Predictive Thermodynamics for Condensed Phases

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Supplementary Information

Table S1: Correlations observed by Westwell et al.[7] between various

thermodynamic parameters fitted to the linear relationship: y = $mx + c$

y^a / kJ mol^{-1}	x^b	m	c	R^c
$\Delta_{sub}H$	T_m	0.188 / kJ mol^{-1} K^{-1}	0.522 / kJ mol^{-1}	0.95
$\Delta_{vap}H$	T_b	0.108 / kJ mol^{-1} K^{-1}	- 5.08 / kJ mol^{-1}	0.99
$\Delta_{vap}H$	T_m	0.166 / kJ mol^{-1} K^{-1}	- 3.99 / kJ mol^{-1}	0.93
$\Delta_{sub}H$	T_b	0.119 / kJ mol^{-1} K^{-1}	1.38 / kJ mol^{-1}	0.98
$\Delta_{vap}H$	$\Delta_{sub}H$	0.889	- 4.75 / kJ mol^{-1}	0.99

^{a} $\Delta_{sub}H$ = sublimation enthalpy / kJ mol^{-1}; $\Delta_{vap}H$ / kJ mol^{-1} = vaporization enthalpy.

^{b} T_m = melting temperature / K; T_b = boiling temperature / K.

^{c} Correlation coefficient.

Table S2: Constants for use in VBT equations[18] (12) and (13) for lattice energy / kJ

mol^{-1}. If U_{POT} < 5 000 kJ mol^{-1} then: $U_{POT} = 2I\,[\alpha/V_m^{1/3} + \beta]$ or $U_{POT} = \gamma\,(\rho_m / M_m)$

$^{1/3} + \delta$. If U_{POT} > 5 000 kJ mol^{-1}, then: $U_{POT} = AI(2I/V_m)^{1/3}$ where $A = 121.4$ kJ mol^{-1}

nm, where I is the lattice ionic strength factor and V_m is the formula unit volume.

Salt (charge ratio)	I, ionic strength factor	α / kJ mol^{-1} nm	β / kJ mol^{-1}	γ /kJ mol^{-1} cm	δ / kJ mol^{-1}
MX (1:1)	1	117.3	51.9	1981.2	103.8
M$_2$X (1:2)	3	165.3	-29.8	8375.6	-178.8
MX$_2$ (2:1)	3	133.5	60.9	6764.3	365.4
MX (2:2)	4	106.3	74.5	7181.5	596.0
general formula: M$_p$X$_q$ (q:p)	$\frac{1}{2}(pq^2 + qp^2)$	138.7	27.6	2342.6 · I	55.2·I

Table S3a: Unconstrained and constrained (c = 0) linear relationships[8] between standard entropy, S^o_{298} / J K^{-1} mol^{-1} and formula unit volume, V_m / nm^3 for inorganic solids.

compound type	number of compounds considered	fitted parameters for equations: $S^o_{298} = kV_m + c$ (6) $S^o_{298} = k'(M/\rho) + c$				S^o_{298} $= kV_m + c$
		k / J K^{-1} mol^{-1} (nm^{-3} formula unit)	k' /J K^{-1} cm^{-3}	c / J K^{-1} mol^{-1}	correlation coefficient . for volume-based equation, R^2	average unsigned % error for S^o_{298}, using equation
anhydrous ionic solids	65	1 360 ± 56	2.258 ± 0.093	15 ± 6	0.90	11.5
		1 481 ± 27	2.458 ± 0.045	0	0.88	12.6
hydrated ionic solids	67	1 579 ± 30	2.621 ± 0.050	6 ± 6	0.98	7.4
		1 606 ± 14	2.666 ± 0.023	0	0.96	7.4

Table S3b: Unconstrained and constrained (c = 0) linear relationships[8] between standard entropy, S^o_{298} / J K^{-1} mol^{-1} and formula unit volume, V_m / nm^3 for minerals.

mineral type	number of compounds considered	$S^o_{298} = kV_m + c$ (6)			
		k / J K^{-1} mol^{-1} (nm^{-3} formula unit)	c / J K^{-1} mol^{-1}	correlation coefficient R^2	average unsigned % error
minerals	99	1 262 ± 28	13 ± 5	0.95	12.6
		1 317 ± 18	0	0.94	11.6
silicates	53	1 303 ± 30	0 ± 5	0.97	9.1

combined, subset of data for minerals		$1\ 305 \pm 16$	0	0.95	9.1
ortho and ring structure silicates subset of data for silicates	20	$1\ 265 \pm 99$ $1\ 338 \pm 39$	10 ± 13 0	0.89 0.84	13.3 12.1
chain and band structure silicates subset of data for silicates	11	$1\ 176 \pm 56$ $1\ 216 \pm 36$	9 ± 9 0	0.98 0.88	9.9 10.9
sheet structure silicates subset of data for silicates	8	$1\ 490 \pm 205$ $1\ 251 \pm 32$	-51 ± 43 0	0.88 0.73	4.8 5.5
framework structure silicates subset of data for silicates	14	$1\ 384 \pm 27$ $1\ 350 \pm 16$	-10 ± 6 0	0.99 0.92	5.1 4.5

Table S3c: Unconstrained linear relationships[9] between standard entropy, S^o_{298} / J K^{-1} mol^{-1}, and volume per molecule, V_m, or density, ρ / g cm^{-3}, for condensed-phase organics.

compound type	number of compounds considered	$S^o_{298} = kV_m + c$ (6) and $S^o_{298} = k'(M/\rho) + c$				average unsigned % error
		[V_m-based] k / J K^{-1} mol^{-1} nm^{-3} molecule	[M/ρ-based] k' / J K^{-1} cm^{-3}	c / J K^{-1} mol^{-1}	correlation coefficient R^2	
Liquid n-paraffins (C$_5$-C$_{16}$)^a	12	$1\ 212.0 \pm 4.2$	2.012 ± 0.007	32.1 ± 1.5	1.00	0.25
Liquid n-alcohols (C$_1$-C$_{11}$)^a	11	$1\ 174.5 \pm 3.5$	1.949 ± 0.006	46.0 ± 0.8	1.00	0.34
Organic liquids	1 496	$1\ 133 \pm 7$	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