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# Volumetric Properties of the Nucleosides Adenosine, Cytidine, and Uridine in Aqueous Solution at $T$ = (288.15 and 313.15) K and $p$ = (10 to 100) MPa

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**Abstract** Speeds of sound have been measured for aqueous solutions of the nucleosides adenosine, cytidine, and uridine at the temperatures $T$ = (288.15 and 313.15) K and at the pressures $p$ = (10, 20, 40, 60, 80, and 100) MPa. Using the methods described in our previous work, the partial molar volumes at infinite dilution, $V_2^{\mathrm{o}}$, the partial molar isentropic compressions at infinite dilution, $K_{S,2}^{\mathrm{o}}$, and the partial molar isothermal compressions at infinite dilution, $K_{T,2}^{\mathrm{o}}\{K_{T,2}^{\mathrm{o}} = -(\partial V_2^{\mathrm{o}}/\partial p)_T\}$, for the nucleosides were derived from the speed of sound data at elevated pressures. The thermodynamic properties $V_2^{\mathrm{o}}$ and $K_{T,2}^{\mathrm{o}}$ were combined with those determined previously for $T$ = 298.15 K to create 3D surfaces that display the pressure and temperature dependences of these properties. The purine nucleoside adenosine displays distinctly different trends in these properties from those of the pyrimidine nucleosides cytidine and uridine. A semi-empirical model was used to rationalize the $K_{T,2}^{\mathrm{o}}$ results in terms of likely changes in hydration as a function of temperature and pressure.

**Keywords** Speed of sound · Partial molar volume · Partial molar isothermal compression · High pressure · Nucleosides · Aqueous solution

## 1 Introduction

One hypothesis for how life may have first emerged from an abiotic world proposes that RNA was the earliest form of both a genetic and catalytic biopolymer [1-3]. This hypothesis, which is commonly referred to as the “RNA world”, was first proposed three decades ago [4] and still remains popular today [5,6]. The primordial conditions of temperature, pressure, and pH under which the polymer RNA could be formed from its basic building blocks such as the nucleic-acid bases, nucleosides and nucleotides are far from established [7-9]. It is useful, therefore, to determine the conditions of temperature and pressure under which RNA and its constituent molecules are both physically and chemically stable so that the boundary conditions necessary for an RNA world to prevail can be defined.

The volumetric properties as a function of pressure for RNA and its constituents are paramount for mapping the physical stabilities of these molecules over the ($p$,$T$) landscape. In our previous work [10,11], the partial molar volumes at infinite dilution, $V_2^{\circ}$, and the partial molar isothermal compressions at infinite dilution, $K_{T,2}^{\circ}\{K_{T,2}^{\circ} = -(\partial V_2^{\circ}/\partial p)_T\}$, were obtained for the nucleosides adenosine, cytidine, and uridine over the pressure range $p$ = (10 to 120) MPa, and for guanosine over the range $p$ = (10 to 100) MPa. Both studies were conducted at the single isotherm $T$ = 298.15 K. In order to construct a functional ($p$,$T$) stability map, volumetric data are required for a range of temperatures. As an initial contribution to this objective, we report herein speed of sound measurements at the temperatures $T$ = (288.15 and 313.15) K and at the pressures $p$ = (10, 20, 40, 60, 80, and 100) MPa for aqueous solutions of the nucleosides adenosine, cytidine, and uridine. Using the methods described previously [10-12], these sound speeds were analysed to obtain the volumetric properties, $V_2^{\circ}$, the partial molar isentropic compressions at infinite dilution, $K_{S,2}^{\circ}$, and $K_{T,2}^{\circ}$.

# 2 Experimental

## 2.1 Materials

The samples of adenosine, cytidine, and uridine were from the same batches of material used in a previous study [13]. Details of the purification and characterization of these samples, and a summary Table that gives the source, purification method, and mass fraction purity for each nucleoside have been reported elsewhere [13].

The water used to prepare solutions and as the reference solvent was purified by reverse osmosis and deionization using an Ondeo Purite Select water purification system, and thoroughly degassed just prior to use. All solutions were prepared by mass using a Mettler Toledo AX205 analytical balance with a readability of 0.01 mg. Corrections were made for the effect of air buoyancy using densities for the crystalline nucleosides taken from the literature [14,15]. The uncertainties for the solution molalities were $< 2 \times 10^{-5}$ $\text{mol}\cdot\text{kg}^{-1}$.

## 2.2 Apparatus and Methods

The instrument used for the sound speed measurements at high pressures was designed and constructed at the University of Bergen. Details of the apparatus and operational procedures used have been described previously [12]. The operating temperatures $T$ = 288.15 K and $T$ = 313.15 K were stable to ± 0.001 K and ± 0.002 K, respectively, and the pressure was adjustable to within ± 0.15 MPa of any nominal value [12]. The estimated uncertainty for a measured sound speed was ± 0.03 $\text{m}\cdot\text{s}^{-1}$.

# 3 Results

## 3.1 Thermodynamic Formalism

The derivation of the relationship for the calculation of solution densities from speed of sound measurements at high pressures is summarized as follows. The difference between the isothermal compressibility, $\kappa_T$ $\{\kappa_T = -(\partial V/\partial p)_T/V\}$, and the isentropic compressibility, $\kappa_S$ $\{\kappa_S = -(\partial V/\partial p)_S/V\}$, which is usually represented by the symbol $\delta$ [16,17], can be written in the form [16-18]:

$$\delta = \kappa_T - \kappa_S = (T\alpha^2 V)/C_p = (T\alpha^2)/\sigma \tag{1}$$

where $C_p$ is the isobaric heat capacity, $\sigma$ is the heat capacity per unit volume, and $\alpha$ is the isobaric expansibility [16], which is defined by the equation:

$$\alpha = (\partial V/\partial T)_p/V \tag{2}$$

Since the difference between $C_p$ and the isochoric heat capacity, $C_v$, is given by [18]:

$$C_p - C_v = (T\alpha^2 V)/\kappa_T \tag{3}$$

it follows from Eqs. 1 and 3 that the ratio of $C_p$ to $C_v$, which is often expressed using the symbol $\gamma$, is given by:

$$\gamma = C_p/C_v = \kappa_T/\kappa_S \tag{4}$$

Isentropic compressibilities of fluids are conveniently evaluated from speed of sound measurements. In the absence of sound dispersion, the isentropic compressibility is related to the speed of sound, $u$, by the Newton-Laplace equation [19]:

$$\kappa_S = 1/(u^2\rho) \tag{5}$$

where $\rho$ is the density of the fluid. Combining the isothermal compressibility recast in terms of density, $\{\kappa_T = (\partial\rho/\partial p)_T/\rho\}$, with Eqs. 4 and 5 leads to the equation:

$$(\partial\rho/\partial p)_T = \gamma/u^2 \tag{6}$$

Integration of Eq. 6 at constant temperature between the limits of $p$ = 0.1 MPa and a pressure $p$ gives the expression:

$$\rho(p) - \rho(p = 0.1) = \int_{p=0.1}^{p} (\gamma/u^2)\,dp \qquad (7)$$

This relationship provides a route for the evaluation of volumetric properties at high pressures. If the quantities $\rho$, $\gamma$, and $u$ are known for a system at $p$ = 0.1MPa, and if the pressure dependence of the quantity $(\gamma/u^2)$ can be determined, then the density $\rho$ at any pressure $p$, $\rho(p)$ can be obtained using Eq. 7.

**3.2 Thermodynamic Quantities at $p$ = 0.1 MPa**

Values of $\gamma$ for aqueous solutions of the nucleosides at $p$ = 0.1 MPa were obtained using the following expression derived by combining Eqs. 1 and 4:

$$\gamma = (\kappa_S + \alpha^2 T/\sigma)/\kappa_S \qquad (8)$$

In a recent paper [20], speeds of sound and specific heat capacities, $c_p$, were reported for aqueous solutions of adenosine, cytidine, and uridine at $T$ = (288.15 and 313.15) K and at ambient pressure. The $c_p$ results were analysed using a power series in molality, $m$, of the generic form:

$$y = y_1^* + a_1(m/m^o) + a_2(m/m^o)^2 \qquad (9)$$

where $a_1$ and $a_2$ are the fitted coefficients, $m^o$ = 1.0 mol·kg$^{-1}$, and $y_1^*$ is the respective property for pure water ($c_{p,1}^*$ = (4.1855 and 4.1783) J·K$^{-1}$·g$^{-1}$ at $T$ = (288.15 and 313.15) K, respectively [21]). Values for the coefficients $a_1$ and $a_2$ together with their estimated uncertainties are given in Table 1. The $a_1$ coefficient for adenosine at $T$ = 288.15 K was obtained using the linear form of Eq. 9 because the value obtained initially for the $a_2$ coefficient was statistically insignificant. Included in Table 1 are the $a_1$ and $a_2$ coefficients obtained previously [10] from analyses using

Eq. 9 of density data reported [22] for solutions of the three nucleosides at four temperatures. Solution densities calculated using Eq. 9 were combined with the reported speed of sound data [20] to obtain isentropic compressibilities for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K. These $\kappa_S$ results were in turn analysed using Eq. 9, with $\kappa_{S,1}^*$ = (4.65762 × $10^{-10}$ and 4.31178 × $10^{-10}$ ) $Pa^{-1}$ at $T$ = (288.15 and 313.15) K, respectively, [23] to give the $a_1$ and $a_2$ coefficients shown in Table 1. For adenosine, the values for $a_2$ were not statistically significant; the $a_1$ values were evaluated using the linear form of Eq. 9. Values of $c_p$ and $\kappa_S$ (calculated using Eq. 9) for aqueous solutions of the nucleosides at $p$ = 0.1 MPa and at the molalities and temperatures used in this work are given in Table 2. Also included in Table 2 are solution densities calculated using Eq. 9 and sound speeds calculated from the $\kappa_S$ and $\rho$ values using Eq. 5.

The isobaric expansibilities, $\alpha$, for the various solutions at $T$ = (288.15 and 313.15) K and $p$ = 0.1 MPa were calculated using Eq. 2 transformed as:

$$\alpha = -(\partial\rho/\partial T)_p/\rho \qquad (10)$$

Solution densities for the molalities used in this study were calculated using Eq. 9 and the $a_1$ and $a_2$ coefficients at the four temperatures given in Table 1. The values of $\rho_1^*$ for water used in the calculations were the same as those used in our previous work, *viz.* $\rho_1^*$ = (999.101, 997.047, 995.650, and 992.219) kg·$m^{-3}$ at $T$ = (288.15, 298.15, 303.15, and 313.15) K, respectively [10,22,24]. For each solution the equation:

$$\rho - \rho_1^* = b_0 + b_1(T - T_m) + b_2(T - T_m)^2 \qquad (11)$$

was fitted to the density data, where $T_m$ is the mid-point temperature of the range used ($T_m$ = 300.65 K), and $b_i$ , i = 0-2, are the fitted coefficients. Differentiation of Eq. 11 with respect to temperature at constant pressure leads to:

$$(\partial\rho/\partial T)_p = (\partial\rho_1^*/\partial T)_p + b_1 + 2b_2(T-T_m) \quad (12)$$

The derivatives $(\partial\rho/\partial T)_p$ obtained using Eq. 12, with $(\partial\rho_1^*/\partial T)_p$ taken as $-150.73 \times 10^{-3}$ kg·m$^{-3}$·K$^{-1}$ at $T = 288.15$ K and $-382.30 \times 10^{-3}$ kg·m$^{-3}$·K$^{-1}$ at $T = 313.15$ K [25], were used to calculate the isobaric expansibilities using Eq. 10. These $\alpha$ values and their uncertainties, which were assessed by the application of propagation of errors methods [26] to Eq. 12, are given in Table 2.

The heat capacities per unit volume, which were obtained by simple multiplication of $c_p$ by $\rho$, were combined with the values of $\alpha$ and $\kappa_S$ to obtain using Eq. 8 the values of $\gamma$ given in Table 2. The uncertainties for $\gamma$ given in Table 2 were estimated by the application of propagation of errors methods to Eq. 8.

### 3.3 Solution Densities at High Pressures

The rigorous application of Eq. 7 to obtain from measured sound speeds the solution densities at high pressures is not possible because the pressure dependence of $\gamma$ is not known. However, solution densities at high pressures can be estimated using Eq. 7, given some suitable assumption about the pressure dependence of $\gamma$ . Since the solutions used in this work are relatively dilute, a reasonable assumption that can be made is that the difference between the $\gamma$ values for a given solution at any two pressures is approximately the same as that for the pure solvent, *i.e.*:

$$\gamma(p) - \gamma(p = 0.1 \text{ MPa}) \approx \gamma_{H2O}(p) - \gamma_{H2O}(p = 0.1 \text{ MPa}), \quad (13)$$

where $\gamma(p)$ and $\gamma_{H2O}(p)$ represent, respectively, the $\gamma$ values for the solution and pure water at the pressure $p$ given in parentheses. The values for $\gamma_{H2O}(p)$ over the range $p$ = (0.1 to 100) MPa were evaluated using the literature data given in Table 3. For consistency with our previous work [10,12,27], the sound speeds were calculated using the equation reported by Chen and Millero [28]. It is worth reiterating [29] that the sound speeds for water at the nominal temperature of 300 K calculated using the equation reported by Chen and Millero differ from those in the comprehensive article by Wagner and Pruss [30] by less than 0.01% at pressures up to 20 MPa and by less than 0.03% at the higher pressures used in this study. The densities and isothermal compressibilities, $\kappa^{*}_{T,1}$, for water were obtained using the equation of state given by Chen *et al.* [31]. The isentropic compressibilities and the $\gamma_{H2O}$ values given in Table 3 were calculated using Eqs. 5 and 4, respectively. Evidence presented in previous work [12] suggests that the underlying assumption upon which Eq. 13 is based is indeed reasonable, at least for dilute solutions and at moderate pressures.

The measured sound speeds for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K and $p$ = (10.0 to 100.0) MPa are given in supporting information Table 4. Following previous work [11,29], the quantity ($\gamma/u^2 - \gamma_1/u_1^2$) for each solution was analysed by weighted least-squares using a second-order polynomial of the form:

$$\gamma/u^2 - \gamma_1/u_1^2 = c_0 + c_1(p - 0.1) + c_2(p - 0.1)^2 \qquad (14)$$

where $\gamma_1/u_1^2$ is the quantity for the pure solvent and $c_i$, i = 0-2, are the fitted coefficients. The weighting factor for each value of ($\gamma/u^2 - \gamma_1/u_1^2$) was taken as $1/(\delta(\gamma/u^2))^2$, where $\delta(\gamma/u^2)$ is the uncertainty for the quantity $\gamma/u^2$. In estimating the uncertainty for $\gamma$, no account was taken of the contribution from the right hand side of Eq. 13. In other words, the estimated errors are relative to those for water. The polynomial coefficients, $c_i$, i = 0-2, and their standard deviations obtained from the least-squares analyses are given in supporting information Table S1. For several solutions of adenosine, three solutions of cytidine, and one solution of uridine all at $T$ = 313.15 K, the values obtained for $c_2$ were not statistically significant. In these cases, the linear form of Eq. 14 was used in the analyses.

The densities for solutions of the nucleosides at $p$ = (10 to 100) MPa were obtained by integration between the limits of $p$ = 0.1 MPa and a pressure $p$ of the expression that follows from combining Eqns. 6 and 14, *viz.*:

$$(\partial\rho/\partial p)_T - (\partial\rho_1^*/\partial p)_T = c_0 + c_1(p - 0.1) + c_2(p - 0.1)^2 \quad (15)$$

The results obtained are given in supporting information Table S2. Included in Table S2 are the estimated uncertainties for the solution densities, which were obtained by the application of propagation of errors to Eq. 15. At the pressures $p$ = (10 to 60) MPa, the uncertainty for the density at $p$ = 0.1 MPa ($3.0 \times 10^{-3}$ kg·m$^{-3}$) is the predominant contributor to the estimated uncertainty for the calculated solution density. At $p$ = (80 and 100) MPa, small contributions arise for some solutions from the estimated uncertainties for the $c_i$ coefficients of Eq. 15.

**3.4 Apparent and Partial Molar Volumes at High Pressures**

The apparent molar volumes, $V_\phi$, of the nucleosides in aqueous solution at $T$ = (288.15 and 313.15) K and $p$ = (10 to 100) MPa were calculated from the solution densities given in Table S2 using the equation:

$$V_\phi = (M_2/\rho) - (\rho - \rho_1^*)/(m\rho\rho_1^*) \quad (16)$$

Where $M_2$ is the solute molar mass and the other symbols used are as defined *vide supra*. The values used for $\rho_1^*$ at the various pressures are those given in Table 3. The $V_\phi$ results, together with their uncertainties estimated using the procedures described previously [32], are given in supporting information Table S3. At each pressure, the molality dependence of $V_\phi$ was analysed using the linear equation:

$$V_\phi = V_2^{\mathrm{o}} + S_{\mathrm{v}}m \quad (17)$$

where $V_2^{\mathrm{o}}$ is the partial molar volume of the solute at infinite dilution and $S_{\mathrm{v}}$ is the experimental slope. The $V_2^{\mathrm{o}}$ and $S_{\mathrm{v}}$ values, together with their standard errors obtained from weighted least-squares analyses of the $V_\phi$ data, are given in Table 5. The inverse squares of the uncertainties of the apparent molar volumes were used as the weighting factors. The molality range accessible for the sparingly soluble adenosine is too narrow for reliable values of $V_2^{\mathrm{o}}$ and $S_{\mathrm{v}}$ to be obtained using Eq. 17. The $V_2^{\mathrm{o}}$ values given in Table 5 are the means of the $V_\phi$ data and the uncertainties are the standard deviations. For cytidine and uridine at $T$ = 288.15 K and $p$ = 100 MPa, the values of $S_{\mathrm{v}}$ obtained from the least-squares analysis were not statistically significant. The $V_2^{\mathrm{o}}$ values reported in Table 5 are the means of the $V_\phi$ data and the uncertainties given are the standard deviations. For completeness, the $V_2^{\mathrm{o}}$ and $S_{\mathrm{v}}$ results for the nucleosides at $p$ = 0.1 MPa that were obtained in previous work [22] are included in Table 5.

### 3.5 Apparent and Partial Molar Isentropic and Isothermal Compressions at High Pressures

The isentropic compressions, $\kappa_S$, for solutions of the nucleosides at $T$ = (288.15 and 313.15) K and over the range $p$ = (10 to 100) MPa were calculated using Eq. 5 and the speeds of sound and solution densities given in Table 4 and supporting information Table S2, respectively. These $\kappa_S$ values were used to calculate the apparent molar isentropic compressions, $K_{S,\phi}$, which are defined by the relation [16,33]:

$$K_{S,\phi} = (M_2\kappa_S/\rho) - (\kappa_{S,1}^{*}\rho - \kappa_S\,\rho_1^{*})/(m\rho\rho_1^{*}) \qquad (18)$$

The values used for the densities and isentropic compressibilities of water at the various pressures are those given in Table 3. The $K_{S,\phi}$ results obtained are given in supporting information Table S4. Included in Table S4 are the uncertainties for the $K_{S,\phi}$ values which were estimated by the application of propagation of errors to Eqs. 5 and 18, but with the exclusion of contributions from the thermodynamic properties of the solvent. The uncertainty for $u$ was taken as ±0.03 $m \cdot s^{-1}$ and the uncertainties used for the solution densities are those given in Table S2.

For dilute solutions of nonelectrolytes, the molality dependence of $K_{S,\phi}$ can usually be represented by the simple linear equation [34-36]:

$$K_{S,\phi} = K^{\mathrm{o}}_{S,2} + S_{k(S)}m \tag{19}$$

where $K^{\mathrm{o}}_{S,2}$ is the partial molar isentropic compression of the solute at infinite dilution and $S_{k(S)}$ is the experimental slope. Values of $K^{\mathrm{o}}_{S,2}$ and $S_{k(S)}$ and their standard deviations obtained from weighted least-squares analyses of the apparent molar isentropic compressions using Eq. 19 are given in Table 6. The weighting factors used were the inverse squares of the uncertainties of the apparent molar isentropic compressions. The $K^{\mathrm{o}}_{S,2}$ values for adenosine given in Table 6 are actually the means of the $K_{S,\phi}$ data because, as outlined in section 3.4, analyses using Eq. 19 are unreliable when the accessible molality range is too narrow. Since the $S_{k(S)}$ values obtained for cytidine at $T$ = 313.15 K and $p$ = (10 to 100) MPa, and for uridine at $T$ = 313.15 K and $p$ =20 MPa were not statistically significant, the $K^{\mathrm{o}}_{S,2}$ values given in Table 6 are the means of the $K_{S,\phi}$ data and the uncertainties given are the standard deviations. Included in Table 6 are the $K^{\mathrm{o}}_{S,2}$ and $S_{k(S)}$ values for the nucleosides at $T$ = (288.15 and 313.15) K and $p$ = 0.1 MPa that were reported recently [20].

The apparent molar isothermal compressions, $K_{T,\phi}$, for the nucleosides at $T$ = (288.15 and 313.15) K and pressures over the range $p$ = (10 to 100) MPa were calculated using the isothermal equivalent of Eq. 18, *i.e.* with $K_{S,\phi}$, $\kappa_S$, and $\kappa^*_{S,1}$ replaced by $K_{T,\phi}$, $\kappa_T$, and $\kappa^*_{T,1}$, respectively. The $\kappa_T$ values were obtained from the $\kappa_S$ and $\gamma$ data using Eqs. 4 and 13. The $\kappa^*_{T,1}$ values used in the calculations are given in Table 3. The $K_{T,\phi}$ results, along with their uncertainties estimated using propagation-of-errors methods applied to Eqs. 4 and 18, are given in the supporting information Table S5. At each pressure, the molality dependence of $K_{T,\phi}$ was analysed by weighted least-squares using the isothermal equivalent of Eq. 19 with the inverse squares of the uncertainties of the apparent molar isothermal compressions as the weighting factors. The partial molar isothermal compressions at infinite dilution, $K_{T,2}^{\text{o}}$, the $S_{k(T)}$ values, and the standard errors obtained from the least-squares analyses are given in Table 6. The $K_{T,2}^{\text{o}}$ values for adenosine given in Table 5 are actually the means of the $K_{T,\phi}$ data, as described above for $K_{S,2}^{\text{o}}$. For cytidine at $T$ = 313.15 K and $p$ = 60 MPa, and for uridine at $T$ = 313.15 K and $p$ = (10, 20, and 40) MPa, analyses using the isothermal equivalent of Eq. 19 gave values for $S_{k(T)}$ that were not statistically significant. The $K_{T,2}^{\text{o}}$ values and their estimated uncertainties given in Table 6 are, respectively, the means of the $K_{T,\phi}$ data and the standard deviations. Included in Table 6 are the $K_{T,2}^{\text{o}}$ results for the nucleosides at $p$ = 0.1 MPa reported previously [20].

## 4 Discussion

It is convenient to combine the results obtained herein with those for $T$ = 298.15 K obtained previously [10] and hence use 3D diagrams to display the pressure and temperature dependences of the partial molar volumes and the partial molar isothermal compressions at infinite dilution for the three nucleosides. The $V_2^{\text{o}}$ and $K_{T,2}^{\text{o}}$ values for adenosine over the pressure and temperature ranges $p$ = (0.1 to 100) MPa and $T$ = (288.15 to 313.15) K are displayed in Figs. 1a and 1b, respectively. At the temperatures $T$ = (313.15 and 298.15) K, $V_2^{\text{o}}$ decreases with increasing pressure as a consequence of the positive values for $K_{T,2}^{\text{o}}$ at these temperatures, as indicated in Fig. 1b. The positive $K_{T,2}^{\text{o}}$ values for $T$ = 298.15 K are smaller than those for $T$ = 313.15 K, hence the trend in $V_2^{\text{o}}$ with pressure at $T$ = 298.15 K is less marked. At

$T = 288.15$ K, the values of $K^{\mathrm{o}}_{T,2}$ are negative which means that $V^{\mathrm{o}}_2$ now increases with increasing pressure.

The temperature and pressure dependences of $V^{\mathrm{o}}_2$ and $K^{\mathrm{o}}_{T,2}$ for cytidine are shown in Fig. 2. At $T = 313.15$ K, there is a small decrease in the value of $V^{\mathrm{o}}_2$ with increasing pressure ($K^{\mathrm{o}}_{T,2}$ values are small and positive) whereas at $T = 298.15$ K there is a small increase in $V^{\mathrm{o}}_2$ with increasing pressure up to $p = 80$ MPa because the values of $K^{\mathrm{o}}_{T,2}$ are negative. The value of $K^{\mathrm{o}}_{T,2}$ at $T = 298.15$ K actually changes sign at about $p = 90$ MPa [10] so the value of $V^{\mathrm{o}}_2$ is essentially constant at the higher pressures used in this study (see Table 5). At $T = 288.15$ K the increase in $V^{\mathrm{o}}_2$ with increasing pressure is more distinct because of the larger negative values for $K^{\mathrm{o}}_{T,2}$.

Figs. 3a and 3b show the temperature and pressure dependences of $V^{\mathrm{o}}_2$ and $K^{\mathrm{o}}_{T,2}$ for uridine, respectively. The $T$ and $p$ dependences of $V^{\mathrm{o}}_2$ are qualitatively similar to those for cytidine. At the highest temperature, $V^{\mathrm{o}}_2$ decreases as the pressure increases because the values of $K^{\mathrm{o}}_{T,2}$ are positive. The changes in $V^{\mathrm{o}}_2$ at $T = 298.15$ K with increasing pressure are small and since the value of $K^{\mathrm{o}}_{T,2}$ changes sign at about $p = 75$ MPa, a maximum in the value of $V^{\mathrm{o}}_2$ occurs for the pressure $p = 80$ MPa [10]. At the lowest temperature the value of $V^{\mathrm{o}}_2$ now increases with increasing pressure because the values of $K^{\mathrm{o}}_{T,2}$ are negative.

Various semi-empirical models are often used to rationalize the volumetric properties of small organic solutes in aqueous solution [37-39]. In previous work [10,20,27], we used a model [37] that involves an interpretation of hydration effects based on the relationship:

$$V^{\mathrm{o}}_2 = V_{\mathrm{int}} + n_{\mathrm{h}} \cdot (V_{\mathrm{h}} - V^*_1) \tag{20}$$

where $V_{\mathrm{int}}$ is the intrinsic volume of the solute molecule, and $V_{\mathrm{h}}$ and $V^*_1$ are, respectively, the partial molar volumes of water in the hydration shell of the solute and in the bulk solvent. The value of the ‘hydration number’, $n_h$, is determined largely by the number of water molecules in the first hydration shell. Assuming that the value of $n_h$ does not vary significantly with pressure, at least for moderate pressure changes, then differentiating Eq. 20 with respect to pressure at constant temperature gives:

$$K_{T,2}^{o} = -(\partial V_2^{o}/\partial p)_T = -(\partial V_{int}/\partial p)_T + n_h \cdot (K_h - K_1^{*}) \qquad (21)$$

where $K_h$ $\{K_h = -(\partial V_h/\partial p)_T\}$ is the partial molar isothermal compression of water in the hydration shell of the solute and $K_1^{*}$ $\{K_1^{*} = -(\partial V_1^{*}/\partial p)_T\}$ is the partial molar isothermal compression of water in the bulk solvent. For solutes of low molar mass, the pressure dependence of the intrinsic volume can be neglected, at least to a first approximation, because it essentially involves the compression of covalent bonds [37,40]. Hence, Eq. 21 reduces to:

$$K_{T,2}^{o} = n_h \cdot (K_h - K_1^{*}) \qquad (22)$$

It follows from this expression that a negative value of $K_{T,2}^{o}$ for a solute in aqueous solution indicates that the water molecules in the hydration shell are, on average, less compressible that those in the bulk solvent. Conversely, positive values for $K_{T,2}^{o}$ arise if the water molecules in the hydration shell of a solute are more compressible than those in the bulk solvent.

As shown in Fig. 1b and Table 6, the $K_{T,2}^{o}$ values for adenosine at $T$ = 288.15 K are negative and increase from around $-10 \times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$ at the lower pressures to $-0.1 \times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$ at $p$ = 100 MPa. These negative values imply that the water of hydration for adenosine at $T$ = 288.15 K is less compressible than bulk water. From the trend in $K_{T,2}^{o}$ with pressure, it is apparent that at a pressure slightly above $p$ = 100 MPa the value of $K_{T,2}^{o}$ will become zero. At this particular pressure, the water molecules in the hydration shell are essentially the same as those in the bulk solvent, as least with regard to isothermal compression.

At the temperatures $T = (298.15$ and $313.15)$ K the $K^{o}_{T,2}$ values for adenosine are positive, which implies that the water molecules in the hydration shell are now more compressible than those in the bulk solvent. Interestingly, for $T = 313.15$ K the values of $K^{o}_{T,2}$ are more or less independent of pressure. This suggests that the value of $K_h$ changes with pressure at approximately the same rate as for $K^{*}_{1}$ (from the data in Table 3, the values for $K^{*}_{1}$ at $T = 313.15$ K are $(8.03$ and $6.11) \times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$ at $p = (0.10$ and $100)$ MPa, respectively).

Nucleosides are composed of just two major structural units, the base moiety and the ribose group. Results from previous studies of nucleosides and their bases [41,42] suggest that intra-interactions between the base and ribose units of a nucleoside in aqueous solution are minimal. Consequently, if volumetric data were available for a compound that models, for example, the ribose group of a nucleoside it would be possible to rationalize the $K^{o}_{T,2}$ results obtained herein in terms of the group contributions. In earlier work [43], we derived from literature data a $K^{o}_{T,2}$ value for D-ribose at $T = 298.15$ K and $p = 0.1$ MPa ($K^{o}_{T,2} = -(7.4_2 \pm 0.4) \times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$). More recently, $K^{o}_{T,2}$ data for D-ribose have become available over the pressure range used in this work, but only at the temperature $T = 298.15$ K. Although D-ribose is not a perfect model for the ribose unit of a nucleoside, it is reasonable to assume that at least the signs for $K^{o}_{T,2}$, and the trends with pressure, ought to be similar for both D-ribose and the ribose moiety of a nucleoside. The $K^{o}_{T,2}$ values for D-ribose at $p = (20, 60, 100)$ MPa are $(-7.78, -3.91, -0.32) \times 10^{-15}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$, respectively (H. Høiland, unpublished results). Since the values of $K^{o}_{T,2}$ for adenosine at these pressures and $T = 298.15$ K are all positive [10], the contribution to $K^{o}_{T,2}$ from the base moiety of adenosine must be positive. Presumably these positive values arise because the "structure-breaking" nature of the planar purine ring is not sufficiently compensated by hydrogen bonding between solvent water molecules and the polar functional groups on the purine ring.

Fig. 2b shows that at each of the three temperatures, the $K_{T,2}^{\mathrm{o}}$ values for cytidine become more positive as the pressure increases, and at any given pressure $K_{T,2}^{\mathrm{o}}$ becomes more positive as the temperature increases. The close proximity of the polar functional groups on the pyrimidine ring for cytidine allows for co-operative hydrogen bonding with water molecules. This type of interaction is expected to make a significant negative contribution to $K_{\mathrm{h}}$ and hence to $K_{T,2}^{\mathrm{o}}$ [38]. The negative values observed for $K_{T,2}^{\mathrm{o}}$ at low temperatures and pressures are indeed consistent with a contribution from such hydrogen bonding. As the temperature increases, the hydrogen bonding networks within the hydration shell should become more flexible, and as such more compressible, *i.e.* $K_{\mathrm{h}}$ would become more positive. The trends in $K_{T,2}^{\mathrm{o}}$ with temperature displayed in Fig. 2b support this view.

The polar functional groups on the pyrimidine ring of uridine are, like cytidine, oriented such that co-operative hydrogen bonding with solvent water molecules is possible. The trends in $K_{T,2}^{\mathrm{o}}$ with temperature and pressure shown in Fig. 3b are indeed similar to those for cytidine, with one exception. Interestingly, the values of $K_{T,2}^{\mathrm{o}}$ at $T$ = 313.15 K are essentially independent of pressure over the range used in this work. As noted above for adenosine, this implies that at this temperature the value of $K_{\mathrm{h}}$ changes with pressure at approximately the same rate as for $K_1^*$.

In conclusion, this paper is the last of a series [10,11,20,27] in which our focus has been to determine reliable volumetric properties of the four constituent building blocks of RNA, adenosine, cytidine, uridine, and guanosine at high pressures and several temperatures. These volumetric properties are, through the thermodynamic relation $(\partial G/\partial p)_T = V$, essential for mapping the physical stability of these solutes over the ($p$-$T$) landscape.

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**Table 1** Coefficients of Eq. 9 used to calculate solution densities, specific heat capacities, and isentropic compressibilities for aqueous solutions of adenosine, cytidine, and uridine at $p$ = 0.1 MPa.

| $T$ (K) | $\rho$ (kg·m$^{-3}$)[a] | | $c_p$ (J·K$^{-1}$·g$^{-1}$) | | $\kappa_S$ (Pa$^{-1}$) | |
|---|---|---|---|---|---|---|
| | $a_1$ | $a_2$ | $a_1$ | $a_2$ | $10^{11}a_1$ | $10^{11}a_2$ |
| Adenosine | | | | | | |
| 288.15 | $98.6_8$ (0.3)[c] | $-54._8$ ($1_7$) | $-0.616_9$ ($0.001_7$) | [b] | $-9.253_4$ (0.007) | [b] |
| 298.15 | 95.81 (0.06) | | | | | |
| 303.15 | 94.90 (0.04) | | | | | |
| 313.15 | 93.18 (0.05) | | $-0.62_2$ ($0.02_4$) | $2.8_8$ ($1._2$) | $-6.772_7$ (0.005) | [b] |
| Cytidine | | | | | | |
| 288.15 | 91.43 (0.02) | $-15.4_3$ (0.18) | $-0.620_4$ (0.003) | $0.22_1$ ($0.04_0$) | $-9.568_8$ (0.008) | $2.32_5$ ($0.06_7$) |
| 298.15 | 89.50 (0.02) | $-13.4_9$ ($0.1_2$) | | | | |
| 303.15 | 88.72 (0.02) | $-13.0_7$ ($0.1_9$) | | | | |
| 313.15 | 87.48 (0.03) | $-12.6_7$ ($0.2_4$) | $-0.552_2$ (0.003) | $0.23_7$ ($0.03_8$) | $-7.208_7$ (0.005) | $1.47_2$ ($0.05_0$) |
| Uridine | | | | | | |
| 288.15 | 93.44 (0.03) | $-15.4_9$ ($0.2_2$) | $-0.639_9$ (0.004) | $0.29_9$ ($0.05_3$) | $-9.268_7$ (0.005) | $2.86_8$ ($0.05_9$) |
| 298.15 | 91.62 (0.02) | $-15.1_3$ ($0.1_2$) | | | | |
| 303.15 | 90.87 (0.02) | $-14.8_3$ ($0.1_3$) | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 313.15 | 89.35 (0.02) | −13.4$_2$ (0.2$_0$) | −0.557$_5$ (0.002) | 0.18$_1$ (0.02$_5$) | −6.728$_5$ (0.004) | 1.33$_2$ (0.03$_7$) |

[a] Ref. [10]

[b] See text

[c] Standard uncertainties are in parentheses

**Table 2** Calculated values of isentropic compressibility, density, speed of sound, specific heat capacity, α and γ for aqueous solutions of adenosine, cytidine, and uridine at $T$ = (288.15 and 313.15) K and $p$ = 0.1 MPa.

| $m$ (mol·kg$^{-1}$) | $10^{10}\kappa_S$[a] (Pa$^{-1}$) | $\rho$[b] (kg·m$^{-3}$) | $u$[c] (m·s$^{-1}$) | $c_p$[d] (J·K$^{-1}$·g$^{-1}$) | $10^6\alpha$ (K$^{-1}$) | $\gamma$[e] |
|---|---|---|---|---|---|---|
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | 4.63918 | 1001.046 | $1467.41_4$ | 4.17321 | $154.18_7$ ($0.06_9$) | 1.003535(3) |
| 0.01957 | 4.63951 | 1001.011 | $1467.38_7$ | 4.17343 | $154.17_4$ ($0.05_8$) | 1.003534(3) |
| 0.01944 | 4.63963 | 1000.998 | $1467.37_7$ | 4.17351 | $154.16_9$ ($0.05_4$) | 1.003533(3) |
| 0.01929 | 4.63977 | 1000.984 | $1467.36_6$ | 4.17360 | $154.16_3$ ($0.05_0$) | 1.003533(2) |
| 0.01904 | 4.64000 | 1000.960 | $1467.34_7$ | 4.17376 | $154.15_2$ ($0.04_3$) | 1.003532(2) |
| 0.01873 | 4.64029 | 1000.930 | $1467.32_3$ | 4.17395 | $154.13_7$ ($0.03_5$) | 1.003531(2) |
| 0.01846 | 4.64053 | 1000.904 | $1467.30_3$ | 4.17411 | $154.12_4$ ($0.02_8$) | 1.003530(1) |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | 4.29833 | 994.068 | $1529.82_6$ | 4.16709 | $388.00_6$ ($0.06_6$) | 1.026478(9) |
| 0.01973 | 4.29841 | 994.057 | $1529.82_1$ | 4.16714 | $387.98_6$ ($0.06_2$) | 1.026474(9) |
| 0.01951 | 4.29856 | 994.037 | $1529.81_0$ | 4.16725 | $387.94_5$ ($0.05_7$) | 1.026468(8) |
| 0.01936 | 4.29865 | 994.023 | $1529.80_3$ | 4.16733 | $387.91_8$ ($0.05_2$) | 1.026463(7) |
| 0.01919 | 4.29877 | 994.007 | $1529.79_5$ | 4.16742 | $387.88_7$ ($0.04_7$) | 1.026458(7) |
| 0.01896 | 4.29893 | 993.986 | $1529.78_3$ | 4.16753 | $387.84_5$ ($0.04_1$) | 1.026451(6) |
| 0.01870 | 4.29910 | 993.961 | $1529.77_1$ | 4.16767 | $387.79_8$ ($0.03_4$) | 1.026444(5) |
| 0.01848 | 4.29925 | 993.941 | $1529.76_0$ | 4.16778 | $387.75_8$ ($0.02_8$) | 1.026437(4) |
| Cytidine, $T$ = 288.15 K | | | | | | |
| 0.09058 | 4.57284 | 1007.257 | $1473.45_5$ | 4.13111 | $167.08_5$($0.02_1$) | 1.004228(1) |
| 0.08214 | 4.58059 | 1006.507 | $1472.75_7$ | 4.13603 | 165.746(0.008) | 1.004151(1) |
| 0.07292 | 4.58908 | 1005.686 | $1471.99_4$ | 4.14144 | 164.244(0.003) | 1.004067(1) |
| 0.06285 | 4.59839 | 1004.787 | $1471.16_1$ | 4.14738 | $162.55_7$($0.01_3$) | 1.003974(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.05387 | 4.60674 | 1003.982 | $1470.41_6$ | 4.15272 | $161.00_9(0.01_9)$ | 1.003889(1) |
| 0.04435 | 4.61563 | 1003.126 | $1469.62_5$ | 4.15842 | $159.32_3(0.02_2)$ | 1.003799(1) |
| 0.03651 | 4.62299 | 1002.418 | $1468.97_3$ | 4.16315 | $157.90_0(0.02_3)$ | 1.003724(1) |
| 0.02857 | 4.63047 | 1001.701 | $1468.31_3$ | 4.16796 | $156.42_9(0.02_2)$ | 1.003647(1) |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.092038 | 4.24667 | 1000.163 | $1534.40_7$ | 4.12948 | $391.64_1(0.02_4)$ | 1.027385(4) |
| 0.082652 | 4.25319 | 999.363 | $1533.84_3$ | 4.13428 | 390.981(0.009) | 1.027241(2) |
| 0.072497 | 4.26028 | 998.494 | $1533.23_3$ | 4.13951 | 390.270(0.004) | 1.027086(2) |
| 0.063041 | 4.26691 | 997.683 | $1532.66_4$ | 4.14443 | $389.61_1(0.01_3)$ | 1.026943(2) |
| 0.053942 | 4.27331 | 996.901 | $1532.11_6$ | 4.14920 | $388.98_0(0.01_9)$ | 1.026806(3) |
| 0.044977 | 4.27964 | 996.128 | $1531.57_7$ | 4.15394 | $388.36_1(0.02_2)$ | 1.026671(4) |
| 0.035446 | 4.28640 | 995.304 | $1531.00_2$ | 4.15902 | $387.70_6(0.02_3)$ | 1.026529(4) |
| 0.027241 | 4.29224 | 994.593 | $1530.50_7$ | 4.16343 | $387.14_5(0.02_1)$ | 1.026407(3) |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | 4.57194 | 1007.860 | $1473.15_9$ | 4.12726 | $167.3_8(0.6_6)$ | 1.00425(3) |
| 0.08466 | 4.58120 | 1006.900 | $1472.37_0$ | 4.13346 | $165.5_5(0.6_0)$ | 1.00414(3) |
| 0.07501 | 4.58970 | 1006.023 | $1471.64_7$ | 4.13918 | $163.8_9(0.5_4)$ | 1.00405(3) |
| 0.06473 | 4.59882 | 1005.084 | $1470.87_4$ | 4.14533 | $162.1_1(0.4_8)$ | 1.00395(2) |
| 0.05522 | 4.60731 | 1004.213 | $1470.15_5$ | 4.15108 | $160.4_6(0.4_1)$ | 1.00386(2) |
| 0.04138 | 4.61976 | 1002.941 | $1469.10_5$ | 4.15953 | $158.0_6(0.3_2)$ | 1.00374(2) |
| 0.03782 | 4.62297 | 1002.612 | $1468.83_4$ | 4.16173 | $157.4_4(0.2_9)$ | 1.00370(1) |
| 0.02942 | 4.63060 | 1001.837 | $1468.19_3$ | 4.16693 | $155.9_9(0.2_3)$ | 1.00363(1) |
| Uridine, $T$ = 313.15 K | | | | | | |
| 0.09524 | 4.24890 | 1000.607 | $1533.66_4$ | 4.12684 | $393.6_8(0.66)$ | 1.02766(9) |
| 0.08191 | 4.25755 | 999.447 | $1532.99_3$ | 4.13385 | $392.6_9(0.59)$ | 1.02745(8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.07492 | 4.26211 | 998.838 | $1532.64_1$ | 4.13754 | $392.1_5$(0.54) | 1.02734(8) |
| 0.06499 | 4.26860 | 997.969 | $1532.14_1$ | 4.14283 | $391.3_5$(0.48) | 1.02718(7) |
| 0.05449 | 4.27550 | 997.047 | $1531.61_1$ | 4.14846 | $390.4_8$(0.41) | 1.02700(6) |
| 0.04992 | 4.27851 | 996.646 | $1531.38_1$ | 4.15092 | $390.0_8$(0.38) | 1.02692(5) |
| 0.04094 | 4.28445 | 995.854 | $1530.92_8$ | 4.15578 | $389.2_8$(0.32) | 1.02676(4) |
| 0.03745 | 4.28676 | 995.546 | $1530.75_2$ | 4.15767 | $388.9_7$(0.29) | 1.02670(4) |

[a] The uncertainties for $\kappa_S$ are typically 6.3-6.5 × $10^{-15}$ $Pa^{-1}$ for $T$ = 288.15 K and 5.7-5.8 × $10^{-15}$ $Pa^{-1}$ for $T$ = 313.15 K

[b] The uncertainty for $\rho$ is ±3.0 × $10^{-3}$ kg·$m^{-3}$

[c] The uncertainty for $u$ is ±0.01 m·$s^{-1}$

[d] The uncertainties for $c_p$ are typically 2 ×$10^{-4}$ J·$K^{-1}$·$g^{-1}$

[e] The digit in parentheses is the uncertainty in the last digit of $\gamma$

**Table 3** Values of sound speed, density, isentropic and isothermal compressibility, and $\gamma$ for water at $T$ = (288.15 and 313.15) K and at $p$ = (0.1 to 100) MPa

| $p$ (MPa) | $u^a$ (m·s$^{-1}$) | $\rho_1^{*b}$ (kg·m$^{-3}$) | $10^{10}\kappa_{S,1}^{*}$ (Pa$^{-1}$) | $10^{10}\kappa_{T,1}^{*b}$(Pa$^{-1}$) | $\gamma_{H2O}$ |
|---|---|---|---|---|---|
| $T$ = 288.15 K | | | | | |
| 0.1 | 1465.931 | 999.101 | 4.65762 | 4.67330 | 1.00337 |
| 10.0 | 1482.118 | 1003.673 | 4.53568 | 4.55467 | 1.00419 |
| 20.0 | 1498.654 | 1008.196 | 4.41624 | 4.43943 | 1.00525 |
| 40.0 | 1532.174 | 1016.964 | 4.18869 | 4.22186 | 1.00792 |
| 60.0 | 1566.112 | 1025.378 | 3.97622 | 4.02004 | 1.01102 |
| 80.0 | 1600.251 | 1033.459 | 3.77860 | 3.83245 | 1.01425 |
| 100.0 | 1634.372 | 1041.227 | 3.59545 | 3.65781 | 1.01735 |
| $T$ = 313.15 K | | | | | |
| 0.1 | 1528.863 | 992.219 | 4.31178 | 4.42400 | 1.02603 |
| 10.0 | 1546.122 | 996.515 | 4.19787 | 4.31239 | 1.02728 |
| 20.0 | 1563.384 | 1000.768 | 4.08823 | 4.20480 | 1.02851 |
| 40.0 | 1597.435 | 1009.013 | 3.88380 | 4.00391 | 1.03093 |
| 60.0 | 1630.930 | 1016.936 | 3.69688 | 3.82029 | 1.03338 |
| 80.0 | 1663.958 | 1024.561 | 3.52515 | 3.65206 | 1.03600 |
| 100.0 | 1696.607 | 1031.911 | 3.36663 | 3.49768 | 1.03893 |

[a] Calculated using the equation given in reference [28]

[b] Calculated using the equation of state given in reference [31]

**Table 4** Sound speeds for aqueous solutions of adenosine, cytidine, and uridine at $T$ = (288.15 and 313.15) K and at $p$ = (10.0 to 100.0) MPa

| $m$/(mol·kg$^{-1}$) | $u^{a}$ /(m·s$^{-1}$) | | | | | |
|---|---|---|---|---|---|---|
| | $p$/MPa | | | | | |
| | 10.0 | 20.0 | 40.0 | 60.0 | 80.0 | 100.0 |
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | 1483.67 | 1500.23 | 1533.75 | 1567.72 | 1601.84 | 1635.93 |
| 0.01957 | 1483.65 | 1500.20 | 1533.74 | 1567.68 | 1601.82 | 1635.92 |
| 0.01944 | | 1500.20 | 1533.72 | 1567.68 | 1601.82 | 1635.90 |
| 0.01929 | 1483.64 | 1500.20 | 1533.73 | 1567.68 | 1601.81 | 1635.89 |
| 0.01904 | 1483.60 | 1500.12 | 1533.66 | 1567.62 | 1601.77 | 1635.85 |
| 0.01873 | 1483.57 | 1500.13 | 1533.66 | 1567.60 | 1601.72 | 1635.82 |
| 0.01846 | 1483.53 | 1500.09 | 1533.62 | 1567.56 | 1601.70 | 1635.79 |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | | 1564.34 | 1598.43 | 1631.95 | 1664.97 | 1697.62 |
| 0.01973 | 1547.08 | 1564.37 | 1598.44 | 1631.94 | 1664.97 | 1697.62 |
| 0.01951 | 1547.05 | 1564.38 | 1598.47 | 1631.94 | 1664.95 | 1697.61 |
| 0.01936 | 1547.06 | 1564.34 | 1598.42 | 1631.90 | 1664.93 | 1697.60 |
| 0.01919 | | 1564.36 | 1598.42 | 1631.91 | 1664.94 | 1697.60 |
| 0.01896 | | 1564.36 | 1598.44 | 1631.90 | 1664.96 | 1697.59 |
| 0.01870 | 1547.03 | 1564.33 | 1598.45 | 1631.89 | 1664.92 | 1697.54 |
| 0.01848 | | 1564.29 | 1598.39 | 1631.89 | 1664.93 | 1697.56 |
| Cytidine, $T$ = 288.15 K | | | | | | |
| 0.09058 | 1489.83 | 1506.41 | 1539.98 | 1573.89 | 1607.92 | 1641.90 |
| 0.08214 | 1489.11 | 1505.72 | 1539.25 | 1573.17 | 1607.21 | 1641.22 |
| 0.07292 | 1488.37 | 1504.97 | 1538.49 | 1572.41 | 1606.46 | 1640.48 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.06285 | 1487.54 | 1504.10 | 1537.64 | 1571.56 | 1605.64 | 1639.65 |
| 0.05387 | 1486.81 | 1503.34 | 1536.91 | 1570.80 | 1604.89 | 1638.93 |
| 0.04435 | 1485.95 | 1502.51 | 1536.04 | 1569.97 | 1604.05 | 1638.11 |
| 0.03651 | 1485.28 | 1501.85 | 1535.38 | 1569.31 | 1603.41 | 1637.47 |
| 0.02857 | 1484.61 | 1501.16 | 1534.69 | 1568.64 | 1602.72 | 1636.80 |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.09204 | 1551.70 | 1569.02 | 1603.12 | 1636.64 | 1669.60 | 1702.22 |
| 0.08265 | 1551.22 | 1568.49 | 1602.56 | 1636.10 | 1669.04 | 1701.64 |
| 0.07250 | 1550.57 | 1567.89 | 1601.92 | 1635.43 | 1668.44 | 1701.04 |
| 0.06304 | 1550.00 | 1567.30 | 1601.31 | 1634.90 | 1667.88 | 1700.47 |
| 0.05394 | 1549.38 | 1566.67 | 1600.79 | 1634.25 | 1667.23 | 1699.86 |
| 0.04498 | 1548.86 | 1566.15 | 1600.22 | 1633.72 | 1666.72 | 1699.34 |
| 0.03545 | 1548.28 | 1565.56 | 1599.62 | 1633.12 | 1666.13 | 1698.76 |
| 0.02724 | 1547.79 | 1565.06 | 1599.11 | 1632.63 | 1665.64 | 1698.29 |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | 1489.46 | 1506.10 | 1539.70 | 1573.60 | 1607.68 | 1641.67 |
| 0.08466 | 1488.67 | 1505.27 | 1538.88 | 1572.79 | 1606.90 | 1640.89 |
| 0.07501 | 1487.95 | 1504.53 | 1538.15 | 1572.04 | 1606.13 | 1640.14 |
| 0.06473 | 1487.19 | 1503.76 | 1537.34 | 1571.25 | 1605.36 | 1639.40 |
| 0.05522 | 1486.45 | 1503.02 | 1536.60 | 1570.54 | 1604.61 | 1638.66 |
| 0.04138 | 1485.36 | 1501.93 | 1535.49 | 1569.42 | 1603.53 | 1637.60 |
| 0.03782 | 1485.06 | 1501.68 | 1535.21 | 1569.15 | 1603.24 | 1637.32 |
| 0.02942 | 1484.44 | 1501.00 | 1534.55 | 1568.46 | 1602.59 | 1636.66 |
| Uridine, $T$ = 313.15 K | | | | | | |
| 0.09524 | 1551.04 | 1568.39 | 1602.46 | 1635.99 | 1669.05 | 1701.61 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.08191 | 1550.36 | 1567.71 | 1601.76 | 1635.30 | 1668.34 | 1700.93 |
| 0.07492 | 1549.99 | 1567.30 | 1601.41 | 1634.94 | 1667.95 | 1700.55 |
| 0.06499 | | 1566.82 | 1600.91 | 1634.42 | 1667.45 | 1700.09 |
| 0.05449 | 1549.03 | 1566.34 | 1600.43 | 1633.92 | 1666.98 | 1699.60 |
| 0.04992 | 1548.69 | 1565.96 | 1600.03 | 1633.62 | 1666.62 | 1699.26 |
| 0.04094 | 1548.29 | 1565.56 | 1599.66 | 1633.20 | 1666.21 | 1698.86 |
| 0.03745 | | 1565.33 | 1599.43 | 1632.97 | 1665.98 | 1698.61 |

[a] The estimated uncertainty of $u$ is ±0.03 $m \cdot s^{-1}$

**Table 5** Partial molar volumes at infinite dilution and the $S_v$ values for adenosine, cytidine, and uridine at $T$ = (288.15 and 313.15) K and at $p$ = (0.1 to 100) MPa

| $p$ (MPa) | $V_2^{o}$ ($cm^3 \cdot mol^{-1}$) | $S_v$ ($cm^3 \cdot kg \cdot mol^{-1}$) | $V_2^{o}$/($cm^3 \cdot mol^{-1}$) | $S_v$ ($cm^3 \cdot kg \cdot mol^{-1}$) |
|---|---|---|---|---|
| Adenosine | $T$ = 288.15 K | | $T$ = 313.15 K | |
| 0.1 | $169.2_6$ ($0.1_3$)[a,b] | | $174.4_2$ ($0.1_7$)[b] | |
| 10 | 169.46 (0.03) | [c] | 174.19 (0.02) | [c] |
| 20 | 169.54 (0.03) | [c] | 174.07 (0.02) | [c] |
| 40 | 169.71 (0.04) | [c] | 173.70 (0.02) | [c] |
| 60 | 169.84 (0.05) | [c] | 173.38 (0.03) | [c] |
| 80 | 169.92 (0.06) | [c] | 173.04 (0.03) | [c] |
| 100 | 169.94 (0.07) | [c] | 172.72 (0.04) | [c] |
| Cytidine | | | | |
| 0.1 | 151.82 (0.03)[b] | 2.1 (0.2)[b] | 156.25 (0.03)[b] | –0.5 (0.2)[b] |
| 10 | 152.031 (0.009) | $1.8_4$ ($0.1_3$) | 156.241 (0.008) | $-0.5_8$ ($0.1_1$) |
| 20 | 152.216 (0.009) | $1.7_5$ ($0.1_3$) | 156.253 (0.008) | $-0.8_5$ ($0.1_0$) |
| 40 | 152.58 (0.01) | $1.2_9$ ($0.1_4$) | 156.18 (0.01) | $-0.7_7$ ($0.1_5$) |
| 60 | 152.88 (0.01) | $0.8_4$ ($0.1_7$) | 156.11 (0.01) | $-0.8_9$ ($0.1_7$) |
| 80 | 153.12 (0.01) | $0.4_2$ ($0.1_9$) | 156.01 (0.02) | $-0.9_9$ ($0.2_0$) |
| 100 | 153.29 (0.02) | [c] | 155.90 (0.02) | $-1.2_0$ ($0.2_4$) |
| Uridine | | | | |
| 0.1 | 150.58 (0.09)[b] | | 155.30 (0.02)b | 0.4 (0.2)[b] |
| 10 | 150.983 (0.008) | $1.5_5$ ($0.1_1$) | 155.29 (0.01) | $-0.2_1$ ($0.1_3$) |
| 20 | 151.142 (0.009) | $1.4_3$ ($0.1_2$) | 155.24 (0.01) | $-0.3_5$ ($0.1_5$) |
| 40 | 151.452 (0.009) | $0.9_7$ ($0.1_2$) | 155.07 (0.02) | $-0.2_4$ ($0.2_2$) |
| 60 | 151.71 (0.01) | $0.5_4$ ($0.1_3$) | 154.92 (0.02) | $-0.3_6$ ($0.3_0$) |
| 80 | 151.91 (0.01) | $0.1_7$ ($0.1_5$) | 154.76 (0.03) | $-0.5_2$ ($0.3_9$) |

| | | | | |
|---|---|---|---|---|
| 100 | 152.03 (0.01) | [c] | 154.59 (0.04) | $-0.8_3$ ($0.5_2$) |

[a] Standard uncertainties are in parentheses

[b] Ref. [22]

[c] See text

**Table 6** Partial molar isentropic and isothermal compressions at infinite dilution and the $S_{k(S)}$ and $Sk_{(T)}$ values for adenosine, cytidine, and uridine $T$ = (288.15 and 313.15) K and at $p$ = (0.1 to 100) MPa

| $p$ (MPa) | $10^{15}\, K^{o}_{S,2}$ (m$^3$·mol$^{-1}$·Pa$^{-1}$) | $10^{15}\, S_{k(S)}$ (m$^3$·kg·mol$^{-2}$·Pa$^{-1}$) | $10^{15}\, K^{o}_{T,2}$ (m$^3$·mol$^{-1}$·Pa$^{-1}$) | $10^{15}\, S_{k(T)}$ (m$^3$·kg·mol$^{-2}$·Pa$^{-1}$) |
|---|---|---|---|---|
| Adenosine, $T$ = 288.15 K | | | | |
| 0.1 | $-14.0_5$ $(0.2_6)$[a,b] | [c] | $-9.8_5$ $(0.2_6)$[a] | [d] |
| 10.0 | $-14.4_2$ $(0.4_1)$ | [c] | $-10.6_2$ $(0.4_6)$ | [c] |
| 20.0 | $-13.2_9$ $(0.5_9)$ | [c] | $-9.6_0$ $(0.6_2)$ | [c] |
| 40.0 | $-10.4_7$ $(0.5_3)$ | [c] | $-7.0_0$ $(0.5_6)$ | [c] |
| 60.0 | $-8.0_9$ $(0.4_8)$ | [c] | $-4.8_5$ $(0.5_3)$ | [c] |
| 80.0 | $-5.7_1$ $(0.3_9)$ | [c] | $-2.6_6$ $(0.4_3)$ | [c] |
| 100.0 | $-3.0_2$ $(0.2_8)$ | [c] | $-0.1_{03}$ $(0.3_3)$ | [c] |
| Adenosine, $T$ = 313.15 K | | | | |
| 0.1 | $6.7_8$ $(0.1_7)$[a] | [c] | $17.0_6$ $(0.2_1)$[a] | [d] |
| 10.0 | $7.4_4$ $(0.2_0)$ | [c] | $17.1_4$ $(0.2_4)$ | [c] |
| 20.0 | $7.0_4$ $(0.5_8)$ | [c] | $16.4_3$ $(0.6_1)$ | [c] |
| 40.0 | $7.1_0$ $(0.6_6)$ | [c] | $15.9_8$ $(0.7_2)$ | [c] |
| 60.0 | $8.2_2$ $(0.2_4)$ | [c] | $16.6_7$ $(0.2_8)$ | [c] |
| 80.0 | $8.8_4$ $(0.3_3)$ | [c] | $16.9_0$ $(0.3_9)$ | [c] |
| 100.0 | $9.4_1$ $(0.2_3)$ | [c] | $17.1_1$ $(0.2_4)$ | [c] |
| Cytidine, $T$ = 288.15 K | | | | |
| 0.1 | $-25.09$ $(0.08)$[a] | $10.3_2$ $(0.7_3)$[a] | $-20.56_9$ $(0.09_2)$[a] | [d] |
| 10.0 | $-25.9_0$ $(0.2_8)$ | $29._0$ $(3._8)$ | $-21.5_4$ $(0.2_8)$ | $26._8$ $(3._8)$ |
| 20.0 | $-23.9_3$ $(0.1_4)$ | $25._0$ $(1._9)$ | $-19.7_1$ $(0.1_4)$ | $22._8$ $(1._9)$ |

| | | | | |
|---|---|---|---|---|
| 40.0 | $-20.2_0$ $(0.2_1)$ | $22._3$ $(2._8)$ | $-16.2_7$ $(0.2_1)$ | $20._3$ $(2._9)$ |
| 60.0 | $-16.7_0$ $(0.1_1)$ | $20._5$ $(1._5)$ | $-13.0_3$ $(0.1_2)$ | $18._7$ $(1._6)$ |
| 80.0 | $-13.2_4$ $(0.1_2)$ | $18._1$ $(1._7)$ | $-9.8_0$ $(0.1_3)$ | $16._5$ $(1._7)$ |
| 100.0 | −10.08 (0.07) | $15._6$ $(1._0)$ | $-6.82_4$ $(0.07_4)$ | $14._1$ $(1._0)$ |
| Cytidine, $T$ = 313.15 K | | | | |
| 0.1 | −5.34 (0.05)[a] | $4.0_1$ $(0.4_9)$[a] | $0.9_7$ $(0.1_2)$[a] | [d] |
| 10.0 | $-4.4_2$ $(0.2_6)$ | [c] | $1.1_5$ $(0.4_4)$ | $6._3$ $(5._8)$ |
| 20.0 | $-3.6_5$ $(0.2_2)$ | [c] | $1.7_5$ $(0.3_7)$ | $6._3$ $(4._9)$ |
| 40.0 | $-1.9_6$ $(0.1_2)$ | [c] | $3.2_2$ $(0.1_7)$ | $5._2$ $(2._3)$ |
| 60.0 | $-0.6_{28}$ $(0.1_9)$ | [c] | $4.6_0$ $(0.2_1)$ | [c] |
| 80.0 | $0.9_{33}$ $(0.1_9)$ | [c] | $5.6_5$ $(0.2_8)$ | $4._9$ $(3._7)$ |
| 100.0 | $2.2_1$ $(0.1_7)$ | [c] | $6.7_8$ $(0.1_8)$ | $4._2$ $(2._4)$ |
| Uridine, $T$ = 288.15 K | | | | |
| 0.1 | −22.55 (0.05)[a] | $16.1_4$ $(0.6_0)$[a] | $-18.3_8$ $(0.5_0)$[a] | [d] |
| 10.0 | $-21.8_3$ $(0.2_4)$ | $20._2$ $(3._1)$ | $-17.9_9$ $(0.2_4)$ | $22._3$ $(3._2)$ |
| 20.0 | $-20.5_4$ $(0.1_6)$ | $20._9$ $(2._1)$ | $-16.9_0$ $(0.1_6)$ | $24._0$ $(2._1)$ |
| 40.0 | −17.41 (0.09) | $17._4$ $(1._1)$ | $-13.97_8$ $(0.08_4)$ | $19._8$ $(1._1)$ |
| 60.0 | $-14.3_0$ $(0.1_4)$ | $17._8$ $(1._8)$ | $-11.1_0$ $(0.1_5)$ | $20._0$ $(2._0)$ |
| 80.0 | $-11.0_6$ $(0.1_3)$ | $12._3$ $(1._7)$ | $-8.0_6$ $(0.1_2)$ | $14._5$ $(1._6)$ |
| 100.0 | $-8.3_5$ $(0.1_2)$ | $12._3$ $(1._5)$ | $-5.5_0$ $(0.1_1)$ | $14._4$ $(1._5)$ |
| Uridine, $T$ = 313.15 K | | | | |
| 0.1 | −0.89 (0.03)[a] | $3.5_8$ $(0.3_5)$[a] | $7.0_1$ $(1._4)$[a] | [d] |
| 10.0 | $-1.6_0$ $(0.5_6)$ | $13._4$ $(7._1)$ | $6.6_9$ $(0.4_1)$ | [c] |
| 20.0 | $-0.2_1$ $(0.4_2)$ | [c] | $7.0_1$ $(0.4_3)$ | [c] |

| | | | | |
|---|---|---|---|---|
| 40.0 | $0.2_0$ ($0.5_1$) | $11._2$ ($6._7$) | $7.7_5$ ($0.4_2$) | [c] |
| 60.0 | $0.7_8$ ($0.2_3$) | $16._3$ ($3._1$) | $7.5_2$ ($0.2_5$) | $12._2$ ($3._7$) |
| 80.0 | $2.2_1$ ($0.3_6$) | $10._5$ ($4._8$) | $8.6_8$ ($0.3_7$) | $6._1$ ($5._4$) |
| 100.0 | $3.0_2$ ($0.3_2$) | $14._3$ ($4._2$) | $9.2_2$ ($0.3_4$) | $9._9$ ($5._0$) |

[a] Reference [20]

[b] Standard uncertainties are in parentheses

[c] See text

[d] The $S_{k(T)}$ value is not available because $K^{\mathrm{o}}_{T,2}$ was evaluated directly from $K^{\mathrm{o}}_{S,2}$. See reference [20]

**Table S1** Coefficients of Eq. 14 for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K

| $m$ (mol·kg$^{-1}$) | $10^9 c_0$ (m$^{-2}$· s$^2$· MPa$^{-1}$) | $10^{12} c_1$ (m$^{-2}$·s$^2$·MPa$^{-2}$) | $10^{14} c_2$ (m$^{-2}$·s$^2$· MPa$^{-3}$) |
|---|---|---|---|
| Adenosine, $T$ = 288.15 K | | | |
| 0.01993 | $-0.878_8$ ($0.008_2$)[b] | $1.0_2$ ($0.4_0$) | $1.1_4$ ($0.3_7$) |
| 0.01957 | $-0.86_7$ ($0.01_1$) | $1.1_3$ ($0.5_1$) | $1.0_0$ ($0.4_8$) |
| 0.01944 | $-0.85_1$ ($0.01_0$) | $0.7_3$ ($0.4_5$) | $1.3_1$ ($0.4_1$) |
| 0.01929 | $-0.85_4$ ($0.01_1$) | $0.6_0$ ($0.5_2$) | $1.5_3$ ($0.4_9$) |
| 0.01904 | $-0.835_1$ ($0.009_5$) | $1.3_8$ ($0.4_6$) | $0.6_9$ ($0.4_3$) |
| 0.01873 | $-0.824_0$ ($0.008_7$) | $1.1_4$ ($0.4_2$) | $0.9_9$ ($0.4_0$) |
| 0.01846 | $-0.806_5$ ($0.006_2$) | $1.4_1$ ($0.3_0$) | $0.6_8$ ($0.2_8$) |
| Adenosine, $T$ = 313.15 K | | | |
| 0.01984 | $-0.357_0$ ($0.005_0$) | $0.82_2$ ($0.07_7$) | [a] |
| 0.01973 | $-0.354_8$ ($0.003_7$) | $0.4_7$ ( $0.1_8$) | $0.3_4$ ($0.1_7$) |
| 0.01951 | $-0.36_3$ ($0.01_0$) | $0.8_6$ ($0.1_6$) | [a] |
| 0.01936 | $-0.352_1$ ($0.003_6$) | $0.84_2$ ($0.05_8$) | [a] |
| 0.01919 | $-0.358_2$ ($0.004_7$) | $0.86_0$ ($0.07_1$) | [a] |
| 0.01896 | $-0.361_2$ ($0.008_8$) | $0.8_5$ ($0.1_3$) | [a] |
| 0.01870 | $-0.35_4$ ($0.01_1$) | $0.9_1$ ($0.1_8$) | [a] |
| 0.01848 | $-0.335_2$ ($0.005_0$) | $0.2_9$ ($0.2_2$) | $0.4_2$ ($0.1_2$) |
| Cytidine, $T$ = 288.15 K | | | |
| 0.09058 | $-4.40_0$ ($0.02_3$) | $9.3_9$ ($1._1$) | $3.0_4$ ($1._0$) |
| 0.08214 | $-3.99_6$ ($0.02_4$) | $8.6_8$ ($1._2$) | $2.6_1$ ($1._1$) |

| | | | |
|---|---|---|---|
| 0.07292 | $-3.56_2$ $(0.02_7)$ | 7.40 $(1._3)$ | $2.6_5$ $(1._2)$ |
| 0.06285 | $-3.07_8$ $(0.02_6)$ | $6.0_9$ $(1._2)$ | $2.5_8$ $(1._2)$ |
| 0.05387 | $-2.65_1$ $(0.02_8)$ | $5.0_8$ $(1._4)$ | $2.3_4$ $(1._3)$ |
| 0.04435 | $-2.17_7$ $(0.01_9)$ | $4.2_7$ $(0.8_9)$ | $1.8_1$ $(0.8_4)$ |
| 0.03651 | $-1.79_6$ $(0.01_7)$ | $3.1_9$ $(0.8_2)$ | $1.7_8$ $(0.7_8)$ |
| 0.02857 | $-1.41_0$ $(0.01_6)$ | $2.3_3$ $(0.7_5)$ | $1.5_7$ $(0.7_1)$ |
| Cytidine, $T$ = 313.15 K | | | |
| 0.09204 | $-2.589_3$ $(0.007_4)$ | $6.2_6$ $(0.3_6)$ | $0.6_3$ $(0.3_4)$ |
| 0.08265 | $-2.34_8$ $(0.01_4)$ | $5.4_1$ $(0.6_5)$ | $1.0_0$ $(0.6_2)$ |
| 0.07250 | $-2.071_9$ $(0.008_8)$ | $5.5_8$ $(0.1_4)$ | [a] |
| 0.06304 | $-1.80_7$ $(0.01_3)$ | $4.7_8$ $(0.2_1)$ | [a] |
| 0.05394 | $-1.526_2$ $(0.009_8)$ | $3.7_1$ $(0.4_8)$ | $0.4_9$ $(0.4_5)$ |
| 0.04498 | $-1.280_4$ $(0.001_7)$ | $3.07_4$ $(0.08_3)$ | $0.38_0$ $(0.07_8)$ |
| 0.03545 | $-1.012_2$ $(0.002_4)$ | $2.5_6$ $(0.1_1)$ | $0.1_7$ $(0.1_1)$ |
| 0.02724 | $-0.783_4$ $(0.003_1)$ | $2.01_3$ $(0.04_9)$ | [a] |
| Uridine, $T$ = 288.15 K | | | |
| 0.09524 | $-4.18_6$ $(0.01_6)$ | $8.4_1$ $(0.7_9)$ | $3.0_1$ $(0.7_5)$ |
| 0.08466 | $-3.73_4$ $(0.01_2)$ | $7.3_9$ $(0.5_8)$ | $2.6_6$ $(0.5_5)$ |
| 0.07501 | $-3.32_3$ $(0.01_4)$ | $6.4_7$ $(0.6_6)$ | $2.6_2$ $(0.6_3)$ |
| 0.06473 | $-2.88_7$ $(0.01_5)$ | $5.8_4$ $(0.7_2)$ | $1.9_5$ $(0.6_8)$ |
| 0.05522 | $-2.46_9$ $(0.01_2)$ | $4.4_6$ $(0.5_9)$ | $2.2_6$ $(0.5_6)$ |
| 0.04138 | $-1.856_5$ $(0.008_3)$ | $3.5_7$ $(0.4_0)$ | $1.4_0$ $(0.3_8)$ |
| 0.03782 | $-1.69_7$ $(0.01_1)$ | $2.9_4$ $(0.5_5)$ | $1.6_6$ $(0.5_2)$ |
| 0.02942 | $-1.329_5$ $(0.009_0)$ | $2.5_2$ $(0.4_3)$ | $1.0_8$ $(0.4_1)$ |

Uridine, $T = 313.15$ K

| | | | |
|---|---|---|---|
| 0.09524 | $-2.06_7$ (0.01$_4$) | 3.4$_9$ (0.7$_1$) | 1.6$_3$ (0.6$_8$) |
| 0.08191 | $-1.77_6$ (0.01$_5$) | 2.9$_0$ (0.7$_4$) | 1.5$_0$ (0.7$_0$) |
| 0.07492 | $-1.614_1$ (0.007$_0$) | 2.4$_8$ (0.3$_5$) | 1.5$_4$ (0.3$_3$) |
| 0.06499 | $-1.40_0$ (0.01$_5$) | 1.9$_5$ (0.6$_8$) | 1.3$_1$ (0.6$_3$) |
| 0.05449 | $-1.21_6$ (0.01$_9$) | 2.6$_9$ (0.3$_1$) | [a] |
| 0.04992 | $-1.06_2$ (0.01$_0$) | 1.8$_9$ (0.5$_0$) | 0.5$_6$ (0.4$_8$) |
| 0.04094 | $-0.88_5$ (0.01$_1$) | 0.7$_6$ (0.5$_4$) | 1.1$_1$ (0.5$_1$) |
| 0.03745 | $-0.792_1$ (0.006$_1$) | 0.7$_5$ (0.2$_7$) | 1.0$_0$ (0.2$_5$) |

[a] See text

[b] Standard uncertainties are in parentheses

**Table S2** Calculated densities for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K and at $p$ = (10.0 to 100.0) MPa

| $m$ (mol·kg$^{-1}$) | $\rho^a$ (kg·m$^{-3}$) | | | | | |
|---|---|---|---|---|---|---|
| | $p$ (MPa) | | | | | |
| | 10.0 | 20.0 | 40.0 | 60.0 | 80.0 | 100.0 |
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | 1005.609 | 1010.124 | 1018.875 | 1027.273(3) | 1035.339(3) | 1043.093(4) |
| 0.01957 | 1005.574 | 1010.089 | 1018.841 | 1027.239(3) | 1035.305(4) | 1043.060(4) |
| 0.01944 | 1005.562 | 1010.077 | 1018.828 | 1027.226(3) | 1035.292(4) | 1043.047(4) |
| 0.01929 | 1005.548 | 1010.063 | 1018.814 | 1027.212(3) | 1035.278(4) | 1043.033(4) |
| 0.01904 | 1005.524 | 1010.039 | 1018.791 | 1027.190(3) | 1035.257(4) | 1043.012(4) |
| 0.01873 | 1005.494 | 1010.009 | 1018.761 | 1027.160(3) | 1035.227(3) | 1042.983(4) |
| 0.01846 | 1005.468 | 1009.984 | 1018.736 | 1027.136(3) | 1035.203(3) | 1042.959(4) |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | 998.361 | 1002.610 | 1010.849 | 1018.765(3) | 1026.384(3) | 1033.728(3) |
| 0.01973 | 998.350 | 1002.599 | 1010.838 | 1018.754(3) | 1026.373(3) | 1033.717(3) |
| 0.01951 | 998.330 | 1002.579 | 1010.817 | 1018.734(3) | 1026.353(3) | 1033.697(3) |
| 0.01936 | 998.316 | 1002.565 | 1010.804 | 1018.721(3) | 1026.340(3) | 1033.684(3) |
| 0.01919 | 998.300 | 1002.549 | 1010.788 | 1018.704(3) | 1026.323(3) | 1033.667(3) |
| 0.01896 | 998.279 | 1002.528 | 1010.766 | 1018.683(3) | 1026.302(3) | 1033.646(3) |
| 0.01870 | 998.254 | 1002.503 | 1010.742 | 1018.659(3) | 1026.278(3) | 1033.622(3) |
| 0.01848 | 998.234 | 1002.483 | 1010.722 | 1018.639(3) | 1026.258(3) | 1033.602(3) |
| Cytidine, $T$ = 288.15 K | | | | | | |
| 0.09058 | 1011.785 | 1016.266 | 1024.952 | 1033.289(4) | 1041.298(5) | 1049.000(8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.08214 | 1011.040 | 1015.525 | 1024.218 | 1032.562(4) | 1040.578(5) | 1048.286(8) |
| 0.07292 | 1010.223 | 1014.712 | 1023.414 | 1031.765(4) | 1039.787(6) | 1047.502(9) |
| 0.06285 | 1009.329 | 1013.822 | 1022.533 | 1030.892(4) | 1038.923(6) | 1046.645(8) |
| 0.05387 | 1008.528 | 1013.026 | 1021.744 | 1030.111(4) | 1038.148(6) | 1045.876(9) |
| 0.04435 | 1007.677 | 1012.179 | 1020.906 | 1029.282(4) | 1037.327(5) | 1045.062(6) |
| 0.03651 | 1006.972 | 1011.478 | 1020.212 | 1028.594(4) | 1036.646(4) | 1044.387(6) |
| 0.02857 | 1006.259 | 1010.769 | 1019.510 | 1027.899(3) | 1035.956(4) | 1043.703(6) |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.09204 | 1004.434 | 1008.661 | 1016.859 | 1024.737(3) | 1032.319(3) | 1039.629(4) |
| 0.08265 | 1003.636 | 1007.866 | 1016.068 | 1023.950(3) | 1031.536(4) | 1038.850(5) |
| 0.07250 | 1002.770 | 1007.002 | 1015.210 | 1023.097(3) | 1030.688(3) | 1038.007(3) |
| 0.06304 | 1001.962 | 1006.196 | 1014.409 | 1022.300(3) | 1029.896(3) | 1037.218(3) |
| 0.05394 | 1001.182 | 1005.420 | 1013.637 | 1021.534(3) | 1029.134(4) | 1036.460(4) |
| 0.04498 | 1000.412 | 1004.652 | 1012.874 | 1020.774(3) | 1028.378(3) | 1035.708(3) |
| 0.03545 | 999.590 | 1003.833 | 1012.060 | 1019.965(3) | 1027.574(3) | 1034.908(3) |
| 0.02724 | 998.882 | 1003.126 | 1011.358 | 1019.267(3) | 1026.879(3) | 1034.216(3) |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | 1012.391 | 1016.874 | 1025.564 | 1033.904(4) | 1041.915(4) | 1049.620(6) |
| 0.08466 | 1011.435 | 1015.923 | 1024.621 | 1032.969(3) | 1040.988(4) | 1048.699(5) |
| 0.07501 | 1010.562 | 1015.054 | 1023.759 | 1032.114(3) | 1040.141(4) | 1047.858(5) |
| 0.06473 | 1009.628 | 1014.123 | 1022.837 | 1031.200(3) | 1039.233(4) | 1046.957(5) |
| 0.05522 | 1008.761 | 1013.260 | 1021.982 | 1030.352(3) | 1038.392(4) | 1046.122(5) |
| 0.04138 | 1007.495 | 1012.000 | 1020.733 | 1029.114(3) | 1037.164(3) | 1044.904(4) |
| 0.03782 | 1007.167 | 1011.674 | 1020.410 | 1028.794(3) | 1036.847(4) | 1044.589(5) |
| 0.02942 | 1006.396 | 1010.906 | 1019.649 | 1028.040(3) | 1036.099(4) | 1043.847(4) |

Uridine, $T$ = 313.15 K

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.09524 | 1004.883 | 1009.115 | 1017.322 | 1025.208(3) | 1032.798(4) | 1040.115(5) |
| 0.08191 | 1003.726 | 1007.961 | 1016.173 | 1024.064(3) | 1031.659(4) | 1038.981(6) |
| 0.07492 | 1003.118 | 1007.355 | 1015.570 | 1023.464(3) | 1031.062(3) | 1038.386(4) |
| 0.06499 | | 1006.490 | 1014.709 | 1022.607(3) | 1030.208(4) | 1037.535(5) |
| 0.05449 | 1001.331 | 1005.572 | 1013.795 | 1021.696(3) | 1029.300(4) | 1036.631(4) |
| 0.04992 | 1000.932 | 1005.174 | 1013.399 | 1021.303(3) | 1028.910(4) | 1036.243(4) |
| 0.04094 | 1000.142 | 1004.385 | 1012.614 | 1020.520(3) | 1028.130(4) | 1035.465(5) |
| 0.03745 | | 1004.079 | 1012.309 | 1020.218(3) | 1027.829(3) | 1035.166(3) |

[a] The estimated uncertainty of $\rho$ for $p$ = 10.0 to 40.0 MPa is $3 \times 10^{-3}$ kg·m$^{-3}$. For $p$ = 60.0 to 100.0 MPa, each number in parentheses is the uncertainty in the last digit, or last two digits, of $\rho$

**Table S3** Apparent molar volumes for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K and at $p$ = (10.0 to 120.0) MPa

| $m$/ (mol·kg$^{-1}$) | $V_\phi$$^{a}$/ (cm$^3$·mol$^{-1}$) | | | | | |
|---|---|---|---|---|---|---|
| | $p$ /MPa | | | | | |
| | 10.0 | 20.0 | 40.0 | 60.0 | 80.0 | 100.0 |
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | 169.47(15) | 169.55(15) | 169.73(15) | 169.86(15) | 169.95(16) | 169.97(18) |
| 0.01957 | 169.48(15) | 169.56(15) | 169.74(15) | 169.87(16) | 169.96(17) | 169.99(21) |
| 0.01944 | 169.49(15) | 169.56(15) | 169.74(15) | 169.88(16) | 169.97(17) | 169.99(20) |
| 0.01929 | 169.47(16) | 169.55(15) | 169.74(15) | 169.89(16) | 169.98(18) | 170.01(21) |
| 0.01904 | 169.43(16) | 169.51(16) | 169.67(16) | 169.79(16) | 169.87(17) | 169.88(20) |
| 0.01873 | 169.42(16) | 169.50(16) | 169.67(16) | 169.79(16) | 169.87(17) | 169.88(20) |
| 0.01846 | 169.43(16) | 169.50(16) | 169.66(16) | 169.78(16) | 169.84(16) | 169.85(18) |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | 174.16(15) | 174.03(15) | 173.66(15) | 173.32(15) | 172.98(15) | 172.66(15) |
| 0.01973 | 174.20(15) | 174.07(15) | 173.70(15) | 173.38(15) | 173.04(15) | 172.72(16) |
| 0.01951 | 174.18(16) | 174.05(15) | 173.69(15) | 173.36(15) | 173.03(15) | 172.71(16) |
| 0.01936 | 174.20(16) | 174.07(16) | 173.70(15) | 173.37(15) | 173.03(15) | 172.70(15) |
| 0.01919 | 174.20(16) | 174.08(16) | 173.71(15) | 173.38(15) | 173.05(15) | 172.73(15) |
| 0.01896 | 174.19(16) | 174.07(16) | 173.71(16) | 173.39(15) | 173.07(16) | 172.76(16) |
| 0.01870 | 174.22(16) | 174.10(16) | 173.74(16) | 173.41(15) | 173.08(16) | 172.76(17) |
| 0.01848 | 174.19(16) | 174.07(16) | 173.71(16) | 173.39(15) | 173.06(16) | 172.75(17) |
| Cytidine, $T$ = 288.15 K | | | | | | |
| 0.09058 | 152.20(3) | 152.38(3) | 152.70(4) | 152.96(4) | 153.16 (6) | 153.30(8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.08214 | 152.18(4) | 152.35(4) | 152.68(4) | 152.94(5) | 153.14(6) | 153.28(9) |
| 0.07292 | 152.16(4) | 152.34(4) | 152.67(4) | 152.94(6) | 153.15(8) | 153.2(11) |
| 0.06285 | 152.14(5) | 152.32(5) | 152.66(5) | 152.93(6) | 153.14(9) | 153.29(12) |
| 0.05387 | 152.13(6) | 152.31(6) | 152.65(6) | 152.93(8) | 153.15(11) | 153.30(15) |
| 0.04435 | 152.11(7) | 152.29(7) | 152.63(7) | 152.90(8) | 153.12(10) | 153.27(13) |
| 0.03651 | 152.11(8) | 152.29(8) | 152.64(8) | 152.92(9) | 153.15(11) | 153.30(15) |
| 0.02857 | 152.08(10) | 152.26(10) | 152.61(10) | 152.90(12) | 153.13(14) | 153.28(18) |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.09204 | 156.19(3) | 156.17(3) | 156.10(3) | 156.02(3) | 155.91(4) | 155.78(4) |
| 0.08265 | 156.19(4) | 156.18(4) | 156.12(4) | 156.04(4) | 155.93(5) | 155.80(6) |
| 0.07250 | 156.21(4) | 156.20(4) | 156.13(4) | 156.05(4) | 155.94(4) | 155.82(4) |
| 0.06304 | 156.21(5) | 156.21(5) | 156.14(5) | 156.06(5) | 155.96(5) | 155.84(5) |
| 0.05394 | 156.21(6) | 156.20(6) | 156.13(6) | 156.05(6) | 155.94(6) | 155.81(7) |
| 0.04498 | 156.21(7) | 156.21(7) | 156.14(7) | 156.06(7) | 155.96(6) | 155.84(6) |
| 0.03545 | 156.22(9) | 156.22(9) | 156.15(8) | 156.07(8) | 155.96(8) | 155.85(8) |
| 0.02724 | 156.21(11) | 156.22(11) | 156.15(11) | 156.08(11) | 155.98(11) | 155.87(10) |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | 151.13(3) | 151.28(3) | 151.54(3) | 151.76(4) | 151.92(4) | 152.03(6) |
| 0.08466 | 151.12(4) | 151.27(4) | 151.54(4) | 151.75(4) | 151.92(4) | 152.03(5) |
| 0.07501 | 151.10(4) | 151.25(4) | 151.52(4) | 151.74(4) | 151.91(5) | 152.02(6) |
| 0.06473 | 151.09(5) | 151.24(5) | 151.52(5) | 151.75(5) | 151.92(6) | 152.04(8) |
| 0.05522 | 151.07(5) | 151.22(5) | 151.51(5) | 151.74(6) | 151.92(6) | 152.04(8) |
| 0.04138 | 151.04(7) | 151.19(7) | 151.48(7) | 151.72(7) | 151.90(8) | 152.02(9) |
| 0.03782 | 151.05(8) | 151.21(8) | 151.50(8) | 151.74(8) | 151.93(9) | 152.04(11) |
| 0.02942 | 151.02(10) | 151.17(10) | 151.47(10) | 151.71(10) | 151.90(11) | 152.02(13) |

Uridine, $T$ = 313.15 K

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.09524 | 155.27(3) | 155.21(3) | 155.05(3) | 154.89(3) | 154.71(4) | 154.52(5) |
| 0.08191 | 155.28(4) | 155.21(4) | 155.06(4) | 154.89(4) | 154.72(5) | 154.53(6) |
| 0.07492 | 155.27(4) | 155.21(4) | 155.05(4) | 154.88(4) | 154.71(4) | 154.52(5) |
| 0.06499 | | 155.21(5) | 155.05(5) | 154.89(5) | 154.72(6) | 154.54(8) |
| 0.05449 | 155.29(6) | 155.23(6) | 155.08(6) | 154.93(6) | 154.76(6) | 154.59(7) |
| 0.04992 | 155.27(6) | 155.21(6) | 155.04(6) | 154.88(6) | 154.70(7) | 154.51(8) |
| 0.04094 | 155.28(7) | 155.23(7) | 155.07(7) | 154.93(8) | 154.76(9) | 154.59(10) |
| 0.03745 | | 155.22(8) | 155.05(8) | 154.90(8) | 154.72(8) | 154.54(9) |

[a] Each number in parentheses is the uncertainty in the last digit, or last two digits, of $V_\phi$

**Table S4** Apparent molar isentropic compressions for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K and at $p$ = (10.0 to 100.0) MPa

| $m$ (mol·kg$^{-1}$) | $K_{S,\phi}$[a] (m$^3$·mol$^{-1}$·Pa$^{-1}$) | | | | | |
|---|---|---|---|---|---|---|
| | $p$ (MPa) | | | | | |
| | 10.0 | 20.0 | 40.0 | 60.0 | 80.0 | 100.0 |
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | $-14.3_{6}(0.92)$ | $-13.3_{3}(0.88)$ | $-10.4_{3}(0.81)$ | $-8.4_{1}(0.75)$ | $-5.7_{7}(0.69)$ | $-3.1_{5}(0.64)$ |
| 0.01957 | $-14.7_{7}(0.94)$ | $-13.4_{0}(0.90)$ | $-10.8_{6}(0.83)$ | $-8.0_{3}(0.76)$ | $-5.9_{6}(0.71)$ | $-3.3_{3}(0.65)$ |
| 0.01944 | | $-13.6_{6}(0.91)$ | $-10.6_{7}(0.83)$ | $-8.4_{0}(0.77)$ | $-6.0_{5}(0.71)$ | $-3.2_{1}(0.66)$ |
| 0.01929 | $-14.9_{0}(0.95)$ | $-14.1_{4}(0.91)$ | $-11.1_{6}(0.84)$ | $-8.7_{7}(0.77)$ | $-6.1_{3}(0.72)$ | $-3.1_{7}(0.67)$ |
| 0.01904 | $-14.5_{2}(0.97)$ | $-12.3_{3}(0.93)$ | $-9.8_{1}(0.85)$ | $-7.8_{2}(0.78)$ | $-5.6_{9}(0.73)$ | $-2.8_{8}(0.67)$ |
| 0.01873 | $-14.2_{7}(0.98)$ | $-13.4_{0}(0.94)$ | $-10.6_{1}(0.87)$ | $-7.8_{6}(0.80)$ | $-5.2_{3}(0.74)$ | $-2.8_{6}(0.68)$ |
| 0.01846 | $-13.7_{4}(0.99)$ | $-12.7_{7}(0.95)$ | $-9.7_{4}(0.88)$ | $-7.3_{4}(0.81)$ | $-5.1_{5}(0.75)$ | $-2.5_{3}(0.69)$ |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | | $7.9_{4}(0.80)$ | $7.8_{9}(0.73)$ | $8.1_{6}(0.68)$ | $9.0_{4}(0.63)$ | $9.5_{3}(0.59)$ |
| 0.01973 | $7.4_{1}(0.83)$ | $7.1_{5}(0.80)$ | $7.5_{1}(0.74)$ | $8.2_{6}(0.68)$ | $8.8_{3}(0.63)$ | $9.4_{5}(0.59)$ |
| 0.01951 | $7.7_{3}(0.84)$ | $6.4_{1}(0.81)$ | $6.5_{0}(0.75)$ | $8.0_{5}(0.69)$ | $9.0_{5}(0.64)$ | $9.3_{8}(0.60)$ |
| 0.01936 | $7.2_{8}(0.85)$ | $7.4_{5}(0.81)$ | $7.5_{6}(0.75)$ | $8.7_{3}(0.70)$ | $9.2_{8}(0.65)$ | $9.4_{0}(0.60)$ |
| 0.01919 | | $6.5_{9}(0.82)$ | $7.4_{6}(0.76)$ | $8.3_{0}(0.70)$ | $8.9_{4}(0.65)$ | $9.1_{8}(0.61)$ |
| 0.01896 | | $6.3_{7}(0.83)$ | $6.5_{3}(0.77)$ | $8.2_{1}(0.71)$ | $8.2_{5}(0.66)$ | $9.1_{7}(0.61)$ |
| 0.01870 | $7.3_{5}(0.88)$ | $6.8_{3}(0.84)$ | $6.0_{1}(0.78)$ | $8.1_{4}(0.72)$ | $8.8_{4}(0.67)$ | $9.8_{7}(0.62)$ |
| 0.01848 | | $7.5_{4}(0.85)$ | $7.3_{4}(0.79)$ | $7.9_{0}(0.73)$ | $8.4_{6}(0.68)$ | $9.3_{0}(0.63)$ |
| Cytidine, $T$ = 288.15 K | | | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.09058 | $-23.3_0$(0.20) | $-21.6_2$(0.19) | $-18.2_3$(0.18) | $-14.8_9$(0.16) | $-11.6_3$(0.15) | $-8.6_7$(0.14) |
| 0.08214 | $-23.4_0$(0.22) | $-21.8_7$(0.21) | $-18.2_6$(0.20) | $-14.9_6$(0.18) | $-11.7_0$(0.17) | $-8.7_8$(0.16) |
| 0.07292 | $-23.7_8$(0.25) | $-22.2_5$(0.24) | $-18.5_8$(0.22) | $-15.1_9$(0.20) | $-11.9_0$(0.19) | $-8.9_6$(0.18) |
| 0.06285 | $-24.2_2$(0.30) | $-22.3_7$(0.28) | $-18.8_2$(0.26) | $-15.4_3$(0.24) | $-12.1_7$(0.22) | $-9.0_7$(0.21) |
| 0.05387 | $-24.7_0$(0.34) | $-22.6_2$(0.33) | $-19.2_9$(0.30) | $-15.5_8$(0.28) | $-12.4_0$(0.26) | $-9.3_5$(0.25) |
| 0.04435 | $-24.3_5$(0.41) | $-22.6_2$(0.40) | $-18.9_9$(0.36) | $-15.6_9$(0.34) | $-12.2_6$(0.31) | $-9.3_1$(0.29) |
| 0.03651 | $-24.5_4$(0.50) | $-23.0_8$(0.48) | $-19.3_1$(0.44) | $-15.9_1$(0.41) | $-12.6_2$(0.38) | $-9.4_8$(0.35) |
| 0.02857 | $-25.0_9$(0.64) | $-23.1_9$(0.62) | $-19.5_7$(0.57) | $-16.4_1$(0.52) | $-12.7_0$(0.48) | $-9.6_6$(0.45) |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.09204 | $-4.1_2$(0.18) | $-3.4_2$(0.17) | $-1.8_9$(0.16) | $-0.53_9$(0.15) | $1.0_5$(0.14) | $2.2_5$(0.13) |
| 0.08265 | $-4.6_7$(0.20) | $-3.7_2$(0.19) | $-2.0_1$(0.18) | $-0.75_1$(0.16) | $0.95_3$(0.15) | $2.2_8$(0.14) |
| 0.07250 | $-4.5_6$(0.23) | $-3.9_0$(0.22) | $-1.9_9$(0.20) | $-0.54_1$(0.19) | $0.81_4$(0.17) | $2.1_8$(0.16) |
| 0.06304 | $-4.6_7$(0.26) | $-3.9_6$(0.25) | $-1.7_8$(0.23) | $-0.98_4$(0.21) | $0.67_2$(0.20) | $2.1_4$(0.18) |
| 0.05394 | $-4.0_7$(0.30) | $-3.3_2$(0.29) | $-2.1_5$(0.27) | $-0.39_0$(0.25) | $1.2_6$(0.23) | $2.4_2$(0.22) |
| 0.04498 | $-4.3_2$(0.36) | $-3.6_0$(0.35) | $-2.0_4$(0.32) | $-0.55_7$(0.30) | $0.94_0$(0.28) | $2.2_9$(0.26) |
| 0.03545 | $-4.3_0$(0.46) | $-3.5_8$(0.44) | $-1.9_6$(0.40) | $-0.52_9$(0.38) | $1.0_4$(0.35) | $2.2_8$(0.33) |
| 0.02724 | $-4.6_9$(0.60) | $-3.6_9$(0.58) | $-1.8_6$(0.53) | $-0.72_9$(0.49) | $0.74_0$(0.46) | $1.8_4$(0.43) |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | $-19.8_5$(0.19) | $-18.6_4$(0.18) | $-15.7_4$(0.17) | $-12.6_1$(0.16) | $-9.8_4$(0.14) | $-7.1_6$(0.14) |
| 0.08466 | $-20.0_9$(0.22) | $-18.7_0$(0.21) | $-15.9_0$(0.19) | $-12.7_9$(0.18) | $-10.1_4$(0.16) | $-7.3_5$(0.15) |
| 0.07501 | $-20.3_5$(0.24) | $-18.8_6$(0.23) | $-16.1_6$(0.21) | $-12.9_3$(0.20) | $-10.0_7$(0.18) | $-7.3_4$(0.17) |
| 0.06473 | $-20.7_4$(0.28) | $-19.1_7$(0.27) | $-16.2_6$(0.25) | $-13.1_4$(0.23) | $-10.3_2$(0.21) | $-7.6_7$(0.20) |
| 0.05522 | $-20.8_8$(0.33) | $-19.3_9$(0.32) | $-16.5_3$(0.29) | $-13.5_1$(0.27) | $-10.3_5$(0.25) | $-7.6_5$(0.23) |
| 0.04138 | $-20.8_5$(0.44) | $-19.5_9$(0.42) | $-16.6_2$(0.39) | $-13.5_2$(0.36) | $-10.5_5$(0.33) | $-7.9_2$(0.31) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.03782 | $-20.6_{0}(0.48)$ | $-20.0_{2}(0.46)$ | $-16.6_{3}(0.43)$ | $-13.7_{1}(0.39)$ | $-10.5_{0}(0.36)$ | $-7.7_{9}(0.34)$ |
| 0.02942 | $-21.2_{4}(0.62)$ | $-20.0_{1}(0.60)$ | $-16.9_{6}(0.55)$ | $-13.4_{3}(0.51)$ | $-10.8_{1}(0.47)$ | $-7.8_{7}(0.43)$ |
| Uridine, $T = 313.15$ K | | | | | | |
| 0.09524 | $-0.3_{67}(0.17)$ | $-0.0_{44}(0.16)$ | $1.2_{6}(0.15)$ | $2.2_{7}(0.14)$ | $3.1_{4}(0.13)$ | $4.3_{2}(0.12)$ |
| 0.08191 | $-0.4_{92}(0.20)$ | $-0.2_{13}(0.19)$ | $1.1_{9}(0.18)$ | $2.1_{6}(0.16)$ | $3.0_{9}(0.15)$ | $4.2_{4}(0.14)$ |
| 0.07492 | $-0.4_{58}(0.22)$ | $0.0_{28}(0.21)$ | $1.0_{7}(0.19)$ | $2.0_{6}(0.18)$ | $3.1_{9}(0.17)$ | $4.2_{5}(0.16)$ |
| 0.06499 | | $-0.3_{18}(0.24)$ | $0.8_{11}(0.22)$ | $1.9_{4}(0.21)$ | $2.9_{5}(0.19)$ | $3.8_{7}(0.18)$ |
| 0.05449 | $-1.3_{9}(0.30)$ | $-1.0_{3}(0.29)$ | $0.1_{28}(0.27)$ | $1.4_{0}(0.25)$ | $2.2_{5}(0.23)$ | $3.4_{2}(0.21)$ |
| 0.04992 | $-0.3_{73}(0.33)$ | $0.3_{02}(0.32)$ | $1.4_{8}(0.29)$ | $1.8_{2}(0.27)$ | $3.0_{7}(0.25)$ | $4.0_{3}(0.23)$ |
| 0.04094 | $-1.2_{4}(0.40)$ | $-0.5_{07}(0.38)$ | $0.4_{29}(0.35)$ | $1.1_{4}(0.33)$ | $2.4_{3}(0.31)$ | $3.3_{0}(0.29)$ |
| 0.03745 | | $0.0_{96}(0.42)$ | $0.9_{30}(0.39)$ | $1.5_{1}(0.36)$ | $2.7_{9}(0.33)$ | $3.8_{9}(0.31)$ |

[a] Estimated uncertainties are in parentheses

**Table S5** Apparent molar isothermal compressions for aqueous solutions of the nucleosides at $T$ = (288.15 and 313.15) K and at $p$ = (10.0 to 100.0) MPa

| $m$ (mol·kg$^{-1}$) | $K_{T,\phi}$[a] (m$^3$·mol$^{-1}$·Pa$^{-1}$) | | | | | |
|---|---|---|---|---|---|---|
| | $p$ (MPa) | | | | | |
| | 10.0 | 20.0 | 40.0 | 60.0 | 80.0 | 100.0 |
| Adenosine, $T$ = 288.15 K | | | | | | |
| 0.01993 | $-10.6_{6}(0.93)$ | $-9.7_{3}(0.89)$ | $-7.0_{5}(0.82)$ | $-5.2_{6}(0.76)$ | $-2.8_{0}(0.71)$ | $-0.3_{15}(0.66)$ |
| 0.01957 | $-11.0_{1}(0.94)$ | $-9.7_{5}(0.91)$ | $-7.4_{4}(0.84)$ | $-4.8_{3}(0.77)$ | $-2.9_{5}(0.72)$ | $-0.4_{60}(0.67)$ |
| 0.01944 | | $-10.0_{0}(0.91)$ | $-7.2_{4}(0.84)$ | $-5.1_{9}(0.78)$ | $-3.0_{2}(0.72)$ | $-0.3_{20}(0.67)$ |
| 0.01929 | $-11.1_{1}(0.96)$ | $-10.4_{6}(0.92)$ | $-7.7_{1}(0.85)$ | $-5.5_{5}(0.78)$ | $-3.0_{9}(0.73)$ | $-0.2_{71}(0.68)$ |
| 0.01904 | $-10.7_{0}(0.97)$ | $-8.6_{1}(0.93)$ | $-6.3_{2}(0.86)$ | $-4.5_{6}(0.79)$ | $-2.6_{2}(0.74)$ | $0.0_{59}(0.69)$ |
| 0.01873 | $-10.4_{0}(0.99)$ | $-9.6_{5}(0.95)$ | $-7.0_{9}(0.87)$ | $-4.5_{6}(0.81)$ | $-2.1_{2}(0.75)$ | $0.1_{11}(0.70)$ |
| 0.01846 | $-9.8_{3}(1.00)$ | $-8.9_{8}(0.96)$ | $-6.1_{8}(0.89)$ | $-4.0_{1}(0.82)$ | $-2.0_{1}(0.76)$ | $0.4_{73}(0.70)$ |
| Adenosine, $T$ = 313.15 K | | | | | | |
| 0.01984 | | $17.4_{6}(0.84)$ | $16.8_{9}(0.78)$ | $16.7_{0}(0.72)$ | $17.1_{9}(0.67)$ | $17.3_{1}(0.63)$ |
| 0.01973 | $17.1_{8}(0.88)$ | $16.6_{2}(0.84)$ | $16.4_{7}(0.78)$ | $16.7_{8}(0.72)$ | $16.9_{6}(0.67)$ | $17.2_{1}(0.63)$ |
| 0.01951 | $17.4_{7}(0.88)$ | $15.8_{3}(0.85)$ | $15.4_{0}(0.78)$ | $16.5_{3}(0.73)$ | $17.1_{6}(0.68)$ | $17.1_{2}(0.63)$ |
| 0.01936 | $16.9_{8}(0.89)$ | $16.8_{7}(0.85)$ | $16.4_{8}(0.79)$ | $17.2_{2}(0.73)$ | $17.3_{8}(0.68)$ | $17.1_{1}(0.64)$ |
| 0.01919 | | $15.9_{6}(0.86)$ | $16.3_{5}(0.79)$ | $16.7_{5}(0.74)$ | $17.0_{1}(0.69)$ | $16.8_{7}(0.64)$ |
| 0.01896 | | $15.7_{0}(0.86)$ | $15.3_{5}(0.80)$ | $16.6_{3}(0.74)$ | $16.2_{6}(0.69)$ | $16.8_{3}(0.65)$ |
| 0.01870 | $16.9_{5}(0.91)$ | $16.1_{4}(0.87)$ | $14.7_{7}(0.81)$ | $16.5_{1}(0.75)$ | $16.8_{4}(0.70)$ | $17.5_{3}(0.65)$ |
| 0.01848 | | $16.8_{3}(0.88)$ | $16.1_{1}(0.82)$ | $16.2_{4}(0.76)$ | $16.4_{1}(0.71)$ | $16.9_{0}(0.66)$ |
| Cytidine, $T$ = 288.15 K | | | | | | |
| 0.09058 | $-19.1_{3}(0.20)$ | $-17.6_{0}(0.19)$ | $-14.4_{8}(0.18)$ | $-11.3_{8}(0.17)$ | $-8.3_{4}(0.16)$ | $-5.5_{5}(0.15)$ |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.08214 | $-19.2_{1}$(0.22) | $-17.8_{2}$(0.21) | $-14.4_{9}$(0.20) | $-11.4_{4}$(0.18) | $-8.3_{9}$(0.17) | $-5.6_{5}$(0.16) |
| 0.07292 | $-19.5_{7}$(0.25) | $-18.1_{9}$(0.24) | $-14.7_{8}$(0.22) | $-11.6_{5}$(0.21) | $-8.5_{8}$(0.19) | $-5.8_{1}$(0.19) |
| 0.06285 | $-19.9_{9}$(0.29) | $-18.2_{8}$(0.28) | $-15.0_{1}$(0.26) | $-11.8_{7}$(0.24) | $-8.8_{3}$(0.23) | $-5.9_{0}$(0.21) |
| 0.05387 | $-20.4_{5}$(0.34) | $-18.5_{1}$(0.33) | $-15.4_{7}$(0.30) | $-12.0_{1}$(0.28) | $-9.0_{5}$(0.26) | $-6.1_{7}$(0.25) |
| 0.04435 | $-20.0_{8}$(0.42) | $-18.4_{9}$(0.40) | $-15.1_{4}$(0.37) | $-12.1_{0}$(0.34) | $-8.8_{9}$(0.32) | $-6.1_{1}$(0.30) |
| 0.03651 | $-20.2_{5}$(0.50) | $-18.9_{4}$(0.48) | $-15.4_{5}$(0.45) | $-12.3_{0}$(0.41) | $-9.2_{4}$(0.39) | $-6.2_{8}$(0.36) |
| 0.02857 | $-20.8_{0}$(0.65) | $-19.0_{3}$(0.62) | $-15.6_{9}$(0.57) | $-12.8_{0}$(0.53) | $-9.3_{1}$(0.49) | $-6.4_{5}$(0.46) |
| Cytidine, $T$ = 313.15 K | | | | | | |
| 0.09204 | $1.9_{8}$(0.18) | $2.5_{0}$(0.18) | $3.7_{3}$(0.16) | $4.8_{1}$(0.15) | $6.1_{7}$(0.14) | $7.1_{5}$(0.13) |
| 0.08265 | $1.3_{9}$(0.20) | $2.1_{7}$(0.20) | $3.5_{8}$(0.18) | $4.5_{6}$(0.17) | $6.0_{5}$(0.16) | $7.1_{6}$(0.15) |
| 0.07250 | $1.4_{7}$(0.23) | $1.9_{6}$(0.22) | $3.5_{7}$(0.21) | $4.7_{5}$(0.19) | $5.8_{7}$(0.18) | $7.0_{4}$(0.17) |
| 0.06304 | $1.3_{2}$(0.27) | $1.8_{6}$(0.26) | $3.7_{6}$(0.24) | $4.2_{6}$(0.22) | $5.7_{0}$(0.20) | $6.9_{6}$(0.19) |
| 0.05394 | $1.9_{0}$(0.31) | $2.4_{8}$(0.30) | $3.3_{4}$(0.28) | $4.8_{4}$(0.26) | $6.2_{8}$(0.24) | $7.2_{3}$(0.23) |
| 0.04498 | $1.5_{9}$(0.38) | $2.1_{5}$(0.36) | $3.4_{0}$(0.33) | $4.6_{3}$(0.31) | $5.9_{1}$(0.29) | $7.0_{5}$(0.27) |
| 0.03545 | $1.5_{5}$(0.48) | $2.1_{1}$(0.46) | $3.4_{2}$(0.42) | $4.6_{0}$ (0.39) | $5.9_{5}$(0.37) | $6.9_{8}$(0.34) |
| 0.02724 | $1.0_{6}$(0.62) | $1.9_{0}$(0.60) | $3.4_{6}$(0.55) | $4.3_{2}$(0.51) | $5.5_{8}$(0.48) | $6.4_{6}$(0.44) |
| Uridine, $T$ = 288.15 K | | | | | | |
| 0.09524 | $-15.7_{9}$(0.25) | $-14.7_{2}$(0.24) | $-12.0_{9}$(0.22) | $-9.1_{8}$(0.21) | $-6.6_{2}$(0.20) | $-4.1_{1}$(0.18) |
| 0.08466 | $-16.0_{6}$(0.27) | $-14.8_{0}$(0.26) | $-12.2_{7}$(0.24) | $-9.3_{9}$(0.22) | $-6.9_{5}$(0.21) | $-4.3_{2}$(0.20) |
| 0.07501 | $-16.3_{5}$(0.29) | $-14.9_{9}$(0.28) | $-12.5_{5}$(0.26) | $-9.5_{5}$(0.24) | $-6.9_{0}$(0.23) | $-4.3_{3}$(0.21) |
| 0.06473 | $-16.7_{7}$(0.33) | $-15.3_{3}$(0.31) | $-12.6_{8}$(0.29) | $-9.7_{9}$(0.27) | $-7.1_{8}$(0.25) | $-4.6_{9}$(0.24) |
| 0.05522 | $-16.9_{3}$(0.37) | $-15.5_{7}$(0.36) | $-12.9_{8}$(0.33) | $-10.1_{9}$(0.31) | $-7.2_{3}$(0.29) | $-4.6_{9}$(0.27) |
| 0.04138 | $-16.9_{4}$(0.47) | $-15.8_{0}$(0.46) | $-13.0_{9}$(0.42) | $-10.2_{3}$(0.39) | $-7.4_{5}$(0.36) | $-4.9_{9}$(0.34) |
| 0.03782 | $-16.7_{0}$(0.51) | $-16.2_{5}$(0.49) | $-13.1_{2}$(0.46) | $-10.4_{3}$(0.42) | $-7.4_{1}$(0.39) | $-4.8_{6}$(0.37) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.02942 | $-17.3_7$(0.65) | $-16.2_6$(0.62) | $-13.4_6$(0.57) | $-10.1_7$(0.53) | $-7.7_5$(0.49) | $-4.9_6$(0.46) |
| Uridine, $T$ = 313.15 K | | | | | | |
| 0.09524 | $6.8_5$(0.45) | $6.9_7$(0.43) | $7.9_1$(0.41) | $8.5_9$(0.38) | $9.1_7$(0.36) | $10.1_0$(0.34) |
| 0.08191 | $6.8_3$(0.47) | $6.8_9$(0.45) | $7.9_2$(0.43) | $8.5_6$(0.40) | $9.2_0$(0.38) | $10.0_9$(0.36) |
| 0.07492 | $6.9_1$(0.48) | $7.1_9$(0.47) | $7.8_5$(0.44) | $8.5_1$(0.41) | $9.3_4$(0.39) | $10.1_3$(0.37) |
| 0.06499 | | $6.9_0$(0.49) | $7.6_5$(0.46) | $8.4_4$(0.43) | $9.1_5$(0.41) | $9.7_9$(0.38) |
| 0.05449 | $6.0_9$(0.54) | $6.2_3$(0.52) | $7.0_0$(0.49) | $7.9_3$(0.46) | $8.4_7$(0.43) | $9.3_7$(0.41) |
| 0.04992 | $7.1_6$(0.56) | $7.6_2$(0.54) | $8.4_3$(0.50) | $8.3_9$(0.47) | $9.3_4$(0.45) | $10.0_3$(0.42) |
| 0.04094 | $6.3_1$(0.61) | $6.8_3$(0.59) | $7.3_7$(0.55) | $7.7_2$(0.52) | $8.7_2$(0.49) | $9.2_9$(0.46) |
| 0.03745 | | $7.4_6$(0.62) | $7.8_9$(0.58) | $8.1_1$(0.54) | $9.0_9$(0.50) | $9.9_2$(0.48) |

[a] Estimated uncertainties are in parentheses

Fig 1

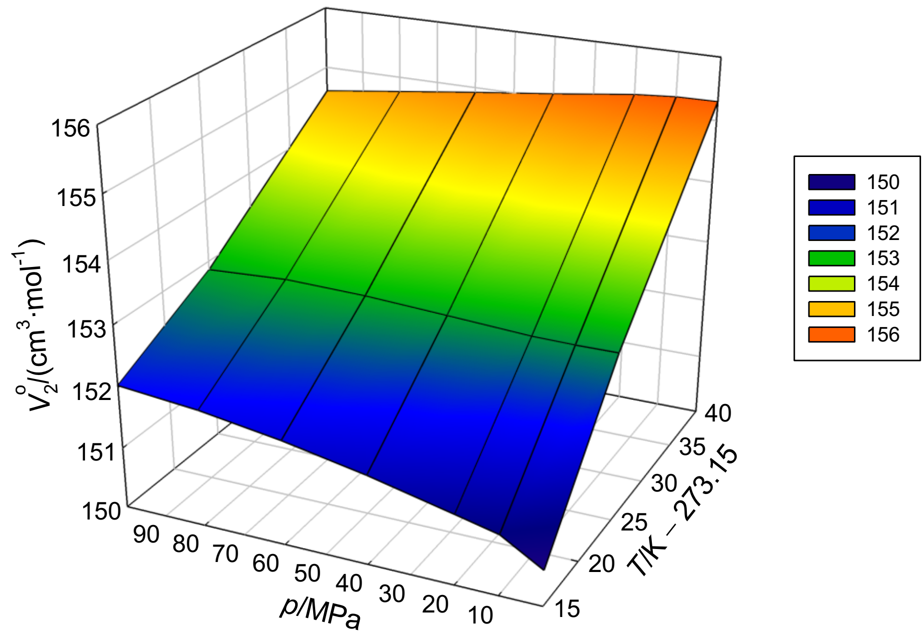
(a)

Fig 2

(a)

Fig 3

(a)

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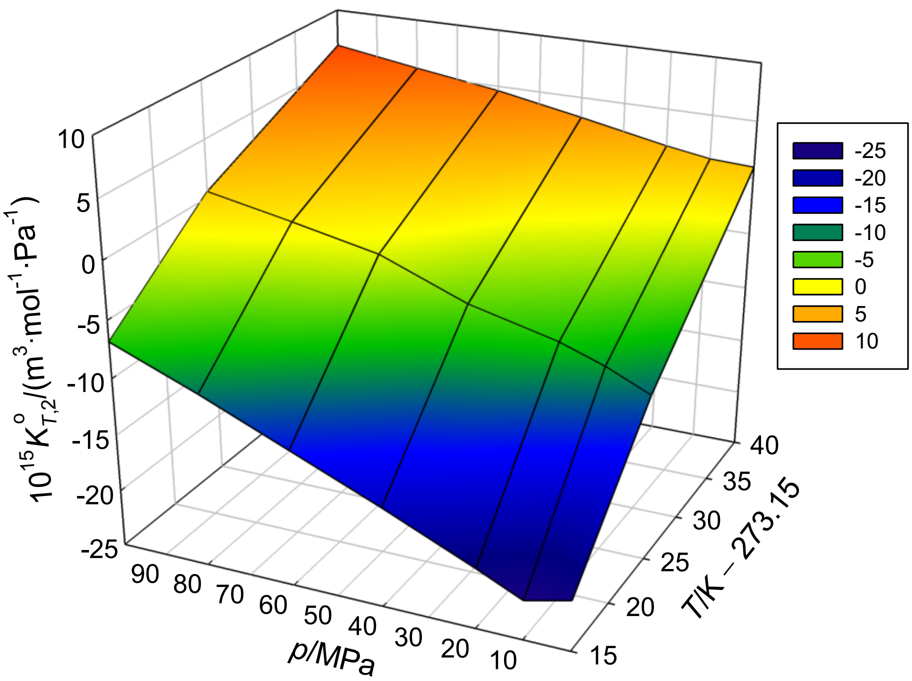

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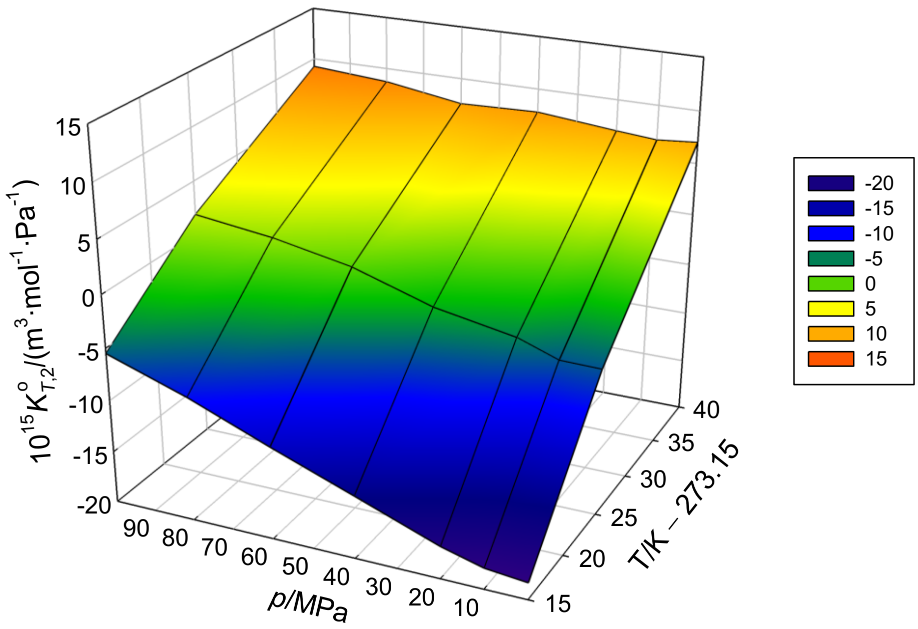


**Figure Captions**

Fig. 1 Volumetric properties as a function of temperature and pressure for adenosine at infinite dilution. **a** Partial molar volume. **b** Partial molar isothermal compression.

Fig. 2 Volumetric properties as a function of temperature and pressure for cytidine at infinite dilution. **a** Partial molar volume. **b** Partial molar isothermal compression.

Fig. 3 Volumetric properties as a function of temperature and pressure for uridine at infinite dilution. **a** Partial molar volume. **b** Partial molar isothermal compression.