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 ^{o}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:

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

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 (^{o}K).

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

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

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 (^{o}K). Thinh et at. (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.

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

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

$$C_p = a + bT + \frac{c}{T^2} \tag{5}$$

$$C_p = a + bT + \frac{e}{\sqrt{T}} \tag{6}$$

$$C_p = a + bT \tag{7}$$

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,

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

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

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

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,

$$C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} x10^{-3}\right)T + \left(\sum_j n_j \Delta_{c,j} x10^{6}\right)\frac{1}{T^2} + \left(\sum_j n_j \Delta_{d,j} x10^{-6}\right)T^2 \tag{10}$$

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 (^oK). 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

$$\boldsymbol{b} = [\boldsymbol{X}^T\boldsymbol{X}]^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{11}$$

where $\boldsymbol{b}$ 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, $\boldsymbol{X}$ is a matrix in which the element in the i^{th} row and j^{th} column contains $(n_{i,j} - \overline{n}_j)$, where $n_{i,j}$ the number of occurrences of group j in compound i and $\overline{n}_j$ is the mean number of occurrences of group j in all salts in the regression, and $\boldsymbol{y}$ 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, $s_{\Delta j}$, which are calculated from the square roots of the diagonal elements of the variance-covariance matrix,

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

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

$$\boldsymbol{e} = \boldsymbol{y} - \boldsymbol{Xb} \tag{13}$$

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 $\Delta_{c,j}$.

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 $\sum_j n_j \Delta_{a,j}$, $\sum_j n_j \Delta_{b,j}$, $\sum_j n_j \Delta_{c,j}$, and $\sum_j n_j \Delta_{d,j}$ 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 (^oK) 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 ^oK found in the literature, predicted heat capacity ($C_{p,predicted}^{298}$) by the proposed method at 298 ^oK, 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 reminder of the 15 compounds are poor. The errors for these poor predictions at their maxium temperature are as follows:

VO (43.53% @ 1973 ^{o}K), UO_2F_2 (49.2% @ 1500 ^{o}K), UO_2 (50.3% @ 2000 ^{o}K), TiO_2 (46.3% @ 2130 ^{o}K), TiF_3 (47.4 @ 1310 ^{o}K), ThO_2 (94.5% @ 2500 ^{o}K), ScF_3 (55.5 % @ 1825 ^{o}K), $NpO_3.H_2O$ (100.4% @ 800 ^{o}K), MoF_3 (93.1% @ 1237 ^{o}K), $MoCl_3$ (52.1 % @ 926 ^{o}K), $MoBr_3$ (60.4% @ 1082 ^{o}K), MgO (43.8% @ 3105 ^{o}K), GeO_2 (68.0% @ 1409 ^{o}K), FeF_3 (46.5% @ 1132 ^{o}K), and Be_2SiO_4 (63.5% @ 1806 ^{o}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 $CaTiO_3$ and $Fe_2(SO_4)_3$ 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 $CaTiO_3$, the predictions are close to experimental values up to 1200 ^{o}K and then the proposed method deviates by predicting higher values. For $Fe_2(SO_4)_3$, predictions are good from 300-600 ^{o}K and then deviates. One of the poorest predictions obtained is shown in Figure 3. Here, for $FeTiO_3$, 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 ^{o}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	$C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j}\, x10^{-3}\right) T + \left(\sum_j n_j \Delta_{c,j}\, x10^{6}\right) \frac{1}{T^2} + \left(\sum_j n_j \Delta_{d,j}\, x10^{-6}\right) T^2$ = 153.6904 + (50.9853)x(10^{-3})x(298) + (-4.26043)x10^6/$(298)^2$ + (-26.71059)x(10^{-6})x$(298)^2$ = 118.54 *J/(g mol °K)*.				

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NOMENCLATURE

$\boldsymbol{b}$ = 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)*.

$\boldsymbol{e}$ = 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.

$\boldsymbol{S}$ = variance-covariance matrix.

$s_{\Delta j}$ = standard deviations of the parameters.

V_b = liquid molar volume at normal boiling point.

$\boldsymbol{X}$ = the matrix the i,j^{th} element of which contains $(n_{i,j} - \bar{n}_j)$.

$\boldsymbol{y}$ = 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 °K)*.

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

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

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

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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 ($s_{\Delta,j}$) associated with them for *a*, *b*, *c*, and *d*.

Group	Number of Occurrences	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
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	$\Delta_{a,j}$	$\Delta_{b,j}$	$\Delta_{c,j}$	$\Delta_{d,j}$	$s_{\Delta,j}$ for $\Delta_{a,j}$	$s_{\Delta,j}$ for $\Delta_{b,j}$	$s_{\Delta,j}$ for $\Delta_{c,j}$	$s_{\Delta,j}$ for $\Delta_{d,j}$
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.
Comparision 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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$ Proposed Method	% Error Proposed Method	$C_{p,predicted}^{298}$ Kopp's Rule	% Error Kopp's Rule
Ag_2CO_3	111.60	109.98	1.45	109.62	1.77
Ag_2SO_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_2TiO_4	149.13	150.56	0.95	144.77	2.93
$Ba_3Al_2O_6$	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_2O_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
$BeAl_2O_4$	104.88	102.55	2.22	144.77	38.03
$BeAl_6O_{10}$	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
$Ca_2B_2O_5$	147.05	140.63	4.37	158.16	7.55
$Ca_2P_2O_7$	187.70	186.21	0.79	214.22	14.13
$Ca_2V_2O_7$	213.88	209.29	2.15	220.92	3.29
$Ca_3Al_2O_6$	209.65	200.54	4.34	230.12	9.76
$Ca_3B_2O_6$	187.77	181.63	3.27	200.83	6.96
Ca_3P_2O8	236.03	227.22	3.73	256.90	8.84
Ca_3WO_6	202.24	200.25	0.99	204.18	0.96
$CaAl_2O_4$	120.55	118.54	1.67	144.77	20.08
$CaAl_4O_7$	193.83	196.07	1.16	246.86	27.36
CaB_2O_4	103.83	99.63	4.05	115.48	11.22
CaB_4O_7	157.74	158.25	0.33	188.28	19.36

COMPOUND	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$ Proposed Method	% Error Proposed Method	$C_{p,predicted}^{298}$ Kopp's Rule	% Error Kopp's Rule
$CaCO_3.MgCO_3$	155.18	156.98	1.16	167.36	7.85
$CaCr_2O_4$	146.59	144.77	1.24	144.77	1.24
$CaFe_2O_5$	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_2O_6	170.74	168.29	1.44	178.24	4.39
$Li_2B_4O_7$	170.34	175.21	2.86	214.22	25.76
Li_2BeF_4	134.97	133.42	1.15	161.50	19.66
Li_2CO_3	97.96	97.68	0.30	109.62	11.90
Li_2HfO_3	111.87	117.59	5.11	128.03	14.44
$Li_2Nb_2O_6$	198.55	204.22	2.86	204.18	2.83
Li_2SO_4	117.14	114.78	2.01	141.42	20.73
$Li_2Ta_2O_6$	200.14	197.02	1.56	204.18	2.02
Li_2WO_4	133.34	135.20	1.39	144.77	8.57
Li_2ZrO_3	110.20	114.01	3.45	128.03	16.18
Li_3AlF_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
$Mg_2V_2O_7$	202.26	200.35	0.94	220.92	9.23
$Mg_3P_2O_8$	213.09	213.82	0.34	256.90	20.56
$MgAl_2O_4$	115.94	114.07	1.61	144.77	24.87
$MgCO_3$	75.40	76.26	1.13	83.68	10.98
$MgFe_2O_4$	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
$MgTi_2O_5$	146.60	152.76	4.21	161.50	10.17
$MgTiO_3$	91.17	94.65	3.82	102.09	11.98
MgV_2O_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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$ Proposed Method	% Error Proposed Method	$C_{p,predicted}^{298}$ 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_2SO_4	144.88	143.47	0.97	148.95	2.81
$UOBr_2$	97.88	96.44	1.47	94.56	3.40

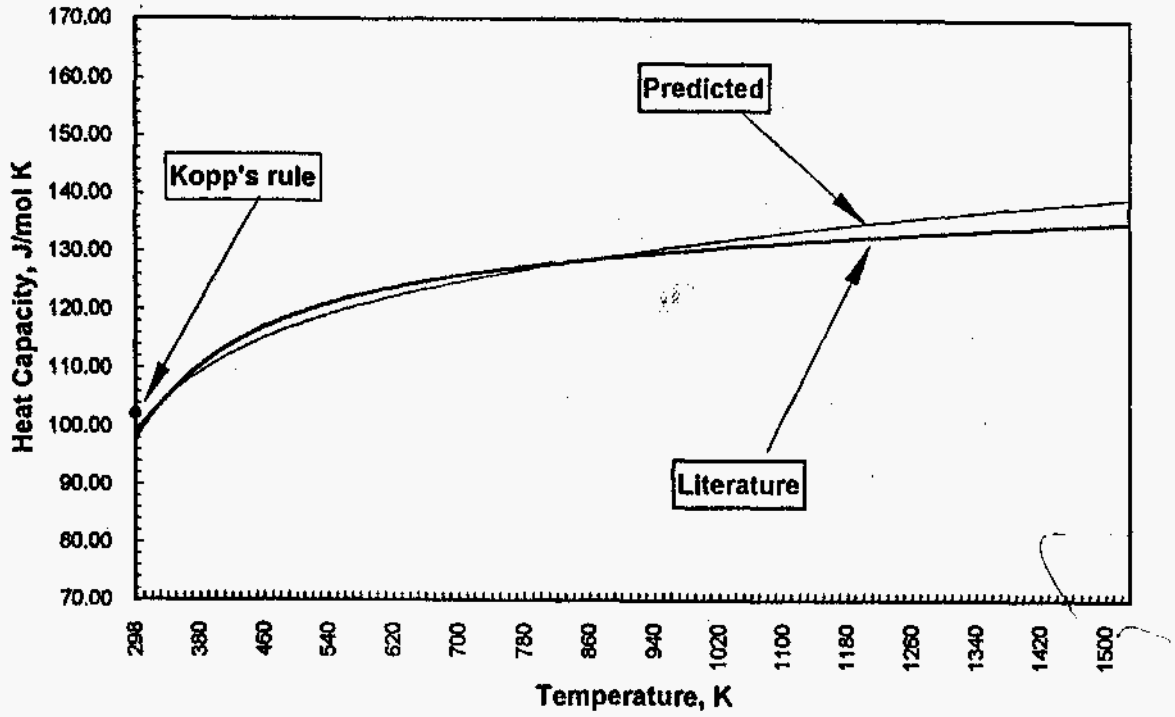

Figure 1. Heat capacity (C_p, *J/mol °K*) vs. temperature (*°K*) of $CaTiO_3$ for literature (From Robie et. al., 1979) and predicted values

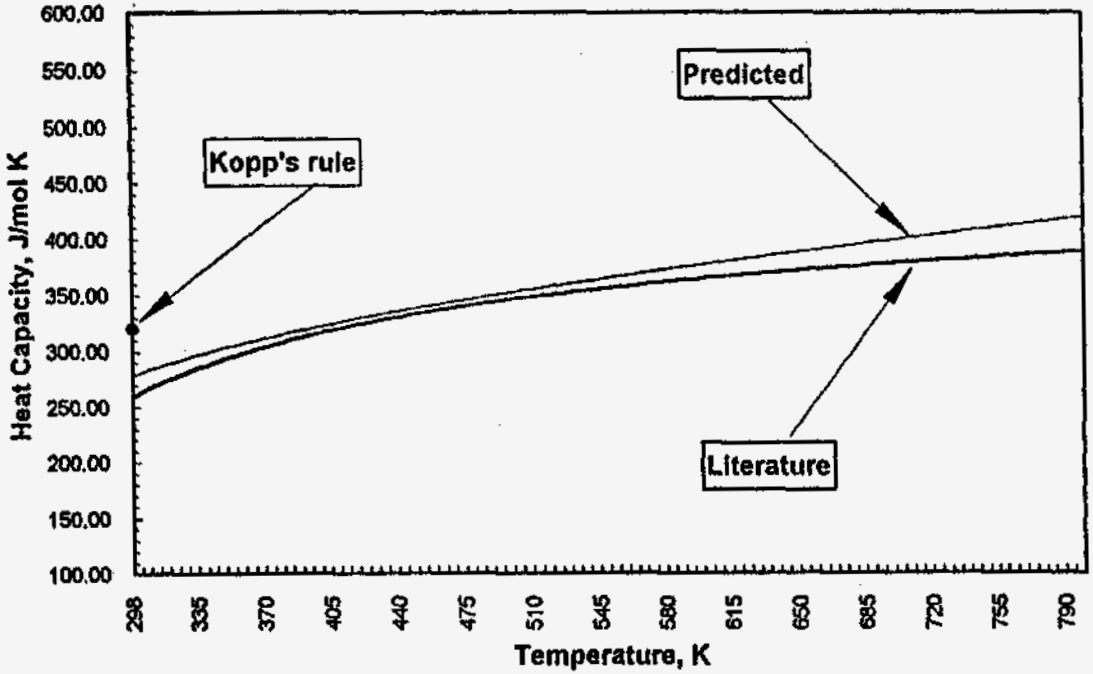

Figure 2. Heat capacity (C_p, *J/mol °K*) vs. temperature (*°K*) of $Fe_2(SO_4)_3$ for literature (From Robie et. al., 1979) and predicted values.

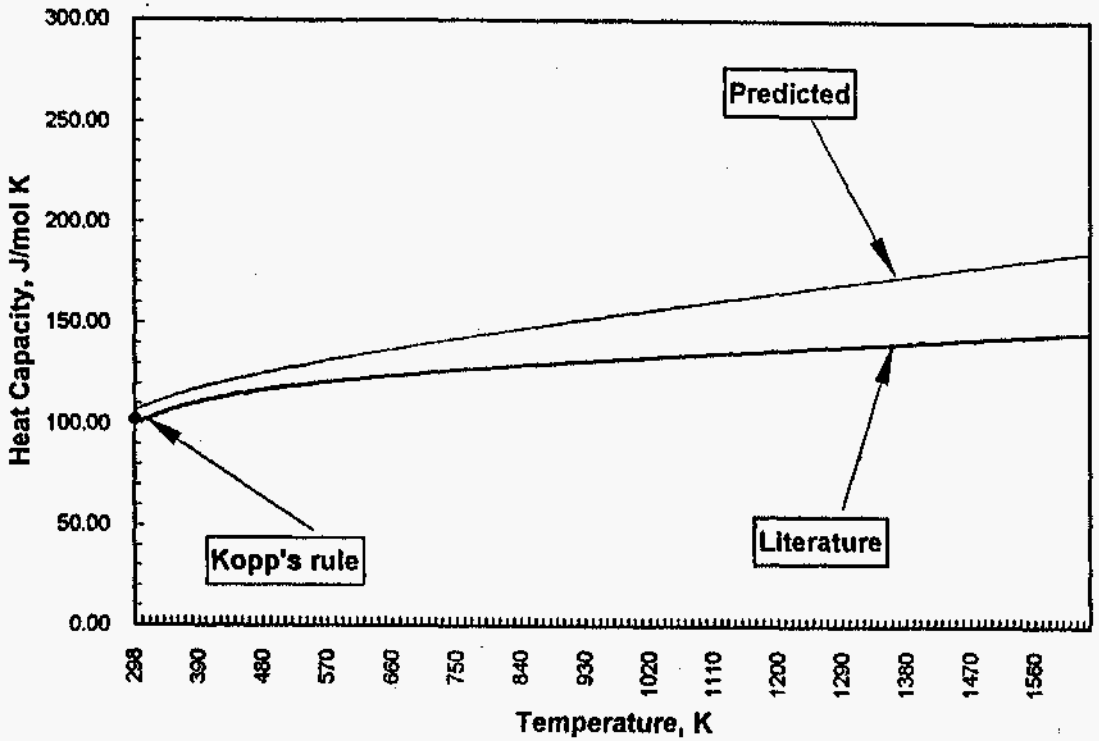

Figure 3. Heat capacity (C_p, *J/mol °K*) vs. temperature (*°K*) of $FeTiO_3$ for literature (From Robie et. al., 1979) and predicted values.

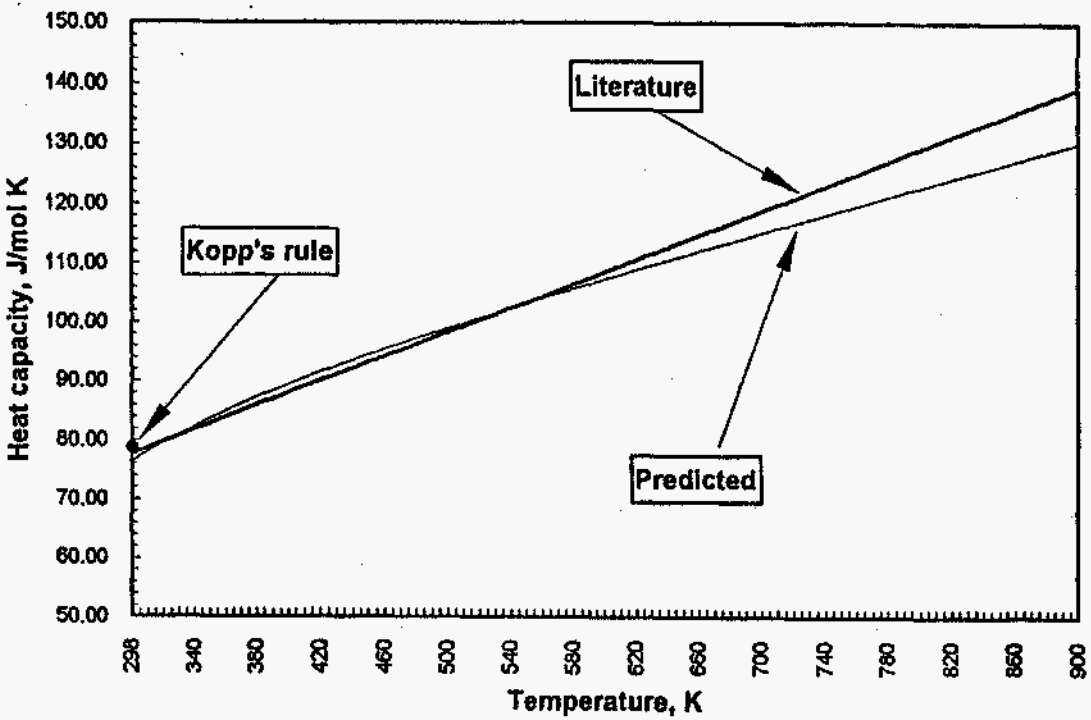

Figure 4. Heat capacity (C_p, *J/mol °K*) vs. temperature (°*K*) of $Mg(OH)_2$ for literature (From Robie et. al., 1979) and predicted values.

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 ^{o}K.

COMPOUNDS	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
Ag_2CO_3	111.60	109.98	1.45	109.62	1.77
Ag_2O	66.31	70.26	5.96	68.62	3.49
Ag_2SO_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_2O_3	78.81	77.53	1.61	102.09	29.55
$Al_2O_3.3H_2O$	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_2O_3	96.95	95.88	1.10	102.09	5.30
As_2O_5	116.54	123.93	6.34	135.56	16.32
As_4O_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_2TiO_4	149.13	150.56	0.95	144.77	2.93
$Ba_3Al_2O_6$	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
$BaO.Al_2O_3$	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	$C_{p,Lawson}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
$BaO.V_2O_5$	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_2SiO_4	93.37	94.21	0.90	134.72	44.30
$BeAl_2O_4$	104.88	102.55	2.22	144.77	38.03
$BeAl_6O_{10}$	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
$BeSO_4.2H_2O$	152.82	155.84	1.97	187.44	22.65
$BeSO_4.4H_2O$	216.42	229.84	6.20	259.41	19.86
$3BeO.B_2O_3$	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_2O_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
$Ca(NO_3)_2.2H_2O$	231.58	229.57	0.87	250.20	8.04
$Ca(NO_3)_2.3H_2O$	267.14	266.57	0.21	286.19	7.13
$Ca(NO_3)_2.4H_2O$	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
$CaO.2Al_2O_3$	193.83	196.07	1.16	246.86	27.36
$CaO.2B_2O_3$	157.74	158.25	0.33	188.28	19.36
$CaO.Al_2O_3$	120.55	118.54	1.67	144.77	20.08
$CaO.Al_2O_3.SiO_2$	156.52	162.72	3.96	194.14	24.03
$CaO.B_2O_3$	103.83	99.63	4.05	115.48	11.22

COMPOUNDS	$C_{p,\text{Literature}}^{298}$	$C_{p,\text{produced}}^{298}$	% Error	$C_{p,\text{Kopp's rule}}^{298}$	% Error
$CaO.Cr_2O_3$	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
$CaO.V_2O_5$	170.74	168.29	1.44	178.24	4.39
$CaSO_4.2H_2O$	185.99	171.83	7.62	187.44	0.78
$CaSO_4.3H_2O$	205.10	208.83	1.82	223.43	8.94
$2CaO.Al_2O_3.SiO_2$	195.74	203.72	4.08	236.81	20.99
$2CaO.B_2O_3$	147.05	140.63	4.37	158.16	7.55
$2CaO.Fe_2O_3$	194.05	188.88	2.66	187.44	3.40
$2CaO.MgO.2SiO_2$	211.99	206.90	2.40	226.77	6.98
$2CaO.P_2O_5$	187.70	186.21	0.79	214.22	14.13
$2CaO.V_2O_5$	213.88	209.29	2.15	220.92	3.29
$3CaO.2TiO_2$	239.57	239.24	0.14	246.86	3.04
$3CaO.Al_2O_3$	209.65	200.54	4.34	230.12	9.76
$3CaO.Al_2O_3.3SiO_2$	323.01	333.09	3.12	378.23	17.10
$3CaO.B_2O_3$	187.77	181.63	3.27	200.83	6.96
$3CaO.P_2O_5$	236.03	227.22	3.73	256.90	8.84
$3CaO.V_2O_5$	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
$CdO.Al_2O_3$	129.87	122.27	5.85	144.77	11.47
$CdO.Ga_2O_3$	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	$C_{p,\text{literature}}^{298}$	$C_{p,\text{predicted}}^{298}$	% 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_2O_3	116.99	108.70	7.09	102.09	12.74
$Ce_2O_3.Al_2O_3$	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
$CoFe_2O_4$	152.54	154.80	1.48	144.77	5.09
$CoO.Al_2O_3$	132.23	125.46	5.12	144.77	9.48
$CoO.Cr_2O_3$	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_2O_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
$Cs_2B_2O_4$	138.91	136.81	1.52	141.42	1.81
$Cs_2Si_2O_5$	176.71	166.54	5.75	167.36	5.29
Cs_2SiO_3	122.22	122.36	0.11	117.99	3.47

COMPOUNDS	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
Cs_2UO_4	152.70	164.83	7.95	144.77	5.19
Cu_2O	63.54	59.93	5.68	68.62	7.99
$Cu_2O.Al_2O_3$	142.15	137.47	3.29	170.71	20.09
$Cu_2O.Ga_2O_3$	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
$CuFe_2O_4$	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
$CuO.Al_2O_3$	127.64	120.45	5.63	144.77	13.42
$CuO.Cr_2O_3$	148.00	146.69	0.88	144.77	2.18
$CuO.CuSO_4$	140.09	142.66	1.83	158.16	12.90
$CuO.Ga_2O_3$	134.98	138.51	2.61	144.77	7.25
$CuSO_4$	98.77	99.74	0.98	115.48	16.92
Dy_2O_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_2O_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
$EuCl_3.6H_2O$	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_2O_3	104.69	106.87	2.08	102.09	2.49
Fe_2SiO_4	132.90	130.06	2.14	134.72	1.37
Fe_3O_4	151.75	149.81	1.27	144.77	4.60
$FeAl_2O_4$	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
$FeCr_2O_4$	133.75	146.71	9.69	144.77	8.24

COMPOUNDS	$C_{p,Laurean}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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_2O_3	93.83	95.59	1.87	102.09	8.80
$GaBr_3$	101.65	97.74	3.84	103.76	2.08
Gd_2O_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_2WO_4	104.08	110.07	5.76	112.13	7.74
H_3BO_3	81.19	78.56	3.25	90.37	11.31
H_3PO_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_2Br_2	104.65	105.33	0.65	103.76	0.85
Hg_2Cl_2	101.54	102.92	1.36	103.76	2.19
Hg_2F_2	100.31	97.26	3.05	93.72	6.57
Hg_2I_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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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_2O_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
$HoCl_3.6H_2O$	347.30	325.06	6.40	319.66	7.96
HoF_3	91.22	94.56	3.67	88.70	2.76
In_2O_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
$K_2B_2O_4$	141.88	136.68	3.67	141.42	0.33
$K_2B_6O_{10}$	265.30	253.93	4.29	287.02	8.19
$K_2B_8O1_3$	318.93	312.55	2.00	359.82	12.82
K_2CO_3	114.25	117.77	3.08	109.62	4.05
K_2CrO_4	146.04	151.46	3.72	144.77	0.87
K_2HPO_4	143.47	144.37	0.63	151.04	5.28
$K_2O.Al_2O_3.2SiO_2$	239.72	243.95	1.76	269.45	12.40
$K_2O.Al_2O_3.4SiO_2$	328.45	332.31	1.18	368.19	12.10
$K_2O.Fe_2O_3$	187.85	184.93	1.56	170.71	9.13
$K_2Si_2O_5$	160.85	166.42	3.46	167.36	4.05
K_2SiO_3	118.62	122.23	3.04	117.99	0.53
K_2SO_4	131.57	134.87	2.52	141.42	7.49
K_2WO_4	150.79	155.29	2.98	144.77	4.00
K_3AlCl_6	249.02	248.52	0.20	259.41	4.17
K_3AlF_6	221.66	231.53	4.45	229.28	3.44
K_3PO_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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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_2PO_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_2O_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
$Li_2B_2O_4$	120.82	126.87	5.01	118.83	1.65
$Li_2B_4O_7$	170.34	175.21	2.86	214.22	25.76
$Li_2B_6O_{10}$	291.00	264.69	9.04	219.24	24.66
Li_2B_8O13	320.65	333.60	4.04	269.45	15.97
Li_2BeF_4	134.97	133.42	1.15	161.50	19.66
Li_2CO_3	97.96	97.68	0.30	109.62	11.90
Li_2HfO_3	111.87	117.59	5.11	128.03	14.44
$Li_2Nb_2O_6$	198.55	204.22	2.86	204.18	2.83
Li_2O	54.07	57.96	7.18	68.62	26.90
$Li_2O.Al_2O_3.2SiO_2$	226.50	220.33	2.72	301.25	33.00
$Li_2O.Al_2O_3.4SiO_2$	317.69	305.18	3.94	431.79	35.91
$Li_2Si_2O_5$	138.62	146.32	5.55	167.36	20.73
Li_2SiO_3	99.90	102.14	2.24	117.99	18.11
Li_2SO_4	117.14	114.78	2.01	141.42	20.73
$Li_2Ta_2O_6$	200.14	197.02	1.56	204.18	2.02
Li_2TiO_3	108.48	116.07	7.00	128.03	18.02
Li_2WO_4	133.34	135.20	1.39	144.77	8.57
Li_2ZrO_3	110.20	114.01	3.45	128.03	16.18
Li_3AlF_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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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_2O_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_2SiO_4	118.43	117.25	1.00	134.72	13.76
Mg_2TiO_4	128.17	131.19	2.35	144.77	12.94
$Mg_2V_2O_7$	202.26	200.35	0.94	220.92	9.23
$Mg_3P_2O_8$	213.09	213.82	0.34	256.90	20.56
$MgAl_2O_4$	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
$MgCr_2O_4$	126.72	140.30	10.72	144.77	14.24
MgF_2	61.33	61.76	0.70	67.78	10.51
$MgFe_2O_4$	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
$MgTi_2O_5$	146.60	152.76	4.21	161.50	10.17
$MgTiO_3$	91.17	94.65	3.82	102.09	11.98
MgV_2O_6	159.87	163.82	2.47	178.24	11.49
$MgWO_4$	109.83	113.78	3.59	118.83	8.19
Mn_2O_3	99.02	99.77	0.76	102.09	3.10
Mn_2SiO_4	129.87	130.45	0.45	134.72	3.74
Mn_2TiO_4	144.52	144.38	0.09	144.77	0.17
Mn_3O_4	140.48	142.90	1.73	144.77	3.05
$MnAl_2O_4$	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
$MnO.Fe_2O_3$	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_2Cl_2	107.65	105.71	1.80	111.29	3.39
MoO_3	75.12	74.82	0.41	76.15	1.37
$Na_2B_2O_4$	131.68	128.50	2.41	141.42	7.40
$Na_2B_4O_7$	186.85	187.12	0.15	214.22	14.65
$Na_2B_6O_{10}$	243.61	245.75	0.88	287.02	17.82
Na_2B_8O13	304.75	304.37	0.12	359.82	18.07
Na_2CO_3	111.30	109.59	1.53	109.62	1.51
$Na_2Cr_2O_4$	178.78	173.64	2.88	170.71	4.52
Na_2CrO_4	142.76	143.29	0.37	144.77	1.41
$Na_2Mo_2O_7$	216.66	219.50	1.31	220.92	1.97
Na_2MoO_4	141.43	144.69	2.30	144.77	2.36
Na_2O	68.54	69.87	1.94	68.62	0.11
$Na_2O.Al_2O_3.4SiO_2$	311.72	324.13	3.98	368.19	18.12
$Na_2O.Al_2O_3.6SiO_2$	409.54	412.50	0.72	466.93	14.02
$Na_2O.UO_3$	146.71	156.52	6.69	144.77	1.33
Na_2O_2	88.92	92.84	4.41	85.35	4.01
$Na_2P_2O_6$	174.44	174.08	0.20	197.48	13.21
$Na_2Si_2O_5$	156.44	158.24	1.15	167.36	6.98
Na_2SiO_3	111.78	114.06	2.04	117.99	5.56
Na_2SO_3	120.08	120.08	0.00	124.68	3.84

COMPOUNDS	$C_{p,Lawrence}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
Na_2SO_4	128.34	126.70	1.28	141.42	10.19
$Na_2Ti_2O_5$	193.11	187.16	3.08	187.44	2.93
$Na_2Ti_3O_7$	252.21	245.69	2.58	246.86	2.12
Na_2TiO_3	131.18	128.62	1.95	128.03	2.40
$Na_2V_2O_6$	195.10	198.42	1.70	204.18	4.65
Na_2WO_4	141.75	147.11	3.78	144.77	2.13
Na_3AlF_6	222.72	219.26	1.55	229.28	2.95
$Na_4P_2O_7$	241.24	243.96	1.13	266.10	10.31
$Na_4V_2O_7$	269.74	268.51	0.46	272.80	1.13
$Na_5Al_3F_{14}$	461.92	467.57	1.22	500.41	8.33
$Na_6As_2O_8$	340.94	333.55	2.17	341.41	0.14
$Na_6P_2O_8$	306.63	313.83	2.35	334.72	9.16
$Na_6V_2O_8$	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_2O_3	111.32	107.16	3.74	102.09	8.29
$Nd_2O_3.2ZrO_2$	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_4ClO_4	128.07	140.15	9.43	157.32	22.83
$(NH_4)_2SO_4$	187.21	184.95	1.21	218.40	16.66

COMPOUNDS	$C_{p,literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
Ni_2SiO_4	126.95	131.75	3.78	134.72	6.13
$NiAl_2O_4$	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
$NiCr_2O_4$	148.77	147.55	0.82	144.77	2.69
$NiFe_2O_4$	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
$NiTiO_3$	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
$NpO_3.H_2O$	118.06	123.41	4.53	112.13	5.02
$NpOCl_2$	92.85	92.62	0.25	94.56	1.84
Pb_2SiO_4	136.90	139.14	1.64	134.72	1.59
Pb_4SiO_6	229.70	234.09	1.91	220.08	4.19
PbB_4O_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	$C_{p,literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
PdO	46.02	43.56	5.34	42.68	7.26
Pr_2O_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_2O_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_2CO_3	117.67	118.37	0.59	109.62	6.84
Rb_2O	73.97	78.65	6.34	68.62	7.23
$Rb_2Si_2O_5$	170.66	167.01	2.14	167.36	1.94
$Rb_2Si_4O_9$	270.85	255.38	5.71	266.10	1.75
Rb_2SiO_3	117.40	122.83	4.63	117.99	0.50
Rb_2SO_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
$ReNH_4O_4$	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_2O_3	103.99	101.47	2.42	102.09	1.82

COMPOUNDS	$C_{p,\text{Literature}}^{298}$	$C_{p,\text{predicted}}^{298}$	% Error	$C_{p,\text{Kopp's rule}}^{298}$	% 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_2O_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_2O_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
SiI_4	108.03	113.73	5.27	119.66	10.77
SiO_2	44.41	44.18	0.52	49.37	11.17
Sm_2O_3	115.80	116.03	0.19	102.09	11.84
$Sm_2O_3.2ZrO_2$	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_2SiO_4	130.75	130.09	0.50	134.72	3.04
Sr_2TiO_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	$C_{p,Lorentzo}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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_2O_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_2O_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_2N_2O	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_2O_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	$C_{p,Literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% 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
TiL_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_2O	78.84	78.14	0.89	68.62	12.97
Tl_2O_3	105.42	107.58	2.04	102.09	3.16
Tl_2SO_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_2O_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
UL_4	134.43	132.69	1.30	129.70	3.52
UO_2	63.57	63.14	0.68	59.41	6.54
UO_2F_2	103.04	111.88	8.58	101.25	1.73
UO_2SO_4	144.88	143.47	0.97	148.95	2.81
UO_3	81.16	86.65	6.76	76.15	6.18
$UO_3.2H_2O$	154.52	160.65	3.97	148.11	4.15
$UO_3.H_2O$	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_2O_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_2O_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_2O_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_2O_3	102.49	100.54	1.90	102.09	0.39
Yb_2O_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_2SiO_4	121.79	124.12	1.91	134.72	10.62
Zn_2TiO_4	137.29	138.05	0.55	144.77	5.45
$Zn_3O(SO_4)_2$	238.35	233.55	2.01	273.63	14.81

COMPOUNDS	$C_{p,literature}^{298}$	$C_{p,predicted}^{298}$	% Error	$C_{p,Kopp's\ rule}^{298}$	% Error
$ZnAl_2O_4$	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
$ZnCr_2O_4$	143.33	143.74	0.28	144.77	1.00
ZnF_2	65.61	65.19	0.64	67.78	3.31
$ZnFe_2O_4$	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