342, 342, 198, 200
$C_5H_9O_5$ (ao8) lyxose ⁻ (ao)	343, 343, 343, 203
$C_5H_{10}O_4$ (cr) ribose (cr)	119, 129, 130, 333, 177
$C_5H_{10}O_5$ (cr2) β -arabinose (cr)	334, 334, 334, 131, 179
$C_5H_{10}O_5$ (cr3) α -xylose (cr)	112, 121, 178, 329, 329, 329, 132
$C_5H_{10}O_5$ (cr4) lyxose (cr)	338, 338, 338, 133, 180
$C_5H_{10}O_4$ (ao) ribose (ao)	11, 80, 82, 129, 130, 177, 182, 184, 83, 317, 317, 317, 116
$C_5H_{10}O_5$ (ao2) ribulose (ao)	82, 92, 319, 319, 319, 12, 94, 83
$C_5H_{10}O_5$ (ao3) xylose (ao)	87, 90, 178, 323, 323, 323, 85, 189, 191, 132
$C_5H_{10}O_5$ (ao4) xylulose (ao)	87, 90, 98, 99, 324, 324, 324, 85
$C_5H_{10}O_5$ (ao5) arabinose (ao)	80, 92, 322, 322, 322, 131, 179, 198, 200, 94
$C_5H_{10}O_5$ (ao8) lyxose (ao)	98, 99, 327, 327, 327, 133, 180, 203
$C_6H_8O_6^{4-}$ (ao) glucose ⁴⁻ (ao)	233
$C_6H_8O_6^{4-}$ (ao3) fructose ⁴⁻ (ao)	260
$C_6H_8O_6^{4-}$ (ao4) galactose ⁴⁻ (ao)	271
$C_6H_9O_6^{3-}$ (ao) glucose ³⁻ (ao)	232
$C_6H_9O_6^{3-}$ (ao3) fructose ³⁻ (ao)	259
$C_6H_9O_6^{3-}$ (ao4) galactose ³⁻ (ao)	270
$C_6H_{10}O_6^{2-}$ (ao) glucose ²⁻ (ao)	228, 229, 230, 231
$C_6H_{10}O_6^{2-}$ (ao2) mannose ²⁻ (ao)	241
$C_6H_{10}O_6^{2-}$ (ao3) fructose ²⁻ (ao)	255, 256, 257, 258
$C_6H_{10}O_6^{2-}$ (ao4) galactose ²⁻ (ao)	269
$C_6H_{10}O_6^{2-}$ (ao5) sorbosose ²⁻ (ao)	274
$C_6H_{11}O_6$ (ao) glucose ⁻ (ao)	222, 228, 229, 230, 226
$C_6H_{11}O_6$ (ao2) mannose ⁻ (ao)	237, 238, 239, 240, 345, 345, 345
$C_6H_{11}O_6$ (ao3) fructose ⁻ (ao)	252, 255, 256, 257, 258, 346, 346, 346, 254
$C_6H_{11}O_6$ (ao4) galactose ⁻ (ao)	347, 347, 347, 268, 266
$C_6H_{11}O_6$ (ao5) sorbosose ⁻ (ao)	272, 273

Table 13. Index to the compounds and their reactions in reference to Tables 11 and 15 — Continued

Compound	Reactions
$C_6H_{12}O_6$ (cr)	113, 122, 135, 136, 137, 138, 139, 140, 141, 142, 143, 168, 330,
α -glucose(cr)	
$C_6H_{12}O_6$ (cr2)	145, 146, 147, 148, 149
β -glucose(cr)	
$C_6H_{12}O_6$ (cr4)	336, 336, 336, 155, 176
mannose(cr)	
$C_6H_{12}O_6$ (cr5)	114, 126, 157, 158, 170, 171, 331, 331, 331
α -galactose(cr)	
$C_6H_{12}O_6$ (cr6)	172, 173, 337, 337, 337, 162
β -fructose(cr)	
$C_6H_{12}O_6$ (cr7)	115, 128, 175, 332, 332, 332, 163
sorbitose(cr)	
$C_6H_{12}O_6$ (cr8)	153
glucose(vit)	
$C_6H_{12}O_6$ (ao)	15, 62, 68, 69, 71, 74, 75, 76, 135, 136, 137, 138, 139, 140, 141, 142, 143,
glucose(ao)	145, 146, 147, 148, 149, 150, 151, 152, 165, 166, 167, 168, 222, 311, 311, 311, 226
$C_6H_{12}O_6$ (ao2)	67, 237, 238, 239, 240, 313, 313, 313, 155, 176
mannose(ao)	
$C_6H_{12}O_6$ (ao3)	8, 10, 62, 68, 69, 71, 74, 75, 76, 172, 173, 252, 315, 315, 315, 162, 254
fructose(ao)	
$C_6H_{12}O_6$ (ao4)	157, 158, 170, 171, 320, 320, 320, 268, 266
galactose(ao)	
$C_6H_{12}O_6$ (ao5)	175, 272, 273, 339, 339, 339, 163
sorbitose(ao)	
$C_6H_{13}O_{6.5}$ (cr)	174
fructose hemihydrate(cr)	
$C_6H_{14}O_7$ (cr)	150, 151, 152, 165, 166, 167, 335, 335, 335
α -glucose monohydrate(cr)	
$C_5H_9O_8P^{3-}$ (ao)	349, 349, 349, 279, 280
ribose 5-phosphate ³⁻ (ao)	
$C_5H_9O_8P^{2-}$ (ao)	11, 117, 275, 276, 277, 316, 316, 316, 37, 278, 279, 280
ribose 5-phosphate ²⁻ (ao)	
$C_5H_9O_8P^{2-}$ (ao2)	318, 318, 318, 12, 37
ribulose 5-phosphate ²⁻ (ao)	
$C_5H_9O_8P^{2-}$ (ao3)	45
xylulose 5-phosphate ²⁻ (ao)	
$C_5H_9O_8P^{2-}$ (ao4)	46
arabinose 5-phosphate ²⁻ (ao)	
$C_5H_9O_8P^{2-}$ (ao5)	15
ribose 1-phosphate ²⁻ (ao)	
$C_5H_{10}O_8P^{1-}$ (ao)	275, 276, 277, 348
ribose 5-phosphate ⁻ (ao)	
$C_6H_{10}O_9P^{3-}$ (ao)	353, 353, 353, 303, 304
glucose 6-phosphate ³⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao)	15, 17, 21, 22, 47, 49, 301, 302, 310, 310, 310, 303, 304
glucose 6-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao2)	47, 49, 287, 321, 321, 321, 289, 290, 291, 293
glucose 1-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao3)	67, 23, 26, 312, 312, 312
mannose 6-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao4)	8, 10, 17, 21, 22, 23, 26, 314, 314, 314
fructose 6-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao5)	13
galactose 6-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao6)	50
galactose 1-phosphate ²⁻ (ao)	
$C_6H_{11}O_9P^{2-}$ (ao7)	14
fructose 1-phosphate ²⁻ (ao)	
$C_6H_{12}O_9P^{-}$ (ao)	296, 297, 298, 301, 302
glucose 6-phosphate ⁻ (ao)	
$C_6H_{12}O_9P^{-}$ (ao2)	283, 284, 287, 350, 350, 350, 289
glucose 1-phosphate ⁻ (ao)	

Table 13. Index to the compounds and their reactions in reference to Tables 11 and 15 — Continued

Compound	Reactions
$C_6H_{12}O_9P^-$ (ao4) fructose 6-phosphate ⁻ (ao)	305
$C_6H_{12}O_9P^-$ (ao6) galactose 1-phosphate ⁻ (ao)	309
$C_6H_{13}O_9P$ (ao) glucose 6-phosphate(ao)	296, 297, 298
$C_6H_{13}O_9P$ (ao2) glucose 1-phosphate(ao)	283, 284
$C_6H_{13}O_9P$ (ao6) galactose 1-phosphate(ao)	308
$NiC_5H_9O_8P$ (ao) Ni-ribose 5-phosphate(ao)	281
$MgC_5H_9O_8P$ (ao) Mg-ribose 5-phosphate(ao)	282
$MgC_6H_{11}O_9P$ (ao2) Mg-glucose 1-phosphate(ao)	352, 352, 352, 293
$MgC_6H_{11}O_9P$ (ao4) Mg-fructose 6-phosphate(ao)	307
$CaC_6H_{11}O_9P$ (ao2) Ca-glucose 1-phosphate(ao)	351, 351, 351, 290
$CaC_6H_{11}O_9P$ (ao4) Ca-fructose 6-phosphate(ao)	306

Table 14. Index to the compounds and their reactions in reference to Table 12 and the heat capacity data in Table 15

Compound	Reactions
C ₅ H ₉ O ₅ ⁻ (ao) ribose ⁻ (ao)	64
C ₅ H ₉ O ₅ ⁻ (ao3) xylose ⁻ (ao)	65
C ₅ H ₉ O ₅ ⁻ (ao5) arabinose ⁻ (ao)	66
C ₅ H ₉ O ₅ ⁻ (ao8) lyxose ⁻ (ao)	67
C ₅ H ₁₀ O ₅ (C) d-ribose(cr)	32, 33
C ₅ H ₁₀ O ₅ (C2) d-arabinose(cr)	34
C ₅ H ₁₀ O ₅ (C3) d-xylose(cr)	16, 17
C ₅ H ₁₀ O ₅ (C4) d-lyxose(cr)	35
C ₅ H ₁₀ O ₅ (ao) ribose(ao)	50
C ₅ H ₁₀ O ₅ (ao3) xylose(ao)	49
C ₅ H ₁₀ O ₅ (ao4) xylulose(ao)	9
C ₅ H ₁₀ O ₅ (ao5) arabinose(ao)	51
C ₅ H ₁₀ O ₅ (ao8) lyxose(ao)	48
C ₆ H ₁₁ O ₅ ⁻ (ao) glucose ⁻ (ao)	68
C ₆ H ₁₁ O ₅ ⁻ (ao2) mannose ⁻ (ao)	69
C ₆ H ₁₁ O ₅ ⁻ (ao3) fructose ⁻ (ao)	70
C ₆ H ₁₁ O ₅ ⁻ (ao4) galactose ⁻ (ao)	71
C ₆ H ₁₂ O ₆ (C) α-D-glucose(cr)	21, 22, 23, 24, 25, 26, 27, 36, 37, 38
C ₆ H ₁₂ O ₆ (C2) β-D-glucose(cr)	39, 40
C ₆ H ₁₂ O ₆ (C4) D-mannose(cr)	30
C ₆ H ₁₂ O ₆ (C5) D-galactose(cr)	18, 19
C ₆ H ₁₂ O ₆ (C6) D-fructose(cr)	31
C ₆ H ₁₂ O ₆ (C7) D-sorbose(cr)	20
C ₆ H ₁₂ O ₆ (Gl) glucose(vit)	28, 29
C ₆ H ₁₂ O ₆ (ao) glucose(ao)	18, 36, 37, 38, 39, 40, 55, 56, 57, 58
C ₆ H ₁₂ O ₆ (ao2) mannose(ao)	2, 60
C ₆ H ₁₂ O ₆ (ao3) fructose(ao)	38, 52
C ₆ H ₁₂ O ₆ (ao4) galactose(ao)	53
C ₅ H ₉ O ₅ P ²⁻ (ao) ribose, 5-phosphate ²⁻ (ao)	4
C ₆ H ₁₁ O ₅ P ²⁻ (ao) glucose, 6-phosphate ²⁻ (ao)	16
C ₆ H ₁₁ O ₅ P ²⁻ (ao3) mannose, 6-phosphate ²⁻ (ao)	27
C ₆ H ₁₁ O ₅ P ²⁻ (ao4) fructose, 6-phosphate ²⁻ (ao)	367

Table 15. Calculated values of thermochemical properties at 298.15 K

Compound	molar mass g mol ⁻¹	$\Delta_f H^\circ$	$\Delta_f G^\circ$	S°	C_p°
		kJ mol ⁻¹		J mol ⁻¹ K ⁻¹	
C ₅ H ₈ O ₅ ²⁻ (ao3) xylose ²⁻ (ao)	148.1166		-599.455±2.4		
C ₅ H ₈ O ₅ ²⁻ (ao5) arabinose ²⁻ (ao)	148.1166		-587.766±6.0		
C ₅ H ₉ O ₅ (ao) ribose ⁻ (ao)	149.1240	-997.903±0.27	-669.666±6.0	93.304±20.	164.0±45.
C ₅ H ₉ O ₅ (ao3) xylose ⁻ (ao)	149.1240	-1008.040±1.6	-681.085±2.3	97.604±9.3	176.0±45.
C ₅ H ₉ O ₅ (ao5) arabinose ⁻ (ao)	149.1240	-1003.787±0.39	-671.786±6.0	80.682±20.	165.0±45.
C ₅ H ₉ O ₅ (ao8) lyxose ⁻ (ao)	149.1240		-680.017±2.3		168.0±45.
C ₅ H ₁₀ O ₅ (cr) ribose(cr)	150.1314	-1047.230±0.22	-730.086±6.0	130.458±20.	185.5±1.5
C ₅ H ₁₀ O ₅ (cr2) β -arabinose(cr)	150.1314	-1057.027±0.39	-737.726±6.0	123.224±20.	184.0±2.0
C ₅ H ₁₀ O ₅ (cr3) α -xylose(cr)	150.1314	-1057.840±1.4	-744.585±2.1	143.500±5.4	184.0±2.0
C ₅ H ₁₀ O ₅ (cr4) lyxose(cr)	150.1314		-740.837±2.4		184.0±2.0
C ₅ H ₁₀ O ₅ (ao) ribose(ao)	150.1314	-1034.003±0.23	-738.786±6.0	204.000±20.	276.0±20.
C ₅ H ₁₀ O ₅ (ao2) ribulose(ao)	150.1314	-1023.015±0.34	-735.936±6.0	231.297±20.	
C ₅ H ₁₀ O ₅ (ao3) xylose(ao)	150.1314	-1045.740±1.5	-750.485±2.2	203.872±8.9	279.0±20.
C ₅ H ₁₀ O ₅ (ao4) xylulose(ao)	150.1314	-1029.650±1.7	-746.152±2.2	243.307±9.4	319.0±28.
C ₅ H ₁₀ O ₅ (ao5) arabinose(ao)	150.1314	-1043.787±0.36	-742.226±6.0	182.725±20.	279.0±20.
C ₅ H ₁₀ O ₅ (ao8) lyxose(ao)	150.1314		-749.137±2.3		285.0±20.
C ₆ H ₈ O ₆ ⁴⁻ (ao) glucose ⁴⁻ (ao)	176.1281		-592.952±2.4		
C ₆ H ₈ O ₆ ⁴⁻ (ao3) fructose ⁴⁻ (ao)	176.1281		-594.236±2.4		
C ₆ H ₈ O ₆ ⁴⁻ (ao4) galactose ⁴⁻ (ao)	176.1281		-584.833±0.23		
C ₆ H ₉ O ₆ ³⁻ (ao) glucose ³⁻ (ao)	177.1355		-679.452±2.2		
C ₆ H ₉ O ₆ ³⁻ (ao3) fructose ³⁻ (ao)	177.1355		-684.436±2.2		
C ₆ H ₉ O ₆ ³⁻ (ao4) galactose ³⁻ (ao)	177.1355		-671.033±0.21		
C ₆ H ₁₀ O ₆ ²⁻ (ao) glucose ²⁻ (ao)	178.1429		-764.752±2.0		
C ₆ H ₁₀ O ₆ ²⁻ (ao2) mannose ²⁻ (ao)	178.1429		-761.239±2.6		
C ₆ H ₁₀ O ₆ ²⁻ (ao3) fructose ²⁻ (ao)	178.1429		-767.436±2.0		
C ₆ H ₁₀ O ₆ ²⁻ (ao4) galactose ²⁻ (ao)	178.1429		-756.033±0.20		
C ₆ H ₁₀ O ₆ ²⁻ (ao5) sorbose ²⁻ (ao)	178.1429		-763.254±6.8		
C ₆ H ₁₁ O ₆ (ao) glucose ⁻ (ao)	179.1503	-1225.494±1.1	-845.802±1.9	159.555±7.5	216.3±28.
C ₆ H ₁₁ O ₆ (ao2) mannose ⁻ (ao)	179.1503	-1225.582±1.8	-842.039±2.4	146.638±9.2	221.0±32.
C ₆ H ₁₁ O ₆ (ao3) fructose ⁻ (ao)	179.1503	-1220.182±1.2	-846.811±1.9	180.756±7.7	366.0±31.
C ₆ H ₁₁ O ₆ (ao4) galactose ⁻ (ao)	179.1503	-1214.503±0.13	-838.433±0.18	171.704±0.77	188.0±44.

Table 15. Calculated values of thermochemical properties at 298.15 K — Continued

Compound	molar mass g mol ⁻¹	$\Delta_f H^\circ$		S° J mol ⁻¹ K ⁻¹	C_p°
		kJ mol ⁻¹			
C ₆ H ₁₁ O ₅ (ao5) sorbitol(ao)	179.1503		-844.454±6.3		
C ₆ H ₁₂ O ₆ (cr) α-glucose(cr)	180.1577	-1273.040±0.87	-908.792±1.8	211.300±5.2	219.1±2.0
C ₆ H ₁₂ O ₆ (cr2) β-glucose(cr)	180.1577	-1266.842±0.91			216.0±3.0
C ₆ H ₁₂ O ₆ (cr4) mannose(cr)	180.1577	-1266.527±1.8	-902.189±2.5	210.998±10.	216.0±3.0
C ₆ H ₁₂ O ₆ (cr5) α-galactose(cr)	180.1577	-1272.340±0.11	-906.333±0.17	205.400±0.45	220.8±2.2
C ₆ H ₁₂ O ₆ (cr6) β-fructose(cr)	180.1577	-1269.462±1.1	-905.645±2.0	212.744±7.6	232.0±3.0
C ₆ H ₁₂ O ₆ (cr7) sorbitol(cr)	180.1577	-1270.240±3.8	-908.854±5.9	220.900±15.	231.4±1.0
C ₆ H ₁₂ O ₆ (cr8) glucose(vit)	180.1577	-1266.594±1.1			372.4±6.6
C ₆ H ₁₂ O ₆ (ao) glucose(ao)	180.1577	-1262.194±0.88	-915.902±1.9	271.525±5.6	336.3±6.5
C ₆ H ₁₂ O ₆ (ao2) mannose(ao)	180.1577	-1258.657±1.7	-910.989±2.4	266.909±9.0	342.0±17.
C ₆ H ₁₂ O ₆ (ao3) fructose(ao)	180.1577	1259.382±1.0	915.511±1.9	279.645±5.9	369.0±14.
C ₆ H ₁₂ O ₆ (ao4) galactose(ao)	180.1577	-1255.203±0.12	-908.933±0.18	271.600±0.49	319.0±20.
C ₆ H ₁₂ O ₆ (ao5) sorbitol(ao)	180.1577	-1263.300±4.2	-911.954±6.2	254.574±25.	
C ₆ H ₁₃ O _{6.5} (cr) fructose hemihydrate(cr)	189.1653		-1024.106±2.1		
C ₆ H ₁₄ O ₇ (cr) α-glucose monohydrate(cr)	198.1730	-1568.897±0.96	-1148.350±1.9	255.567±5.9	
C ₅ H ₉ O ₈ P ³⁻ (ao) ribose 5-phosphate ³⁻ (ao)	227.0891	-2015.983±0.37	-1508.068±0.61	-95.293±2.4	
C ₅ H ₉ O ₈ P ²⁻ (ao) ribose 5-phosphate ²⁻ (ao)	228.0965	-2041.483±0.34	-1582.568±0.60	69.000±1.7	9.6±45.
C ₅ H ₉ O ₈ P ²⁻ (ao2) ribulose 5-phosphate ²⁻ (ao)	228.0965	-2023.755±0.42	-1581.368±0.61	124.437±2.5	
C ₅ H ₉ O ₈ P ²⁻ (ao3) xylulose 5-phosphate ²⁻ (ao)	228.0965		-1582.578±0.62		
C ₅ H ₉ O ₈ P ²⁻ (ao4) arabinose 5-phosphate ²⁻ (ao)	228.0965		-1585.168±0.64		
C ₅ H ₉ O ₈ P ²⁻ (ao5) ribose 1-phosphate ²⁻ (ao)	228.0965		-1575.697±6.0		
C ₅ H ₁₀ O ₈ P ⁻ (ao) ribose 5-phosphate ⁻ (ao)	229.1039	-2030.183±0.37	-1620.748±0.61	234.903±2.4	
C ₆ H ₁₀ O ₉ P ³⁻ (ao) glucose 6-phosphate ³⁻ (ao)	257.1154	-2241.236±1.4	-1697.142±2.1	22.198±8.4	
C ₆ H ₁₁ O ₉ P ²⁻ (ao) glucose 6-phosphate ²⁻ (ao)	258.1228	-2276.436±1.2	-1763.942±2.0	128.130±6.9	48.3±17.
C ₆ H ₁₁ O ₉ P ²⁻ (ao2) glucose 1-phosphate ²⁻ (ao)	258.1228		-1756.867±2.1		
C ₆ H ₁₁ O ₉ P ²⁻ (ao3) mannose 6-phosphate ²⁻ (ao)	258.1228	-2273.227±1.3	-1760.820±2.1	128.420±7.3	56.6±19.
C ₆ H ₁₁ O ₉ P ²⁻ (ao4) fructose 6-phosphate ²⁻ (ao)	258.1228	-2264.767±1.2	-1760.795±2.0	156.711±6.9	88.9±17.
C ₆ H ₁₁ O ₉ P ²⁻ (ao5) galactose 6-phosphate ²⁻ (ao)	258.1228		-1756.694±0.21		
C ₆ H ₁₁ O ₉ P ²⁻ (ao6) galactose 1-phosphate ²⁻ (ao)	258.1228		-1754.067±2.1		
C ₆ H ₁₁ O ₉ P ²⁻ (ao7) fructose 1-phosphate ²⁻ (ao)	258.1228		-1764.192±2.2		
C ₆ H ₁₂ O ₉ P ⁻ (ao) glucose 6-phosphate ⁻ (ao)	259.1302		-1800.592±2.1		

Table 15. Calculated values of thermochemical properties at 298.15 K — Continued

Compound	molar mass g mol ⁻¹	$\Delta_f H^\circ$	$\Delta_f G^\circ$	S°	C_p°
		kJ mol ⁻¹		J mol ⁻¹ K ⁻¹	
C ₆ H ₁₂ O ₆ P ⁻ (ao2) glucose 1-phosphate ⁻ (ao)	259.1302		-1793.977±2.1		
C ₆ H ₁₂ O ₉ P ⁻ (ao4) fructose 6-phosphate ⁻ (ao)	259.1302		-1796.595±2.1		
C ₆ H ₁₂ O ₉ P ⁻ (ao6) galactose 1-phosphate ⁻ (ao)	259.1302		-1791.767±2.2		
C ₆ H ₁₃ O ₉ P(ao) glucose 6-phosphate(ao)	260.1376		-1809.375±2.1		
C ₆ H ₁₃ O ₉ P(ao2) glucose 1-phosphate(ao)	260.1376		-1800.707±2.2		
C ₆ H ₁₃ O ₉ P(ao6) galactose 1-phosphate(ao)	260.1376		-1798.727±2.3		
NiC ₅ H ₉ O ₈ P(ao) Ni-ribose 5-phosphate(ao)	286.7854		-1643.068±0.64		
MgC ₅ H ₉ O ₈ P(ao) Mg-ribose 5-phosphate(ao)	252.4004		-2051.568±0.63		
MgC ₆ H ₁₁ O ₈ P(ao2) Mg-glucose 1-phosphate(ao)	282.4267		-2226.317±2.2		
MgC ₆ H ₁₁ O ₈ P(ao4) Mg-fructose 6-phosphate(ao)	282.4267		-2230.195±2.2		
CaC ₆ H ₁₁ O ₈ P(ao2) Ca-glucose 1-phosphate(ao)	298.2017		-2323.907±2.3		
CaC ₆ H ₁₁ O ₈ P(ao4) Ca-fructose 6-phosphate(ao)	298.2017		-2326.995±2.2		

Auxiliary Data

C(cr)	12.0110	0	0	5.74 ± 0.10	
CO ₂ (g)	44.0098	-393.51 ± 0.13	-394.37 ± 0.13	213.676 ± 0.01	
O ₂ (g)	31.9988	0	0	205.043 ± 0.005	
H ⁺ (ao)	1.0074	0	0	0	0
H ₂ (g)	2.0159	0	0	130.571 ± 0.003	
H ₂ O(l)	18.0153	-285.830 ± 0.040	-237.189 ± 0.04	69.95 ± 0.03	75.359
N ₂ (g)	28.0134	0	0	191.500 ± 0.004	
P(cr)	30.9738	0	0	41.09 ± 0.25	
HPO ₄ ²⁻ (ao)	95.9804	-1299.0 ± 1.5	-1096.1 ± 1.5	-33.5 ± 1.5	-254.
H ₂ PO ₄ ⁻ (ao)	96.9878	-1302.6 ± 1.5	-1137.3 ± 1.5	92.5 ± 1.5	-34.
Ni ²⁺ (ao)	58.6889	-54.0	-45.6	-128.9	
Mg(cr)	24.3050	0	0	32.67 ± 0.10	
Mg ²⁺ (ao)	24.3039	-467.0 ± 0.6	-455.30 ± 1.4	-137 ± 4	-16.0
Ca(cr)	40.0800	0	0	41.59 ± 0.40	
Ca ²⁺ (ao)	40.0789	-543.0 ± 1.0	-552.8 ± 1.0	-56.2 ± 1.0	-27.0

TABLE 16. Ranges of property values

Quantity	Range of values
V^* (pentose(cr))	$(91.7 \text{ to } 99.4) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
V^* (hexose(cr))	$(108.9 \text{ to } 118.3) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
V_2^* (pentose(ao))	$(93.7 \text{ to } 95.7) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
V_2^* (hexose(ao))	$(110.5 \text{ to } 112.0) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
$\{V_2^*$ (pentose(ao)) - V^* (pentose(cr)) $\}$	$(-3.5 \text{ to } 1.7) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
$\{V_2^*$ (hexose(ao)) - V^* (hexose(cr)) $\}$	$(-2.7 \text{ to } 0.8) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$
E^* (hexose(cr))	$\approx 0.028 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1} \text{ K}^{-1}$
E_2^* (hexose(ao))	$(0.09 \text{ to } 0.15) \times 10^{-6} \text{ m}^3 \text{ mol}^{-1} \text{ K}^{-1}$
$K_{T,2}^*$ (pentose(ao))	$(-8.4 \text{ to } -15.2) \times 10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1}$
$K_{T,2}^*$ (hexose(ao))	$(-12.7 \text{ to } -16.7) \times 10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1}$
$(\partial K_{T,2}^*/\partial T)_p$ (hexose(ao))	$(0.64 \text{ to } 0.80) \times 10^{-15} \text{ m}^3 \text{ mol}^{-1} \text{ Pa}^{-1} \text{ K}^{-1}$
C_p^* (pentose(cr))	$(184 \text{ to } 186) \text{ J mol}^{-1} \text{ K}^{-1}$
C_p^* (hexose(cr))	$(205 \text{ to } 232) \text{ J mol}^{-1} \text{ K}^{-1}$
$C_{p,2}^*$ (pentose(ao))	$(276 \text{ to } 319) \text{ J mol}^{-1} \text{ K}^{-1}$
$C_{p,2}^*$ (hexose(ao))	$(319 \text{ to } 369) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{C_{p,2}^*$ (pentose(ao)) - C_p^* (pentose(cr)) $\}$	$(98 \text{ to } 137) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{C_{p,2}^*$ (hexose(ao)) - C_p^* (hexose(cr)) $\}$	$(90 \text{ to } 101) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{C_{p,2}^*$ (sugar(ao)) - $C_{p,2}^*$ (sugar-phosphate(ao)) $\}$	$(266 \text{ to } 288) \text{ J mol}^{-1} \text{ K}^{-1}$
S^* (pentose(cr))	$(123 \text{ to } 144) \text{ J mol}^{-1} \text{ K}^{-1}$
S^* (hexose(cr))	$(205 \text{ to } 221) \text{ J mol}^{-1} \text{ K}^{-1}$
S_2^* (pentose(ao))	$(204 \text{ to } 231) \text{ J mol}^{-1} \text{ K}^{-1}$
S_2^* (hexose(ao))	$(255 \text{ to } 280) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{S_2^*$ (pentose(ao)) - S^* (pentose(cr)) $\}$	$(60 \text{ to } 108) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{S_2^*$ (hexose(ao)) - S^* (hexose(cr)) $\}$	$(34 \text{ to } 67) \text{ J mol}^{-1} \text{ K}^{-1}$
$\{S_2^*$ (sugar(ao)) - S_2^* (sugar-phosphate(ao)) $\}$	$(107 \text{ to } 144) \text{ J mol}^{-1} \text{ K}^{-1}$
$\Delta_f H^*$ (pentose(cr))	$(-1047 \text{ to } -1058) \text{ kJ mol}^{-1}$
$\Delta_f H^*$ (hexose(cr))	$(-1266 \text{ to } -1272) \text{ kJ mol}^{-1}$
$\Delta_f H^*$ (pentose(ao))	$(-1023 \text{ to } -1046) \text{ kJ mol}^{-1}$
$\Delta_f H^*$ (hexose(ao))	$(-1255 \text{ to } -1263) \text{ kJ mol}^{-1}$
$\{\Delta_f H^*$ (pentose(ao)) - $\Delta_f H^*$ (pentose(cr)) $\}$	$(-13 \text{ to } +14) \text{ kJ mol}^{-1}$
$\{\Delta_f H^*$ (hexose(ao)) - $\Delta_f H^*$ (hexose(cr)) $\}$	$(4.6 \text{ to } 17.1) \text{ kJ mol}^{-1}$
$\{\Delta_f H^*$ (sugar(ao)) - $\Delta_f H^*$ (sugar-phosphate(ao)) $\}$	$(1001 \text{ to } 1015) \text{ kJ mol}^{-1}$
$\Delta_f G^*$ (pentose(cr))	$(-730 \text{ to } -745) \text{ kJ mol}^{-1}$
$\Delta_f G^*$ (hexose(cr))	$(-902 \text{ to } -909) \text{ kJ mol}^{-1}$
$\Delta_f G^*$ (pentose(ao))	$(-739 \text{ to } -751) \text{ kJ mol}^{-1}$
$\Delta_f G^*$ (hexose(ao))	$(-909 \text{ to } -916) \text{ kJ mol}^{-1}$
$\{\Delta_f G^*$ (pentose(ao)) - $\Delta_f G^*$ (pentose(cr)) $\}$	$(-4.5 \text{ to } -8.7) \text{ kJ mol}^{-1}$
$\{\Delta_f G^*$ (hexose(ao)) - $\Delta_f G^*$ (hexose(cr)) $\}$	$(-2.6 \text{ to } -9.9) \text{ kJ mol}^{-1}$
$\Delta_f G^*$ (sugar(ao)) - $\Delta_f G^*$ (sugar-phosphate(ao))	$(836 \text{ to } 850) \text{ kJ mol}^{-1}$

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88TEW/STE	Tewari, Y. B.; Steckler, D. K.; Goldberg, R. N.; J. Biol. Chem.; 263 , 3664 (1988)
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<i>R</i>	gas constant (8.314 51 J mol ⁻¹ K ⁻¹)
<i>S</i>	entropy
<i>T</i>	thermodynamic temperature
<i>V</i>	volume

Greek

α	cubic expansion coefficient: $V^{-1}(\partial V/\partial T)_p$
γ	activity coefficient
η	viscosity
κ_S	cubic isentropic compressibility coefficient: $V^{-1}(\partial V/\partial p)_S$
κ_T	cubic isothermal compressibility coefficient: $V^{-1}(\partial V/\partial p)_T$
ρ	(mass) density/ kg m ⁻³
ϕ	osmotic coefficient
Δ	change in a property

superscripts

^o	standard state quantity
*	the property of the pure substance
∞	the limit of a property as the concentration of solute approaches zero
ex	excess
id	ideal

subscripts

<i>f</i>	formation property
1, 2	designate solvent and solute, respectively; the subscript 2 is frequently omitted for the solute
1, 2, ...	subscripts for virial parameters
ϕ	apparent molar quantity

physical states

am	amorphous solid
ao	aqueous, standard state of the indicated species
aq	aqueous solution, concentration not specified
cr	crystalline solid
<i>g</i>	gaseous
<i>l</i>	liquid
vit	vitreous (glassy) liquid

12. Glossary of Symbols and Terminology^a*Roman*

<i>c</i>	concentration/mol L ⁻¹ ; or parameter in expression for the excess heat capacity; or specific heat capacity/J kg ⁻¹
<i>e</i>	parameter in expression for the excess expansivity
<i>g</i>	parameter in expression for the excess Gibbs energy
<i>h</i>	parameter in expression for the excess enthalpy
<i>k</i>	parameter in expression for the excess compressibility
<i>m</i>	molality/mol kg ⁻¹
<i>n</i>	amount of substance
<i>p</i>	pressure/Pa
<i>u</i>	speed of sound/m s ⁻¹
<i>v</i>	parameter in expression for the excess volume
<i>x</i>	mole fraction
<i>C</i>	heat capacity
<i>D</i>	diffusion coefficient
<i>E</i>	expansivity: $(\partial V/\partial T)_p$
<i>G</i>	Gibbs energy
<i>H</i>	enthalpy
<i>K</i>	equilibrium constant
K_S	isentropic compressibility: $(\partial V/\partial p)_S$
K_T	isothermal compressibility: $(\partial V/\partial p)_T$
<i>L</i>	relative enthalpy ($H - H^\circ$)
<i>M</i>	molar mass/kg mol ⁻¹

^a When more than one meaning is attached to a given symbol, the context will serve to clarify the meaning of the symbol at that point in the text.