due to covalent bonds. For crystals whose enthalpy of formation (ΔH_f°) is known, the difference between calculations based on ionic theory and the measured (known) value of ΔH_f° give an apparent value for the covalent enthalpy in the lattice. There will, however, be some error in taking the actual enthalpy and the calculated ionic enthalpy equal to the covalent bond energy. This is because the lattice parameters and bulk moduli used to calculate the ionic enthalpy do themselves reflect the actual potentials within the crystal and not just the ionic portion of the potential. Also the "resonance" between ionic and covalent bonding arrangements will contribute to the lattice energy. However, in general the difference between the calculated ionic enthalpy and the actual enthalpy should be a good index of the relative proportion of covalent bonding involved.

In some of the crystal structures considered, notably rutile, α-quartz and corundum, non-radially-symmetric electric fields are known to be present at some of the lattice sites. In such cases the charge distribution associated with the ion occupying that site will be deformed into a dipole or higher order multipole. As a result interactions other than monopole interactions should be included in calculating the ionic lattice energy. We have taken such interaction into account only for SiO_2 (stishovite), TiO_2 (rutile), and Al_2O_3 (corundum). In the first, the permanent dipole effect can be estimated to be about 62 kcal/mole (by analogy with KINGSBURY's (1968) calculation of this same effect in rutile). For rutile it is 51 kcal/mole (KINGSBURY (1968)) and for Al_2O_3 multipole interactions account for about 25 kcal/mole (HAFNER and RAYMOND (1968)).

3. Results

Equations (3) and (4) were used to calculate the lat-

TABLE 1

Data for calculation of lattice energies

Compound	Structure	$V(Å^3)$	$R_0(Å)$	α_R [1]	K_T(Mb)	$q^2(e^2)$
FeO	halite	20.197	2.723	2.2018	1.42 [2]	2
SiO_2	α-quartz	37.672	3.352	9.168 [3]	0.374 [4]	4
SiO_2	rutile	23.269	2.855	7.7219	3.627 [5]	4
TiO_2	rutile	31.225	3.149	7.7191 [6]	2.125 [7]	4
Al_2O_3	corundum	42.466	3.489	45.7726	2.505 [4]	1
Cr_2O_3	corundum	48.30	3.64	45.282	2.237	1
$Fe_2^{3+}O_3$	corundum	50.268	3.691	45.679	2.027 [4]	1
$Fe_2^{3+}O_3$	perovskite	45.716 [5]	3.576	44.5549	3.814 [5]	1
$Fe^{2+}Fe^{4+}O_3$	perovskite	45.716 [5]	3.576	12.3775	3.814 [5]	4
$MgSiO_3$ - (a)	perovskite	39.225 [5]	3.398	12.3775	4.188 [5]	4
$MgSiO_3$ - (b)	perovskite	40.957	3.4	12.3775	3.49 [5]	4
$MgSiO_3$ - (c)	perovskite	44.36	3.54	12.3775	2.6 [5]	4
$SrTiO_3$	perovksite	59.558	3.905	12.3775	1.787 [8]	4
$CaTiO_3$	perovskite	55.8325	3.822	12.3775	1.633 [9]	4
Al_2MgO_4	spinel	65.939	4.040	67.535	1.95 [10]	1
Mg_2SiO_4	spinel	65.817	4.038	71.99	2.02 [9]	1
Fe_2SiO_4	spinel	69.782	4.117	72.225	2.12 [2]	1
Ni_2SiO_4	spinel	65.0376	4.0215	72.1 (est.)	2.11 [11]	1
$Fe_2Cr_2O_4$	spinel	73.455	4.188	64.30	1.87	1
Fe_2TiO_4	spinel	76.766	4.25	68.25	1.76	1
Fe_3O_4	spinel	73.982	4.198	65.475	1.872	1

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