

Prediction of Heat Capacities of Solid Inorganic Salts from Group

Contributions.

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ABSTRACT

A group contribution technique is proposed to predict the coefficients in the heat capacity correlation, $C_p = a + bT + \frac{c}{T^2} + dT^2$, for solid inorganic salts. The results from this work are compared with fits to experimental data from the literature. It is shown to give good predictions for both simple and complex solid inorganic salts. Literature heat capacities for a large number (664) of solid inorganic salts covering a broad range of cations (129), anions (17) and ligands (2) have been used in regressions to obtain group contributions for the parameters in the heat capacity temperature function. A mean error of 3.18% is found when predicted values are compared with literature values for heat

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capacity at 298 °K. Estimates of the error standard deviation from the regression for each additivity constant are also determined.

INTRODUCTION

Group Contribution techniques are well studied and implemented to predict thermophysical properties such as heats of formation, ΔH_f^{298} , free energies of formation, ΔG_f^{298} , heat capacities, C_p , and liquid molar volume at normal boiling point, V_b , for organic compounds. Mostafa (1995) has previously described a group contribution method for predicting ΔH_f^{298} and ΔG_f^{298} of solid inorganic salts.

Read et al. (1987) describe a large number of the group contribution methods available in the literature for predicting heat capacity correlation coefficients for organic compounds. Joback (1984) used the following functional form to predict C_p of organic ideal gases:

$$C_p = \left(\sum_j n_j \Delta_{a,j} - 37.93 \right) + \left(\sum_j n_j \Delta_{b,j} + 0.210 \right) T + \left(\sum_j n_j \Delta_{c,j} - 3.91 \times 10^{-4} \right) T^2 + \left(\sum_j n_j \Delta_{d,j} + 2.06 \times 10^{-7} \right) T^3 \quad (1)$$

where, n_j is the number of groups of the j^{th} type, $\Delta_{k,j}$, contributions for the k^{th} ($k=a$, or b , or c , or d) coefficient and the j^{th} atomic or molecular group where T is in Kelvin (°K).

Yoneda (1979) uses the same concept but a different equation for ideal gases

$$C_p = \sum_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} \right) \left(\frac{T}{1000} \right) + \left(\sum_j n_j \Delta_{c,j} \right) \left(\frac{T}{1000} \right)^2 \quad (2)$$

where, n_j , is the number of groups of the j^{th} type, $\Delta_{k,j}$, contributions for the k^{th} ($k=a$, or b , or c , or d) coefficient and the j^{th} atomic or molecular group where T is in Kelvin ($^{\circ}\text{K}$).

Thinh et al. (1976) and Benson et al. (1969) also used the same idea but different functional form of Equation 1 and 2 to predict C_p for organic substances.

The following functional forms have been used by Robie et. al. (1979) to describe heat capacity of different inorganic solids.

$$C_p = a + bT + \frac{c}{T^2} + dT^2 + \frac{e}{\sqrt{T}} \quad (3)$$

$$C_p = a + bT + \frac{c}{T^2} + dT^2 \quad (4)$$

$$C_p = a + bT + \frac{c}{T^2} \quad (5)$$

$$C_p = a + bT + \frac{e}{\sqrt{T}} \quad (6)$$

$$C_p = a + bT \quad (7)$$

ASPEN PLUS[™] (1990), the interactive flowsheet simulator for process modeling, developed by Aspen Technology, Inc., Cambridge, MA, uses the following functional form for the heat capacities of solids,

$$C_p = a + bT + \frac{c}{T^2} + dT^2 + \frac{f}{T} + \frac{g}{\sqrt{T^3}} \quad (8)$$

where a , b , c , d , e , f , and g are constants. Kanacke and Kubaschewski (1990) used the functional form of Equation 4 for solid inorganic salts which is shown to fit experimental data well.

The inverse square of the absolute temperature functionality which appears in many of these relationship comes from Einstein's (McQuarrie, 1976) theory of the specific heat of crystals, which is

$$C_v = 3Nk \left(\frac{h\nu_E}{kT} \right)^2 \frac{e^{-h\nu_E/kT}}{\left(1 - e^{-h\nu_E/kT} \right)^2} \quad (9)$$

where, C_v , heat capacity at constant volume, N , number of atoms, k , Boltzmann constant, h , Plank constant, ν_E , Einstein frequency, and T , absolute temperature. The inverse square term appears as a dominant temperature functionality in the Taylor series expansion of Equation 9.

DEVELOPMENT OF METHOD

In the present work the functional form of Equation 4 has been selected and written as follows,

$$C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} \times 10^{-3} \right) T + \left(\sum_j n_j \Delta_{c,j} \times 10^6 \right) \frac{1}{T^2} + \left(\sum_j n_j \Delta_{d,j} \times 10^{-6} \right) T^2 \quad (10)$$

where, n_j , is the number of groups of the j^{th} type, $\Delta_{k,j}$, contributions for the k^{th} ($k=a$, or b , or c , or d) coefficient and the j^{th} atomic or molecular group where T is in Kelvin ($^{\circ}\text{K}$).

The values of the group contributions are obtained by regressing on C_p data from a number of (664) solid inorganic salts.

The parameters are predicted using the multiple linear regression relationship

$$\mathbf{b} = [\mathbf{X}^T \mathbf{X}]^{-1} \mathbf{X}^T \mathbf{y} \quad (11)$$

where $\mathbf{b}$ is a vector the j^{th} element of which contains $\Delta_{k,j}$, the calculated prediction for the k^{th} coefficient ($k=a$, or b , or c , or d) the j^{th} group contributions, $\mathbf{X}$ is a matrix in which the element in the i^{th} row and j^{th} column contains $(n_{i,j} - \bar{n}_j)$, where $n_{i,j}$ the number of occurrences of group j in compound i and $\bar{n}_j$ is the mean number of occurrences of group j in all salts in the regression, and $\mathbf{y}$ is a vector the i^{th} element of which contains the experimental values found for C_p , heat capacity for compound i . Estimates of the error in each of the calculated group contributions are obtained from the standard deviations of the parameters, s_{Δ_j} , which are calculated from the square roots of the diagonal elements of the variance-covariance matrix,

$$\mathbf{S} = \left(\frac{\mathbf{e}^T \mathbf{e}}{n - p - 1} \right) [\mathbf{X}^T \mathbf{X}]^{-1} \quad (12)$$

where n is the number of salts in the regression, p is the number of group contribution parameters being estimated, and $\mathbf{e}$ is the error vector,

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{b} \quad (13)$$

The reader is referred to Himmelblau (1970) for a discussion of regression and statistical parameter estimation.

The data for inorganic solid salt heat capacities used in the regression are obtained from Kanacke and Kubaschewski (1990). Data for Neptunium and the hydrates are collected from Barin (1989) at different temperatures and fitted in the functional form of Equation 4

to get the coefficients a , b , c , and d . Table II gives all the groups and their contributions, $\Delta_{k,j}$, estimated by the regression for a , b , c , and d . The columns in this table list, in order, the group being estimated, the number of occurrences of that group in the regression, the contribution of that group to $\Delta_{a,j}$, the contribution of that group to $\Delta_{b,j}$, the contribution of that group to $\Delta_{c,j}$, the contribution of that group to $\Delta_{d,j}$, the standard deviations of the estimate of $\Delta_{a,j}$, the standard deviations of the estimate of $\Delta_{b,j}$, the standard deviations of the estimate of $\Delta_{c,j}$, and the standard deviations of the estimate of $\Delta_{d,j}$.

PROCEDURE FOR PREDICTION BY THE PROPOSED METHOD

A stepwise procedure for the prediction of C_p by the proposed method is described below. Table I gives an illustrative example of this sequence of calculations. The successive steps are as follows:

- Step 1: Write the molecular structural formula for the solid inorganic salt.
- Step 2: Break the molecular structural formula into appropriate ionic, atomic, or ligand molecule structural groups as given in Table II. Then calculate the numerical contributions of each group by picking the numerical value of that specific group from Table II and multiplying it by the number of occurrences of the same group in the molecular structural formula.

- Step 3: Sum of the numerical values of the various groups to yield prediction for

$$\sum_j n_j \Delta_{a,j}, \sum_j n_j \Delta_{b,j}, \sum_j n_j \Delta_{c,j}, \text{ and } \sum_j n_j \Delta_{d,j} \text{ for Equation 10.}$$

- Step 4: Calculated C_p by plugging $\sum_j n_j \Delta_{a,j}$, $\sum_j n_j \Delta_{b,j}$, $\sum_j n_j \Delta_{c,j}$, and $\sum_j n_j \Delta_{d,j}$ in Equation 10 and using any absolute temperature T ($^{\circ}\text{K}$) as required.

Dean (1979) discusses the historical Kopp's simple rule for estimating heat capacity of a liquid or solid, which states that the heat capacity of a solid inorganic compound is approximately equal to the sum of the heat capacities of the constituent elements and that an approximate value expressed in gram calories per gram formula weight can be calculated by assigning atomic heat capacities to the elements.

Table III gives a comparison of predictions of heat capacities (C_p^{298}) for different solid inorganic salts using Kopp's rule and by the proposed method with the corresponding fits to experimental values. The columns in this table list, in order, the solid inorganic compound being considered, experimental values of heat capacity ($C_{p,Literature}^{298}$) at 298 $^{\circ}\text{K}$ found in the literature, predicted heat capacity ($C_{p,predicted}^{298}$) by the proposed method at 298 $^{\circ}\text{K}$, percent error associated with the prediction by the proposed method as compared to the experimental values, predicted heat capacity ($C_{p,predicted}^{298}$) by Kopp's rule, and percent error associated with the prediction by Kopp's rule. It can be seen that the proposed method gives better prediction. Heat capacities at the maximum temperature for which each correlation is valid (Kanacke and Kubaschewski (1990), Barin (1989)) are also predicted. A mean error of 8.17% is calculated for 649 of the 664 salts. The predictions for the remainder of the 15 compounds are poor. The errors for these poor predictions at their maximum temperature are as follows:

VO (43.53% @ 1973 °K), UO₂F₂ (49.2% @ 1500 °K), UO₂ (50.3% @ 2000 °K), TiO₂ (46.3% @ 2130 °K), TiF₃ (47.4 @ 1310 °K), ThO₂ (94.5% @ 2500 °K), ScF₃ (55.5 % @ 1825 °K), NpO₃.H₂O (100.4% @ 800 °K), MoF₃ (93.1% @ 1237 °K), MoCl₃ (52.1 % @ 926 °K), MoBr₃ (60.4% @ 1082 °K), MgO (43.8% @ 3105 °K), GeO₂ (68.0% @ 1409 °K), FeF₃ (46.5% @ 1132 °K), and Be₂SiO₄ (63.5% @ 1806 °K). Essentially all of these higher error levels are for oxides and helides of single cations.

SUMMARY AND CONCLUSION

As mentioned earlier C_p values predicted by the proposed method are in good agreement with the literature values at low and moderate temperatures. In Figures 1 and 2, the literature and predicted heat capacities of CaTiO₃ and Fe₂(SO₄)₃ have been plotted as a function of absolute temperatures. The temperature range used in each of the figures (Figure 1, 2, 3, & 4) are the range given by Robie et. al. (1979) over which their fit of experimental heat capacity data is said to be valid. For CaTiO₃, the predictions are close to experimental values up to 1200 °K and then the proposed method deviates by predicting higher values. For Fe₂(SO₄)₃, predictions are good from 300-600 °K and then deviates. One of the poorest predictions obtained is shown in Figure 3. Here, for FeTiO₃, the predictions begin to deviate at much lower temperature. Figure 4 illustrate one of cases found for under prediction at high temperature. Here, for Mg(OH)₂, predictions and the experimental values are almost the same from 298-600 °K and then the predictions deviate. In general, it can be said that the proposed method gives estimates of heat capacity with in an acceptable range of accuracy at most temperatures.

In the regression of heat capacity 664 solid inorganic salts have been used and their corresponding C_p^{298} values are predicted. A mean error of 3.18%, a maximum error of 13.63% is found for these salts. This method can not be used for single metallic carbides, sulfides, hydrides, and nitrides such as CaC_2 , CaS , CaH_2 , and Mg_3N_2 . This method is also not applicable for metallic solutions such as Al_2Se_3 , ScAs , NiSe , NiTe , PbTe , etc..

Table I. Estimation of C_p from Equation 6.

Step Number	C_p				
1	CaAl_2O_4				
	Group	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$
2	Ca^{++}	1(20.4698)	1(-6.2249)	1(-0.02629)	1(-3.21927)
2	Al^{+++}	2(10.3059)	2(4.5183)	2(-0.62271)	2(-3.7007)
2	O^-	4(28.1522)	4(12.0434)	4(-0.74718)	4(-4.02248)
3	$\sum_j n_j \Delta_{i,j}$	153.6904	50.9853	-4.26043	-26.71059
4	$C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} \times 10^{-3} \right) T + \left(\sum_j n_j \Delta_{c,j} \times 10^6 \right) \frac{1}{T^2}$ $+ \left(\sum_j n_j \Delta_{d,j} \times 10^{-6} \right) T^2$ $= 153.6904 + (50.9853) \times (10^{-3}) \times (298) + (-4.26043) \times 10^6 / (298)^2 +$ $(-26.71059) \times (10^{-6}) \times (298)^2 = 118.54 \text{ J/(g mol } ^\circ\text{K)}.$				

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NOMENCLATURE

- b = the vector the j^{th} element of which contains $\Delta_{i,j}$, the calculated estimates for the j^{th} group contributions.
- C_p^{298} = heat capacity at 298 °K, J/(g mol °K).
- C_p = heat capacity, J/(g mol °K).
- C_v = heat capacity at constant volume, J/(g mol °K).
- e = the vector containing the errors between the experimental values and those predicted by regression.
- h = Plank constant.
- k = Boltzmann constant.
- N = number of atoms.
- n = total number of salts in the regression.
- $n_{i,j}$ = number of occurrences of group j in compound i .
- $\bar{n}_j$ = mean number of occurrences of group j in all salts in the regression.
- n_j = number of groups of the j^{th} type.
- p = number of group contribution parameters being estimated.
- S = variance-covariance matrix.
- s_{Δ_j} = standard deviations of the parameters.
- V_b = liquid molar volume at normal boiling point.
- X = the matrix the i,j^{th} element of which contains $(n_{i,j} - \bar{n}_j)$.
- y = the vector the i^{th} element of which contains the experimental values found for C_p for compound i .
- ν_E = Einstein frequency.

ΔH_f^{298} = heat of formation, $KJ/(g\ mol)$.

ΔG_f^{298} = free energy of formation, $KJ/(g\ mol)$.

$\Delta_{k,j}$ = group contribution for k of i^{th} ionic, atomic or ligand molecule group.

$\Delta_{a,j}$ = group contribution for a of i^{th} ionic, atomic or ligand molecule group.
 $J/(g\ mol\ ^\circ K)$.

$\Delta_{b,j}$ = group contribution for b of i^{th} ionic, atomic or ligand molecule group.
 $J/(g\ mol\ (^\circ K)^2)$.

$\Delta_{c,j}$ = group contribution for c of i^{th} ionic, atomic or ligand molecule group.
 $(J\ ^\circ K)/(g\ mol)$.

$\Delta_{d,j}$ = group contribution for d of i^{th} ionic, atomic or ligand molecule group.
 $J/(g\ mol\ (^\circ K)^3)$.

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Table II. Solid inorganic Salt Groups.

Cationic, anionic, ligand molecule groups, their contributions, number of occurrences in the regression, standard deviation (s_{Δ_j}) associated with them for a , b , c , and d .

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	s_{Δ_j} for $\Delta_{a,j}$	s_{Δ_j} for $\Delta_{b,j}$	s_{Δ_j} for $\Delta_{c,j}$	s_{Δ_j} for $\Delta_{d,j}$
Cations									
Ag ⁺	8	11.398	24.063	0.434	2.106	5.613	12.287	0.269	8.322
Al ⁺⁺⁺	81	10.306	4.518	-0.623	-3.701	3.420	7.485	0.164	5.069
As ⁺⁺⁺	6	-18.849	69.121	0.995	6.034	5.785	12.663	0.277	8.576
As ⁺⁺⁺⁺	4	-16.941	25.671	1.183	5.796	2.715	5.943	0.130	4.025
B ⁺⁺⁺	59	-13.188	16.765	0.273	-0.219	14.813	32.424	0.710	21.960
Ba ⁺⁺	23	26.676	-15.773	0.054	7.523	1.546	3.384	0.074	2.292
Be ⁺⁺	16	-5.164	22.314	-0.002	6.544	2.783	6.092	0.133	4.126
Bi ⁺⁺⁺	9	-3.363	14.344	1.658	2.171	1.257	2.753	0.060	1.864
Ca ⁺⁺	64	20.470	-6.225	-0.026	-3.219	2.384	5.217	0.114	3.534
Cd ⁺⁺	14	21.910	-23.495	0.561	6.178	4.737	10.369	0.227	7.023
Ce ⁺⁺⁺	9	13.011	-7.089	0.762	4.687	3.088	6.760	0.148	4.579
Ce ⁺⁺⁺⁺	1	8.506	-6.387	0.734	8.045	3.010	6.589	0.144	4.462
Cm ⁺⁺⁺	1	-5.346	10.658	0.076	-3.166	6.906	15.116	0.331	10.238
Co ⁺⁺	17	26.552	-19.272	0.327	5.245	18.490	40.473	0.887	27.411
Co ⁺⁺⁺	1	34.158	-42.075	-0.149	-4.614	12.259	26.834	0.588	18.174
Cr ⁺⁺	4	16.779	-8.351	0.152	0.073	1.353	2.962	0.065	2.006
Cr ⁺⁺⁺	22	21.086	-16.392	0.067	5.298	3.272	7.162	0.157	4.851
Cr ⁺⁺⁺⁺	4	-23.112	27.266	1.662	8.719	3.228	7.066	0.155	4.786
Cs ⁺	8	20.779	-0.058	0.520	11.137	10.108	22.126	0.485	14.985
Cu ⁺	7	11.289	12.683	0.270	4.246	13.191	28.874	0.633	19.555

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	s_{Δ_j} for $\Delta_{a,j}$	s_{Δ_j} for $\Delta_{b,j}$	s_{Δ_j} for $\Delta_{c,j}$	s_{Δ_j} for $\Delta_{d,j}$
Cu ⁺⁺	11	19.179	3.018	-0.002	-1.275	9.051	19.811	0.434	13.418
Dy ⁺⁺⁺	4	21.060	-15.320	0.476	2.925	5.094	11.151	0.244	7.552
Er ⁺⁺⁺	2	17.635	-17.241	1.542	-3.292	13.191	28.874	0.633	19.555
Eu ⁺⁺	2	22.957	-9.764	0.500	3.050	11.995	26.256	0.575	17.782
Eu ⁺⁺⁺	6	35.717	-36.906	0.298	18.834	15.374	33.652	0.737	22.791
Fe ⁺⁺	15	20.486	-5.415	0.055	5.393	6.074	13.295	0.291	9.004
Fe ⁺⁺⁺	26	16.618	3.328	0.082	5.002	13.171	28.830	0.632	19.525
Ga ⁺⁺⁺	9	16.577	-11.146	-0.034	5.207	4.675	10.233	0.224	6.930
Gd ⁺⁺⁺	7	20.474	-20.495	0.163	3.088	14.364	31.441	0.689	21.294
Ge ⁺⁺	2	17.815	-5.864	0.556	3.312	6.528	14.289	0.313	9.678
Ge ⁺⁺⁺	2	-7.106	41.113	0.226	6.623	9.494	20.782	0.455	14.075
H ⁺	12	-5.217	25.754	0.232	2.576	6.839	14.969	0.328	10.138
Hf ⁺⁺	1	8.841	-27.084	0.280	2.601	4.451	9.744	0.213	6.599
Hf ⁺⁺⁺⁺	9	20.580	-22.025	-0.050	2.633	6.366	13.935	0.305	9.438
Hg ⁺	8	23.601	0.155	0.078	0.036	25.914	56.722	1.243	38.416
Hg ⁺⁺	6	8.228	19.740	0.585	2.319	2.770	6.063	0.133	4.106
Ho ⁺⁺⁺	6	33.919	-49.884	0.133	19.321	6.964	15.244	0.334	10.324
In ⁺	3	15.693	13.602	0.212	0.561	7.036	15.401	0.337	10.430
In ⁺⁺	1	5.362	29.459	0.502	-1.314	7.587	16.607	0.364	11.247
In ⁺⁺⁺	5	13.433	-4.548	0.310	2.953	7.675	16.800	0.368	11.378
Ir ⁺⁺⁺	2	13.108	-18.124	0.469	0.573	5.394	11.808	0.259	7.997
Ir ⁺⁺⁺⁺	1	5.576	-3.667	0.394	8.045	6.983	15.285	0.335	10.352
K ⁺	48	25.309	-2.284	0.218	5.174	18.426	40.333	0.884	27.316
La ⁺⁺⁺	8	15.803	-11.296	0.458	3.344	18.643	40.808	0.894	27.638
Li ⁺	47	15.639	4.124	-0.007	7.973	6.207	13.585	0.298	9.201
Lu ⁺⁺⁺	3	18.605	-16.153	0.172	3.904	10.230	22.392	0.491	15.166

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
Mg ⁺⁺	32	14.639	-0.637	-0.074	-0.609	11.283	24.698	0.541	16.727
Mn ⁺⁺	15	21.419	-15.908	0.265	5.652	13.410	29.352	0.643	19.879
Mn ⁺⁺⁺	4	8.913	3.070	0.454	5.448	19.073	41.749	0.915	28.275
Mo ⁺⁺	3	22.549	-9.633	0.289	1.122	1.575	3.447	0.076	2.335
Mo ⁺⁺⁺	4	-28.076	84.735	1.976	0.108	5.333	11.673	0.256	7.906
Mo ⁺⁺⁺⁺	3	19.349	-24.670	0.62	0.855	6.632	14.516	0.318	9.831
Mo ⁺⁺⁺⁺⁺	2	-48.550	202.730	1.237	-5.487	25.970	56.846	1.245	38.500
Mo ⁺⁺⁺⁺⁺⁺	11	-7.473	-7.423	1.279	13.430	10.108	22.125	0.485	14.985
Na ⁺	91	14.186	9.665	0.529	4.851	13.171	28.830	0.632	19.526
Nb ⁺⁺⁺	1	20.593	-14.387	0.043	-1.971	13.265	29.036	0.636	19.665
Nb ⁺⁺⁺⁺	3	12.016	-14.823	0.494	2.709	7.278	15.931	0.349	10.789
Nb ⁺⁺⁺⁺⁺	5	19.843	-33.720	0.517	1.065	25.907	56.707	1.242	38.406
Nd ⁺⁺⁺	9	15.042	-4.286	0.450	3.311	15.349	33.597	0.736	22.754
NH4 ⁺	4	4.205	116.120	1.206	2.166	10.477	22.932	0.502	15.531
Ni ⁺⁺	14	22.497	-6.671	-0.022	6.234	15.110	33.074	0.725	22.400
Np ⁺⁺⁺	2	23.683	-10.822	0.742	-3.274	13.265	29.036	0.636	19.665
Np ⁺⁺⁺⁺	3	-12.661	62.760	1.250	-48.715	15.378	33.662	0.737	22.798
Np ⁺⁺⁺⁺⁺	2	-19.545	-43.129	1.616	356.929	18.835	41.228	0.903	27.922
P ⁺⁺⁺⁺⁺	12	-39.486	50.248	1.686	2.325	8.664	18.965	0.415	12.844
Pb ⁺⁺	26	14.632	7.448	0.642	4.828	25.970	56.846	1.245	38.500
Pb ⁺⁺⁺⁺	1	0.7457	4.913	1.076	8.045	26.165	57.272	1.255	38.789
Pd ⁺⁺	3	15.727	-2.973	0.496	1.895	25.907	56.707	1.242	38.406
Pr ⁺⁺⁺	6	20.343	-11.940	0.213	2.084	25.970	56.846	1.245	38.500
Pr ⁺⁺⁺⁺	1	21.266	0.933	0.419	8.045	10.836	23.719	0.520	16.064
Pt ⁺⁺	2	14.033	4.772	0.453	0.382	15.136	33.131	0.726	22.439
Pt ⁺⁺⁺	2	28.058	-25.164	0.679	0.573	7.393	16.183	0.355	10.960

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
Pt ⁺⁺⁺	2	43.127	-50.286	0.905	0.764	7.690	16.832	0.369	11.400
Pu ⁺⁺	7	31.509	-15.262	0.127	3.352	10.108	22.126	0.485	14.985
Pu ⁺⁺⁺	2	35.028	-39.982	-0.268	-1.420	25.819	56.515	1.238	38.276
Pu ⁺⁺⁺⁺⁺	2	-17.410	43.930	0.385	-1.932	15.111	33.076	0.725	22.402
Rb ⁺	16	19.747	5.160	0.526	7.198	10.959	23.987	0.526	16.246
Re ⁺⁺⁺	1	11.056	-11.407	0.201	8.045	25.970	56.846	1.245	38.500
Re ⁺⁺⁺⁺	1	3.204	-19.960	0.492	12.067	9.768	21.382	0.468	14.481
Re ⁺⁺⁺⁺⁺	2	-7.326	6.207	1.683	15.007	18.569	40.645	0.890	27.528
Rh ⁺⁺⁺	4	10.964	3.8319	0.338	4.214	1.660	3.634	0.080	2.461
Ru ⁺⁺	1	35.233	-31.127	0.754	-1.971	6.705	14.676	0.322	9.940
Ru ⁺⁺⁺	1	20.326	-13.287	-0.920	8.045	5.090	11.141	0.244	7.545
Sb ⁺⁺	6	-11.375	36.678	1.780	0.090	6.772	14.823	0.325	10.039
Sc ⁺⁺	5	12.644	-15.208	0.330	2.953	6.171	13.507	0.296	9.148
Se ⁺⁺⁺	6	-14.644	16.581	1.731	5.589	18.623	40.763	0.893	27.607
Se ⁺⁺⁺⁺	2	0.120	-8.773	0.697	10.056	8.016	17.547	0.384	11.884
Se ⁺⁺⁺⁺⁺	2	-63.818	110.803	2.335	10.990	18.623	40.763	0.893	27.607
Si ⁺⁺⁺	79	-2.308	4.382	-0.041	-3.301	7.003	15.329	0.336	10.382
Sm ⁺⁺	1	24.182	-4.011	0.502	-1.314	6.803	14.892	0.326	10.086
Sm ⁺⁺⁺	8	22.693	-10.606	0.327	3.826	18.411	40.299	0.883	27.294
Sn ⁺⁺	6	16.189	5.634	0.378	1.586	7.268	15.908	0.349	10.774
Sn ⁺⁺⁺	1	10.166	-7.447	-0.180	8.045	13.249	29.000	0.635	19.641
Sr ⁺⁺	14	15.410	-0.275	0.381	4.159	6.889	15.079	0.330	10.213
Sr ⁺⁺⁺	1	17.666	-6.047	1.494	8.045	7.441	16.287	0.357	11.030
Ta ⁺⁺	1	16.373	-14.807	0.043	-1.971	18.623	40.763	0.893	27.607
Ta ⁺⁺⁺	1	27.033	-41.503	-0.208	-2.628	7.932	17.361	0.380	11.758
Ta ⁺⁺⁺⁺	9	12.959	-20.800	0.439	4.567	7.475	16.363	0.358	11.082

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
Tb ⁺⁺⁺	5	18.899	-10.177	0.342	3.065	15.232	33.340	0.730	22.580
Tb ⁺⁺⁺⁺	1	8.506	-6.387	0.733	8.045	8.228	18.010	0.395	12.198
Tc ⁺⁺⁺	1	12.316	-12.577	0.038	8.045	25.819	56.515	1.238	38.276
Tc ⁺⁺⁺⁺	1	23.493	-36.130	2.242	12.067	7.932	17.361	0.380	11.758
Te ⁺⁺⁺	2	20.470	-25.515	0.999	2.709	18.411	40.299	0.883	27.294
Th ⁺⁺⁺	11	20.291	-28.458	0.351	-1.633	8.577	18.773	0.411	12.715
Ti ⁺⁺	4	21.321	-9.603	0.209	1.847	25.871	56.630	1.241	38.353
Ti ⁺⁺⁺	7	0.689	23.784	0.839	3.471	8.857	19.388	0.425	13.131
Ti ⁺⁺⁺⁺	34	10.043	-7.562	0.299	11.414	25.907	56.707	1.242	38.406
Tl ⁺	7	15.850	20.050	0.507	0.635	26.065	57.054	1.250	38.641
Tl ⁺⁺⁺	3	25.172	-13.439	-0.203	5.087	8.112	17.756	0.389	12.025
Tm ⁺⁺⁺	4	23.189	-19.727	0.482	3.370	18.959	41.499	0.909	28.106
U ⁺⁺	4	17.864	-10.375	0.780	0.108	18.569	40.645	0.890	27.528
U ⁺⁺⁺	7	26.669	-29.923	-0.066	2.171	25.819	56.515	1.238	38.276
U ⁺⁺⁺⁺	4	13.890	-31.178	0.627	-2.126	19.886	43.528	0.954	29.480
U ⁺⁺⁺⁺⁺	11	-14.769	50.875	1.654	-14.399	26.165	57.272	1.255	38.789
V ⁺⁺	4	20.124	-11.173	0.087	1.847	25.970	56.846	1.245	38.500
V ⁺⁺⁺	4	20.671	-27.881	0.199	0.867	25.970	56.846	1.245	38.500
V ⁺⁺⁺⁺	3	2.121	2.604	1.214	1.988	18.487	40.466	0.887	27.407
V ⁺⁺⁺⁺⁺	20	-1.279	-5.243	0.697	13.608	18.386	40.246	0.882	27.257
W ⁺⁺	1	18.062	1.149	0.502	-1.314	18.487	40.466	0.887	27.407
W ⁺⁺⁺	2	6.405	3.023	0.790	2.709	18.679	40.886	0.896	27.691
W ⁺⁺⁺⁺	2	-6.784	42.333	1.062	0.956	6.585	14.415	0.316	9.763
W ⁺⁺⁺⁺⁺	20	-23.788	35.451	1.836	9.893	11.045	24.177	0.530	16.374
Y ⁺⁺⁺	5	22.197	-22.411	0.002	3.065	3.823	8.368	0.183	5.667
Yb ⁺⁺	1	14.772	0.169	0.502	-1.314	25.970	56.846	1.245	38.500

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
Yb ⁺⁺⁺	4	23.895	-21.427	0.346	2.925	7.762	16.991	0.372	11.507
Zn ⁺⁺	18	12.599	-0.744	0.377	4.203	12.729	27.863	0.610	18.871
Zr ⁺⁺	4	30.330	-18.041	0.077	0.072	8.019	17.554	0.385	11.888
Zr ⁺⁺⁺	4	26.864	-34.755	-0.144	0.108	11.751	25.722	0.564	17.421
Zr ⁺⁺⁺⁺	13	17.188	-23.478	-0.063	7.098	7.905	17.304	0.379	11.720
Anions									
Br ⁻	166	26.093	14.767	-0.201	-1.039	9.698	21.228	0.465	14.377
Cl ⁻	295	26.609	10.376	-0.251	0.657	8.392	18.368	0.402	12.440
ClO3 ⁻	2	56.325	104.045	-1.043	-5.013	11.537	25.253	0.553	17.103
ClO4 ⁻	4	113.901	46.380	-3.511	-6.944	8.502	18.611	0.408	12.605
CO3 ⁻	15	47.278	86.757	-0.887	-5.133	18.462	40.411	0.885	27.369
F ⁻	247	22.041	15.652	-0.244	1.538	15.349	33.597	0.736	22.754
HCO3 ⁻	2	26.758	138.905	-0.373	-5.013	18.958	41.497	0.909	28.105
I ⁻	132	26.999	13.542	-0.182	-1.300	7.373	16.138	0.354	10.930
N ⁻⁻⁻	2	24.083	31.806	-0.764	3.644	15.410	33.732	0.739	22.845
NO2 ⁻	1	18.307	126.388	0.596	-4.044	19.692	43.103	0.944	29.192
NO3 ⁻	120	49.766	83.928	-0.478	-7.040	26.387	57.758	1.265	39.118
O ⁻	36	34.706	3.050	-1.052	-6.604	4.844	10.604	0.232	7.182
O ⁺	1155	28.152	12.043	-0.747	-4.023	18.490	40.473	0.887	27.411
OH ⁻	16	28.917	30.730	-0.628	3.257	4.780	10.462	0.229	7.086
PO4 ⁻⁻⁻	6	95.827	56.863	-2.462	-7.691	26.695	58.433	1.280	39.575
SO3 ⁻	1	78.739	24.184	-1.058	-9.702	11.282	24.694	0.541	16.725
SO4 ⁻	49	85.866	52.357	-1.925	-0.047	2.270	4.969	0.109	3.365
Ligand Molecules									

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
CO	18	36.332	20.257	-0.265	-1.780	26.181	57.306	1.256	38.812
H2O	39	15.458	66.593	0.470	-40.518	3.561	7.794	0.171	5.278

Table III. Predicted and Experimental Values, Percent Error.

Comparison of heat capacities by the proposed method, Kopp's rule with the corresponding experimental values and the percent errors (% Error) associated with some selected solid inorganic salts.

COMPOUND	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$ Proposed Method	% Error Proposed Method	$C_{p, \text{predicted}}^{298}$ Kopp's Rule	% Error Kopp's Rule
Ag ₂ CO ₃	- 111.60	109.98	1.45	109.62	1.77
Ag ₂ SO ₄	131.44	127.08	3.31	141.42	7.59
AgNO ₂	81.34	85.97	5.70	85.35	4.94
AgNO ₃	93.01	92.41	0.64	102.09	9.76
Al(OH) ₃	93.05	98.19	5.53	105.02	12.87
Al ₂ (SO ₄) ₃	260.15	248.00	4.67	320.49	23.20
AlOCl	56.83	54.21	4.61	68.62	20.74
AlPO ₄	92.98	88.67	4.63	115.48	24.19
Ba(NO ₃) ₂	151.32	160.79	6.25	178.24	17.79
Ba ₂ TiO ₄	149.13	150.56	0.95	144.77	2.93
Ba ₃ Al ₂ O ₆	215.35	216.20	0.39	230.12	6.86
BaCO ₃	87.97	85.94	2.31	83.68	4.88
BaHfO ₃	108.25	105.86	2.21	102.09	5.69
BaSO ₄	101.67	103.04	1.35	115.48	13.58
BaTiO ₃	102.38	104.34	1.91	102.09	0.29
BaV ₂ O ₆	172.78	173.51	0.42	178.24	3.16
BaZrO ₃	105.39	102.27	2.95	102.09	3.13
Be(OH) ₂	65.55	64.63	1.40	78.66	20.01
BeAl ₂ O ₄	104.88	102.55	2.22	144.77	38.03
BeAl ₆ O ₁₀	261.81	257.61	1.60	348.95	33.28
BeSO ₄	85.60	81.84	4.40	115.48	34.90
Bi ₂ (SO ₄) ₃	278.82	278.93	0.04	320.49	14.95
BiOCl	70.16	69.67	0.70	68.62	2.20
Ca(NO ₃) ₂	149.29	155.57	4.20	178.24	19.39
Ca(OH) ₂	87.56	80.62	7.92	78.66	10.16
Ca ₂ B ₂ O ₅	147.05	140.63	4.37	158.16	7.55
Ca ₂ P ₂ O ₇	187.70	186.21	0.79	214.22	14.13
Ca ₂ V ₂ O ₇	213.88	209.29	2.15	220.92	3.29
Ca ₃ Al ₂ O ₆	209.65	200.54	4.34	230.12	9.76
Ca ₃ B ₂ O ₆	187.77	181.63	3.27	200.83	6.96
Ca ₃ P ₂ O ₈	236.03	227.22	3.73	256.90	8.84
Ca ₃ WO ₆	202.24	200.25	0.99	204.18	0.96
CaAl ₂ O ₄	120.55	118.54	1.67	144.77	20.08
CaAl ₄ O ₇	193.83	196.07	1.16	246.86	27.36
CaB ₂ O ₄	103.83	99.63	4.05	115.48	11.22
CaB ₄ O ₇	157.74	158.25	0.33	188.28	19.36

COMPOUND	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$ Proposed Method	% Error Proposed Method	$C_{p, \text{predicted}}^{298}$ Kopp's Rule	% Error Kopp's Rule
CaCO ₃ .MgCO ₃	155.18	156.98	1.16	167.36	7.85
CaCr ₂ O ₄	146.59	144.77	1.24	144.77	1.24
CaFe ₂ O ₅	194.05	188.88	2.66	187.44	3.40
CaMgO ₂	79.61	77.54	2.60	85.35	7.22
CaMoO ₄	117.06	115.82	1.06	118.83	1.51
CaO.HfO ₂	105.71	100.64	4.80	102.09	3.42
CaUO ₄	130.44	127.65	2.13	118.83	8.90
CaV ₂ O ₆	170.74	168.29	1.44	178.24	4.39
Li ₂ B ₄ O ₇	170.34	175.21	2.86	214.22	25.76
Li ₂ BeF ₄	134.97	133.42	1.15	161.50	19.66
Li ₂ CO ₃	97.96	97.68	0.30	109.62	11.90
Li ₂ HfO ₃	111.87	117.59	5.11	128.03	14.44
Li ₂ Nb ₂ O ₆	198.55	204.22	2.86	204.18	2.83
Li ₂ SO ₄	117.14	114.78	2.01	141.42	20.73
Li ₂ Ta ₂ O ₆	200.14	197.02	1.56	204.18	2.02
Li ₂ WO ₄	133.34	135.20	1.39	144.77	8.57
Li ₂ ZrO ₃	110.20	114.01	3.45	128.03	16.18
Li ₃ AlF ₆	202.30	201.38	0.45	229.28	13.34
LiBeF ₃	92.61	91.83	0.84	114.64	23.79
LiClO ₄	104.94	105.06	0.12	118.83	13.24
LiNO ₃	89.11	86.26	3.20	102.09	14.56
LiOH	49.75	48.79	1.93	52.30	5.13
Mg(NO ₃) ₂	141.90	151.10	6.48	178.24	25.61
Mg(OH) ₂	77.49	76.15	1.73	78.66	1.50
Mg ₂ V ₂ O ₇	202.26	200.35	0.94	220.92	9.23
Mg ₃ P ₂ O ₈	213.09	213.82	0.34	256.90	20.56
MgAl ₂ O ₄	115.94	114.07	1.61	144.77	24.87
MgCO ₃	75.40	76.26	1.13	83.68	10.98
MgFe ₂ O ₄	137.76	143.41	4.10	144.77	5.09
MgMoO ₄	110.88	111.35	0.42	118.83	7.16
MgSO ₄	95.57	93.36	2.31	115.48	20.83
MgTi ₂ O ₅	146.60	152.76	4.21	161.50	10.17
MgTiO ₃	91.17	94.65	3.82	102.09	11.98
MgV ₂ O ₆	159.87	163.82	2.47	178.24	11.49
MgWO ₄	109.83	113.78	3.59	118.83	8.19
UBr ₃	108.73	107.96	0.71	103.76	4.57
UBr ₄	128.11	129.74	1.27	129.70	1.24
UCl ₃	102.52	104.35	1.79	103.76	1.21
UCl ₄	120.77	124.93	3.44	129.70	7.40
UCl ₅	144.57	146.12	1.08	155.64	7.66

COMPOUND	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$ Proposed Method	% Error Proposed Method	$C_{p, \text{predicted}}^{298}$ Kopp's Rule	% Error Kopp's Rule
UCl ₆	175.53	179.32	2.16	181.59	3.45
UF ₃	95.08	95.86	0.82	88.70	6.71
UF ₄	116.01	113.60	2.08	109.62	5.51
UF ₅	132.30	131.96	0.26	130.54	1.33
UF ₆	167.43	162.33	3.05	151.46	9.54
UI ₃	112.02	110.18	1.65	103.76	7.37
UI ₄	134.43	132.69	1.30	129.70	3.52
UO ₂	63.57	63.14	0.68	59.41	6.54
UO ₂ SO ₄	144.88	143.47	0.97	148.95	2.81
UOBr ₂	97.88	96.44	1.47	94.56	3.40

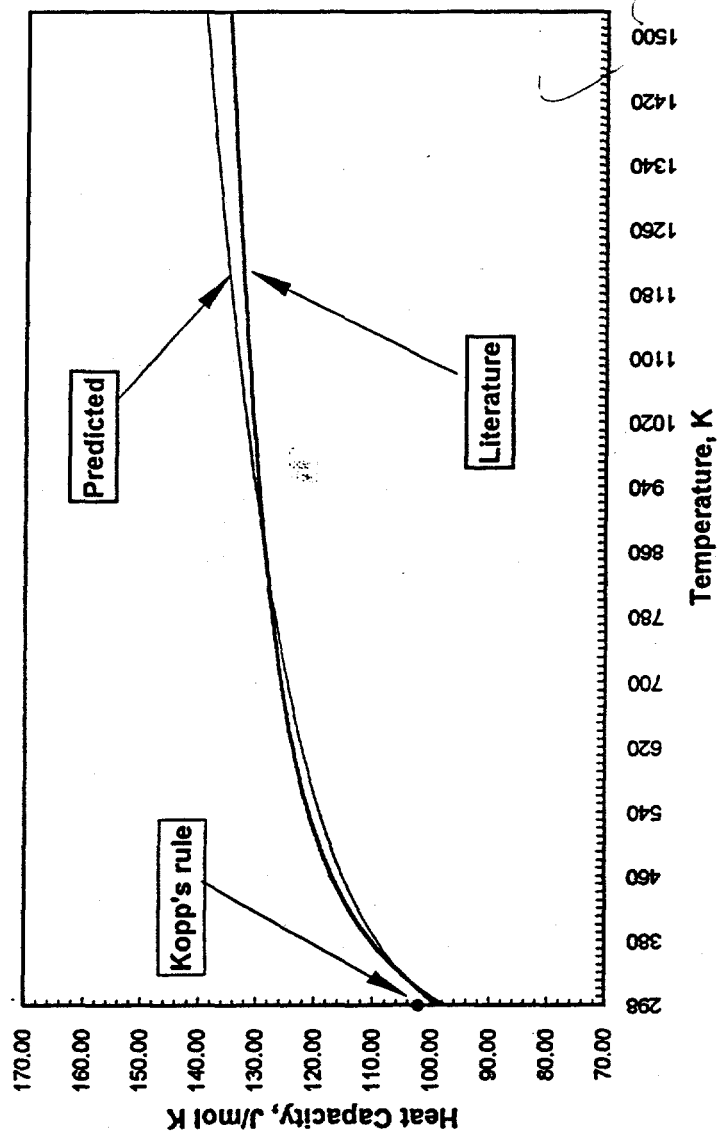


Figure 1. Heat capacity (C_p , J/mol °K) vs. temperature (°K) of CaTiO_3 for literature (From Robie et. al., 1979) and predicted values

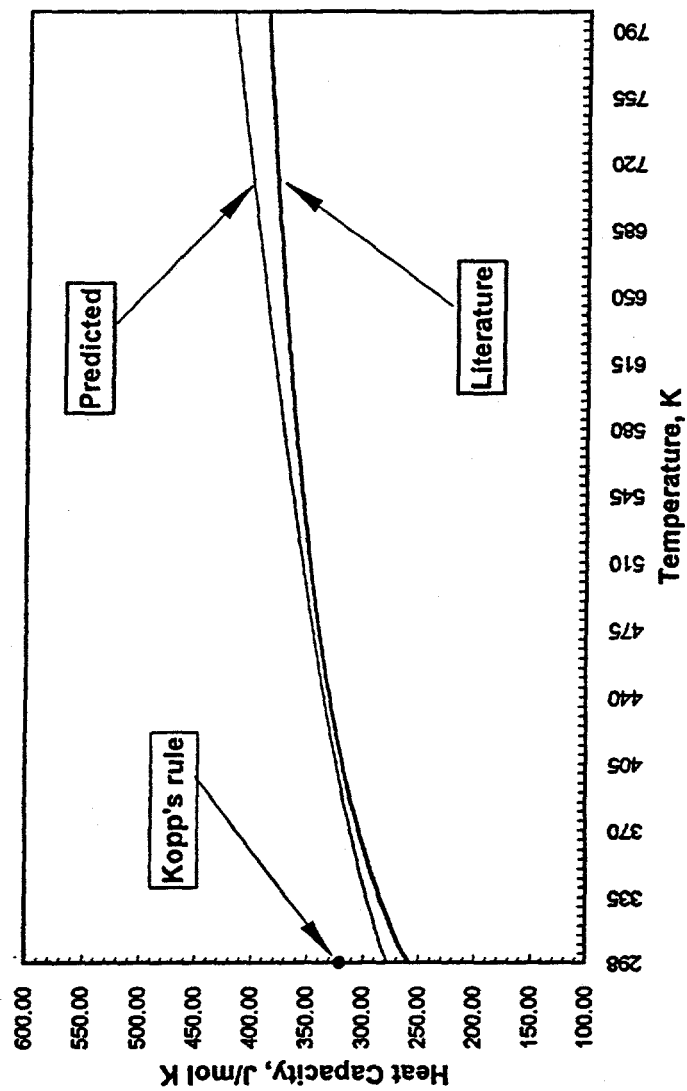


Figure 2. Heat capacity (C_p , J/mol °K) vs. temperature (°K) of $\text{Fe}_2(\text{SO}_4)_3$ for literature (From Robie et. al., 1979) and predicted values.

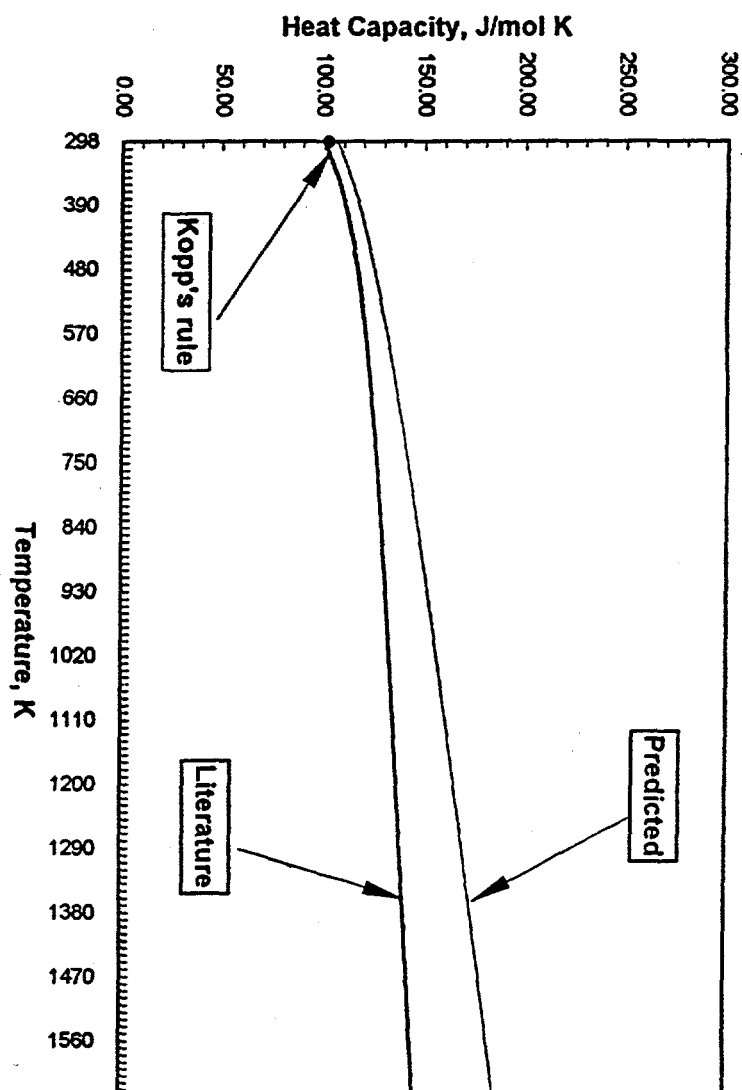


Figure 3. Heat capacity (C_p , J/mol K) vs. temperature (°K) of FeTiO_3 for literature (From Robie et. al., 1979) and predicted values.

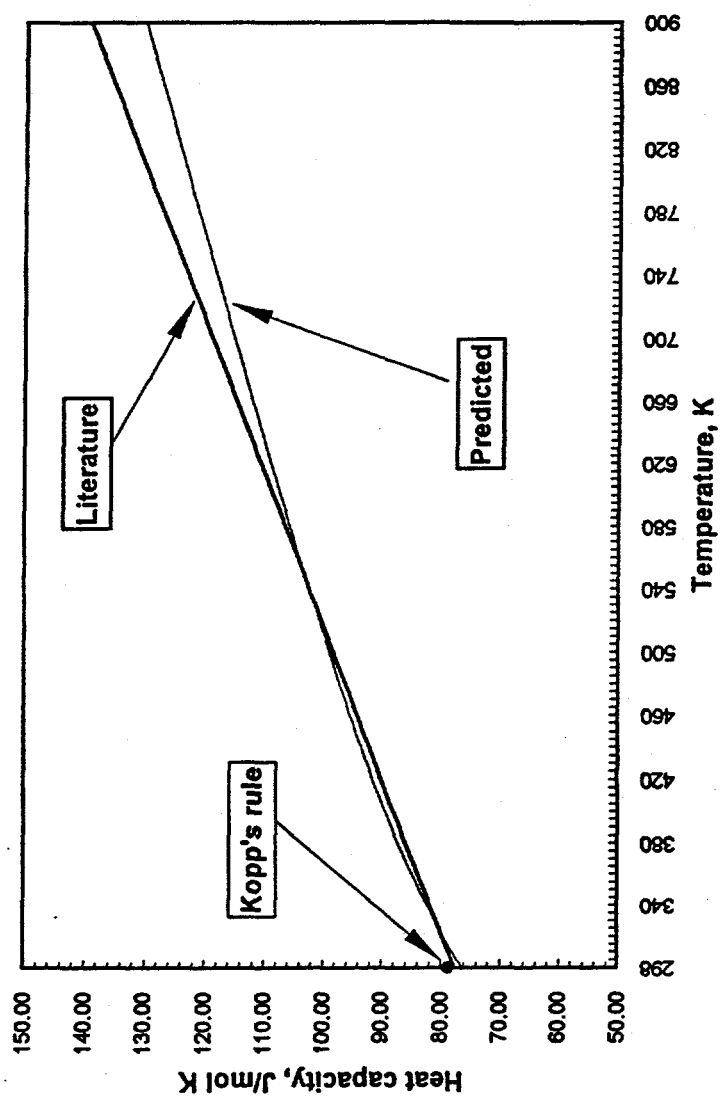


Figure 4. Heat capacity (C_p , J/mol °K) vs. temperature (°K) of $\text{Mg}(\text{OH})_2$ for literature (From Robie et. al., 1979) and predicted values.

SUPPLEMENTARY MATERIAL.

List of all the solid inorganic salts used in the regression, corresponding experimental values from the literature, prediction by the proposed method, percent error for the proposed method, prediction by Kopp's rule, and percent error for Kopp's rule for heat capacity at 298 °K.

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
Ag ₂ CO ₃	111.60	109.98	1.45	109.62	1.77
Ag ₂ O	66.31	70.26	5.96	68.62	3.49
Ag ₂ SO ₄	131.44	127.08	3.31	141.42	7.59
AgNO ₂	81.34	85.97	5.70	85.35	4.94
AgNO ₃	93.01	92.41	0.64	102.09	9.76
Al(OH) ₃	93.05	98.19	5.53	105.02	12.87
Al ₂ (SO ₄) ₃	260.15	248.00	4.67	320.49	23.20
Al ₂ O ₃	78.81	77.53	1.61	102.09	29.55
Al ₂ O ₃ ·3H ₂ O	183.44	188.53	2.77	210.04	14.50
AlCl ₃	91.12	85.10	6.61	103.76	13.87
AlF ₃	75.45	76.61	1.54	88.70	17.57
AlI ₃	98.89	90.93	8.05	103.76	4.93
AlOCl	56.83	54.21	4.61	68.62	20.74
AlPO ₄	92.98	88.67	4.63	115.48	24.19
As ₂ O ₃	96.95	95.88	1.10	102.09	5.30
As ₂ O ₅	116.54	123.93	6.34	135.56	16.32
As ₄ O ₆	191.23	191.77	0.28	204.18	6.77
Ba(NO ₃) ₂	151.32	160.79	6.25	178.24	17.79
Ba ₂ TiO ₄	149.13	150.56	0.95	144.77	2.93
Ba ₃ Al ₂ O ₆	215.35	216.20	0.39	230.12	6.86
BaBr ₂	76.91	79.52	3.39	77.82	1.18
BaCl ₂	75.17	77.11	2.59	77.82	3.53
BaCO ₃	87.97	85.94	2.31	83.68	4.88
BaF ₂	72.34	71.45	1.24	67.78	6.31
BaHfO ₃	108.25	105.86	2.21	102.09	5.69
BaI ₂	77.43	80.99	4.60	77.82	0.50
BaO	46.80	46.22	1.23	42.68	8.80
BaO·Al ₂ O ₃	113.63	123.76	8.91	144.77	27.40
BaO·SiO ₂	88.99	90.40	1.59	92.05	3.44
BaO·TiO ₂	102.38	104.34	1.91	102.09	0.29
BaO·UO ₃	146.81	132.87	9.50	118.83	19.06

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
BaO.V ₂ O ₅	172.78	173.51	0.42	178.24	3.16
BaO ₂	70.69	69.19	2.12	59.41	15.96
BaSO ₄	101.67	103.04	1.35	115.48	13.58
BaZrO ₃	105.39	102.27	2.95	102.09	3.13
2BaO.SiO ₂	134.06	134.87	0.60	150.62	12.36
Be(OH) ₂	65.55	64.63	1.40	78.66	20.01
Be ₂ SiO ₄	93.37	94.21	0.90	134.72	44.30
BeAl ₂ O ₄	104.88	102.55	2.22	144.77	38.03
BeAl ₆ O ₁₀	261.81	257.61	1.60	348.95	33.28
BeBr ₂	65.05	58.31	10.36	77.82	19.64
BeCl ₂	62.43	55.90	10.45	77.82	24.65
BeF ₂	51.83	50.24	3.07	67.78	30.77
BeSO ₄	85.60	81.84	4.40	115.48	34.90
BeSO ₄ .2H ₂ O	152.82	155.84	1.97	187.44	22.65
BeSO ₄ .4H ₂ O	216.42	229.84	6.20	259.41	19.86
3BeO.B ₂ O ₃	138.36	152.57	10.28	230.12	66.32
Bi ₂ (SO ₄) ₃	278.82	278.93	0.04	320.49	14.95
Bi ₂ O ₃	113.46	108.46	4.40	102.09	10.02
BiBr ₃	100.82	104.17	3.33	103.76	2.92
BiCl ₃	100.42	100.57	0.14	103.76	3.33
BiF ₃	85.81	92.07	7.30	88.70	3.37
BiI ₃	105.88	106.39	0.48	103.76	1.99
BiOCl	70.16	69.67	0.70	68.62	2.20
Ca(NO ₃) ₂	149.29	155.57	4.20	178.24	19.39
Ca(NO ₃) ₂ .2H ₂ O	231.58	229.57	0.87	250.20	8.04
Ca(NO ₃) ₂ .3H ₂ O	267.14	266.57	0.21	286.19	7.13
Ca(NO ₃) ₂ .4H ₂ O	300.62	303.57	0.98	322.17	7.17
Ca(OH) ₂	87.56	80.62	7.92	78.66	10.16
CaBr ₂	73.89	74.30	0.55	77.82	5.32
CaCl ₂	72.62	71.89	1.01	77.82	7.16
CaCO ₃ .MgCO ₃	155.18	156.98	1.16	167.36	7.85
CaF ₂	67.16	66.23	1.38	67.78	0.93
CaI ₂	77.16	75.78	1.80	77.82	0.86
CaO.2Al ₂ O ₃	193.83	196.07	1.16	246.86	27.36
CaO.2B ₂ O ₃	157.74	158.25	0.33	188.28	19.36
CaO.Al ₂ O ₃	120.55	118.54	1.67	144.77	20.08
CaO.Al ₂ O ₃ .SiO ₂	156.52	162.72	3.96	194.14	24.03
CaO.B ₂ O ₃	103.83	99.63	4.05	115.48	11.22

COMPOUNDS	C_p^{298} <i>p, literature</i>	C_p^{298} <i>p, predicted</i>	% Error	C_p^{298} <i>p, Kopp's rule</i>	% Error
CaO.Cr ₂ O ₃	146.59	144.77	1.24	144.77	1.24
CaO.HfO ₂	105.71	100.64	4.80	102.09	3.42
CaO.MgO	79.61	77.54	2.60	85.35	7.22
CaO.MgO.2SiO ₂	156.05	165.90	6.31	184.10	17.97
CaO.MgO.SiO ₂	123.22	121.72	1.22	134.72	9.34
CaO.MoO ₃	117.06	115.82	1.06	118.83	1.51
CaO.TiO ₂	97.66	99.12	1.50	102.09	4.54
CaO.TiO ₂ .SiO ₂	138.89	143.30	3.18	151.46	9.05
CaO.UO ₃	130.44	127.65	2.13	118.83	8.90
CaO.V ₂ O ₅	170.74	168.29	1.44	178.24	4.39
CaSO ₄ .2H ₂ O	185.99	171.83	7.62	187.44	0.78
CaSO ₄ .3H ₂ O	205.10	208.83	1.82	223.43	8.94
2CaO.Al ₂ O ₃ .SiO ₂	195.74	203.72	4.08	236.81	20.99
2CaO.B ₂ O ₃	147.05	140.63	4.37	158.16	7.55
2CaO.Fe ₂ O ₃	194.05	188.88	2.66	187.44	3.40
2CaO.MgO.2SiO ₂	211.99	206.90	2.40	226.77	6.98
2CaO.P ₂ O ₅	187.70	186.21	0.79	214.22	14.13
2CaO.V ₂ O ₅	213.88	209.29	2.15	220.92	3.29
3CaO.2TiO ₂	239.57	239.24	0.14	246.86	3.04
3CaO.Al ₂ O ₃	209.65	200.54	4.34	230.12	9.76
3CaO.Al ₂ O ₃ .3SiO ₂	323.01	333.09	3.12	378.23	17.10
3CaO.B ₂ O ₃	187.77	181.63	3.27	200.83	6.96
3CaO.P ₂ O ₅	236.03	227.22	3.73	256.90	8.84
3CaO.V ₂ O ₅	257.02	250.29	2.62	263.59	2.56
3CaO.WO ₃	202.24	200.25	0.99	204.18	0.96
4CaO.3TiO ₂	337.70	338.36	0.20	348.95	3.33
Cd(NO ₃) ₂	179.91	159.30	11.45	178.24	0.93
CdBr ₂	76.67	78.04	1.78	77.82	1.50
CdCl ₂	74.59	75.63	1.39	77.82	4.33
CdCO ₃	82.38	84.46	2.53	83.68	1.58
CdF ₂	66.90	69.97	4.59	67.78	1.32
CdI ₂	79.94	79.51	0.54	77.82	2.65
CdO	44.17	44.74	1.30	42.68	3.37
CdO.Al ₂ O ₃	129.87	122.27	5.85	144.77	11.47
CdO.Ga ₂ O ₃	138.47	140.33	1.34	144.77	4.54
CdO.SiO ₂	88.75	88.92	0.19	92.05	3.71
CdO.TiO ₂	98.48	102.85	4.44	102.09	3.66
CdSeO ₃	94.66	100.96	6.66	102.09	7.85

COMPOUNDS	$C_{p, \text{Lennard-Jones}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
CdSeO ₄	99.81	110.12	10.34	118.83	19.06
CdWO ₄	124.49	121.98	2.01	118.83	4.55
Ce ₂ (SO ₄) ₃	280.75	279.16	0.57	320.49	14.15
Ce ₂ O ₃	116.99	108.70	7.09	102.09	12.74
Ce ₂ O ₃ .Al ₂ O ₃	189.57	186.23	1.76	204.18	7.71
CeBr ₃	100.83	104.29	3.43	103.76	2.91
CeF ₃	93.14	92.19	1.02	88.70	4.76
CeI ₃	100.43	106.51	6.05	103.76	3.32
CeO ₂	61.53	61.53	0.00	59.41	3.44
Co(NO ₃) ₂	156.74	162.49	3.67	178.24	13.72
Co(OH) ₂	97.05	87.54	9.80	78.66	18.95
CoBr ₂	79.62	79.62	0.00	103.76	30.32
CoCl ₂	78.50	78.82	0.41	77.82	0.86
CoCO ₃	79.61	87.65	10.10	83.68	5.12
CoF ₂	68.78	73.16	6.36	67.78	1.45
CoF ₃	91.82	91.82	0.00	88.70	3.40
CoFe ₂ O ₄	152.54	154.80	1.48	144.77	5.09
CoO.Al ₂ O ₃	132.23	125.46	5.12	144.77	9.48
CoO.Cr ₂ O ₃	157.17	151.70	3.48	144.77	7.89
CoO.TiO ₂	107.78	106.04	1.61	102.09	5.28
CoSeO ₃	97.74	104.15	6.56	102.09	4.45
CoSO ₄	103.07	104.75	1.63	115.48	12.04
CoWO ₄	129.93	125.17	3.66	118.83	8.55
2CoO.SiO ₂	133.90	140.04	4.58	134.72	0.61
2CoO.TiO ₂	160.41	153.97	4.01	144.77	9.75
Cr(CO) ₆	240.13	239.84	0.12	171.54	28.56
Cr ₂ (SO ₄) ₃	280.64	274.24	2.28	320.49	14.20
Cr ₂ O ₃	114.26	103.77	9.18	102.09	10.65
CrBr ₂	72.51	72.27	0.33	77.82	7.33
CrCl ₂	69.27	69.86	0.86	77.82	12.35
CrCl ₃	91.73	98.22	7.07	103.76	13.12
CrF ₂	64.63	64.20	0.67	67.78	4.87
CrI ₂	73.67	73.75	0.10	77.82	5.63
CrI ₃	111.67	104.04	6.83	103.76	7.08
CrO ₃	79.07	73.41	7.16	76.15	3.70
Cs ₂ B ₂ O ₄	138.91	136.81	1.52	141.42	1.81
Cs ₂ Si ₂ O ₅	176.71	166.54	5.75	167.36	5.29
Cs ₂ SiO ₃	122.22	122.36	0.11	117.99	3.47

COMPOUNDS	C_p^{298} <i>C_p, literature</i>	C_p^{298} <i>C_p, predicted</i>	% Error	C_p^{298} <i>C_p, Kopp's rule</i>	% Error
Cs ₂ UO ₄	152.70	164.83	7.95	144.77	5.19
Cu ₂ O	63.54	59.93	5.68	68.62	7.99
Cu ₂ O.Al ₂ O ₃	142.15	137.47	3.29	170.71	20.09
Cu ₂ O.Ga ₂ O ₃	139.97	155.52	11.11	170.71	21.96
CuBr ₂	75.77	76.21	0.59	77.82	2.71
CuCl ₂	71.74	73.81	2.89	77.82	8.48
CuF ₂	65.12	66.68	2.39	67.78	4.08
CuFe ₂ O ₄	148.75	149.79	0.70	144.77	2.68
CuI	54.18	48.82	9.89	51.88	4.24
CuO	42.26	42.92	1.57	42.68	1.00
CuO.Al ₂ O ₃	127.64	120.45	5.63	144.77	13.42
CuO.Cr ₂ O ₃	148.00	146.69	0.88	144.77	2.18
CuO.CuSO ₄	140.09	142.66	1.83	158.16	12.90
CuO.Ga ₂ O ₃	134.98	138.51	2.61	144.77	7.25
CuSO ₄	98.77	99.74	0.98	115.48	16.92
Dy ₂ O ₃	116.21	113.14	2.64	102.09	12.15
DyCl ₃	97.03	102.91	6.06	103.76	6.94
DyF ₃	94.15	94.41	0.28	88.70	5.79
ErCl ₃	103.29	110.36	6.85	103.76	0.46
ErF ₃	111.53	101.87	8.67	88.70	20.47
Eu ₂ O ₃	124.65	128.41	3.02	102.09	18.10
EuBr ₂	82.39	82.21	0.21	77.82	5.54
EuBr ₃	110.66	114.15	3.15	103.76	6.24
EuCl ₃	106.92	110.54	3.39	103.76	2.95
EuCl ₃ .6H ₂ O	366.91	332.54	9.37	319.66	12.88
EuF ₃	99.49	102.05	2.57	88.70	10.84
EuO	48.74	48.92	0.36	42.68	12.45
Fe(OH) ₂	86.23	82.56	4.26	78.66	8.78
Fe ₂ (SO ₄) ₃	257.80	277.34	7.58	320.49	24.32
Fe ₂ O ₃	104.69	106.87	2.08	102.09	2.49
Fe ₂ SiO ₄	132.90	130.06	2.14	134.72	1.37
Fe ₃ O ₄	151.75	149.81	1.27	144.77	4.60
FeAl ₂ O ₄	123.46	120.47	2.42	144.77	17.25
FeBr ₂	80.23	76.24	4.98	77.82	3.00
FeCl ₂	76.50	73.83	3.48	77.82	1.73
FeCl ₃	96.90	99.77	2.96	103.76	7.08
FeCO ₃	82.06	82.66	0.73	83.68	1.97
FeCr ₂ O ₄	133.75	146.71	9.69	144.77	8.24

COMPOUNDS	C_p^{298} <i>p. Literature</i>	C_p^{298} <i>p. predicted</i>	% Error	C_p^{298} <i>p. Kopp's rule</i>	% Error
FeF ₂	68.17	68.17	0.01	67.78	0.58
FeF ₃	91.64	91.28	0.40	88.70	3.21
FeMoO ₄	117.59	117.76	0.14	118.83	1.05
FeO	48.02	42.94	10.58	42.68	11.12
FeO(OH)	74.31	73.24	1.43	69.04	7.09
FeOCl	77.03	68.88	10.58	68.62	10.92
FeSO ₄	100.29	99.76	0.52	115.48	15.15
FeTiO ₃	99.52	106.41	6.92	102.09	2.58
FeWO ₄	114.26	120.18	5.18	118.83	4.00
Ga ₂ O ₃	93.83	95.59	1.87	102.09	8.80
GaBr ₃	101.65	97.74	3.84	103.76	2.08
Gd ₂ O ₃	105.50	101.85	3.46	102.09	3.23
GdBr ₃	96.91	100.87	4.09	103.76	7.07
GdCl ₃	97.75	97.26	0.50	103.76	6.15
GdF ₃	88.38	88.77	0.43	88.70	0.36
GdI ₃	98.66	103.08	4.49	103.76	5.17
GdOCl	68.34	66.37	2.87	68.62	0.41
GeI ₂	81.62	80.36	1.55	77.82	4.66
GeI ₄	126.05	123.76	1.82	129.70	2.89
GeO	44.32	45.59	2.85	42.68	3.71
GeO ₂	51.93	54.22	4.41	59.41	14.42
H ₂ WO ₄	104.08	110.07	5.76	112.13	7.74
H ₃ BO ₃	81.19	78.56	3.25	90.37	11.31
H ₃ PO ₄	106.23	99.15	6.66	118.41	11.47
HfBr ₄	127.60	126.23	1.08	129.70	1.65
HfCl ₄	120.53	121.42	0.74	129.70	7.61
HfF ₄	100.43	110.09	9.62	109.62	9.16
HfI ₂	61.89	61.89	0.00	77.82	25.73
HfI ₄	144.32	129.18	10.49	129.70	10.13
HfO ₂	60.28	59.63	1.07	59.41	1.44
Hg ₂ Br ₂	104.65	105.33	0.65	103.76	0.85
Hg ₂ Cl ₂	101.54	102.92	1.36	103.76	2.19
Hg ₂ F ₂	100.31	97.26	3.05	93.72	6.57
Hg ₂ I ₂	105.81	106.81	0.94	103.76	1.93
HgBr ₂	75.35	77.17	2.42	77.82	3.28
HgCl ₂	73.91	74.77	1.16	77.82	5.30
HgI ₂	77.75	78.65	1.16	77.82	0.10
HgO	43.91	43.88	0.07	42.68	2.81

COMPOUNDS	$C_{p, \text{Laurance}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
HgSeO ₃	102.13	100.10	1.99	102.09	0.04
HgSO ₄	102.22	100.70	1.49	115.48	12.97
Ho ₂ O ₃	114.96	113.44	1.32	102.09	11.20
HoBr ₃	98.79	106.67	7.98	103.76	5.04
HoCl ₃	96.18	103.06	7.15	103.76	7.88
HoCl ₃ .6H ₂ O	347.30	325.06	6.40	319.66	7.96
HoF ₃	91.22	94.56	3.67	88.70	2.76
In ₂ O ₃	100.33	100.58	0.25	102.09	1.75
InBr	50.99	50.31	1.33	51.88	1.75
InBr ₃	98.22	100.23	2.05	103.76	5.65
InCl	47.62	49.11	3.13	51.88	8.95
InCl ₂	73.54	73.54	0.00	77.82	5.82
InCl ₃	95.24	96.63	1.45	103.76	8.94
InF ₃	92.02	88.13	4.23	88.70	3.60
InI	51.86	51.05	1.56	51.88	0.04
IrBr ₃	105.44	97.44	7.59	103.76	1.59
IrCl ₃	85.82	93.83	9.33	103.76	20.91
IrO ₂	55.58	55.58	0.00	59.41	6.90
K ₂ B ₂ O ₄	141.88	136.68	3.67	141.42	0.33
K ₂ B ₆ O ₁₀	265.30	253.93	4.29	287.02	8.19
K ₂ B ₈ O ₁₃	318.93	312.55	2.00	359.82	12.82
K ₂ CO ₃	114.25	117.77	3.08	109.62	4.05
K ₂ CrO ₄	146.04	151.46	3.72	144.77	0.87
K ₂ HPO ₄	143.47	144.37	0.63	151.04	5.28
K ₂ O.Al ₂ O ₃ .2SiO ₂	239.72	243.95	1.76	269.45	12.40
K ₂ O.Al ₂ O ₃ .4SiO ₂	328.45	332.31	1.18	368.19	12.10
K ₂ O.Fe ₂ O ₃	187.85	184.93	1.56	170.71	9.13
K ₂ Si ₂ O ₅	160.85	166.42	3.46	167.36	4.05
K ₂ SiO ₃	118.62	122.23	3.04	117.99	0.53
K ₂ SO ₄	131.57	134.87	2.52	141.42	7.49
K ₂ WO ₄	150.79	155.29	2.98	144.77	4.00
K ₃ AlCl ₆	249.02	248.52	0.20	259.41	4.17
K ₃ AlF ₆	221.66	231.53	4.45	229.28	3.44
K ₃ PO ₄	164.60	166.99	1.45	167.36	1.68
KAl(SO ₄) ₂	192.91	191.44	0.77	230.96	19.72
KAlCl ₄	156.48	139.57	10.80	155.64	0.53
KBF ₄	114.70	118.79	3.57	120.92	5.42
KCl	51.58	54.47	5.60	51.88	0.58

COMPOUNDS	C_p^{298} <i>C_p, Literature</i>	C_p^{298} <i>C_p, predicted</i>	% Error	C_p^{298} <i>C_p, Kopp's rule</i>	% Error
KClO ₃	100.45	102.68	2.22	102.09	1.63
KClO ₄	112.37	115.11	2.44	118.83	5.74
KH ₂ PO ₄	116.49	121.76	4.53	134.72	15.65
KHCO ₃	90.05	91.04	1.11	93.30	3.62
KHF ₂	76.89	80.67	4.91	77.40	0.66
KI	52.96	56.41	6.51	51.88	2.04
KNO ₃	95.87	96.31	0.46	102.09	6.49
KO ₂	78.23	73.48	6.07	59.41	24.05
KOH	64.93	58.83	9.39	52.30	19.45
La ₂ O ₃	108.77	104.68	3.76	102.09	6.14
LaBr ₃	99.59	102.29	2.70	103.76	4.19
LaCl ₃	98.13	98.68	0.56	103.76	5.74
LaF ₃	90.36	90.18	0.20	88.70	1.84
LaI ₃	99.10	104.50	5.45	103.76	4.71
LaOCl	68.97	67.79	1.72	68.62	0.52
LaPO ₄	101.64	102.25	0.60	115.48	13.62
Li ₂ B ₂ O ₄	120.82	126.87	5.01	118.83	1.65
Li ₂ B ₄ O ₇	170.34	175.21	2.86	214.22	25.76
Li ₂ B ₆ O ₁₀	291.00	264.69	9.04	219.24	24.66
Li ₂ B ₈ O ₁₃	320.65	333.60	4.04	269.45	15.97
Li ₂ BeF ₄	134.97	133.42	1.15	161.50	19.66
Li ₂ CO ₃	97.96	97.68	0.30	109.62	11.90
Li ₂ HfO ₃	111.87	117.59	5.11	128.03	14.44
Li ₂ Nb ₂ O ₆	198.55	204.22	2.86	204.18	2.83
Li ₂ O	54.07	57.96	7.18	68.62	26.90
Li ₂ O.Al ₂ O ₃ .2SiO ₂	226.50	220.33	2.72	301.25	33.00
Li ₂ O.Al ₂ O ₃ .4SiO ₂	317.69	305.18	3.94	431.79	35.91
Li ₂ Si ₂ O ₅	138.62	146.32	5.55	167.36	20.73
Li ₂ SiO ₃	99.90	102.14	2.24	117.99	18.11
Li ₂ SO ₄	117.14	114.78	2.01	141.42	20.73
Li ₂ Ta ₂ O ₆	200.14	197.02	1.56	204.18	2.02
Li ₂ TiO ₃	108.48	116.07	7.00	128.03	18.02
Li ₂ WO ₄	133.34	135.20	1.39	144.77	8.57
Li ₂ ZrO ₃	110.20	114.01	3.45	128.03	16.18
Li ₃ AlF ₆	202.30	201.38	0.45	229.28	13.34
LiBeF ₃	92.61	91.83	0.84	114.64	23.79
LiBr	49.06	45.63	7.00	51.88	5.75
LiCl	48.10	44.42	7.64	51.88	7.87

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
LiClO ₄	104.94	105.06	0.12	118.83	13.24
LiF	41.85	41.59	0.61	46.86	11.98
LiI	51.80	46.36	10.50	51.88	0.15
LiNO ₃	89.11	86.26	3.20	102.09	14.56
LiOH	49.75	48.79	1.93	52.30	5.13
Lu ₂ O ₃	101.72	101.05	0.65	102.09	0.36
LuF ₃	87.04	88.37	1.53	88.70	1.91
Mg(NO ₃) ₂	141.90	151.10	6.48	178.24	25.61
Mg(OH) ₂	77.49	76.15	1.73	78.66	1.50
Mg ₂ SiO ₄	118.43	117.25	1.00	134.72	13.76
Mg ₂ TiO ₄	128.17	131.19	2.35	144.77	12.94
Mg ₂ V ₂ O ₇	202.26	200.35	0.94	220.92	9.23
Mg ₃ P ₂ O ₈	213.09	213.82	0.34	256.90	20.56
MgAl ₂ O ₄	115.94	114.07	1.61	144.77	24.87
MgBr ₂	74.67	69.83	6.48	77.82	4.23
MgCl ₂	71.29	67.43	5.41	77.82	9.17
MgCO ₃	75.40	76.26	1.13	83.68	10.98
MgCr ₂ O ₄	126.72	140.30	10.72	144.77	14.24
MgF ₂	61.33	61.76	0.70	67.78	10.51
MgFe ₂ O ₄	137.76	143.41	4.10	144.77	5.09
MgI ₂	74.78	71.31	4.65	77.82	4.07
MgMoO ₄	110.88	111.35	0.42	118.83	7.16
MgO	37.25	36.54	1.91	42.68	14.58
MgSiO ₃	81.85	80.72	1.39	92.05	12.45
MgSO ₄	95.57	93.36	2.31	115.48	20.83
MgTi ₂ O ₅	146.60	152.76	4.21	161.50	10.17
MgTiO ₃	91.17	94.65	3.82	102.09	11.98
MgV ₂ O ₆	159.87	163.82	2.47	178.24	11.49
MgWO ₄	109.83	113.78	3.59	118.83	8.19
Mn ₂ O ₃	99.02	99.77	0.76	102.09	3.10
Mn ₂ SiO ₄	129.87	130.45	0.45	134.72	3.74
Mn ₂ TiO ₄	144.52	144.38	0.09	144.77	0.17
Mn ₃ O ₄	140.48	142.90	1.73	144.77	3.05
MnAl ₂ O ₄	124.60	120.67	3.16	144.77	16.18
MnBr ₂	75.30	76.43	1.50	77.82	3.35
MnCl ₂	73.01	74.03	1.39	77.82	6.59
MnF ₂	62.71	68.36	9.01	67.78	8.09
MnMoO ₄	124.07	117.95	4.93	118.83	4.22

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
MnO.Fe ₂ O ₃	149.19	150.01	0.55	144.77	2.97
MnSiO ₃	86.32	87.32	1.15	92.05	6.63
MnSO ₄	100.37	99.96	0.41	115.48	15.06
MnTiO ₃	99.78	101.25	1.48	102.09	2.32
MnWO ₄	124.07	120.37	2.98	118.83	4.22
Mo(CO) ₆	241.96	241.24	0.30	171.54	29.10
MoBr ₂	79.69	79.30	0.49	77.82	2.35
MoBr ₃	105.37	103.84	1.46	103.76	1.52
MoBr ₄	133.02	131.50	1.15	129.70	2.49
MoCl ₂	74.58	76.89	3.10	77.82	4.35
MoCl ₃	94.87	100.23	5.65	103.76	9.38
MoCl ₄	124.40	126.68	1.84	129.70	4.26
MoCl ₅	156.13	159.96	2.45	155.64	0.31
MoF ₃	95.21	91.73	3.65	88.70	6.84
MoF ₄	125.04	115.36	7.74	109.62	12.33
MoF ₅	149.63	145.80	2.56	130.54	12.76
MoI ₂	82.70	80.77	2.32	77.82	5.89
MoI ₃	106.40	106.05	0.33	103.76	2.47
MoO ₂ Cl ₂	107.65	105.71	1.80	111.29	3.39
MoO ₃	75.12	74.82	0.41	76.15	1.37
Na ₂ B ₂ O ₄	131.68	128.50	2.41	141.42	7.40
Na ₂ B ₄ O ₇	186.85	187.12	0.15	214.22	14.65
Na ₂ B ₆ O ₁₀	243.61	245.75	0.88	287.02	17.82
Na ₂ B ₈ O ₁₃	304.75	304.37	0.12	359.82	18.07
Na ₂ CO ₃	111.30	109.59	1.53	109.62	1.51
Na ₂ Cr ₂ O ₄	178.78	173.64	2.88	170.71	4.52
Na ₂ CrO ₄	142.76	143.29	0.37	144.77	1.41
Na ₂ Mo ₂ O ₇	216.66	219.50	1.31	220.92	1.97
Na ₂ MoO ₄	141.43	144.69	2.30	144.77	2.36
Na ₂ O	68.54	69.87	1.94	68.62	0.11
Na ₂ O.Al ₂ O ₃ .4SiO ₂	311.72	324.13	3.98	368.19	18.12
Na ₂ O.Al ₂ O ₃ .6SiO ₂	409.54	412.50	0.72	466.93	14.02
Na ₂ O.UO ₃	146.71	156.52	6.69	144.77	1.33
Na ₂ O ₂	88.92	92.84	4.41	85.35	4.01
Na ₂ P ₂ O ₆	174.44	174.08	0.20	197.48	13.21
Na ₂ Si ₂ O ₅	156.44	158.24	1.15	167.36	6.98
Na ₂ SiO ₃	111.78	114.06	2.04	117.99	5.56
Na ₂ SO ₃	120.08	120.08	0.00	124.68	3.84

COMPOUNDS	$C_{p, \text{Laurance}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
Na ₂ SO ₄	128.34	126.70	1.28	141.42	10.19
Na ₂ Ti ₂ O ₅	193.11	187.16	3.08	187.44	2.93
Na ₂ Ti ₃ O ₇	252.21	245.69	2.58	246.86	2.12
Na ₂ TiO ₃	131.18	128.62	1.95	128.03	2.40
Na ₂ V ₂ O ₆	195.10	198.42	1.70	204.18	4.65
Na ₂ WO ₄	141.75	147.11	3.78	144.77	2.13
Na ₃ AlF ₆	222.72	219.26	1.55	229.28	2.95
Na ₄ P ₂ O ₇	241.24	243.96	1.13	266.10	10.31
Na ₄ V ₂ O ₇	269.74	268.51	0.46	272.80	1.13
Na ₅ Al ₃ F ₁₄	461.92	467.57	1.22	500.41	8.33
Na ₆ As ₂ O ₈	340.94	333.55	2.17	341.41	0.14
Na ₆ P ₂ O ₈	306.63	313.83	2.35	334.72	9.16
Na ₆ V ₂ O ₈	329.62	338.59	2.72	341.41	3.58
NaBF ₄	119.94	114.70	4.37	120.92	0.82
NaBr	51.43	51.59	0.31	51.88	0.88
NaClO ₃	100.82	98.59	2.21	102.09	1.26
NaClO ₄	111.03	111.02	0.01	118.83	7.02
NaF	46.91	47.55	1.36	46.86	0.11
NaHCO ₃	87.95	86.95	1.13	93.30	6.09
NaI	49.53	52.32	5.65	51.88	4.76
NaNO ₃	93.00	92.22	0.84	102.09	9.77
NaO ₂	72.17	69.39	3.85	59.41	17.68
NbCl ₃	97.40	97.40	0.00	103.76	6.53
NbCl ₄	119.81	121.12	1.10	129.70	8.26
NbCl ₅	147.90	150.36	1.66	155.64	5.24
NbF ₅	149.66	136.20	9.00	130.54	12.78
NbO ₂	57.68	59.34	2.89	59.41	3.01
NbOCl ₂	93.21	90.23	3.19	94.56	1.45
NbOCl ₃	119.81	119.47	0.28	120.50	0.57
Nd ₂ O ₃	111.32	107.16	3.74	102.09	8.29
Nd ₂ O ₃ ·2ZrO ₂	223.33	219.26	1.82	220.92	1.08
NdBr ₃	104.13	103.52	0.58	103.76	0.35
NdCl ₃	99.16	99.92	0.76	103.76	4.64
NdF ₃	92.43	91.42	1.09	88.70	4.03
NdI ₃	98.73	105.74	7.09	103.76	5.10
NdOCl	69.85	69.02	1.18	68.62	1.76
NH ₄ ClO ₄	128.07	140.15	9.43	157.32	22.83
(NH ₄) ₂ SO ₄	187.21	184.95	1.21	218.40	16.66

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
Ni ₂ SiO ₄	126.95	131.75	3.78	134.72	6.13
NiAl ₂ O ₄	131.53	121.32	7.76	144.77	10.06
NiBr ₂	75.40	77.08	2.23	77.82	3.21
NiCl ₂	71.68	74.68	4.17	77.82	8.56
NiCO ₃	86.40	83.51	3.35	83.68	3.15
NiCr ₂ O ₄	148.77	147.55	0.82	144.77	2.69
NiFe ₂ O ₄	159.14	150.66	5.33	144.77	9.03
NiI ₂	77.41	78.56	1.48	77.82	0.53
NiO	44.28	43.78	1.13	42.68	3.63
NiSeO ₃	97.33	100.01	2.75	102.09	4.89
NiSO ₄	97.48	100.61	3.21	115.48	18.47
NiTlO ₃	99.25	101.90	2.66	102.09	2.86
NiWO ₄	121.60	121.02	0.47	118.83	2.28
NpCl ₃	101.61	109.32	7.58	103.76	2.11
NpCl ₄	120.86	123.51	2.19	129.70	7.32
NpF ₃	108.52	100.82	7.10	88.70	18.26
NpF ₆	167.44	162.09	3.20	151.46	9.54
NpO ₂	64.14	61.73	3.77	59.41	7.37
NpO ₃ .H ₂ O	118.06	123.41	4.53	112.13	5.02
NpOCl ₂	92.85	92.62	0.25	94.56	1.84
Pb ₂ SiO ₄	136.90	139.14	1.64	134.72	1.59
Pb ₄ SiO ₆	229.70	234.09	1.91	220.08	4.19
PbB ₄ O ₇	151.71	164.73	8.58	188.28	24.10
PbBr ₂	79.47	80.77	1.64	77.82	2.08
PbCl ₂	77.14	78.37	1.59	77.82	0.88
PbF ₂	72.29	72.70	0.57	67.78	6.24
PbI ₂	77.57	82.25	6.03	77.82	0.32
PbO.PbCO ₃	133.23	134.68	1.09	126.36	5.16
PbO ₂	60.99	60.99	0.00	59.41	2.58
PbSiO ₃	89.10	91.66	2.88	92.05	3.31
PbSO ₄	102.98	104.30	1.28	115.48	12.13
PbSO ₄ .2PbO	205.84	199.26	3.20	200.83	2.43
PbSO ₄ .3PbO	251.55	246.73	1.91	243.51	3.19
PbSO ₄ .PbO	160.15	151.78	5.23	158.16	1.24
PbTiO ₃	104.38	105.59	1.16	102.09	2.20
PbWO ₄	119.62	124.72	4.26	118.83	0.67
PdCl ₂	75.27	74.45	1.09	77.82	3.39
PdI ₂	75.06	78.33	4.37	77.82	3.68

COMPOUNDS	C_p^{298} <i>C_p, literature</i>	C_p^{298} <i>C_p, predicted</i>	% Error	C_p^{298} <i>C_p, Kopp's rule</i>	% Error
PdO	46.02	43.56	5.34	42.68	7.26
Pr ₂ O ₃	116.61	107.65	7.69	102.09	12.46
PrBr ₃	101.65	103.77	2.08	103.76	2.08
PrCl ₃	98.92	100.16	1.25	103.76	4.90
PrF ₃	92.48	91.66	0.88	88.70	4.09
PrI ₃	99.55	105.98	6.46	103.76	4.23
PrO ₂	72.92	72.92	0.00	59.41	18.52
PtBr ₂	75.90	76.85	1.26	77.82	2.54
PtBr ₃	100.36	112.65	12.25	103.76	3.39
PtBr ₄	150.62	150.94	0.21	129.70	13.89
PtCl ₂	75.40	74.45	1.27	77.82	3.21
PtCl ₃	121.34	109.05	10.13	103.76	14.49
PtCl ₄	146.44	146.13	0.22	129.70	11.43
Pu ₂ O ₃	133.01	126.28	5.06	102.09	23.25
PuBr ₃	107.86	113.08	4.84	103.76	3.80
PuCl ₃	102.86	109.48	6.43	103.76	0.88
PuF ₃	92.63	100.98	9.01	88.70	4.25
PuF ₄	116.18	116.36	0.16	109.62	5.64
PuF ₆	137.52	144.44	5.03	151.46	10.13
PuO ₂	66.28	65.91	0.56	59.41	10.36
PuOBr	87.79	79.79	9.12	68.62	21.84
PuOCl	83.64	78.58	6.05	68.62	17.96
Rb ₂ CO ₃	117.67	118.37	0.59	109.62	6.84
Rb ₂ O	73.97	78.65	6.34	68.62	7.23
Rb ₂ Si ₂ O ₅	170.66	167.01	2.14	167.36	1.94
Rb ₂ Si ₄ O ₉	270.85	255.38	5.71	266.10	1.75
Rb ₂ SiO ₃	117.40	122.83	4.63	117.99	0.50
Rb ₂ SO ₄	133.96	135.47	1.13	141.42	5.56
RbBr	52.55	55.97	6.52	51.88	1.27
RbCl	51.36	54.77	6.65	51.88	1.02
RbF	50.47	51.94	2.92	46.86	7.14
RbI	51.45	56.71	10.23	51.88	0.84
ReAgO ₄	116.24	106.69	8.22	92.88	20.09
ReCl ₃	92.22	80.79	12.39	77.82	15.61
ReNH ₄ O ₄	149.71	159.27	6.38	157.32	5.08
ReO ₂	56.58	56.58	0.00	59.41	5.01
ReO ₃	72.77	72.77	0.00	76.15	4.64
Rh ₂ O ₃	103.99	101.47	2.42	102.09	1.82

COMPOUNDS	C_p^{298} <i>p. Literature</i>	C_p^{298} <i>p. predicted</i>	% Error	C_p^{298} <i>p. Kopp's rule</i>	% Error
RhBr ₃	100.54	100.68	0.14	103.76	3.21
RhCl ₃	92.18	97.07	5.31	103.76	12.57
RuCl ₃	115.06	115.06	0.00	103.76	9.82
RuO ₂	52.66	52.66	0.00	59.41	12.81
Sb ₂ (SO ₄) ₃	275.44	278.59	1.15	320.49	16.36
SbBr ₃	112.97	104.01	7.93	103.76	8.15
SbCl ₃	107.50	100.40	6.61	103.76	3.48
SbF ₃	90.29	91.90	1.79	88.70	1.76
SbI ₃	98.08	106.22	8.30	103.76	5.79
Sc ₂ O ₃	93.93	93.08	0.91	102.09	8.68
ScBr ₃	95.34	96.49	1.20	103.76	8.84
ScCl ₃	92.04	92.88	0.91	103.76	12.74
ScF ₃	84.67	84.38	0.34	88.70	4.76
Se ₂ O ₅	127.33	127.33	0.00	135.56	6.46
SeCl ₄	133.90	118.00	11.87	129.70	3.13
SeO ₃	75.69	65.38	13.63	76.15	0.60
SiL ₄	108.03	113.73	5.27	119.66	10.77
SiO ₂	44.41	44.18	0.52	49.37	11.17
Sm ₂ O ₃	115.80	116.03	0.19	102.09	11.84
Sm ₂ O ₃ .2ZrO ₂	224.23	228.13	1.74	220.92	1.48
SmCl ₂	82.39	82.39	0.00	77.82	5.54
SmCl ₃	99.52	104.35	4.86	103.76	4.27
SmF ₃	106.75	95.85	10.21	88.70	16.91
SmOCl	71.10	73.46	3.31	68.62	3.50
SmOF	69.56	70.63	1.54	63.60	8.57
SnBr ₂	78.97	78.53	0.56	77.82	1.46
SnCl ₂	78.02	76.13	2.43	77.82	0.26
SnF ₂	72.39	70.46	2.66	67.78	6.37
SnI ₂	79.02	80.01	1.25	77.82	1.51
SnI ₄	131.96	137.75	4.39	129.70	1.71
SnO	47.76	45.24	5.28	42.68	10.65
SnO ₂	52.58	52.58	0.00	59.41	13.00
Sr ₂ SiO ₄	130.75	130.09	0.50	134.72	3.04
Sr ₂ TiO ₄	143.66	144.02	0.26	144.77	0.77
SrBr ₂	76.86	76.25	0.79	77.82	1.26
SrCl ₂	75.60	73.85	2.32	77.82	2.94
SrF ₂	69.92	68.18	2.48	67.78	3.06
SrHfO ₃	103.91	102.59	1.27	102.09	1.75

COMPOUNDS	C_p^{298} <i>p. literature</i>	C_p^{298} <i>p. predicted</i>	% Error	C_p^{298} <i>p. Kopp's rule</i>	% Error
SrI ₂	77.96	77.73	0.30	77.82	0.18
SrMoO ₄	117.03	117.77	0.64	118.83	1.54
SrO	45.49	42.95	5.57	42.68	6.18
SrO ₂	79.35	79.35	0.00	59.41	25.12
SrSiO ₃	87.05	87.14	0.10	92.05	5.74
SrTiO ₃	99.04	101.07	2.05	102.09	3.08
SrZrO ₃	100.79	99.01	1.77	102.09	1.29
Ta ₂ O ₅	131.44	139.07	5.80	135.56	3.14
TaBr ₅	155.69	152.77	1.87	155.64	0.03
TaCl ₃	93.06	93.06	0.00	103.76	11.51
TaCl ₄	119.81	119.81	0.00	129.70	8.26
TaCl ₅	147.90	146.76	0.77	155.64	5.24
TaF ₅	133.89	132.60	0.96	130.54	2.50
TaI ₅	156.21	156.46	0.16	155.64	0.36
TaOCl ₃	119.81	115.87	3.29	120.50	0.57
Tb ₂ O ₃	115.03	108.90	5.33	102.09	11.25
TbCl ₃	97.47	100.79	3.40	103.76	6.45
TbF ₃	92.94	92.29	0.70	88.70	4.56
TbI ₃	97.89	106.61	8.90	103.76	5.99
TbO ₂	61.52	61.52	0.00	59.41	3.42
TcO ₂	55.65	55.65	0.00	59.41	6.75
TcO ₃	107.95	107.95	0.00	76.15	29.46
TeCl ₄	138.49	132.07	4.63	129.70	6.34
TeO ₂	63.88	70.29	10.04	59.41	6.99
Th ₂ N ₂ O	104.77	104.77	0.00	120.50	15.01
ThBr ₄	125.17	128.15	2.38	129.70	3.62
ThCl ₄	120.28	123.34	2.55	129.70	7.83
ThF ₄	110.53	112.01	1.34	109.62	0.82
ThI ₄	145.98	131.11	10.19	129.70	11.15
ThO ₂	61.80	61.56	0.39	59.41	3.87
ThOBr ₂	93.46	94.86	1.50	94.56	1.18
ThOCl ₂	91.00	92.45	1.59	94.56	3.91
ThOF ₂	86.24	86.79	0.63	84.52	2.00
ThOI ₂	103.82	96.33	7.21	94.56	8.92
Ti ₂ O ₃	101.78	103.97	2.16	102.09	0.31
TiBr ₂	78.73	77.24	1.89	77.82	1.15
TiBr ₃	100.03	101.93	1.91	103.76	3.74
TiBr ₄	131.48	124.71	5.15	129.70	1.35

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
TiCl ₂	69.84	74.84	7.16	77.82	11.44
TiCl ₃	97.07	98.32	1.29	103.76	6.90
TiF ₃	91.63	89.83	1.97	88.70	3.20
TiF ₄	114.19	108.57	4.92	109.62	4.00
TiI ₂	86.24	78.72	8.72	77.82	9.76
TiI ₃	116.79	104.15	10.83	103.76	11.16
TiI ₄	125.62	127.66	1.63	129.70	3.25
TiO	39.93	43.94	10.04	42.68	6.87
TiO ₂	55.28	58.11	5.12	59.41	7.47
Tl ₂ O	78.84	78.14	0.89	68.62	12.97
Tl ₂ O ₃	105.42	107.58	2.04	102.09	3.16
Tl ₂ SO ₄	137.82	134.96	2.08	141.42	2.61
TlBr	50.47	55.72	10.39	51.88	2.79
TlCl	50.93	54.52	7.04	51.88	1.87
TlF	53.38	51.68	3.18	46.86	12.21
TlI	52.51	48.20	8.20	51.88	1.20
Tm ₂ O ₃	116.71	114.99	1.48	102.09	12.53
TmCl ₃	97.67	103.83	6.31	103.76	6.23
TmF ₃	94.97	95.34	0.38	88.70	6.60
UBr ₃	108.73	107.96	0.71	103.76	4.57
UBr ₄	128.11	129.74	1.27	129.70	1.24
UCl ₃	102.52	104.35	1.79	103.76	1.21
UCl ₄	120.77	124.93	3.44	129.70	7.40
UCl ₅	144.57	146.12	1.08	155.64	7.66
UCl ₆	175.53	179.32	2.16	181.59	3.45
UF ₃	95.08	95.86	0.82	88.70	6.71
UF ₄	116.01	113.60	2.08	109.62	5.51
UF ₅	132.30	131.96	0.26	130.54	1.33
UF ₆	167.43	162.33	3.05	151.46	9.54
UI ₃	112.02	110.18	1.65	103.76	7.37
UI ₄	134.43	132.69	1.30	129.70	3.52
UO ₂	63.57	63.14	0.68	59.41	6.54
UO ₂ F ₂	103.04	111.88	8.58	101.25	1.73
UO ₂ SO ₄	144.88	143.47	0.97	148.95	2.81
UO ₃	81.16	86.65	6.76	76.15	6.18
UO ₃ ·2H ₂ O	154.52	160.65	3.97	148.11	4.15
UO ₃ ·H ₂ O	117.46	123.65	5.27	112.13	4.54
UOBr ₂	97.88	96.44	1.47	94.56	3.40

COMPOUNDS	$C_{p, \text{Literature}}^{298}$	$C_{p, \text{predicted}}^{298}$	% Error	$C_{p, \text{Kopp's rule}}^{298}$	% Error
UOBr ₃	121.11	118.84	1.87	120.50	0.50
UOCl ₂	94.97	94.03	0.98	94.56	0.43
UOCl ₃	115.40	115.23	0.15	120.50	4.42
V ₂ O ₅	127.33	127.28	0.04	135.56	6.46
VBr ₂	77.38	74.20	4.11	77.82	0.57
VBr ₃	101.65	99.08	2.52	103.76	2.08
VCl ₂	71.86	71.79	0.09	77.82	8.29
VCl ₃	93.17	95.47	2.47	103.76	11.37
VF ₃	89.84	86.98	3.19	88.70	1.27
VF ₄	107.03	113.14	5.71	109.62	2.42
VI ₂	74.80	75.68	1.17	77.82	4.04
VI ₃	99.73	101.30	1.57	103.76	4.04
VO	38.53	40.90	6.17	42.68	10.77
VO ₂	56.87	62.69	10.23	59.41	4.48
VOSO ₄	131.44	119.51	9.07	132.21	0.59
W(CO) ₆	242.65	243.67	0.42	171.54	29.30
WBr ₅	155.47	158.55	1.98	155.64	0.11
WBr ₆	181.40	177.13	2.35	181.59	0.10
WCl ₂	77.81	77.81	0.00	77.82	0.02
WCl ₂ O ₂	104.35	108.13	3.63	111.29	6.66
WCl ₄	129.72	124.16	4.29	129.70	0.01
WCl ₅	155.61	152.53	1.98	155.64	0.02
WCl ₆	175.40	169.91	3.13	181.59	3.53
WH ₂ O ₄	104.08	100.21	3.71	92.88	10.75
WO ₂	56.82	62.38	9.79	59.41	4.57
WO ₃	72.78	77.24	6.12	76.15	4.62
WOCl ₄	146.24	139.02	4.94	146.44	0.13
Y ₂ O ₃	102.49	100.54	1.90	102.09	0.39
Yb ₂ O ₃	115.34	112.25	2.68	102.09	11.49
YbCl ₂	74.22	74.22	0.00	77.82	4.85
YbCl ₃	95.34	102.46	7.47	103.76	8.83
YbF ₃	94.56	93.96	0.63	88.70	6.20
YCl ₃	92.01	96.61	4.99	103.76	12.77
YF ₃	95.24	88.11	7.48	88.70	6.86
YI ₃	96.00	102.43	6.69	103.76	8.08
Zn ₂ SiO ₄	121.79	124.12	1.91	134.72	10.62
Zn ₂ TiO ₄	137.29	138.05	0.55	144.77	5.45
Zn ₃ O(SO ₄) ₂	238.35	233.55	2.01	273.63	14.81

COMPOUNDS	C_p^{298} <i>C_p, literature</i>	C_p^{298} <i>C_p, predicted</i>	% Error	C_p^{298} <i>C_p, Kopp's rule</i>	% Error
ZnAl ₂ O ₄	119.31	117.50	1.52	144.77	21.33
ZnBr ₂	65.69	73.26	11.54	77.82	18.48
ZnCl ₂	71.05	70.86	0.27	77.82	9.53
ZnCO ₃	80.06	79.69	0.46	83.68	4.53
ZnCr ₂ O ₄	143.33	143.74	0.28	144.77	1.00
ZnF ₂	65.61	65.19	0.64	67.78	3.31
ZnFe ₂ O ₄	137.27	146.84	6.97	144.77	5.46
ZnI ₂	74.43	74.74	0.42	77.82	4.56
ZnO	41.06	39.97	2.66	42.68	3.94
ZnSeO ₃	93.66	96.19	2.71	102.09	9.00
ZnWO ₄	125.50	117.21	6.61	118.83	5.32
ZrBr ₂	86.71	82.09	5.33	77.82	10.25
ZrBr ₃	99.47	99.30	0.17	103.76	4.32
ZrBr ₄	124.80	122.64	1.72	129.70	3.93
ZrCl ₂	72.60	79.69	9.76	77.82	7.19
ZrCl ₃	96.20	95.69	0.53	103.76	7.86
ZrCl ₄	119.83	117.83	1.67	129.70	8.24
ZrF ₂	65.93	74.03	12.29	67.78	2.81
ZrF ₃	83.66	87.19	4.23	88.70	6.03
ZrF ₄	102.98	106.51	3.43	109.62	6.45
ZrI ₂	94.14	83.57	11.23	77.82	17.33
ZrI ₃	104.37	101.51	2.73	103.76	0.58
ZrI ₄	125.11	125.60	0.39	129.70	3.67
ZrO ₂	56.19	56.05	0.24	59.41	5.74
ZrSiO ₄	98.54	100.23	1.72	108.78	10.40