

Table 2

## Additivity Calculation of Physical and Thermodynamic Parameters

Parameter	Spinel MgO·Al <sub>2</sub> O <sub>3</sub>	Garnet ZnO·Al <sub>2</sub> O <sub>3</sub>	Hercynite FeO·Al <sub>2</sub> O <sub>3</sub>	Chrysoberyl BeO·Al <sub>2</sub> O <sub>3</sub>	Magnetite FeO·Fe <sub>2</sub> O <sub>3</sub>	Ilmenite FeO·TiO <sub>2</sub>
	Oxides					
$M/\rho$ , cm <sup>3</sup> /mole	36.85/ 38.8	39.94/ 40.0	37.65/ 39.4	33.92/ 34.22	42.25/ 44.3	31.3/ 31.71
$\rho$ , g/cm <sup>3</sup>	3.86/ 3.64	4.59/ 4.59	4.54/ 4.4	3.73/ 3.70	5.42/ 5.24	4.83/ 4.78
$K \cdot 10^5$ , kg/cm <sup>2</sup>	22.6/ 6.20	21/ —	22/ —	28/ 27	19.1/ 18	19.1/ 18.5
$l$ , (Å) <sup>-3</sup>	8.4/ 8.2	8.2/ 8.3	6.72/ 6.2	9.6/ 9.4	6.07/ 5.7	7.9/ 7.7
$b$	4.9/ 4.6	4.52/ 4.50	4.8/ 4.4	5.3/ 5.3	4.92/ 4.06	4.74/ 3.8
$S_{298}^{\circ}$ , cal/mole-deg	19.2/ 19.3	23.2/ —	25.0/ 25.4	15.55/ —	34.4/ 35	24.9/ 25.3
$\Delta Z_{298}^{\circ}$ , kcal/mole	512.8/ 517.5	452.7/ —	435.1/ 441.9	515.7/ 515.5	235.5/ 242	269.4/ 277.5
$C_{p,298}^{\circ}$ , cal/mole-deg	27.82/ —	28.50/ —	31.08/ —	24.9/ —	37.2/ 34.2	25.8/ 23.78

## Silicates

Parameter	Forsterite 2MgO·SiO <sub>2</sub>	Fayalite 2FeO·SiO <sub>2</sub>	Enstatite MgO·SiO <sub>2</sub>	Ferrosilite FeO·SiO <sub>2</sub>	Phenakite 2BeO·SiO <sub>2</sub>	Kyanite Al <sub>2</sub> O <sub>3</sub> ·SiO <sub>2</sub>
$M/\rho$ , cm <sup>3</sup> /mole	42.50/ 43.67	44.1/ 46.4	31.95/ 32.5	32.0/ 33	36.6/ 37.2	44.1/ 44.1
$\rho$ , g/cm <sup>3</sup>	3.32/ 3.22	4.62/ 4.39	3.27/ 3.20	4.1/ 3.99	3.0/ 2.97	3.66/ 3.66
$K \cdot 10^5$ , kg/cm <sup>2</sup>	12.5/ 13	11.5/ 11	11/ 11.0	10.7/ —	21/ —	19/ —
$l$ , (Å) <sup>-3</sup>	7.5/ 7.5	7.2/ 7.0	7.7/ 7.8	7.5/ 7.4	8.5/ 8.7	—
$b$	4.1/ 4.1	3.9/ 3.9	3.7/ 3.8	3.7/ 3.7	4.87/ 4.9	—
$S_{298}^{\circ}$ , cal/mole-deg	22.8/ 22.7	35/ 34.7	15.4/ 16.2	21.9/ 23	15.7/ 15.4	—
$\Delta Z_{298}^{\circ}$ , kcal/mole	472/ 480	317/ 316	336/ 337	258/ 257.7	478/ 470	—
$C_{p,298}^{\circ}$ , cal/mole-deg	28.4/ 28.2	35/ 31.7	19/ 19.6	21.2/ —	22.7/ 22.8	—

or enstatite and ferrosilite with the ilmenite structure. In that case we should use stishovite (6:3 coordination) as the basis. Table 1 gives the results.

It is not important as regards the additivity principle whether a substance occurs in the depths of the Earth as simple oxides or

as a compound of spinel, garnet, etc. type; but the chemical composition and the cation coordination (in an oxygen environment) are important. The principle can give reasonably reliable results for the properties of a substance of known composition, provided that we have a clear conception of the stability ranges of oxides and silicates at the P and T prevailing within the Earth.