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Standard absolute entropies, S°_{298}, from volume or density Part II. Organic liquids and solids

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Abstract

The standard absolute entropies of many materials are unknown, which precludes a full understanding of their thermodynamic stabilities. We show, for both organic liquids and solids, that entropies are reliably linearly correlated with volume per molecule, V_m (nm^3 per molecule) (or molar volume, M/ρ (cm^3 mol^{-1})); thus, permitting simple evaluation of standard entropies (J K^{-1} mol^{-1}) at 298 K. The regression lines generally pass close to the origin, with formulae:

For organic liquids:

$$S^\circ_{298}(\mathrm{l})\ (\mathrm{J\,K^{-1}\,mol^{-1}}) = 1133(V_\mathrm{m}\ (\mathrm{nm^3\ per\ molecule})) + 44$$

or

$$S^\circ_{298}(\mathrm{l})\ (\mathrm{J\,K^{-1}\,mol^{-1}}) = 1.881\left[\frac{M}{\rho}\ (\mathrm{cm^3\,mol^{-1}})\right] + 44$$

For organic solids:

$$S^\circ_{298}(\mathrm{s})\ (\mathrm{J\,K^{-1}\,mol^{-1}}) = 774(V_\mathrm{m}\ (\mathrm{nm^3\ per\ molecule})) + 57$$

or

$$S^\circ_{298}(\mathrm{s})\ (\mathrm{J\,K^{-1}\,mol^{-1}}) = 1.285\left[\frac{M}{\rho}\ (\mathrm{cm^3\,mol^{-1}})\right] + 57$$

These results complement similar studies (by ourselves and others) demonstrating linear entropy–volume correlations for ionic solids (including minerals, simple ionic solids and ionic hydrates and solvates), but are now—for the first time—demonstrated for organic materials. Part I of this series of papers [22] applies a similar analysis to ionic solids.

Keywords: Entropy; Density; Volume; Thermodynamic estimation

1. Introduction

In order to make a thermodynamic prediction on the stability of a material, and to select among synthetic procedures, it is necessary to have information on its Gibbs energy, G, which itself depends upon its enthalpy, H, and entropy, S, through its definition as:

$$G \equiv H - TS \tag{1}$$

Whilst values for standard enthalpies of formation are readily available, being widely tabulated in thermochemical tables and databases [1–5], there is a paucity of standard

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entropy values[1] in these sources, with as much as 70% of the entropy data unavailable. We here report simple but reliable procedures (based on thermodynamic considerations) for the estimation of standard entropy values, S°_{298}, of organic liquids and solids. Only the chemical formula and its molar volume, V_m (available from crystal structure and powder diffraction data [6]; or indirectly calculated from simple, non-intrusive density, ρ, measurements[2] or estimated using group additivities [7]), are needed in order to estimate unknown standard entropy values. Furthermore, the $T\Delta S$ term in ΔG for these condensed phases is generally quite small relative to ΔH at or near room temperature[3] where much of chemistry (and of biochemistry and biology) is studied, so that rule-of-thumb procedures are likely to prove suitable even when the entropy estimate may be somewhat in error.

There is a long and honorable history of thermodynamic estimation procedures, from theoretically-based statistical mechanical analyses [3,8] (requiring the assignment of spectroscopically observed absorptions to specific intra-atomic vibrations, and essentially suitable for materials in the gas phase) to empirical additivity schemes [9]; the latter range from simple, zero-order [10] atom additivity (for example, additivity of ion molar refraction and of magnetic susceptibility [11]) through to first-order bond energy contributions [12], or of oxide components of a mineral [13], to the considerably more complex, second-order group additivity schemes which may contain dozens of specific group contributions. Group contribution schemes exist for heat capacities [14], energies (and enthalpies) of formation [15], absolute entropies [16], enthalpies and entropies of fusion [17,18],[4,5] vaporization [19] and dissolution [20], densities [7] (and, hence, molar volumes),[2] and many others.

In an independent but parallel vein, successful broad predictive procedures have been developed for lattice energies and enthalpies of formation of ionic solids [21]; our present results now demonstrate—for the first time—simple linear entropy–volume correlations for organic materials, complementing studies (by ourselves [22] and others [13,23,24]) showing similar linear correlations for ionic solids (including minerals, simple ionic solids and ionic hydrates and solvates [22]). The advantage of these correlations is that of extreme simplicity—only one or two empirical constants are required beyond the basic information of chemical formula—instead of multiple, special fitted group constants; this means that we are able to predict the entropies of materials as yet to be synthesized, or even hypothetical. On the other hand, this simplicity does also imply that our method cannot distinguish among the consequences of secondary features of the molecular structure (such as flexibility or rigidity, or the possibilities of hydrogen bonding, etc.) except insofar as those features are reflected in a known molecular volume of the material under consideration. For this reason, while drawing attention to the extreme simplicity of our procedure, we warn against over-interpretation of the results of our predictions (cf. Section 3, below).

2. Statistical analysis of literature data

On the basis of thermodynamic indications for a linear entropy–volume correlation (see Appendix A), we have plotted reported values of absolute entropies against molar volumes, V_m, for organic liquids and for organic solids, and find very satisfactory linear regressions. (In practice, we use volume per molecule for V_m rather than molar volume, in order to ease the transition from crystal structure data.) The volume-based fitted equation is of the form:

$$\begin{aligned} S^\circ_{298}\,(\mathrm{J\,K^{-1}\,mol^{-1}}) &= k\,(V_m(\mathrm{nm^3\ per\ molecule})) + c \\ &= 1.66\times10^{-3}\times k(V_m(\mathrm{cm^3\,mol^{-1}}))+c \end{aligned} \qquad (2)$$

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[1] As an illustration, the *Handbook of Chemistry and Physics* [1] tabulates thermodynamic data for 1526 organic compounds, the majority of which exist as liquids. We might anticipate at least one entropy value entry being recorded against each compound, corresponding to its usual physical state (solid, liquid or gas). In fact, only 476 (31%) individual entropy values are listed. In the HSC database [5] of about 2800 organic liquid entries, only about 1500 room temperature entropies are given.

[2] The relationship between molar volume, V_m, and density, ρ, is:

$$\begin{aligned} V_m\,(\mathrm{cm^3\,mol^{-1}}) &= \frac{M\,(\mathrm{g\,mol^{-1}})}{\rho\,(\mathrm{g\,cm^{-3}})} = \frac{M\,(\mathrm{g\,mol^{-1}})\times(10^7)^3(\mathrm{nm^3\,cm^{-3}})}{N_A\,(\mathrm{molecules\,mol^{-1}})\times\rho\,(\mathrm{g\,cm^{-3}})} \\ &= \frac{10^{21}M}{6.023\times10^{23}\times\rho} \\ &= \left[1.66\times10^{-3}\frac{M}{\rho}\,(\mathrm{nm^3\ per\ molecule})\right] \end{aligned}$$

where N_A is Avogadro's constant, M is the chemical formula mass, and ρ is the density. Consider hexane as an example: its liquid density at 298 K is reported [1] as $0.6548\,\mathrm{g\,cm^{-3}}$ and $M = 86.18\,\mathrm{g\,mol^{-1}}$; V_m is thus evaluated as $131.6\,\mathrm{cm^3\,mol^{-1}}$ or $0.2185\,\mathrm{nm^3}$ per molecule, leading to an estimated value for S°_{298} of $290\,\mathrm{J\,K^{-1}\,mol^{-1}}$—the reported [1] experimental value is $296\,\mathrm{J\,K^{-1}\,mol^{-1}}$, thus an error of −2%.

[3] In the estimation of the $T\Delta S^\circ$ contribution to the ΔG° term (in $\mathrm{kJ\,mol^{-1}}$) at 298 K, the value of ΔS° (in $\mathrm{J\,K^{-1}\,mol^{-1}}$), derived from absolute standard entropy differences of products and reactants, is multiplied by the factor $T\,(\mathrm{K\,kJ\,J^{-1}}) = 0.298$. Effectively, any error there might be in the S°_{298} values used to obtain ΔS° is reduced by 30%, thereby rendering the correlations reported here of enhanced value. With an average unsigned error of 6.1%, this corresponds to an error of 1.8% in the $T\Delta S^\circ$ term for the Gibbs energy, ΔG°.

[4] Note: the reported group additivity method for estimation of fusion entropies yields a biased estimate; the bias may be reduced by reversing the reported linear regression equation between calculated and experimental fusion entropies, thus: $\Delta_{\mathrm{tpce}}S(\mathrm{calc,\ reduced\ bias}) = [\Delta_{\mathrm{tpce}}S(\mathrm{calc}) - b]/m$, where $\Delta_{\mathrm{tpce}}S$ is the 'total phase change entropy', while m and b are the linear regression coefficients reported in Fig. 3 of the referenced paper.

[5] Note: the reported symmetry- and flexibility-based method for estimation of fusion entropies yields a biased estimate, as may be observed in Fig. 2 of the paper; the bias may be reduced by reversing a linear regression through the data, as in our Footnote 4 (above). We have determined the coefficients of such a linear regression through 1269 of their data points as being $m = 0.9036$, $b = 8.62$, and $R^2 = 0.885$.

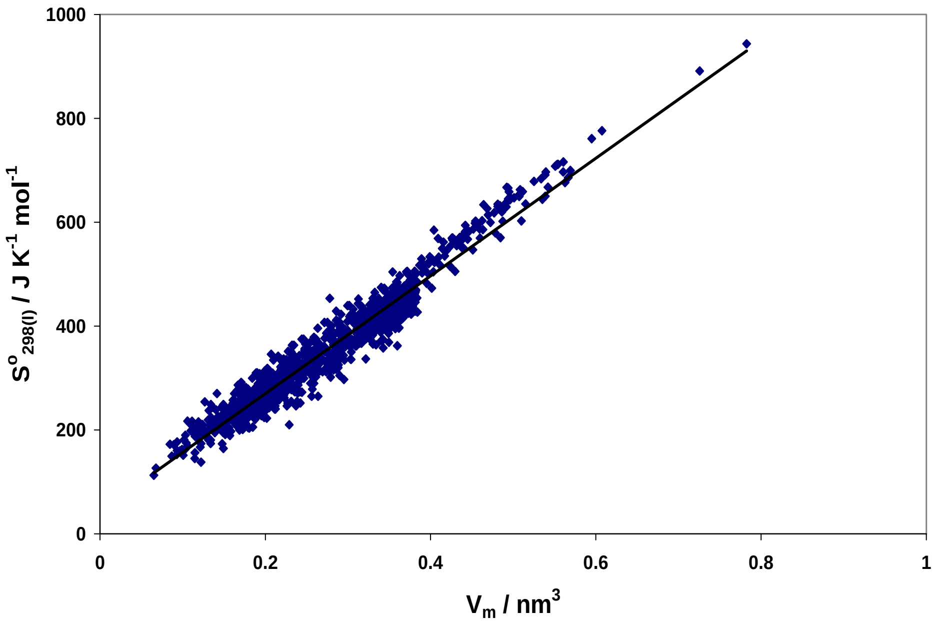

Fig. 1. Standard absolute molar entropies, S°_{298}(l) (J K^{-1} mol^{-1}) vs. volume, V_m (nm^3 per molecule) for a set [5] of 1496 organic liquids.

where V_m may be determined from experimental X-ray crystallographic measurements, from density[2], ρ, or from group additivity [7]. Results are displayed in Figs. 1 and 2, and tabulated in Table 1. Based on the inverse relation between volume and density[2] we can also parameterize Eq. (2) as a function of the molar mass, M (g mol^{-1}), and density, ρ (g cm^{-3}), to give an equivalent, density-based equation:

$$S^\circ_{298}\,(\mathrm{J\,K^{-1}\,mol^{-1}}) = k'\left[\frac{M}{\rho}\,(\mathrm{cm^3\,mol^{-1}})\right] + c \qquad (3)$$

where the values of k' cited in Table 1 are obtained[2] from:

$$k' = 1.66 \times 10^{-3} k \qquad (4)$$

One observes in Table 1 that:

- The correlations have small but non-zero intercepts; these intercepts correspond to the zero-volume entropy contributions of the entities concerned.

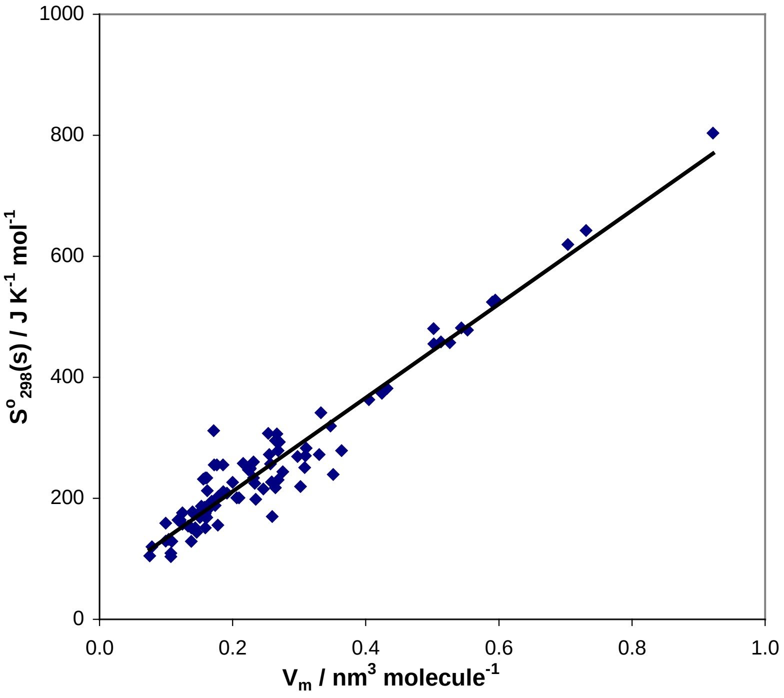

Fig. 2. Standard absolute molar entropies, S°_{298}(s) (J K^{-1} mol^{-1}) vs. volume, V_m (nm^3 per molecule) for a set [5] of 100 organic solids.

Table 1
Unconstrained linear relationships between standard entropy, S°_{298} ($\mathrm{J\,K^{-1}\,mol^{-1}}$), and volume, V_m ($\mathrm{nm^3}$ per molecule), or density, ρ ($\mathrm{g\,cm^{-3}}$)

Compound type	number of compounds considered	$S^{\circ}_{298} = kV_m + c$ and $S^{\circ}_{298} = k'(M/\rho) + c$				Average unsigned % error
		[V_m-based]k ($\mathrm{J\,K^{-1}\,mol^{-1}\,nm^{-3}}$ molecule)	[M/ρ-based]k' ($\mathrm{J\,K^{-1}\,cm^{-3}}$)	c ($\mathrm{J\,K^{-1}\,mol^{-1}}$)	Correl. coeff. R^2	
Liquid *n*-paraffins (C_5-C_{16})[a]	12	1212.0 ± 4.2	2.012 ± 0.007	32.1 ± 1.5	1.00	0.25
Liquid *n*-alcohols (C_1-C_{11})[a]	11	1174.5 ± 3.5	1.949 ± 0.006	46.0 ± 0.8	1.00	0.34
Organic liquids	1496	1133 ± 7	1.881 ± 0.011	44 ± 2	0.95	5.7
Organic solids	100	774 ± 21	1.285 ± 0.035	57 ± 6	0.93	10.4

[a] The intercepts correspond to the zero-volume entropy contribution of the terminal pair of H's or H and OH, respectively. The difference of $-13.9\,\mathrm{J\,K^{-1}\,mol^{-1}}$ on the substitution of a terminal H by OH differs slightly from the 1932-based published value [8] of $-6.3\,\mathrm{J\,K^{-1}\,mol^{-1}}$. From this data, also the insertion of a methylene ($-CH_2-$) group into the hydrocarbon chain involves an increase in entropy of $32.4\,\mathrm{J\,K^{-1}\,mol^{-1}}$ (which agrees well with the 1932-based published value [8] of $32.2\,\mathrm{J\,K^{-1}\,mol^{-1}}$).

- The correlations hold for both organic condensed phases, which include a variety of materials, including organometallics, but less well for the solids.
- For new (or even hypothetical) materials, we can utilize extrapolation–interpolation procedures, or else group additivity methods [6,7] to infer missing volumes and thence use the correlation between S and V_m to obtain standard entropies for new organic materials.

Alternative correlations which have also been investigated by us are: absolute entropies against number of atoms (n) (possibly relevant on statistical mechanical grounds); and absolute entropies against formula masses (M). Analysis of the former shows very poor correlation; any correlation of entropy with M is essentially non-existent.

3. Discussion

We have here demonstrated (Figs. 1 and 2; Table 1) that there is a close linear relation between the entropies and volumes of a wide range of condensed organic phases, both solids and liquids. The mean unsigned errors of the predicted entropies relative to the literature values are as low as 6% for organic liquids.

However, users are cautioned against over-interpretation of the estimated results; for example, organic isomers may differ considerably in their flexibility and crowding—this will be little reflected in their molar volumes and so in their predicted entropies. As a pertinent example, consider Table 2 for the methylheptanes, having 2-, 3- and 4-isomers, where 3-methylheptane has a rigid-rotational symmetry number, σ_r, of 1 and its gas-phase entropy [3] at 298 K is larger than that of its isomers with values of σ_r of 2.

The gas-phase differences of $6.3\,\mathrm{J\,K^{-1}\,mol^{-1}}$ between the entropies of the 3- and 2-isomers, and of $8.3\,\mathrm{J\,K^{-1}\,mol^{-1}}$ between those of the 3- and 4-isomers, carries over into the liquid phase; thus, the error in the volume-based prediction for the 3-isomer may be considerably reduced by correcting for this chiral difference (as in the final row of Table 2).

In principle, the difference between the entropy–volume regression lines for liquids and solids yields the entropy of fusion (assuming little or no change in molar volume) and, together with the fusion temperature, T_{fus}, also the enthalpy of fusion:

$$\Delta_{\mathrm{fus}} S^{\circ}_{298}\ (\mathrm{J\,K^{-1}\,mol^{-1}}) \approx 399(V_m\ (\mathrm{nm^3\ per\ molecule})) - 7 = \Delta_{\mathrm{fus}} \frac{H^{\circ}}{T_{\mathrm{fus}}} \qquad (5)$$

This result complements very extensive studies on group additivity measures of entropies and enthalpies of fusion of organic materials [17],[4] as well as shape-based correlations [18].[5] However, the results obtained by this difference calculation are very poor, being generally up to twice larger than the experimental values of fusion entropies; this reflects various problems with this procedure, including that of dealing with a relatively small difference of much larger quantities

Table 2
Experimental [3] and predicted entropies (and % errors) of the methylheptanes, demonstrating and correcting for the effects of secondary factors

Isomer	2-Methylheptane	3-Methylheptane[a]	4-Methylheptane
Gas-phase experimental S°_{298}(g) ($\mathrm{J\,K^{-1}\,mol^{-1}}$)	455.3	461.6	453.3
Liquid-phase experimental S°_{298}(l) ($\mathrm{J\,K^{-1}\,mol^{-1}}$)	352.1	358.4	350.3
V_m(l) ($\mathrm{nm^3}$ per molecule)	0.273	0.268	0.269
predicted from Eq. (2) S°_{298}(l) ($\mathrm{J\,K^{-1}\,mol^{-1}}$)	350.9 (−0.6%)	345.4 (−3.6%)	346.5 (−1.1%)
corrected for symmetry number difference[b] S°_{298}(l) ($\mathrm{J\,K^{-1}\,mol^{-1}}$)		358.5 (0.0%)	

[a] 3-Methylheptane has a chiral centre and, consequently, a smaller rigid-rotational symmetry number, σ_r, than its achiral structural isomers.

[b] Correction applied by subtracting the mean entropy of condensation of the 2- and 4-isomers ($103.1\,\mathrm{J\,K^{-1}\,mol^{-1}}$) from the gas-phase entropy of the 3-isomer [25].

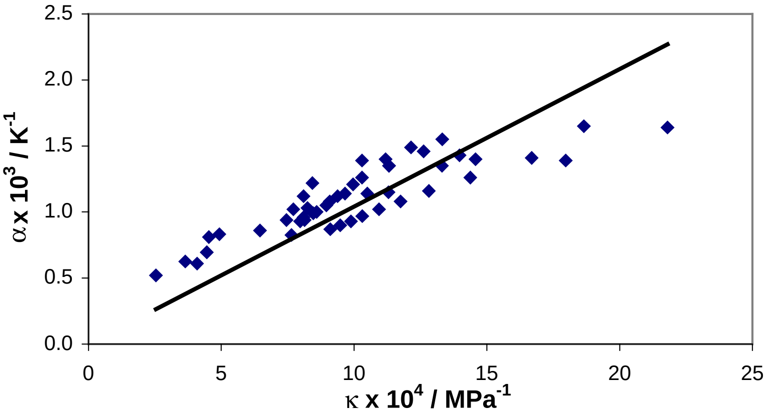

Fig. 3. Linear regression plot of cubic thermal expansivity ($\alpha \times 10^3$ (K^{-1})) vs. isothermal compressibility ($\kappa \times 10^4$ (MPa^{-1})) for 33 organic liquids [29] at 20–25 °C. Slope = 1.04 MPa K^{-1}.

and using average values from the correlations, together with the assumption of little change in molar volume. In practice, therefore, this procedure should be avoided.

The entropy–volume slopes, which represent the entropy gain per unit volume, increase in the sequence: organics < minerals ≈ ionic solids < ionic hydrates [22]. This sequence may be rationalised by reference to Eq. (A.1), which suggests that the slopes represent the isochoric (i.e., constant pressure) increase in pressure with rising temperature (cf. Appendix A). This increase in pressure is smallest for the soft organics, with their weak van der Waals intermolecular forces; larger for the ionics with their non-directional central coulombic forces; and largest for the ionic hydrates which also contain directed hydrogen bonds.

The net effect of our present results on entropy estimation, together with our earlier work on the estimation of enthalpies of ionic solids [6,21,26–28], is that estimations of the Gibbs energies of organic liquids and solids, as well as of a wide range of ionic solids and their hydrates, are now readily accessible, even to the occasional user.

Appendix A. Thermodynamic considerations

Standard thermodynamics demonstrates a close connection between the entropy and volume of a given closed, non-reacting thermodynamic system (independent of composition, whether containing a single component or even a mixture, although this is seldom, if ever, noted) through one of the set of Maxwell relations, namely:

$$\left(\frac{\partial S}{\partial V_\mathrm{m}}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V = \frac{\alpha}{k} \qquad \text{(A.1)}$$

where α is the coefficient of cubic thermal expansion:

$$\left(\frac{\partial V_\mathrm{m}}{\partial T}\right)_p = V_\mathrm{m}\alpha \qquad \text{(A.2)}$$

and κ is the coefficient of isothermal compressibility:

$$\left(\frac{\partial V_\mathrm{m}}{\partial p}\right)_T = -V_\mathrm{m}\kappa \qquad \text{(A.3)}$$

This relation has earlier been noted by Fyfe et al. [13] (see also Holland [23]) who observed that the two coefficients, α and κ, are approximately constant for ionic solids over a small temperature and pressure range, implying a linear relation between entropy, S°_{298}, and volume, V_m, at ambient conditions. Furthermore, for a given *class of materials* in a given phase—in this case, organics—the coefficients vary by less than an order of magnitude, and may be considered to be very roughly constant within their class (see Fig. 3). For organic liquids, typical values [29] near room temperature (20–25 °C) of α are of the order of 10^{-3} K^{-1} whilst values of κ lie near 10^{-9} Pa^{-1}. So that[6]

$$\left(\frac{\partial S}{\partial V_\mathrm{m}}\right)_T \approx 1\,\mathrm{MPa\,K^{-1}} \approx 600\,\mathrm{J\,K^{-1}\,mol^{-1}\,(nm^3\ per\ molecule)^{-1}} \qquad \text{(A.4)}$$

Fig. 3 shows, from the linear plot, that α/κ has a value of 1.04 MPa K^{-1} ≈ 624 J K^{-1} mol^{-1} (nm^3 per molecule)$^{-1}$ ≈ 1 J K^{-1} cm^{-3} for the group [29] of 33 organic liquids (for comparison, Fyfe et al. [13] report values between about 1.3 and 5.5 J K^{-1} cm^{-3} for most oxides and silicates); alternatively, the average value of α/κ for the same set of organic liquids is 713 J K^{-1} mol^{-1}/(nm^3 per molecule). In broad terms, larger values of α/κ for this data set are associated with materials having stronger intermolecular forces (such as hydrogen bonded alcohols exhibit) while weakly-bonded materials (such as hydrocarbons) have smaller values of α/κ—by up to a factor of three.

It is noticeable that these values of α/κ differ quite considerably from the correlational result which we obtain (Table 1) for the value of $(\partial S/\partial V_\mathrm{m})_T$, namely about 1200 J K^{-1} mol^{-1}/(nm^3 per molecule). We ascribe this difference to the different circumstances pertaining to α/κ and $(\partial S/\partial V_\mathrm{m})_T$ through their relation to $(\partial p/\partial T)_\mathrm{V}$ in Eq. (A.1), as follows. $(\partial p/\partial T)_V$ represents the pressure generated by a

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[6] 1 J K^{-1} mol^{-1} (nm^3 per molecule)$^{-1}$ = 1.66 × 10^3 Pa K^{-1}; 1 J K^{-1} cm^{-3} = 1 MPa K^{-1}.

material with increasing temperature (at fixed volume), the rising temperature resulting in increased anharmonicity in the intermolecular vibrations. Thus, this pressure arises from the compression of the *free volume* between the molecules since the *excluded volume* of the molecules themselves hardly themselves alters in volume with temperature. (The fact that it is the free volumes which are relevant has an analogy in the derivation of van der Waals gas equation of state where the term $[V - b]$ represents the volume between the molecules, and b is the excluded volume.) By contrast, our plot of S versus V_m represents the effect of adding *new material* to increase the volume; this new material represents largely excluded volume, and so the value of $(\partial p/\partial T)_V$ [and also of $(\partial S/\partial V_\mathrm{m})_T$] is increased beyond that of α/κ.

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