structure is viewed along the *b* axis. This projection illustrates very clearly that the external shape of a crystal – in this case the prominence of $\{10\bar{1}\}$ – is a function of the packing of the molecules in the crystal lattice.

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Effective Ionic Radii in Oxides and Fluorides*

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An empirical set of 'effective' ionic radii has been compiled by the use of techniques similar to those of Goldschmidt. The actual radius values were derived from: (1) 1000 experimental interatomic distances and (2) an approximately linear relationship between ionic volume and unit cell volume of over 60 isotypic series of oxides and fluorides. These radii take into account electronic spin state and the coordination of both cations and anions and have been found to reproduce closely the experimental interatomic distances in most oxides and fluorides. The choice of absolute values for anion radii and certain deviations from additivity are important and must be taken into consideration.

Introduction

The traditional sets of ionic radii of Goldschmidt, Barth, Lunde & Zachariasen (1926), Pauling (1927), Zachariasen (1931), and Ahrens (1952) have been used with considerable success by chemists, physicists, mineralogists, and crystallographers alike. Ionic radii have been important to the crystal chemist because structure types and cation coordination numbers are determined principally by cation/anion radius ratios. The ability to substitute one cation for another in a particular structure is largely dependent upon matching ionic radii; thus, good values of ionic radii have been important to the chemist synthesizing inorganic compounds. The crystallographer has found radii helpful in comparing experimental interatomic distances with those calculated for other structures.* These interatomic distances in turn can help the chemist to infer oxidation states.

There are, however, several deficiencies in these traditional sets of radii: (1) they do not reproduce interatomic distances to the accuracy now possible in modern structural analyses; (2) although several papers (Pauling, 1927; Zachariasen, 1931) present techniques for calculating the effect of coordination number on *interatomic distances*, no provision is made for determining

* Contribution No. 1454.

* Goldschmidt's & Pauling's radii and correction factors for coordination number (CN) ≠ VI were included in Volume II of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). Interatomic distances in numerous inorganic compounds were published in Volume III of *International Tables for X-Ray Crystallography* (1962) and in *Tables of Interatomic Distances and Configuration in Molecules and Ions* (1958, 1965).

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values of the *radii* in other than octahedral coordination; (3) the effect of variations in electronic spin state on radii has not been included.

This paper presents an extensive table of empirical radii that can be used to closely reproduce average observed cation–anion distances in most oxide and fluoride crystal structures. These radii, which take into consideration both anion and cation coordination and electronic spin state, were derived from over 1000 average interatomic distances. Certain radii were made consistent with regular plots of effective ionic radii (r) or volume (r^3) *vs.*(1) unit cell volumes for over 60 isotypic series of compounds, (2) electron configuration, (3) coordination number (CN), and/or (4) valence.

Background of ionic radii

Crystal chemists have tried for many years to treat atoms and ions as hard spheres and to calculate atomic and ionic radii that would closely reproduce interatomic distances. Approximate additivity of atomic and ionic radii was noted by the earliest investigators (Goldschmidt *et al.*, 1926; Pauling, 1927; Zachariasen, 1931). However, since the additivity of a given set of radii was not found applicable to all bond types, separate tables of radii were derived for ionic, covalent, and metallic bonding. The history of radii determinations for ionic compounds, treated in detail by Pauling (1927), Ahrens (1952), Slater (1964), and Tosi (1964), will be reviewed here only briefly to point out similarities and differences in the methods.

The first attempt at such determinations was by Bragg (1920) who derived a set of atomic radii which reproduced interatomic distances in both ionic and metallic crystals to an average deviation of about 0·06 Å. Bragg & West (1927) later revised these radii so as to be more in accord with Wasastjerna's (1923) conclusion that $r(O^{2-}) = 1{\cdot}32$ Å.* Bragg & West arrived at a value of $r(O^{2-}) = 1{\cdot}35$ Å from close-packed oxygen structures. Goldschmidt *et al.* (1926) derived a set of radii to be used only in ionic crystals. Goldschmidt's radii were obtained from average interatomic distances using Wasastjerna's radii of $r(O^{2-}) = 1{\cdot}32$ Å and $r(F^-) = 1{\cdot}33$ Å. Because structural data were scarce, Goldschmidt's table was necessarily limited. However he was able to extend the able to cover radii for which there were no experimental interatomic distances by interpolation or extrapolation of unit-cell dimensions of isotypic series *e.g.* In^{3+}, Y^{3+}, and Tl^{3+} from the *C* rare earth oxide structure type. If his radii are based on $r(O^{2-}) = 1{\cdot}40$ Å, the value generally used by later investigators, they agree well with more recent sets of radii. Goldschmidt was the first to note that radii varied with coordination number and provided a few examples of this variation.

Pauling (1927) calculated a set of radii based on an inverse variation with effective nuclear charge in isoelectronic series of the alkali ions. The radii of the alkali ions were determined from interatomic distances in alkali halides assuming $r(O^{2-}) = 1{\cdot}40$ Å and $r(F^-) = 1{\cdot}36$ Å. Pauling prepared two tables of radii: (1) a univalent set from which radii of ions of any charge could be calculated and (2) a table of ionic octahedral crystal radii (ionic radii for multivalent ions). A correction factor was provided to allow calculation of interatomic distances in crystals where the CN of the cation differed from six. However, the coordination of the anion was neglected. Pauling (1928) noted that additivity in the alkali halides alone was poor and introduced extra terms in the expression for interatomic distance to correct for cation–cation and anion–anion repulsion. With these corrections, calculated and observed distances agreed to within about 0·001 Å.

Subsequently, Zachariasen (1931) derived a set of radii from the best available interatomic distances, assuming $r(K^+) = 1{\cdot}33$ Å and $r(Cl^-) = 1{\cdot}81$ Å. He calculated univalent radii using Pauling's (1927) method and provided equations with which interatomic distances could be calculated if valence and CN of the cation were known. Zachariasen's radii differed considerably from Pauling's but not from Goldschmidt's corrected radii using $r(O^{2-}) = 1{\cdot}40$ Å. Although Zachariasen's radii reproduced interatomic distances quite accurately, they seem to have been used less than some of the other sets of radii. Ahrens' or Pauling's radii were probably preferred because of the simplicity of extracting radii directly from a table rather than of calculation from univalent radii with corrections for valence and CN. However, even Zachariasen's table did not allow direct comparison of cation radii when the cation CN was different from 6, nor did it differentiate between high and low spin ions.

The next extensive list of radii was prepared by Ahrens (1952) who revised Pauling's radii by the use of slightly different values for the alkali ions. His method utilized the regularities found by plotting radii *vs.* ionization potentials. The regular curves obtained by Ahrens were used to estimate the radii of ions for which no values previously existed. Ahrens' table was thus the most complete table for many years and consequently was widely used. However, Ahrens considered only octahedral radii and made no provision for variation of radius with electronic spin state.

More recently, two further sets of radii were introduced. Slater (1964) extended the idea of Bragg (1920) and published a table of atomic radii in which $r(^{VI}O^{2-}) = 0{\cdot}60$ Å, which reproduced interatomic distances in 1200 metallic, covalent, and ionic solids to a deviation of $\pm 0{\cdot}12$ Å. These radii have not proved to be particularly useful in oxide and fluoride crystal chemistry. Fumi & Tosi (1964) derived a set of ionic radii for the alkali halides based on (1) a correlation between Born repulsive parameters and the ratio r_c/r_a in alkali halides and (2) the minimum in the LiF and NaCl electron

* Throughout this paper a Roman numeral at the upper left of the element will be used to designate CN. Thus, $^{X}Ba^{2+}$ refers to the ten-coordinated barium ion. If no symbol for CN is present, six coordination is implied.

density maps. Their most significant conclusion was that the ratio r_c/r_a is much larger than that found in all the other traditional sets of radii. Fumi & Tosi's cation and anion crystal radii are larger and smaller respectively by ~0·2 Å than the traditional radii. These radii will be considered in more detail in the discussion.

The advent of accurate structure analysis by the use of Guinier *d*-value data, intensities collected with counter diffractometers, and least-squares refinements of crystal structures has provided a wealth of new accurate cell dimensions and interatomic distances. These data have been used in our derivation of an empirical set of 'effective' ionic radii by an extension of Goldschmidt's (1926) method, with the further assumption that the radii of the anions also vary with CN. This derivation uses approximately 1000 interatomic distances in oxides and fluorides, assumes $r(^{VI}O^{2-}) = 1{\cdot}40$ Å and $r(^{VI}F^{-}) = 1{\cdot}33$Å, and takes into consideration both coordination number and electronic spin state of first-row transition metal ions. Low-spin tetrahedrally coordinated ions and high-spin second-row transition-metal ions are not included because of their infrequent occurrence. The term 'effective' ionic radii is used to emphasize the fact that these radii are empirical and include effects of covalence in specific metal–oxygen or metal–fluorine bonds. We feel these radii more closely reproduce interatomic distances in solids than the previous sets of radii and will be more useful to those who wish to compare radii rather than interatomic distances.

Methods of determining 'effective' ionic radii

Assumptions

It has already been shown that interatomic distances (and therefore 'effective' ionic radii) depend on CN (Goldschmidt, 1926), electronic spin state (van Santen & van Wieringen, 1952; Blasse, 1965), covalency (Pauling, 1927), and the presence of strong anion–anion or cation–cation repulsive forces (Pauling, 1928). Changes due to CN variation are of the order of 0·0–0·3 Å; those due to change in magnetic spin state are ~0·1 Å. The changes due to covalency effects are unknown but are probably reasonably constant for combinations of cations with anions whose electronegativities are approximately the same. Repulsive forces cause changes in the order of 0·0–0·1 Å.

In deriving the set of 'effective' ionic radii listed in Table 1(*a*) the following assumptions were made:

(1) The principle of additivity of both cation and anion radii to accurately reproduce interatomic distances is valid if one takes into consideration CN, electronic spin, covalency, and repulsive forces. (Repulsive forces are discussed further in another section.)

(2) The effect of covalency in shortening *M*–*X* bonds is comparable in all *M*–F or *M*–O bonds (Phillips & Williams, 1965).

(3) With the exceptions noted in assumption 1, radii are independent of structure type.

(4) The radii of both *cation* and *anion* vary with coordination number. (The variation in anion radii with CN is discussed in detail in another section.)

(5) Although individual cation–anion distances vary in a polyhedron, the average cation–anion distance over all similar polyhedra in one structure is constant.

(6) With a constant anion, the volume of the unit cells of isostructural series is proportional to the volume of the cations.

Assumption 5 is not basically different from 6 in that it says an ion can be deformed in any fashion but the total volume of the polyhedron will not change.* The test of assumptions 1–6 is the consistency of radii derived from different structures.

The principle of obtaining radii from relative unit volumes for a particular structure type was originated by Grimm & Wolff (1926) and Goldschmidt *et al.* (1926). Goldschmidt estimated the radii of numerous rare earth ions by comparing cell volumes of rare earth oxides with those of Sc_2O_3 and Y_2O_3 for which interatomic distances were known. A similar procedure was used by others to obtain sets of radii applicable to certain structures: Templeton & Dauben (1954) – rare earth fluorides, chlorides, oxychlorides, and oxides; Geller (1957) – oxide perovskites; Geller &Mitchell (1959) – garnets; Roth & Schneider (1960) – rare earth oxides; Sasvári (1960) – rocksalt, rutile, fluorite, and, antifluorite compounds; Knox (1961) – fluoride perovskites; and Espinosa (1962) – garnets.

Procedure

As a first approximation, anion radii (O^{2-} and F^{-}) with CN = III, IV, and VI were determined by subtracting Ahrens' sixfold radii from interatomic distances in simple oxide structures: III – rutile; IV – corundum and *C* rare earth; VI – rocksalt. In a second step, cation radii for various CN's were determined. These radii were in turn used to obtain anion radii with CN = II, III, IV, and VIII. The results are listed in Table 2. The values in parentheses represent anion radii obtained at a later stage by repeating this procedure with appropriate refined cation radii, *e.g.* in quartz $r(^{II}O^{2-}) = R_{av}(Si{-}O) - r(^{IV}Si^{4+}) = 1{\cdot}607 - 0{\cdot}26 = 1{\cdot}347$ Å. The consistency of these values can be taken as a measure of their validity.

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* The approximate linearity of radii-volume plots has been shown by Bertaut & Forrat (1957) for $A_3B_5O_{12}$ garnets, by Whinfrey, Eckart & Tauber (1960), and Brisse & Knop (1968) for $A_2B_2O_7$ pyrochlores, by Gattow (1963, 1964) for A_2BX_4 compounds, by Pannetier & Courtine (1966) for ABO_4, by Giglio (1963) for ABX_6, by Sasvári (1960) for AX_2 and by Roth & Schneider (1960) for A_2O_3. Sasvári also corrected certain radii of Ahrens to comply with this regularity and derived a set of eight-coordinated radii from the fluorite structures. Although Giglio, Gattow, and Pannetier & Courtine plotted *r vs. V*, we feel that it is more correct to plot r^3 *vs. V* or *r vs. A* (cubic). The excellent linearity in simple oxide structures (rocksalt, rutile, corundum and *C* rare-earth) supports this view.

Table 1(*a*). *Effective ionic radii*

ION	EC	CN	SP	A-IR	CR	'IR'	
AC+3	6P 6	VI		1.18			
AG+1	4D10	II			.81	.67	
		IVSQ			1.16	1.02	
		V			1.26	1.12	
		VI		1.26	1.29	1.15	
		VII			1.38	1.24	
		VIII			1.44	1.30	
AG+2	4D 9	VI		.89			
AG+3	4D 8	IVSQ			.79	.65	
AL+3	2P 6	IV			.53	.39	*
		V			.62	.48	
		VI		.51	.670	.530	R*
AM+3	5F 6	VI		1.07	1.15	1.01	R
AM+4	5F 5	VI		.92			
		VIII			1.09	.95	
AS+3	4S 2	VI		(.58)			
AS+5	3D10	IV			.475	.335	R*
		VI		.46	.64	.50	
AT+7	5D10	VI		.62			
AU+1	5D10	VI		1.37			
AU+3	5D 8	IVSQ			.84	.70	
		VI		(.85)			
B +3	1S 2	III			.16	.02	
		IV			.26	.12	*
		VI		.23			
BA+2	5P 6	VI		1.34	1.50	1.36	
		VII			1.53	1.39	
		VIII			1.56	1.42	
		IX			1.61	1.47	
		X			1.66	1.52	?
		XII			1.74	1.60	
BE+2	1S 2	III			.31	.17	
		IV			.41	.27	*
		VI		.35			
BI+3	6S 2	V			1.13	.99	
		VI		(.96)	1.16	1.02	
		VIII			1.25	1.11	R
BI+5	5D10	VI		.74			
BK+3	5F 8	VI			1.10	.96	R
BK+4	5F 7	VIII			1.07	.93	R
BR-1	4P 6	VI		1.96			
BR+7	3D10	VI		.39			
C +4	1S 2	III			.06	-.08	
		IV		.15P			
		VI		.16			
CA+2	3P 6	VI		.99	1.14	1.00	
		VII			1.21	1.07	
		VIII			1.26	1.12	*
		IX			1.32	1.18	
		X			1.42	1.28	
		XII			1.49	1.35	
CD+2	4D10	IV			.98	.84	
		V			1.01	.87	
		VI		.97	1.09	.95	
		VII			1.14	1.00	
		VIII			1.21	1.07	
		XII			1.45	1.31	
CE+3	6S 1	VI		1.07	1.174	1.034	R
		VIII			1.28	1.14	R
		XII			1.43	1.29	
CE+4	5P 6	VI		.9	.94	.80	?
		VIII			1.11	.97	R
CF+3	6D 1	VI			1.09	.95	R
CL-1	3P 6	VI		1.81			
CL+5	3S 2	III			.26	.12	
CL+7	2P 6	IV			.34	.20	
		VI		.27			
CM+3	5F 7	VI			1.12	.98	R
CM+4	5F 6	VIII			1.09	.95	R
CO+2	3D 7	VI	LS		.79	.65	R
			HS	.72	.875	.735	R*
CO+3	3D 6	VI	LS		.665	.525	R
			HS	.63	.75	.61	
CR+2	3D 4	VI	LS		.87	.73	E
			HS		.96	.82	R
CR+3	3D 3	VI		.63	.755	.615	R*
CR+4	3D 2	IV			.58	.44	
		VI			.69	.55	R
CR+5	3D 1	IV			.490	.350	R
		VIII			.71	.57	
CR+6	3P 6	IV			.44	.30	
		VI		.52			
CS+1	5P 6	VI		1.67	1.84	1.70	
		IX			1.92	1.78	
		X			1.95	1.81	
CS+1	5P 6	XII			2.02	1.88	
CU+1	3D10	II			.60	.46	
		VI		.96			
CU+2	3D 9	IVSQ			.76	.62	
		V			.79	.65	
		VI		(.72)	.87	.73	
DY+3	4F 9	VI		.92	1.048	.908	R
		VIII			1.17	1.03	R
ER+3	4F11	VI		.89	1.021	.881	R
		VIII			1.14	1.00	R
EU+2	4F 7	VI			1.31	1.17	
		VIII			1.39	1.25	
EU+3	4F 6	VI		.98	1.090	.950	R
		VIII			1.21	1.07	R
F -1	2P 6	II			1.145	1.285	
		III			1.16	1.30	
		IV			1.17	1.31	
		VI		1.33	1.19	1.33	
F +7	1S 2	VI		.08			
FE+2	3D 6	IV	HS		.77	.63	
		VI	LS		.75	.61	E
			HS	.74	.910	.770	R*
FE+3	3D 5	IV	HS		.63	.49	*
		VI	LS		.69	.55	R
			HS	.64	.785	.645	R*
FR+1	6P 6	VI		1.80			
GA+3	3D10	IV			.61	.47	*
		V			.69	.55	
		VI		.62	.760	.620	R*
GD+3	4F 7	VI		.97	1.078	.938	R
		VIII			1.20	1.06	R
GE+2	4S 2	VI		(.73)			
GE+4	3D10	IV			.54	.40	*
		VI		.53	.680	.540	R*
H +1	1S 0	I			-.24	-.38	
		II			-.04	-.18	
HF+4	4F14	VI		.78	.85	.71	R
		VIII			.97	.83	
HG+1	6S 1	III			1.11	.97	
HG+2	5D10	II			.83	.69	
		IV			1.10	.96	
		VI		1.10	1.16	1.02	
		VIII			1.28	1.14	R
HO+3	4F10	VI		.91	1.034	.894	R
		VIII			1.16	1.02	R
I -1	5P 6	VI		2.20			
I +5	5S 2	VI		.62	1.09	.95	?
I +7	4D10	VI		.50			
IN+3	4D10	VI		.81	.930	.790	R*
		VIII			1.063	.923	R
IR+3	5D 6	VI			.87	.73	?
IR+4	5D 5	VI		.68	.77	.63	R
K +1	3P 6	VI		1.33	1.52	1.38	
		VII			1.60	1.46	?
		VIII			1.65	1.51	?
		IX			1.69	1.55	?
		X			1.73	1.59	?
		XII			1.74	1.60	?
LA+3	4D10	VI		1.14	1.201	1.061	R
		VII			1.24	1.10	
		VIII			1.32	1.18	R
		IX			1.34	1.20	?
		X			1.42	1.28	
		XII			1.46	1.32	?
LI+1	1S 2	IV			.73	.59	
		VI		.68	.88	.74	
LU+3	4F14	VI		.85	.988	.848	R
		VIII			1.11	.97	R
MG+2	2P 6	IV			.63	.49	
		VI		.66	.860	.720	R*
		VIII			1.03	.89	
MN+2	3D 5	VI	LS		.81	.67	E
			HS	.80	.960	.820	R*
		VIII			1.07	.93	R
MN+3	3D 4	V			.72	.58	
		VI	LS		.72	.58	R
			HS	(.66)	.79	.65	R
MN+4	3D 3	VI		(.60)	.680	.540	R
MN+6	3D 1	IV			.41	.27	
MN+7	3P 6	IV			.40	.26	
		VI		.46			
MO+3	4D 3	VI			.81	.67	
MO+4	4D 2	VI		.70	.790	.650	R
MO+5	4D 1	VI			.77	.63	E
MO+6	4P 6	IV			.56	.42	*

Table 1(*a*) (*cont.*)

ION	EC	CN	SP	A-IR	CR	'IR'	
MO+6	4P 6	V			.64	.50	
		VI		.62	.74	.60	*
		VII			.85	.71	
N +3	2S 2	VI		(.16)			
N +5	1S 2	III			.02	-.12	
		VI		.13			
NA+1	2P 6	IV			1.13	.99	?
		V			1.14	1.00	?
		VI		.97	1.16	1.02	
		VII			1.27	1.13	?
		VIII			1.30	1.16	?
		IX			1.46	1.32	?
NB+2	4D 3	VI			.85	.71	?
NB+3	4D 2	VI			.84	.70	E
NB+4	4D 1	VI		(.74)	.83	.69	R
NB+5	4P 6	IV			.46	.32	?
		VI		.69	.78	.64	
		VII			.80	.66	
ND+3	4F 3	VI		1.04	1.135	.995	R
		VIII			1.26	1.12	R
		IX			1.23	1.09	?
NI+2	3D 8	VI		.69	.840	.700	R*
NI+3	3D 7	VI	LS		.70	.56	R
			HS		.74	.60	E
NP+2	5F 5	VI			1.24	1.10	
NP+3	5F 4	VI		1.10	1.18	1.04	R
NP+4	5F 3	VI		.95			
		VIII			1.12	.98	R
NP+7	6P 6	VI		.71			
O -2	2P 6	II			1.21	1.35	
		III			1.22	1.36	
		IV			1.24	1.38	
		VI		1.40	1.26	1.40	
		VIII			1.28	1.42	
OS+4	5D 4	VI		.69	.770	.630	R
P +3	3S 2	VI		(.44)			
P +5	2P 6	IV			.31	.17	*
		VI		.35			
PA+3	5F 2	VI		1.13			
PA+4	6D 1	VI		.98			
		VIII			1.15	1.01	
PA+5	6P 6	VI		.89			
		IX			1.09	.95	
PB+2	6S 2	IVPY			1.08	.94	
		VI		1.20	1.32	1.18	
		VIII			1.45	1.29	
		IX			1.47	1.33	
		XI			1.53	1.39	
		XII			1.63	1.49	
PB+4	5D10	VI		.84	.915	.775	R
		VIII			1.08	.94	R
PD+1	4D 9	II			.73	.59	
PD+2	4D 8	IVSQ			.78	.64	
		VI		(.80)	1.00	.86	
PD+3	4D 7	VI			.90	.76	?
PD+4	4D 6	VI		.65	.76	.62	R
PM+3	4F 4	VI		1.06	1.119	.979	R
PO+4	6S 2	VIII			1.24	1.10	R
PO+6	5D10	VI		.67			
PR+3	4F 2	VI		1.06	1.153	1.013	R
		VIII			1.28	1.14	R
PR+4	4F 1	VI		.92	.92	.78	?
		VIII			1.13	.99	
PT+2	5D 8	VI		(.80)			
PT+4	5D 6	VI		(.65)	.77	.63	R
PU+3	5F 5	VI		1.08	1.14	1.00	R
PU+4	5F 4	VI		.93	.94	.80	?
		VIII			1.10	.96	
RA+2	6P 6	VI		1.43			
RB+1	4P 6	VI		(1.47)	1.63	1.49	
		VII			1.70	1.56	?
		VIII			1.74	1.60	
		XII			1.87	1.73	
RE+4	5D 3	VI		(.72)	.77	.63	R
RE+5	5D 2	VI			.66	.52	?
RE+6	5D 1	VI			.66	.52	
RE+7	5P 6	IV			.54	.40	
		VI		.56	.71	.57	
RH+3	4D 6	VI		.68	.805	.665	R
RH+4	4D 5	VI			.755	.615	R
RU+3	4D 5	VI			.82	.68	
RU+4	4D 4	VI		.67	.760	.620	R
S -2	3P 6	VI		1.84P			
S +4	3S 2	VI		(.37)			
S +6	2P 6	IV			.26	.12	*
S +6	2P 6	VI		.30			
SB+3	5S 2	IVPY			.91	.77	
		V			.94	.80	
		VI		(.76)			
SB+5	4D10	VI		.62	.75	.61	
SC+3	3P 6	VI		.81	.870	.730	R*
		VIII			1.01	.87	R
SE-2	4P 6	VI		1.98P			
SE+4	4S 2	VI		(.50)			
SE+6	3D10	IV			.43	.29	
		VI		.42			
SI+4	2P 6	IV			.40	.26	*
		VI		.42	.540	.400	R*
SM+3	4F 5	VI		1.00	1.104	.964	R
		VIII			1.23	1.09	R
SN+2	5S 2	VI		.93			
		VIII			1.36	1.22	R
SN+4	4D10	VI		.71	.830	.690	R*
SR+2	4P 6	VI		1.12	1.30	1.16	
		VII			1.35	1.21	
		VIII			1.39	1.25	
		X			1.46	1.32	
		XII			1.58	1.44	
TA+3	5D 2	VI			.81	.67	
TA+4	5D 1	VI			.80	.66	R
TA+5	5P 6	VI		.68	.78	.64	
		VIII			.83	.69	
TB+3	4F 8	VI		.93	1.063	.923	R
		VIII			1.18	1.04	R
TB+4	4F 7	VI		.81	.90	.76	R
		VIII			1.02	.88	
TC+4	4D 3	VI			.78	.64	R
TC+7	4P 6	VI		.56			
TE-2	5P 6	VI		2.21P			
TE+4	5S 2	III			.66	.52	
		IV					
		VI		(.70)			
TE+6	4D10	VI		.56			
TH+4	6P 6	VI		1.02	1.14	1.00	
		VII			1.20	1.06	
		IX			1.23	1.09	
TI+2	3D 2	VI			1.00	.86	E
TI+3	3D 1	VI		(.76)	.81	.67	R
TI+4	3P 6	V			.67	.53	
		VI		.68	.745	.605	R*
TL+1	6S 2	VI		1.47	1.64	1.50	R
		VIII			1.74	1.60	R
		XII			1.90	1.76	R
TL+3	5D10	VI		.95	1.020	.880	R
		VIII			1.14	1.00	R
TM+3	4F12	VI		.87	1.009	.869	R
		VIII			1.13	.99	R
U +3	5F 3	VI			1.20	1.06	R
U +4	5F 2	VI		.97			
		VII			1.12	.98	
		VIII			1.14	1.00	R*
		IX			1.19	1.05	
U +5	5F 1	VI			.90	.76	
		VII			1.10	.96	
U +6	6P 6	II			.59	.45	
		IV			.62	.48	
		VI		.80	.89	.75	
		VII			1.02	.88	
V +2	3D 3	VI		(.88)	.93	.79	
V +3	3D 2	VI		(.74)	.780	.640	R
V +4	3D 1	VI		(.63)	.73	.59	R
V +5	3P 6	IV			.495	.355	R
		V			.60	.46	*
		VI		.59	.68	.54	
W +4	5D 2	VI		.70	.790	.650	R
W +6	5P 6	IV			.55	.41	*
		VI		.62	.72	.58	
Y +3	4P 6	VI		.92	1.032	.892	R*
		VIII			1.155	1.015	R*
		IX			1.24	1.10	
YB+3	4F13	VI		.86	.998	.858	R
		VIII			1.12	.98	R
ZN+2	3D10	IV			.74	.60	*
		V			.82	.68	
		VI		.74	.885	.745	R*
ZR+4	4P 6	VI		.79	.86	.72	R
		VII			.92	.78	
		VIII			.98	.84	

EC – electron configuration, CN – coordination number, SP – electronic spin, A–IR – Ahrens ionic radii (CN = VI) (Ahrens, 1952), CR – crystal radii based on $r(^{VI}F^{-}) = 1{\cdot}19$ Å, 'IR' – effective ionic radii based on $r(^{VI}O^{2-}) = 1{\cdot}40$ Å.

Table 1(*b*). *References for Table* 1(*a*)*

AC+3 VI

AG+1 II
PREWITT,C.T. AND R.D.SHANNON, TO BE PUBLISHED. AG FF 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AG2 O

AG+1 IVSQ
BYSTROM,A. AND L.EVERS, ACTA CHEM.SCAND. 4:613(1950) AG2 PB O2
DONOHUE,J. AND L.HELMHOLZ, J.AM.CHEM.SOC. 66:295(1944) K AG C O3
SCATTURIN,V. AND P.L.BELLON, J. ELECTROCHEM.SOC. 108:819(1961) AG O

AG+1 V
JOST,K.H., ACTA CRYST. 14:779(1961) (AG P O3)X

AG+1 VI
RODE,H., Z.ANORG.ALLGEM.CHEM. 267,62(1951) AG SB F6
KIERKEGAARD,P. AND S.HOLMEN, ARKIV KEMI 23:213(1965) AG MO P O6
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AG F
ZACHARIASEN,W.H., Z.KRIST. 82:161(1932) AG2 S O4

AG+1 VII
KIERKEGAARD,P. AND S. HOLMEN, ARKIV KEMI 23:213(1965) AG MO P O6

AG+1 VIII
KROGH-MOE,J., ACTA CRYST.18:77(1965) AG2 BE O13
WELLS,A.F., Z.KRIST. 95,74(1936) AG CO (N H3)2 (N O2)4

AG+2 VI

AG+3 IVSQ
SCATTURIN,V. AND P.L.BELLON, J.ELECTROCHEM.SOC. 108:819(1961) AG+1 AG+3 O2

AL+3 IV
BROWN,P.E. AND S.W.BAILEY, ACTA CRYST. 17:1391(1964) K AL SI3 O8
BURNHAM,C.W., Z.KRIST. 118:127(1963) AL2 SI O5
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) MG AL2 O12
MACHATSCHKI,F., Z.KRIST. 94:222(1936) AL AS O4
MOONEY,R.C.L., ACTA CRYST. 9,728(1956) AL P O4
SCHWARZENBACH,D., Z.KRIST. 123,161(1966) AL P O4
SMITH,J.V. AND S.W.BAILEY, ACTA CRYST. 16:801(1963) AL-O
WILLIAMS,P.P. AND H.D.MEGAW, ACTA CRYST. 17:882(1965) ALBITES
LIEBAU,F., ACTA CRYST. 14,389(1961) LI AL SI4 O10
MAREZIO,M., ACTA CRYST. 19:396(1965) LT AL O2

AL+3 V
BERTAUT,F. AND J.MARESCHAL, COMPT.REND. 257:867(1963) Y AL O3
BURNHAM,C.W. AND M.J.BUERGER, Z.KRIST. 115:269(1961) AL2 SI O5

AL+3 VI
BURNHAM,C.W., Z.KRIST. 118:337(1963) AL2 SI O5
CROMER,D.T. ET AL., ACTA CRYST. 22:182(1967) NA AL (S O4)2.12 H2 O
CROMER,D.T. ET AL., ACTA CRYST. 21:383(1966) CS AL (S O4)2.12 H2 O
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) MG AL2 O12
FARRELL,E.F. ET AL., AM. MINERALOGIST 48,804(1963) BE AL2 O4
GIBBS,G.V. AND J.V.SMITH, AM. MINERALOGIST 50:2023(1965) MG3 AL2 SI3 O12
JACK,K.H. AND V.GUTMANN, ACTA CRYST. 4,246(1951) AL F3
MAREZIO,M. AND J.P.REMEIKA, J.CHEM.PHYS. 44:3143(1966) LI AL O2
NARAY-SZABO,ST.V. AND K.SASVARI, Z.KRIST. 99,27(1938) NA3 AL F6
NEWNHAM,R.E. AND Y.M.DEHAAN, Z.KRIST. 117:235(1962) AL2 O3
PEDERSEN,B.F., ACTA CHEM.SCAND. 16:921(1962) AL NB O4
PRANDL,W., Z.KRIST. 123,81(1966) AL2 CA3 (SI O4)3
SADANAGA,R. ET AL., ACTA CRYST. 15:65(1962) AL4 SI O8

AM+3 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (LA F3)

AM+4 VI

AM+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AM O2

AS+3 VI

AS+5 IV
FINNEY,J.J., AM. MINERALOGIST 48,1(1963) PB FE2 (AS O4)2 (O H)2
FINNEY,J.J., ACTA CRYST. 21:437(1966) CU2 (AS O4) (O H).3 H2 O
HILMER,W., ACTA CRYST. 9:87(1956) (LI AS O3)X
JOST,K.H. ET AL., ACTA CRYST. 21:808(1966) AS2 O5.5/3 H2 O
LIEBAU,F., ACTA CRYST. 9:811(1956) (NA AS O3)X
LUKASZEWICZ,K., BULL.ACAD.POLON.SCI.SER.SCI.CHIM. 11:361(1963) MG2 AS2 O7
MACHATSCHKI,F., Z.KRIST. 94:222(1936) AL AS O4
MOONEY,R.C.L., ACTA CRYST. 1,163(1948) BI AS O4
MORI,H. AND T.ITO, ACTA CRYST. 3:1(1950) FE3 AS O4.8 H2 O
PLIETH,K. AND G.SANGER, Z.KRIST. 124,91(1967) ZN2 CU AS2 O8
POULSEN,S.J. AND C.CALVO, CAN.J.CHEM. 46:917(1968) CU3 AS2 O8
SCHULZE,G.E.R., Z.PHYSIK CHEM. 24B:215(1934) B AS O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (ZIPCON)

AS+5 VI
IBERS,J.A., ACTA CRYST. 9,967(1956) K AS F6
JOST,K.H. ET AL., ACTA CRYST. 21:808(1966) AS2 O5.5/3 H2 O

AT+7 VI

AU+1 VI

AU+3 IVSQ
EINSTEIN,F.W.B. ET AL., J.CHEM.SOC. A1967:478 AU F3

AU+3 VI

B +3 III
BLOCK,S. AND A.PERLOFF, ACTA CRYST. 19,297(1965) BA B4 O7
IHARA,M. AND J.KROGH-MOE, ACTA CRYST. 20:132(1966) CD BA O7
KROGH-MOE,J., ACTA CRYST. 13,889(1960) CS2 B6 O10
KROGH-MOE,J., ACTA CRYST. 15,190(1962) LI2 B4 O7
KROGH-MOE,J., ACTA CRYST. 18,77(1965) AG2 BA O13
KROGH-MOE,J., ACTA CRYST. 18,1088(1965) K B5 O8
MAREZIO,M. ET AL., ACTA CRYST. 16,390(1963) CA B2 O4
MAREZIO,M. ET AL., ACTA CRYST. 16,975(1963) K2 B4 O7.4 H2 O
ZACHARIASEN,W.H. ET AL., ACTA CRYST. 16,1144(1963) BE2 B O3 (O H)

B +3 IV
BLOCK,S. AND A.PERLOFF, ACTA CRYST. 19,297(1965) BA B4 O7
CLARK,J.R., AM. MINERALOGIST 40:1549(1964) SR B6 O9 (O H)2.3 H2 O
HOARD,J.L. AND V.BLAIR, J.AM.CHEM.SOC. 57:1949(1935) BA B B4
IHARA,M. AND J.KROGH-MOE, ACTA CRYST. 20:132(1966) CD BA O7
KROGH-MOE,J., ACTA CHEM.SCAND. 18:2055(1964) SR BA O7
KROGH-MOE,J., ACTA CRYST. 13,889(1960) CS2 B6 O10
KROGH-MOE,J., ACTA CRYST. 15,190(1962) LI2 B4 O7
KROGH-MOE,J., ACTA CRYST. 18,77(1965) AG2 BA O13
KROGH-MOE,J., ACTA CRYST. 18,1088(1965) K B5 O8
MAREZIO,M. ET AL., ACTA CRYST. 16,975(1963) K2 B4 O7.4 H2 O
MAREZIO,M. AND J.P.REMEIKA, J.CHEM.PHYS. 44:3348(1966) LI B O2
PANT,A.K. AND D.W.J.CRUICKSHANK, Z.KRIST. 125,286(1967) CA B SI O4.O H
PERLOFF,A. AND S.BLOCK, ACTA CRYST. 20:274(1966) SR B4 O7
PREWITT,C.T. AND R.D.SHANNON, ACTA CRYST. B24:869(1968) B2 O3
REMEIKA,J.P. AND M.MAREZIO, J.PHYS.CHEM.SOLIDS 26:2083(1965) LI B O2
ZACHARIASEN,W.H., ACTA CRYST. 16:380(1963) H B O2
ZACHARIASEN,W.H., ACTA CRYST. 16:385(1963) H B O2

B +3 VI

BA+2 VI
MANI,N.V. AND S.RAMASESHAN, Z.KRIST. 114,200(1960) BA (CL O4)2.3 H2 O
MIGHELL,A.D. ET AL., ACTA CRYST. 20:A19(1966) BA B2 O4
SCHNERING,H.G. ET AL., Z.ANORG ALLGEM.CHEM. 305,241(1960) BA ZN O2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) BA O
ZACHARIASEN,W.H., Z.KRIST. 74:139(1930) BA TI SI3 O9

BA+2 VII
HILMER,W., ACTA CRYST. 15:1101(1962) BA GE O3
SCHNERING,H.G., Z.ANORG.ALLGEM.CHEM. 314:144(1962) BA CD O2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 3,(1965) BA3 NI O4

BA+2 VIII
BLAND,J.A., ACTA CRYST. 14:875(1961) BA2 TI O4
HILMER,W., ACTA CRYST. 15:1101(1962) BA GE O3
LANDER,J.J., ACTA CRYST. 4:148(1951) BA NI O2
MANOHAR,H. AND J.RAMASESHAN, Z.KRIST. 119:357(1964) BA (O H)2.8 H2 O
NARDELLI,M. AND G.FAVA, ACTA CRYST. 15:477(1962) BA S2 O3.H2 O
RAO,R.V.G.S. ET AL., Z.KRIST. 110:231(1958) CU BA2 (C O O H)6.4 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) BA F2

BA+2 IX
BLOCK,S. AND A.PERLOFF, ACTA CRYST. 19,297(1965) BA B4 O7
COLBY,M.Y. AND L.J.B.LACOSTE, Z.KRIST 90:1(1935) BA C O3
FOSS,O. AND O.TJOMSLAND, ACTA CHEM.SCAND. 10,288(1956) BA S (S2 O3)2.2 H2 O
FOSS,O. AND O.TJOMSLAND, ACTA CHEM.SCAND. 12,52(1958) RA TE (S2 O3)2.2 H2 O
MIGHELL,A.D. ET AL., ACTA CRYST. 20:819(1966) BA B2 O4

BA+2 X
BLOCK,S. AND A.PERLOFF, ACTA CRYST. 19,297(1965) BA B4 O7
BURLEY,G., J.RES.NATL.BUR.STD. 60:23(1958) BA H P O8
NEWNHAM,R.E. AND H.D.MEGAW, ACTA CRYST. 13:303(1960) BA AL2 SI2 O8
ROBBINS,C. ET AL., J.RES.NATL.BUR.STD. 70A:385(1966) BA GE4 O9
TEMPLETON,D.H. AND C.H.DAUBEN, J.CHEM.PHYS. 32:1515(1960) BA TI4 O9
ZACHARIASEN,W.H., ACTA CRYST. 1:265(1948) BA3 (P O4)2

BA+2 XII
EVANS, H.T.,JR., ACTA CRYST. 4:377(1951) BA TI O3
HOARD,J.L. AND W. VINCENT, J.AM.CHEM.SOC. 62:3126(1940) BA SI F6.BA GE F6
SAHL,K., BEITR.MINERAL.PETROG. 9:111(1963) BA S O4
SCHNERING,H.G., Z. ANORG.ALLGEM.CHEM. 353:13(1967) BA2 M F6
SHIRANE,G. ET AL., PHYS.REV. 105:856(1957) BA TI O3
ZACHARIASEN,W.H., ACTA CRYST. 1:265(1948) BA3 (P O4)2

BE+2 III
HARRIS,L.A. AND H.L.YAKEL, ACTA CRYST. 22:354(1967) Y2 BE O4

BE+2 IV
BEEVERS,C.A. AND H.LIPSON, Z.KRIST. 82,297(1932) BE S O4.4 H2 O
BURNS,J.H. AND E.K.GORDON, ACTA CRYST. 20:135(1966) LI2 BE F4
FARRELL,E.F. ET AL., AM. MINERALOGIST 48:804(1963) BE AL2 O4
GOLOVASTIKOV,N.I., SOVIET PHYS.-CRYST. 6:733(1962) NA BE P O4
HARRIS,L.A. AND H.L.YAKEL, ACTA CRYST.20:295(1966) CA12 BE17 O29
MROSE,M.E. AND D.E.APPLEMAN, Z.KRIST. 117:16(1962) AL BE SI O4 O H
SEARS,D.R. AND J.H.BURNS, J.CHEM.PHYS. 41:3478(1964) LI6 BE F6 ZR F8
SMITH,D.K. ET AL., J.ELECTROCHEM.SOC. 111:78(1964) BE O
ZACHARIASEN,W.H. ET AL., ACTA CRYST. 16:1144(1963) BE2 B O3 (O H)

BE+2 VI

BI+3 V
ABRAHAMS,S.C. ET AL., J.CHEM.PHYS. 47:4034(1967) BI12 GE O20
AURIVILLIUS,B. ACTA CHEM.SCAND. 18:2375(1964) BI2 O2 S O4.H2 O

BI+3 VI
AURIVILLIUS,B., ACTA CHEM.SCAND. 18:2375(1964) BI2 O2 S O4.H2 O
AURIVILLIUS,B. AND I.JONSSON, ARKIV KEMI 19:271(1962) BI O H CR O4
AURIVILLIUS,B. ET AL., ACTA CHEM.SCAND. 18:1555(1964) BI2 GE O5
SEGAL,D.J. ET AL., Z.KRIST. 123,73(1966) BI4 SI3 O12
ZEMANN,J., HEIDELBERGER BEITR.MINERAL.PETROG.MITT. 5:139(1956) BI2 MO O6

BI+3 VIII
AURIVILLIUS,B., ARKIV KEMI 3:153(1951) BI SB O4
MOONEY,R.C.L., ACTA CRYST. 1:163(1948) BI AS O4
MOONEY-SLATER,R.C.L., Z.KRIST. 117:371(1962) BI P O4
QURASHI,M.M. AND W.H.BARNES, AM.MINERALOGIST 38:489(1953) BI V O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (ZIPCON)
TOMASHPOL'SKII,Y. ET AL., SOVIET PHYS.-CRYST. 9,715(1965) BI FE O3

BI+5 VI

BK+3 VI
PETERSON,J.R. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967) BK2 O3

BK+4 VIII
PETERSON,J.R. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967) BK O2

BR-1 VI

BR+7 VI

C +4 III
CHESSIN,H., W.C.HAMILTON, AND B.POST, ACTA CRYST. 18:689(1965) CA C O3

C +4 IV

C +4 VI

CA+2 VI
BUERGER,M.J., Z.KRIST. 108:248(1956) CA2 NA H SI3 O9
CLARK,J.R. ET AL., ACTA CRYST. 15,207(1962) CA B3 O5 O H
CRUICKSHANK,D.W.J., ACTA CRYST. 17:685(1964) CA2 SI O4
GARD,J.A. AND H.F.W.TAYLOR, ACTA CRYST. 13:785(1960) CA4 (SI3 O9) (O H)2
HARRIS,L.A. AND H.L.YAKEL, ACTA CRYST. 20:295(1966) CA12 BE17 O29
ITO,T. ET AL., ACTA CRYST. 5,209(1952) K2 CA4 BE4 AL2 SI24 O60.H2 O
RIETVELD,H.M., ACTA CRYST. 20:508(1966) CA3 U O6
SMITH,D.K. ET AL., ACTA CRYST. 18:787(1965) CA2 SI O4
STEINFINK,H. AND F.J.SANS, AM.MINERALOGIST 44:679(1959) CA MG (C O3)2
TAKEUCHI,Y. AND G.DONNAY, ACTA CRYST. 12:465(1959) CA AL2 SI2 O8
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CA O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CS CA F3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) RB CA F3

CA+2 VII
BAKAKIN,V.V. AND N.V.BELOV, DOKL.AKAD.NAUK SSSR 135:587(1960) CA BE2 (P O4)2
CHRIST,C.L. ET AL., ACTA CRYST. 11:761(1958) CA B3 O4 (O H)3.H2 O
MEGAW,H.D. ACTA CRYST. 5:477(1952) CA3 (SI O3 O H)2.2 H2 O
POSNER,A.S. ET AL., ACTA CRYST. 11:308(1958) CA10 (P O4)6 F2
PRANDL,W., Z.KRIST. 123:81(1966) AL2 CA3 (SI O4)3
RUMANOVA,I.M., M.N.ZNAMENSKAYA, SOV.PHYS.-CRYST. 5:650(1961) CA2 FE (P O4)2.H2 O
SWALLOW,A.G. ET AL., ACTA CRYST. 21:397(1966) CA3 V10 O28.17 H2 O
WEBB,N.C., ACTA CRYST. 21:942(1966) CA2 P2 O7
ZACHARIASEN,W.H., Z.KRIST. 73:7(1930) CA TI SI O5

CA+2 VIII
BERTAUT,E.F. AND P.BLUM, ACTA CRYST. 9:121(1956) CA TI2 O4
BURBANK,R.D., ACTA CRYST. 18:88(1965) CA W O4
CLARK,J.R. AND C.L.CHRIST, Z.KRIST. 112:213(1964) CA B3 O3.(O H)5.2 H2 O
CRUICKSHANK,D.W.J., ACTA CRYST. 17:685(1964) CA2 SI O4
DECKER,B.F. AND J.S.KASPER, ACTA CRYST. 10:332(1957) CA FE2 O4

Table 1(*b*) (*cont.*)

HARRIS,L.A. AND H.L.YAKEL, ACTA CRYST. 20,295(1966) CA12 BF17 O29
HILL,P.W. ET AL., ACTA CRYST. 9,981(1956) CA FF2 O4
HOHNE,E., SOVIET PHYS.-CRYST. 7,559(1963) CA S O4
JAHNBERG,L., ACTA CHEM.SCAND. 17,2548(1963) CA TA2 O6
MAREZIO,M. ET AL., ACTA CRYST. 16,390(1963) CA B2 O4
MULLER-BUSCHBAUM,H., H.G.SCHNERING, Z.ANORG.ALLGEM.CHEM. 336,295(1965) CA SC2 O4
PAVLOV,P.V. AND N.V.BELOV, SOVIET PHYS.-CRYST. 4,300(1960) CA BE P O4 F
PEACOR,D.R. AND M.J.BUERGER, Z.KRIST. 117,331(1962) CA MN SI2 O6
PRANDL,W., Z.KRIST. 123,81(1966) AL2 CA3 (SI O4)3
WEBB,N.C., ACTA CRYST. 21,942(1966) CA2 P2 O7
WILHELMI,K. AND O.JONSSON, ACTA CHEM.SCAND. 19,177(1965) CA5 O H (CR O4)3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CA F2
ZALKIN,A. AND D.H.TEMPLETON, J.CHEM.PHYS. 40,501(1964) CA W O4

CA+2 IX
JOHANSSON,G., ACTA CRYST. 12,522(1959) CA B2 SI2 O8
POSNER,A.S. ET AL., ACTA CRYST. 11,308(1958) CA10 (P O4)6 F2
RODI,F. AND D.BABEL, Z.ANORG,ALLGEM, CHEM. 336,17(1965) CA IR O3

CA+2 X
MAREZIO,M. ET AL., TO BE PUBLISHED CA B2 O4

CA+2 XII
MAREZIO,M. ET AL., TO BE PUBLISHED CA B2 O4

CD+2 IV
KOKKOROS,P.A. AND P.J.RENTZEPERIS, Z.KRIST. 119,234(1963) CD S O4
SCHNERING,H.G., Z.ANORG.ALLGEM.CHEM. 314,144(1962) BA CD O2

CD+2 V
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM. 46,903(1968) A CD 7N2 (P O4)2 6
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM. 46,903(1968) A CD2 7N (P O4)2 6

CD+2 VI
AU,P.K.L. AND C.CALVO, CAN.J.CHEM. 45,2287(1967) CD2 V2 O7
DEWOLFF,P.M., ACTA CRYST. 21,438(1966) CD (O H)2
LIPSON,H., PROC.ROY.SOC.(LONDON)SER.A 156,462(1936) 3CD S O4.8 H2 O
POSNJAK,E. AND T.F.W.BARTH, Z.KRIST. 88,271(1934) CD TT O3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CD O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K CD F3

CD+2 VII
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM. 46,903(1968) CD 7N2 (P O4)2
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM. 46,903(1968) CD2 7N (P O4)2

CD+2 VIII
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) CD2 TA2 O7
DONOHUE,P.C. ET AL., INORG.CHEM. 4,1152(1965) CD2 RE2 O7
MATKOVIC,B. ET AL., ACTA CRYST. 21,719(1966) CD (N O3)2.4 H2O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CD F2

CD+2 XII
POSNJAK,E. AND R.F.W.BARTH, Z.KRIST. 88,265(1934) CD TT O3

CE+3 VI
SLEIGHT,A.W., TO BE PUBLISHED (RE)2 S3
TEMPLETON,D.H. AND C.H. DAUBEN, J.AMER.CHEM.SOC. 76,5237(1954)

CE+3 VIII
MOONEY,R.C.L., ACTA CRYST. 3,337(1950) CE P O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 V5 V (ZIRCON)

CE+3 XII
ZALKIN,A. ET AL., J.CHEM.PHYS. 39,2881(1963) CF2 MG3 (N O3)12.24 H2 O

CE+4 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) BA CE O3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) SR CE O3

CE+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CE O2

CF+3 VI
GREEN,J.L. AND B.B.CUNNINGHAM, INORG,NUCL.CHEM,LETTERS 3,343(1967) CF2 O3
PETERSON,J.R. AND B.B. CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967) CF2 O3

CL-1 VI

CL+5 III
ZACHARIASEN,W.H., Z.KRIST. 71,517(1929) K CL O3

CL+7 IV
GOTTFRIED,C. AND C.SCHUSTERIUS, Z.KRIST. 84,65(1932) K CL O4
ZACHARIASEN,W.H., Z.KRIST. 73,141(1930) NA CL O4

CL+7 VI

CM+3 VI
PETERSON,J.R. AND B.B.CUNNINGHAM, INORG,NUCL.CHEM,LETTERS 3,327(1967) CM2 O3

CM+4 VIII
PETERSON,J.R. AND B.B.CUNNINGHAM, INORG,NUCL.CHEM,LETTERS 3,327(1967) CM O2

CO+2 VI LS

CO+2 VI HS
BAUR,W.H., ACTA CRYST. 11,488(1958) CO F2
IBERS,J.A. AND G.W.SMITH, ACTA CRYST. 17,190(1964) NA CO2.3 MO3 O12
MONTGOMERY,H. ET AL., ACTA CRYST. 22,775(1967) CO (N H4)2 (S O4)2.6 H2 O
RENTZEPERIS,P.J., NEUES JAHRB,MINERAL.MONATSH. 226(1958) CO S O4
SCHNERING,H.G., Z.ANORG.ALLGEM,CHEM. 353:13(1967) BA2 CO F6
SMITH,G.W, AND J.A.IBERS, ACTA CRYST. 19,269(1965) CO MO O4
VAN NIEKERK,J.N., F.R.SCHOENING, ACTA CRYST. 6,609(1953) NI (C H3 C O O)2.4 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CO O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) M CO F3
ZALKIN,A. ET AL., ACTA CRYST. 15,1219(1962) CO S O4.6 H2 O

CO+3 VI LS
BLASSE,G., J.INORG. NUCL. CHEM. 27,748(1965) LI CO O2
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 V5 V (PEROVSKITE)

CO+3 VI HS
BLASSE,G., J.INORG. NUCL. CHEM. 27,748(1965) K3 CO F6
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) CO F3

CR+2 VI LS

CR+2 VI HS
JACK,K.H. AND R. MAITLAND, PROC.CHEM.SOC.LONDON 232(1957) CR F2
SHANNON,R.D. AND C.T. PREWITT, TO BE PUBLISHED, R3 V5 V (RUTILE)
STEINFINK,H. AND J.H.BURNS, ACTA CRYST. 17,823(1964) CR2 F6

CR+3 VI
DOUGLASS,R.M., ACTA CRYST. 10,423(1957) H CR O2
KNOX,K., ACTA CRYST. 13,507(1960) CR F3
NEWNHAM,R.E. AND Y.E.DEHAAN, Z.KRIST. 117,235(1962) CR2 O3
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 V5 V (PEROVSKITE)
STEINFINK,H. AND J.H.BURNS, ACTA CRYST. 17,823(1964) CR2 F6
WILHELMI,K., ACTA CHEM.SCAND. 12,1965(1958) K CR (CR O4)2
WILHELMI,K., ACTA CHEM.SCAND. 19,165(1965) CR5 O12
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CE CR O3

CR+4 IV
WILHELMI,K.A., ARKIV KEMI 26,157(1967) SR2 CR O4

CR+4 VI
CHAMBERLAND,B.L., SOLID STATE COMMUN, 5,663(1967) SR CR O3
CLOUD,W.H. ET AL., J.APPL.PHYS.,SUPPL. 33:1193(1962) CR O2
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R3 V5 V (RUTILE)

CR+5 IV
GREENBLATT,M. ET AL., ACTA CRYST. 23,166(1967) CA2 CR O4 CL
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R3 V5 V (7TOCON)
WILHELMI,K.A. AND O.JONSSON, ACTA CHEM.SCAND. 19,177(1965) CA5 O H (CR O4)3

CR+5 VIII
STROMBERG,R. AND C.BROSSET, ACTA CHEM.SCAND. 14,441(1960) K3 CR O8

CR+6 IV
AURIVILLIUS,B. AND I.JONSSON, ARKIV KEMI 19,271(1962) 9I O H CR O4
BYSTROM,A. AND K.WILHELMI, ACTA CHEM.SCAND. 4,1131(1950) CR O3
COLLOTTI,G. ET AL., ACTA CRYST. 12,416(1959) PB CR O4
LUNDGREN,G. AND L.G.SILLEN, ARKIV KEMI 1,277(1949) TH (O H)2 CR O4 H2 O
LUNDGREN,G., ARKIV KEMI 13,59(1958) ZR4 (O H)16 (CR O4)5,2 H2 O
MILLER,J.J., Z.KRIST. 99,32(1938) CS2 CR O4
NARAY-SZABO,I. AND G.ARGAY, ACTA CHIM.ACAD.SCI.HUNG. 40,283(1964) PB CR O4
QUARENI,S. AND R.DEPIERI, ACTA CRYST. 19,287(1965) PB CR O4
WILHELMI,K., ACTA CHEM.SCAND. 12,1955(1958) K CR3 O8
WILHELMI,K., ACTA CHEM.SCAND. 19,165(1965) CR5 O12
WILHELMI,K., ARKIV KEMI 26,131(1967) LI CR3 O8
WILHELMI,K., ARKIV KEMI 26,141(1967) CS CR3 O8
ZACHARIASEN,W.H. AND G.E.ZIEGLER, Z.KRIST. 80,164(1931) K2 CR O4
ZHUKOVA,L.A. AND Z.G.PINSKER, SOVIET PHYS.-CRYST. 9,31(1964) K2 CR2 O7

CR+6 VI

CS+1 VI
BURNS,J.H. AND W.R.BUSING, INORG.CHEM. 4,1510(1965) CS LI F2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CS F

CS+1 IX
MILLER,J.J., Z.KRIST. 99,32(1938) CS2 CR O4

CS+1 X
BYSTROM,A. AND K.WILHELMI, ARKIV KEMI 3,373(1951) CS SR2 F7
KROGH-MOE,J. AND M.IHARA, ACTA CRYST. 23,427(1967) CS BA O14
MILLER,J.J., Z.KRIST. 99,32(1938) CS2 CR O4

CS+1 XII
CROMER,D.T. ET AL., ACTA CRYST. 21,383(1966) CS AL (S O4)2.12 H2 O
EVANS,H.T.,JR. AND S.BLOCK, INORG.CHEM. 5,1808(1966) CS V3 O8
ROSENZWEIG,A. AND D.T.CROMER, ACTA CRYST. 23,865(1967) CS U F6
ZALKIN,A. ET AL., J.CHEM.PHYS. 37,697(1962) CS MN F3

CU+1 II
PABST,A., AM.MINERALOGIST 31,539(1946) CU FE O2
PREWITT,C.T. AND R.D.SHANNON, TO BE PUBLISHED. CU FE O2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) CU2 O

CU+1 VI

CU+2 IVSQ
BACHMANN,H.G. AND J.ZEMANN, ACTA CRYST. 14,747(1961) PB CU S O4 (O H)2
BRUNTON,G. ET AL., ACTA CRYST. 11,169(1958) CU2 MGR (C O3)4 (O H)24 .8 H2 O
BUKOWSKA-STRZYZEWSKA,M., ACTA CRYST. 19,357(1965) CU (H C O O)2.2 H2 O
FINNEY,J.J. AND T.ARAKI, NATURE 197,70(1963) CU3 (S O4) O H4
FLUGEL-KAHLER,E., ACTA CRYST. 16,1006(1963) CU2 O(S O4)
GATTOW,G., ACTA CRYST. 11,377(1958) CU SE O3.2 H2 O
GATTOW,G. AND J.ZEMANN, ACTA CRYST. 11,866(1958) CU3 (O H)2 (C O3)2
GHOSE,S., ACTA CRYST. 15,1105(1962) CU I O3 O H
GHOSE,S., ACTA CRYST. 16,124(1963) CU5 (P O4)2 (O H)4
JAGGI,H. AND H.R.OSWALD, ACTA CRYST. 14,1041(1961) CU (O H)2
KIRFEL,A.R. ET AL., ACTA CRYST. 7,482(1954) CU (H C O2)2.4 H2 O
PLIETH,K. AND G.SANGER, Z.KRIST.124:401(1967) ZN2 CU (AS O4)2
RAO,B.RAMA, ACTA CRYST. 14,738(1961) NA2 CU (S O4)2.2 H2 O
TUNELL,G. ET AL., Z.KRIST. 90:120(1935) CU O
VAN NIEKERK,J.N., F.R.SCHOENING, ACTA CRYST. 6,227(1953) CU2 (C H3 C O O)4.2 H2O

CU+2 V
ABRAHAMS,S.C. ET AL., J.CHEM.PHYS. 48,2619(1968) CU MO O4
FLUGEL-KAHLER,E., ACTA CRYST. 16,1006(1963) CU2 O(S O4)
HERITSH,H., Z.KRIST. 99,466(1938) CU2 O H AS O4
HERITSH,H., Z.KRIST. 102,1(1939) CU2 O H P O4
POULSEN,S.J. AND C.CALVO, CAN.J.CHEM. 46,917(1968) CU3 AS2 O8

CU+2 VI
BACHMANN,H.G. AND J.ZEMANN, ACTA CRYST. 14,747(1961) PB CU S O4 (O H)2
BILLY,C. AND H.M.HAENDLER, J.AM. CHEM.SOC. 79,1049(1957) CU F2
BUKOWSKA-STRZYZEWSKA,M., ACTA CRYST. 19,357(1965) CU (H C O O)2.2 H2 O
FINNEY,J.J., ACTA CRYST. 21,837(1966) CU2 (AS O4) (O H).3 H2 O
FLUGEL-KAHLER,E., ACTA CRYST. 16,1006(1963) CU2 O(S O4)
GINETTI,Y., BULL.SOC.CHIM.BELGES 63,209(1954) CU BF O3
HERITSCH,H., Z.KRIST. 99,466(1938) CU2(O H)(AS O4)
HERITSCH,H., Z.KRIST. 102,1(1939) CU2 (O H) (P O4)
JAGGI,H. AND H.R.OSWALD, ACTA CRYST. 14,1041(1961) CU (O H)2
KNOX,K., J.CHEM.PHYS. 30,991(1959) K2 CU F4
NOWACKI,W. AND R.SCHEIDEGGER, HELV.CHIM.ACTA 35,375(1952) CU2 (O H)3 N O3
RAO,R.V.G.,SONDRA, ET AL., Z.KRIST. 110:231(1958) CU BA2 (C O O H)6.4 H2 O
RAO,B.RAMA, ACTA CRYST. 14:321(1961) CU S O4
RAO,B.RAMA, ACTA CRYST. 14,738(1961) NA2 CU (S O4)2.2 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K CU F3

DY+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) DY2 O3

DY+3 VIII
ABRAHAMS,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 46,3776(1967) DY MN2 O5
EULER,F. AND BRUCE,J.A., ACTA CRYST. 19,971(1965) DY3 FE2 FE3 O12
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R V5 A (PYROCHLORE)

ER+3 VI
FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85,267(1962) ER2 O3
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) ER2 O3

ER+3 VIII
KNOP,O. ET AL., CAN.J.CHEM. 43,2812(1965) ER2 TI2 O7
PATSCHEKE,E. ET AL., CHEM.PHYS.LETTERS 2,47(1968) ER N O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R V5 A (PYROCHLORE)

EU+2 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) EU O

EU+2 VIII
RAU,R.C., ACTA CRYST. 20,716(1966) EU3 O4
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) EU F2

EU+3 VI
RAU,R.C., ACTA CRYST. 20,716(1966) EU3 O4
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) EU2 O3

EU+3 VIII
MAREZIO,M. ET AL., J.CHEM.PHYS. 48,1094(1968) EU3 FE2 GA3 O12
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R V5 A (PYROCHLORE)
TEMPLETON,D.H. AND A.ZALKIN, ACTA CRYST. 16,762(1963) EU2 (W O4)3

Table 1(*b*) (*cont.*)

F -1 II

F -1 III

F -1 IV

F -1 VI

F +7 VI

FE+2 IV HS
HANISCH,K.NEUES JAHRB.MINERAL.MONATSH. 128,362(1966) H FE2 AL8 SI4 024

FE+2 VI LS

FE+2 VI HS
BAUR,W.H., ACTA CRYST. 11,488(1958) FE F2
BAUR,W.H., ACTA CRYST. 15,815(1962) FE S 08.4 H2 O
BURNHAM,C.W., CARNEGIE INST.WASH.YEAR BOOK 65,285(1966) FE SI 03
GIBBS,G.V. ET AL., AM.MINERALOGIST, IN PRESS. FE2 SI 04
HAMILTON,W.C., ACTA CRYST. 15,353(1962) FE SI F6.6 H2 O
KESTIGIAN,M. ET AL., INORG.CHEM. 5,1462(1966) RB FE F3
RUMANOVA,I.M., M.N.ZNAMENSKAYA, SOV.PHYS.-CRYST. 5,650(1961) CA2 FE (P 08)2,H2 O
SMITH,D.K. ET AL., ACTA CRYST. 18,787(1965) FE2 SI 04
STRUNZ,H. AND M.GIGLIO, ACTA CRYST. 14,205(1961) FE GE (O H)6
ULKU,D., Z.KRIST. 124,192(1967) FE W 04
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) FE O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K FE F3
ZEMANN,J., NEUES JAHRB. MINERAL.MONATSH. 67(1959) FE GF (O H)6

FE+3 IV HS
BATT,A. AND B.POST, ACTA CRYST. 15,1268(1962) Y3 FE5 012
BERTAUT,E.F. ET AL., ACTA CRYST. 12,149(1959) CA2 FE2 05
BERTAUT,F. ET AL., COMPT.REND. 257,821(1963) NA FE 02
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) M3 FE5 012
GELLER,S. AND M.A.GILLEO, ACTA CRYST. 10,239(1957) Y3 FE5 012
ROMERS,C. ET AL., ACTA CRYST. 22,766(1967) NA3 FE5 09
WEIDENBORNER,J.E., ACTA CRYST. 14,1051(1961) GD3 FE5 012

FE+3 VI LS
BLASSE,G., J.INORG,NUCL.CHEM. 27,748(1965)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (K3 MIII (CN)6)

FE+3 VI HS
ABRAHAMS,S.C. ET AL., J.CHEM.PHYS. 42,3957(1965) GA FE 03
BATT,A. AND B.POST, ACTA CRYST. 15,1268(1962) Y3 FE5 012
BERTAUT,E.F. ET AL., ACTA CRYST. 12,149(1959) CA2 FE2 05
BLAKE,R.L. ET AL., AM.MINERALOGIST 51,123(1966) FE2 03
BLASSE,G., J.INORG.NUCL.CHEM. 27,748(1965)
COPPENS,P. AND M.EIBSCHUTZ, ACTA CRYST. 19,528(1965) GD FE 03
EULER,F. AND J.R.BRUCE, ACTA CRYST. 19,971(1965) M3 FE5 012
FINNEY,J.J., AM.MINERALOGIST 48,1(1963) PB FE2 (AS 04)2 (O H)2
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) FE F3
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (PEROVSKITE)
TOMASHPOL'SKII,Y. ET AL., SOVIET PHYS.-CRYST. 9,715(1965) RI FE 03
WEIDENBORNER,J.E., ACTA CRYST. 14,1051(1961) GD3 FE5 012

FR+1 VI

GA+3 IV
ABRAHAMS,S.C. ET AL., J.CHEM.PHYS. 42,3957(1965) GA FE 03
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) M3 GA5 012
GELLER,S., J.CHEM.PHYS. 33,676(1960) GA2 03
MAREZIO,M., ACTA CRYST. 18,481(1965) LI GA 02
MOONEY,R.C.L., ACTA CRYST. 9,728(1956) GA P 04

GA+3 V
SHANNON,R.D. AND C.T.PREWITT, J.INORG.NUCL.CHEM. IN PRESS. IN GA 03

GA+3 VI
BREWER,F.M. ET AL., J.INORG.NUCL.CHEM. 9,55(1959) GA F3
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) M3 GA5 012
GELLER,S., J.CHEM.PHYS. 33,676(1960) GA2 03
MAREZIO,M. AND J.P.REMEIKA, J.PHYS.CHEM.SOLIDS 26,1277(1965) GA2 03
MOONEY-SLATER,R.C.L., ACTA CRYST. 20,526(1966) GA P 04,2 H2 O
MOROSIN,B. AND A.ROSENZWEIG, ACTA CRYST. 18,878(1965) GA NR 04
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CE GA 03

GD+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) GD2 03

GD+3 VIII
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) GD2 TI2 07
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) GD3 AL2 AL3 012
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
WEIDENBORNER,J.E., ACTA CRYST. 14,1051(1961) GD3 FE5 012

GE+2 VI

GE+4 IV
ABRAHAMS,S.C. ET AL., J.CHEM.PHYS. 47,4034(1967) BI12 GE 020
DURIF,A., ACTA CRYST. 9,533(1956) GE U 04
GINETTI,Y., BULL.SOC.CHIM,BELGES 63,209(1954) CU GE 03
HILMER,W., ACTA CRYST. 15,1101(1962) BA GE 03
HILMER,W., SOVIET PHYS.-CRYST. 7,573(1963) SR GE 03
INGRI,N. AND G.LUNDGREN, ACTA CHEM.SCAND. 17,617(1963) NA4 GE9 020
JAMIESON,P.B. AND L.S.D. GLASSER, ACTA CRYST. 22,507(1967) NA2 GE 03.6 H2 O
LARSEN,F.K. ET AL., ACTA CHEM.SCAND. 21,1281(1967) NA8 SN8 GE10 030 (O H)4
ROBBINS,C. ET AL., J.RES.NATL.BUR.STD. 70A,385(1966) BA3 GE4 09
SMITH,G.S. AND P.B.ISAACS, ACTA CRYST. 17,842(1964) GE 02

GE+4 VI
BAUR,W.H., ACTA CRYST. 9,515(1956) GE 02
HOARD,J.L. AND W.B.VINCENT, J.AM.CHEM.SOC. 61,2849(1939) K2 GE F6
INGRI,N. AND G.LUNDGREN, ACTA CHEM.SCAND. 17,617(1963) NA9 GE9 020
ROBBINS,C. ET AL., J.RES.NATL.BUR.STD. 70A,385(1966) BA GE4 09
SHANNON,R.D. AND C.T.PREWITT, TO BE PUB. R3 VS V (RUTILE)
STRUNZ,H. AND M.GIGLIO, ACTA CRYST. 14,205(1961) FE GE (O H)6
ZEMANN,J., NEUES JAHRB.MINERAL.MONATSH. 67,(1959) FE GE (O H)6

H +1 I
ABRAHAMS,S.C., J.CHEM.PHYS. 36,56(1962) CU F2.2 H2 O
ABRAHAMS,S.C., J.CHEM.PHYS. 44,2230(1966) FE3 P2 O8.4 H2 O
CROMER,D.T. ET AL., ACTA CRYST. 21,383(1966) ALUM
KUIPERS, ET AL., J.CHEM.PHYS. 25,275(1956) HF
PIMENTEL,G.C. AND A.L.MC CLELLAN, THE HYDROGEN BOND, REINHOLD (NEW YORK) 1960

H +1 II
ELLISON,R.D. AND H.A.LEVY, ACTA CRYST. 19,260(1965) K H (C2 H O4 CL)
HAMILTON,W.C. AND J.A.IBERS, ACTA CRYST. 16,1209(1963) H CR 02
MC DONALD,T.R.R., ACTA CRYST. 13,113(1960) (N H4) H F2
MC GAW,B.L. AND J.A.IBERS, J.CHEM.PHYS. 39,2677(1963) NA H F2
PETERSON,S.W. AND H.A.LEVY, J.CHEM.PHYS. 20,704(1952) K H F2
PETERSON,S.W. AND H.A. LEVY, J.CHEM.PHYS. 29,948(1958) K H (C2 H2 04)

HF+4 VI
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 HF2 07
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

HF+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) HF 02

HG+1 III
GRDENIC,D. J.CHEM.SOC. 1312(1956) HG2 (N 03)2.2H2 O

HG+2 II
AURIVILLIUS,K., ACTA CRYST. 9,685(1956) HG O
AURIVILLIUS,K., ACTA CHEM.SCAND. 18,1305(1964) HG O
ROTH,W.L., ACTA CRYST. 9,277(1956) HG O

HG+2 IV
BONEFACIC,A., ACTA CRYST. 14,116(1961) HG S 04,H2 O
KOKKOROS,P.A. AND P.J.RENTZEPERIS, Z.KRIST. 119,234(1963) HG S 04

HG+2 VI
BONEFACIC,A., ACTA CRYST. 14,116(1961) HG S 04,H2 O

HG+2 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
SLEIGHT,A.W., TO BE PUBLISHED. HG2 M2 07
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) HG F2

HO+3 VI
FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85,267(1962) HO2 03
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) HO2 03

HO+3 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

I -1 VI

I +5 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CS I 03
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) RB I 03

I +7 VI

IN+3 VI
BERGERHOFF,G. AND H.KASPER, ACTA CRYST. B24,388(1968) CU2 IN2 05
JOHANSSON,G., ACTA CHEM,SCAND. 15,1437(1961) IN O H S 04 (H2 O)2
MAREZIO,M., ACTA CRYST. 20,723(1966) IN2 03
MOONEY,R.C.L., ACTA CRYST. 9,113(1956) IN P 04
MOONEY-SLATER,R.C.L., ACTA CRYST. 14,1140(1961) IN P 04,2 H2 O
REID,A.F., INORG.CHEM. 6,631(1967) CA IN2 04
ROTH,R.S., S.J.SCHNEIDER, J.RES.NATL.BUR.STD. 64A,309(1960) R3 VS V (MN2 O3)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. IN2 03

IN+3 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

IR+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) IR F3

IR+4 VI
BABEL,D. ET AL., Z.ANORG.ALLGEM.CHEM. 347,282(1966) CA2 IR 06
RODI, F. AND D.BABEL, Z.ANORG.ALLGEM.CHEM. 336,17(1965) CA IR 03
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

K +1 VI
BODE,H. AND E.VOSS, Z.ANORG.ALLGEM.CHEM. 264,144(1951) K SB F6
HOPPE,R. AND H.SABROWSKY, Z.ANORG.ALLGEM.CHEM. 339,144(1965) K SC 02
STANLEY,E., ACTA CRYST. 9,897(1956) K2 S2 06
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) K F
ZACHARIASEN,W.H., ACTA CRYST. 7,783(1954) K3 U 02 F5
ZACHARIASEN,W.H., ACTA CRYST. 7,792(1954) K3 U F7
ZIEGLER,G.E., Z.KRIST. 94,491(1936) K N 02

K +1 VII
EANES,E.D. AND H.M.ONDIK, ACTA CRYST. 15,1280(1962) LI K2 P3 09,H2 O
EDWARDS,D.A., Z.KRIST. 80,154(1931) K N 03
LINDQVIST,I. AND M.MORTSELL, ACTA CRYST. 10,406(1957) K2 S2 05
MAREZIO,M. ET AL., ACTA CRYST. 16,975(1963) K2 B4 07,4 H2 O
ZACHARIASEN,W.H., J.CHEM,PHYS. 5,919(1937) K B 02
ZHUKOVA,L.A. AND Z.G.PINSKER, SOVIET PHYS.-CRYST. 9,31(1964) K2 CR2 07

K +1 VIII
ANDERSSON,S. AND A.D.WADSLEY, ACTA CHEM,SCAND. 15,663(1961) K2 TI2 05
BELT,R.F. AND N.C.BAENZIGER, J.AM.CHEM.SOC. 79,316(1957) K S 03 (N H O H)
CHRIST,C.L. ET AL., ACTA CRYST. 7,801(1954) K V 03,H2 O
EANES,E.D. AND H.M.ONDIK, ACTA CRYST. 15,1280(1962) LI K2 P3 09,H2 O
FORRESTER,J.D. ET AL., ACTA CRYST. 16,58(1963) K M2 F3
LINDQVIST,I. AND M.MORTSELL, ACTA CRYST. 10,406(1957) K2 S2 05
MORROW,J.C., ACTA CRYST. 13,443(1960) K RE 04
PALENIK,G.J., INORG.CHEM. 6,503(1967) K MN 04
SIEGEL,S., ACTA CRYST. 9,493(1956) K BR F4
SUTOR,D.J. ET AL., ACTA CRYST. 7,105(1954) K2 C2 H N 04
WADSLEY,A.D., ACTA CRYST. 17,623(1964) K TI NB 05
ZACHARIASEN,W.H., ACTA CRYST. 7,783(1954) K3 U 02 F5
ZACHARIASEN,W.H., ACTA CRYST. 7,792(1954) K3 U F7
ZACHARIASEN,W.H. AND H.A.PLETTINGER, ACTA CRYST. 16,376(1963) K B5 08.4 H2 O

K +1 IX
ARAVINDAKSHAN,C., Z.KRIST. 111,35(1958) K CL 03
BALZ,D. AND K.PLIETH, Z.ELEKTROCHEM. 59,545(1955) K2 NI F4
BODE,H. AND G.TEUFER, ACTA CRYST. 9,929(1956) K2 HF F6
BROWN,G.M. AND L.A.WALKER, ACTA CRYST. 20,220(1966) K2 NB F7
DONOHUE,J. AND L.HELMHOLZ, J.AM,CHEM,SOC. 66,295(1944) K AG C 03
HOARD,J.L., J.AM.CHEM.SOC. 61,1252(1939) K2 NB F7
KNOX,K., J.CHEM,PHYS. 30,991(1959) K2 CU F4
KROGH-MOE,J., ACTA CRYST. 18,1088(1965) K2 B10 016
LOOPSTRA,L.H. AND C.H.MACGILLAVRY, ACTA CRYST. 11,349(1958) K H S 04
PALENIK,G.J., INORG.CHEM. 6,507(1967) K2 MN 04
SCHNEIDER,W., ACTA CRYST. 14,784(1961) K2 MN (S 04)2.4 H2 O
ZACHARIASEN,W.H., SKRIFT.NORSKE VID.-AKAD. OSLO.I.MAT.NATUR.KLASSE(1928) K BR 03
ZACHARIASEN,W.H., Z.KRIST. 71,501(1929) K CL 03
ZACHARIASEN,W.H., Z.KRIST. 89,529(1934) K2 S3 06
ZACHARIASEN,W.H. AND G.E.ZIEGLER, Z.KRIST. 80,164(1931) K2 CR 04

K +1 X
BYSTROM,A. ET AL., ARKIV KEMI 4,175(1952) K SB F4
CANNILLO,F. ET AL., ACTA CRYST. 21,200(1966) K NA3 FE2 TI2 (SI4 012)2
EVANS,H.T.,JR., Z.KRIST. 114,257(1960) K V 03
KEEN,R.C., Z.KRIST. 91,129(1935) K2 S2 08
PALENIK,G.J., INORG.CHEM. 6,507(1967) K2 MN 04
ZACHARIASEN,W.H. AND G.E.ZIEGLER, Z.KRIST. 80,164(1931) K2 CR 04

K +1 XII
BODE,H. AND H.V.DOHREN, ACTA CRYST. 11,80(1958) K TA F6
BODE,H. AND H.V.DOHREN, ACTA CRYST. 11,80(1958) K NB F6
ELLINGER,F.H. AND ZACHARIASEN,W.H., J.PHYS.CHEM. 58,405(1954) K PU 02 C 03
EVANS,H.T.,JR., AND S.BLOCK, INORG.CHEM. 5,1808(1966) K V3 08
GOTTFRIED,C. AND C. SCHUSTERIUS, Z.KRIST. 84,65(1932) K CL 04
HEPWORTH,M.A. ET AL., J.INORG.NUCL.CHEM. 2,79(1956) K O5 F6
HOARD,J.L. AND W.B.VINCENT, J.AM.CHEM.SOC. 61,2849(1934) K2 GE F6
IBERS,J.A., ACTA CRYST. 9,967(1956) K AS F6
ITO,T. ET AL., ACTA CRYST. 5,209(1952) K2 CA4 BE4 AL2 SI24 060,H2 O
KATZ,L. AND H.D.MEGAW, ACTA CRYST. 22,639(1967) K NB 03
SIEGEL,S., ACTA CRYST. 5,683(1952) K2 TI F6
VOUSDEN,P., ACTA CRYST. 4,373(1951) K TA 03
WILHELMI,K., ACTA CHEM,SCAND. 12,1965(1958) K CR3 08
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 3,(1965) K AL3 (O H)6 (S 04)2

LA+3 VI

Table 1(*b*) (*cont.*)

SILLEN+L.G. AND K.LUNDBORG, Z.ANORG.ALLGEM.CHEM, 252,2(1943) LA2 MO O6
TEMPLETON+D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC, 76,5237(1954) LA2 O3

LA+3 VII
GUILLEN+M. AND E.F.BERTAUT, COMPT.REND. SER.A+B 262B,962(1966) LA2 TI O5

LA+3 VIII
BRISSE+F., PH.D.THESIS+DALHOUSIE UNIV.+HALIFAX+N.S.(1967) LA2 M2 O7
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

LA+3 IX
HUNT+E.B.+JR.+ ET AL.+ ACTA CRYST. 7,106(1954) LA2 (S O4)3,9 H2 O
ZALKIN+A. ET AL.+ INORG.CHEM. 5+1466(1966) LA F3

LA+3 X
LONGO+J.M. AND A.W.SLEIGHT+ INORG.CHEM. 7+108(1968) LA4 REG O19

LA+3 XII
HUNT+E.B.+JR.+ ET AL.+ ACTA CRYST. 7,106(1954) LA2 (S O4)3,9 H2 O

LI+1 IV
BURNS+J.H. AND W.R.BUSING+ INORG.CHEM. 4+1510(1965) RB LI F2
BURNS+J.H. AND W.R.BUSING+ INORG.CHEM. 4+1510(1965) CS LI F2
BURNS+J.H. AND E.K. GORDON+ ACTA CRYST. 20+135(1966) LI2 BE F4
EANES+E.D. AND H.W.ONDIK+ ACTA CRYST. 15+1280(1962) LI K2 P3 O9,H2 O
GALY+J. AND A.HARDY+ ACTA CRYST. 19+432(1965) LI V2 O5
KEFFER+C. ET AL.+ INORG.CHEM. 6+119(1967) LI3 P O4
LARSON+A.C.+ ACTA CRYST. 18+717(1965) LI2 S O4,H2 O
LIEBAU+F.+ ACTA CRYST. 14+389(1961) LI2 SI2 O5
LIEBAU+F.+ ACTA CRYST. 14+399(1961) LI AL SI4 O10
MAREZIO+M.+ ACTA CRYST. 18+481(1965) LI GA O2
MAREZIO+M.+ ACTA CRYST. 19+396(1965) LI AL O2
MAREZIO+M. AND J.P.REMEIKA+ J.CHEM.PHYS. 44+3348(1966) LI R O2
REMEIKA+J.P. AND M.MAREZIO+ J.PHYS.CHEM.SOLIDS 26,2083(1965) LI B O2
SEARS+D.R. AND J.H.BURNS+ J.CHEM.PHYS. 41+3478(1964) LI6 BE F4 ZR F8
ZACHARIASEN+W.H. AND H.A.PLETTINGER+ ACTA CRYST. 14+229(1961) LI2 W O4
ZEMANN+J.+ ACTA CRYST. 13+863(1960) LI3 P O4
ZINTL+E. ET AL.+ Z.ELEKTROCHEM. 40+548(1934) LI2 O

LI+1 VI
ABRAHAMS+S.C. AND J.L.BERNSTEIN+ J.PHYS.CHEM.SOLIDS 28+1685(1967) LI TA O3
ABRAHAMS+S.C. AND H.J.WILLIAMS+ J.CHEM.PHYS. 39+2923(1963) LI CU CL3.2 H2 O
ABRAHAMS+S.C. ET AL.+ J.PHYS.CHEM.SOLIDS 27+997(1966) LI NB O3
ABRAHAMS+S.C. ET AL.+ J.PHYS.CHEM.SOLIDS 28+1693(1967) LI TA O3
BRUNTON+G.+ ACTA CRYST. 21+814(1966) LI U F5
BRUNTON+G.+ J.INORG.NUCL.CHEM. 29+1631(1967) LI4 U F8
BURNS+J.H.+ ACTA CRYST. 15+1098(1962) LI SR F6
CANNILLO+F. ET AL.+ ACTA CRYST. 21+200(1966) K NA3 FE2 TI2 (SI4 O12)2
GALY+ J. AND A.HARDY+ ACTA CRYST. 19,432(1965) LI V2 O5
GELLER+S. AND J.L.DURAND+ ACTA CRYST. 13+325(1960) LI MN P O4
MAREZIO+M. AND J.P.REMEIKA+ J.PHYS.CHEM.SOLIDS 26+1277(1965) LI GA O2
MAREZIO+M. AND J.P.REMEIKA+ J.CHEM.PHYS. 44+3143(1966) LI AL O2
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 1,(1963) LI F

LU+3 VI
BARTRAM+S.F.+ INORG.CHEM. 5+749(1966) LU6 U O12
TEMPLETON+D.H. AND C.H.DAUBEN+ J.AM.CHEM.SOC. 76+5237(1954) LU2 O3

LU+3 VIII
BRISSE+F.+ PH.D.THESIS+DALHOUSIE UNIV.+HALIFAX+N.S.(1967) LU2 TI2 O7
EULER+F. AND J.A.BRUCE+ ACTA CRYST. 19,971(1965) LU3 ME5 O12
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

MG+2 IV
SMITH+J.V.+ AM.MINERALOGIST 38+643(1953) CA2 MG SI2 O7

MG+2 VI
BAUR+W.H.+ ACTA CRYST. 9+515(1956) MG F2
BAUR+W.H.+ ACTA CRYST. 15+815(1962) FE S O4.4 H2 O
BRUNTON+G. ET AL.+ ACTA CRYST. 11+169(1958) CU8 MG8 (C O3)8 (O H)24.8 H2 O
CALVO+C.+ CAN.J.CHEM. 43+1139(1965) MG2 P2 O7
CORBRIDGE+D.E.C.+ ACTA CRYST. 9+991(1956) MG H P O3.6 H2 O
GIBBS+G.V. ET AL.+ AM.MINERALOGIST. IN PRESS. MG2 SI O4
KASPER+J.S. AND J.S.PRENER+ ACTA CRYST. 7+246(1954) MG6 MN O8
LUKASZEWICZ+K.+ BULL.ACAD.POLON.SCI.SER.SCI.CHIM. 11+361(1963) MG2 AS2 O7
RENTZEPERIS+P.J. AND C.T.SOLDATOS+ ACTA CRYST. 11+686(1958) MG S O4
STEINFINK+H. AND F.J.SANS+ AM.MINERALOGIST 44+679(1959) CA MG (C O3)2
SUTOR+D.J.+ ACTA CRYST. 23+418(1967) MG H P O4.3H2 O
TAKEUCHI+Y.+ ACTA CRYST. 5+574(1952) MG2 B2 O5
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 1,(1963) MG O
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 2,(1964) K MG F3
ZACHARIASEN+W.H.+ ACTA CRYST. 7,788(1954) MG U O4
ZEMANN+A. AND J.ZEMANN+ ACTA CRYST. 10,409(1957) K2 MG2 (S O4)3

MG+2 VIII
GIBBS+G.V. AND J.V.SMITH+ AM.MINERALOGIST 50,2023(1965) MG3 AL2 SI3 O12
ZEMANN+A. AND J.ZEMANN+ ACTA CRYST. 14+835(1961) MG3 AL2 SI3 O12

MN+2 VI LS

MN+2 VI HS
ABRAHAMS+S.C. AND J.M.REDDY+ J.CHEM.PHYS. 43,2533(1965) MN MO O4
BAUR+W.H.+ ACTA CRYST. 11+488(1958) MN F2
GELLER+S. AND J.L.DURAND+ ACTA CRYST. 13+325(1960) LI MN P O4
HROSE+W.E. AND D.E.APPLEMAN+ Z.KRIST. 117+16(1962) (MN,FE) BE (P O4) (O H)
PEACOR+D.R. AND M.J.BUERGER+ Z.KRIST. 117+331(1962) CA MN SI2 O6
RENTZEPERIS+P.J.+ NEUES JAHRB.MINERAL.MONATSH. 210(1958) MN S O4
RENTZEPERIS+P.J.+ Z.KRIST. 119+117(1963) ZN2 MN (O H)2 SI O4
SCHNEIDER+W.+ ACTA CRYST. 14+784(1961) K2 MN (S O4)2.4 H2 O
SHIRANE+G. ET AL.+ J.PHYS.SOC.JAPAN 14+1352(1959) MN TI O3
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 1,(1963) MN O
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 2,(1964) K MN F3
ZALKIN+A. ET AL.+ J.CHEM.PHYS. 37,697(1962) CS MN F3

MN+2 VIII
SHANNON+R.D. AND C.T.PREWITT, UNPUBLISHED DATA. R VS A (GARNET)

MN+3 V
ABRAHAMS+S.C. AND J.L.BERNSTEIN+ J.CHEM.PHYS. 46+3776(1967) DY MN2 O5
YAKEL+H.L. ET AL.+ ACTA CRYST. 16+957(1963) Y MN O3

MN+3 VI LS
BLASSE+G.+ J.INORG.NUCL.CHEM. 27+748(1965)
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (K3 MIII (C N)6)

MN+3 VI HS
COLLIN+R.L. AND W.N.LIPSCOMB+ ACTA CRYST. 2+104(1949) H MN O2
DACHS+H.+ Z.KRIST. 118+303(1963) MN O O H
FERT+A.+ BULL.SOC.FRANC.MINERAL.CRIST. 85+267(1962) MN2 O3
HASE+M. ET AL.+ Z.KRIST. 124+428(1967) MN2 O3
HEPWORTH+M.A. AND K.H.JACK+ ACTA CRYST. 10+345(1957) MN F3
NORRESTAM+R.+ ACTA CHEM.SCAND. 21+2871(1967) MN2 O3
ROTH+R.S.+ S.J.SCHNEIDER+ J.RES.NATL.BUR.STD. 64A+309(1960) R3 V5 V (MN2 O5)
SHANNON+R.D.+ INORG.CHEM. 6+1474(1967) R3 V5 V (PEROVSKITE)
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (MN2 O3)

MN+4 VI
ABRAHAMS+S.C. AND J.L.BERNSTEIN+ J.CHEM.PHYS. 46+3776(1967) DY MN2 O5
BODE+H. AND W.WENDT+ Z.ANORG.ALLGEM.CHEM. 269+165(1952) RB2 MN F6
KASPER+J.S. AND J.S.PRENER+ ACTA CRYST. 7+246(1954) MG6 MN O8
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 V5 V (RUTILE)
WADSLEY+A.D.+ ACTA CRYST. 8+165(1955) ZN MN3 O7,3 H2 O

MN+6 IV
PALENIK+G.J.+ INORG.CHEM. 6+507(1967) K2 MN O4

MN+7 IV
FERRARI+A. ET AL.+ ACTA CRYST. 21+681(1966) SR (MN O4)2,3 H2 O
JAVAN+A. AND A. ENGELBRECHT+ PHYS.REV. 96+649(1954) MN O3 F
MOONEY+R.C.L.+ PHYS.REV. 37+1306(1931) K MN O4
PALENIK+G.J.+ INORG.CHEM. 6+503(1967) K MN O4
SASVARI+K.+ Z.KRIST. 99+9(1938) AG MN O4

MN+7 VI

MO+3 VI
HEPWORTH+M.A. ET AL.+ ACTA CRYST. 10+63(1957) MO F3

MO+4 VI
ANSELL+G.B. AND L.KATZ+ ACTA CRYST. 21+482(1966) ZN2 MO3 O8
BRANDT+B.G. AND A.C.SKAPSKI+ ACTA CHEM.SCAND. 21+661(1967) MO O2
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 V5 V (RUTILE)
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 2,(1964) BA MO O3
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 2,(1964) SR MO O3

MO+5 VI
EDWARDS+A.J. AND R.D.PEACOCK+ J.CHEM.SOC. 1961+4253 NA MO F6
KIERKEGAARD+P. AND M.WESTERLUND+ ACTA CHEM.SCAND. 18+2217(1964) MO P O5

MO+6 IV
ABRAHAMS+S.C.+ J.CHEM.PHYS. 46+2052(1967) ZN MO O4
ABRAHAMS+S.C. AND J.M. REDDY+ J.CHEM.PHYS. 43+2533(1965) MN MO O4
ABRAHAMS+S.C. ET AL.+ J.CHEM.PHYS. 48+2619(1968) CU MO O4
IBERS+J.A. AND G.W.SMITH+ ACTA CRYST. 17+190(1964) NA C02.3 MO3 O12
KIHLBORG+L.+ ARKIV KEMI 21+357(1963) MO O3
KIHLBORG+L.+ ARKIV KEMI 21+365(1963) MO4 O11 (MON),MO4 O11 (O-RH)
LECIEJEWICZ+J.+ Z.KRIST. 121+158(1965) PB MO O4
SELEBORG+M.+ ACTA CHEM.SCAND. 20+2195(1966) K2 MO3 O10
SELEBORG+M.+ ACTA CHEM.SCAND. 21+499(1967) NA2 MO2 O7
SILLEN+L.G. AND K.LUNDBORG+ Z.ANORG.ALLGEM.CHEM. 252,2(1943) LA2 MO O6

MO+6 V
EICK+H.A. AND L.KIHLBORG+ ACTA CHEM.SCAND. 20+1658(1966) V2 MO O8
GATEHOUSE+B.M. AND P.LEVERETT+ CHEM.COMM. 1967+374 K2 MO3 O10
SELEBORG+M.+ ACTA CHEM.SCAND. 20+2195(1966) K2 MO3 O10

MO+6 VI
GATEHOUSE+B.M. AND P.LEVERETT+ CHEM.COMM. 1967+374 K2 MO3 O10
KIERKEGAARD+P.+ ARKIV KEMI 18+521(1962) MO P2 O8
KIERKEGAARD+P.+ ARKIV KEMI 18+553(1962) NA MO O2 P O4
KIERKEGAARD+P.+ ARKIV KEMI 19+1(1963) (MO O2)2 P2 O7
KIERKEGAARD+P. AND S.HOLMEN+ ARKIV KEMI 23+213(1965) AG MO P O6
KIHLBORG+L.+ ARKIV KEMI 21+357(1963) MO O3
KIHLBORG+L.+ ARKIV KEMI 21+365(1963) MO4 O11 (MON),MO4 O11 (O-RH)
KIHLBORG+L.+ ARKIV KEMI 21+427(1964) MO5 O14
KIHLBORG+L.+ ARKIV KEMI 21+443(1964) MO18 O52
KIHLBORG+L.+ ARKIV KEMI 21+461(1964) MO8 O23
SELEBORG+M.+ ACTA CHEM.SCAND. 20+2195(1966) K2 MO3 O10
SMITH+G.W. AND J.A.IBERS+ ACTA CRYST. 19+269(1965) CO MO O4

MO+6 VII
KIHLBORG+L.+ ARKIV KEMI 21+427(1964) MO5 O14

N +3 VI

N +5 III
CHERIN+P. ET AL.+ ACTA CRYST. 23+455(1967) NA N O3

N +5 VI

NA+1 IV
CORBRIDGE+D.E.C.+ ACTA CRYST. 13+263(1960) NA5 P3 O10
WUNDERLICH+J.A.+ ACTA CRYST. 10+462(1957) NA O H+H2 O
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 1,(1963) NA2 O

NA+1 V
HEMILY+P.W.+ ACTA CRYST. 10+37(1954) NA O H+H2 O
LARSEN+F.K. ET AL.+ ACTA CHEM.SCAND. 21+1281(1967) NA3 SN4 GE10 O30 (O H)4
MCDONALD+W.S. AND D.W.J.CRUICKSHANK+ ACTA CRYST. 22+37(1967) NA2 SI O3
ONDIK+H.M.+ ACTA CRYST. 18+226(1965) NA3 P3 O9
ONDIK+H.M.+ ACTA CRYST. 18+226(1965) NA3 P3 O9.H2 O
PANT+A.K. AND D.W.J.CRUICKSHANK+ ACTA CRYST. B24+13(1968) NA2 SI2 O5
ROMERS+C. ET AL.+ ACTA CRYST. 22+766(1967) NA3 FE5 O9

NA+1 VI
BURNS+ J.H.+ INORG.CHEM. 4+881(1965) NA MO F4
CORBRIDGE+D.E.C.+ ACTA CRYST. 13+263(1960) NA5 P3 O10
CROMER+D.T. ET AL.+ ACTA CRYST. 22+182(1967) NA AL (S O4)2.12 H2 O
CRUICKSHANK+D.W.J.+ ACTA CRYST. 17+677(1964) NA8 P2 O7.10 H2 O
DYER+L.D. ET AL.+ J.AM.CHEM.SOC. 76+1499(1954) NA NI O2
GIESE+R.F.+JR.+ SCIENCE 154+1453(1966) NA2 BA O6 (O H)2.3 H2 O
KIERKEGAARD+P.+ ARKIV KEMI 18+553(1962) NA MO O2 P O4
MCDONALD+R.R. ET AL.+ ACTA CRYST. 17,1104(1964) NA SN2 F5
ONDIK+H.M. ET AL.+ ACTA CRYST. 14+555(1961) NA8 P8 O12.8 H2 O
SHARMA+B.D.+ ACTA CRYST. 18+818(1965) NA H C O3
WEISS+R. ET AL.+ ACTA CRYST. 20+534(1966) NA3 H TI F8
WYCKOFF+R.W.G.+ CRYSTAL STRUCTURES 1,(1963) NA F
ZACHARIASEN+W.H.+ ACTA CRYST. 2+390(1949) NA TH2 F9
ZACHARIASEN+W.H.+ ACTA CRYST. 2+390(1949) NA2 TH F6
ZALKIN+A. ET AL.+ ACTA CRYST. 17+1408(1964) NA2 SI F6

NA+1 VII
ANDERSSON+S. AND A.D.WADSLEY+ ACTA CRYST. 14+1245(1961) NA2 TI3 O7
CANNILLO+F. ET AL.+ ACTA CRYST. 21+200(1966) K NA3 FE2 TI2 (SI4 O12)2
FANG+S.M.+ Z.KRIST. 99A+1(1938) NA B O2
KIERKEGAARD+P.+ ARKIV KEMI 18+553(1962) NA W O2 P O4
KOKKOROS+P.+ Z.KRIST. 99A+38(1938) NA AL F AS O4
MAREZIO+M. ET AL.+ ACTA CRYST. 16+594(1963) NA B O2
RAO+B.RAMA+ ACTA CRYST. 14+738(1961) NA2 CU (S O4)2.2 H2

NA+1 VIII
MCDONALD+R.R. ET AL.+ ACTA CRYST. 17,1104(1964) NA SN2 F5
MENZER+G.+ Z.KRIST. 75+265(1930) NA3 LI3 AL2 F12
RUMANOVA+I.M.+ G.F.VOLODIN+ DOKL.AKAD.NAUK SSSR 123,78(1958) NA CU2 O H (S O4)2.H2
WEISS+R. ET AL.+ ACTA CRYST. 20+534(1966) NA3 H TI F8
ZACHARIASEN+W.H.+ Z.KRIST. 73A,141(1930) NA CL O4

NA+1 IX
ANDERSSON+S. AND A.D.WADSLEY+ ACTA CRYST. 14+1245(1961) NA2 TI3 O7

NB+2 VI
ANDERSSON+G. AND A.MAGNELI+ ACTA CHEM.SCAND. 11+1065(1957) NB O

NB+3 VI
HEPWORTH+M.A. ET AL.+ ACTA CRYST. 10+63(1957) NB F3

NB+4 VI
MARINDER+B.+ ARKIV KEMI 19+435(1962) NB O2
SHANNON+R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 V5 V (RUTILE)

NB+5 IV
GATEHOUSE+B.M. AND A.D.WADSLEY+ ACTA CRYST. 17+1545(1964) NB2 O5

NB+5 VI
ABRAHAMS+S.C. ET AL.+ J.PHYS.CHEM.SOLIDS 27+997(1966) LI NB O3

Table 1(*b*) (*cont.*)

ANDERSSON,S., ACTA CHEM.SCAND. 18,2339(1964) NB3 O7 F
BODE,H. AND H. DOHREN, ACTA CRYST. 11,80(1958) K NB F6
GATEHOUSE,B.M. AND A.D.WADSLEY, ACTA CRYST. 17,1545(1964) NB2 O5
KATZ,L. AND H.D. MEGAW, ACTA CRYST. 22,639(1967) K NB O3
MOROSIN,B. AND A.ROSENZWEIG, ACTA CRYST. 18,874(1965) GA NB O4
PEDERSEN,B.F., ACTA CHEM.SCAND. 16,1421(1962) AL NB O4
SKAPSKI,A.C. AND D.ROGERS, CHEM.COMM. (1965)611 SB NB O4
SLEIGHT,A.W., TO BE PUBLISHED. HG2 NB2 O7

NB+5 VII
BROWN,G.M. AND L.A.WALKER, ACTA CRYST. 20,220(1966) K2 NB F7
HOARD,J.L., J.AM.CHEM.SOC. 61,1252(1939) K2 NB F7

ND+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) ND2 O3

ND+3 VIII
MILLIGAN,W.O. AND L.W.VERNON, J.PHYS.CHEM. 56,145(1952) ND V O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

ND+3 IX
BURNS,J.H., INORG.CHEM. 4,881(1965) NA ND F4

NI+2 VI
BALZ,D. AND K.PLIETH, Z.ELEKTROCHEM. 59,545(1955) K2 NI F4
BAUR,W.H., ACTA CRYST. 11,488(1958) NI F2
BILLY,C. AND H.M.HAENDLER, J.AM.CHEM.SOC. 79,1049(1957) NI F2
DYER,L.D. ET AL., J.AM.CHEM.SOC. 76,1499(1954) NA NI O2
KEELING,R.O.,JR., ACTA CRYST. 10,209(1957) NI W O4
LANDER,J.J., ACTA CRYST. 4,148(1951) BA NI O2
O'CONNOR,B.H. AND D.M.DALE, ACTA CRYST. 21,705(1966) NI 5 O4.6 H2 O
SCHNERING,H.P., Z.ANORG.ALLGEM.CHEM. 353,13(1967) RA2 NI F6
SHIRANE,G, ET AL., J.PHYS.SOC.JAPAN 14,1352(1959) NI TI O3
VAN NIEKERK,J.N., F.R.SCHOENING, ACTA CRYST. 6,609(1953) NI(C H3 C O O)2.4 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) NI O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K NI F3

NI+3 VI LS
BLASSE,G., J.INORG.NUCL.CHEM. 27,748(1965) K3 NI F6
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (PEROVSKITE)

NI+3 VI HS
BLASSE,G., J.INORG.NUCL.CHEM. 27,748(1965)

NP+2 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) NP O

NP+3 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (LA F3)

NP+4 VI

NP+4 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (FLUORITE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) NP O2

NP+7 VI

O -2 II

O -2 III

O -2 IV

O -2 VI

O -2 VIII

OS+4 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)

P +3 VI

P +5 IV
CRUICKSHANK,D.W.J., ACTA CRYST. 17,671(1964) NA P O3 N H3
CRUICKSHANK,D.W.J., ACTA CRYST. 17,672(1964) NA4 P2 O7.10 H2 O
CRUICKSHANK,D.W.J., ACTA CRYST. 17,674(1964) NA5 P3 O10
CRUICKSHANK,D.W.J., ACTA CRYST. 17,675(1964) (N H4)4 P4 O12
CRUICKSHANK,D.W.J., ACTA CRYST. 17,679(1964) P2 O5
CRUICKSHANK,D.W.J., ACTA CRYST. 17,681(1964) RR P O3
FEHLMANN,H. AND S,GHOSE, J.CHEM.PHYS. 41,1910(1964) CU3 P O4 (O H)3
GELLER,S. AND J.L.DURAND, ACTA CRYST. 13,325(1960) LI MN P O4
JARCHOW,O.H., ACTA CRYST. 17,1253(1964) NA2 H2 P4 O12
KEFFER,C. ET AL., INORG.CHEM. 6,119(1967) LI3 P O4
KIERKEGAARD,P., ARKIV KEMI, 18,521(1961) MO P2 O8
KIERKEGAARD,P., ARKIV KEMI, 18,553(1961) NA MO O2 P O4
KIERKEGAARD,P. AND S.HOLMEN, ARKIV KEMI 23,213(1965) AG MO P O6
KIERKEGAARD,P. AND M.WESTERLUND, ACTA CHEM.SCAND. 18,2217(1964) MO P O5
KRSTANOVIC,I., Z.KRIST. 121,315(1965) Y P O4
PAULING,L. AND J.SHERMAN, Z.KRIST. 96,481(1937) AL P3 O9
SCHWARZENBACH,D., Z.KRIST. 123,161(1966) AL P O4
WEBB,N.C., ACTA CRYST. 21,942(1966) CA2 P2 O7
ZEMANN,J., ACTA CRYST. 13,863(1960) LI3 P O4

P +5 VI

PA+3 VI

PA+4 VI

PA+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PA O2

PA+5 VI

PA+5 IX
BROWN,D. ET AL., J.CHEM.SOC. 1967A,1429 K2 PA F7

PB+2 IVPY
BOUCHER,M.L. AND D.R.PEACOR, Z.KRIST. 126,98(1968) PB SI O3
BYSTROM,A. AND L.EVERS, ACTA CHEM.SCAND. 4,613(1950) AG2 PB O2
KAY,M.I., ACTA CRYST. 14,80(1961) PB O

PB+2 VI
MAGNELI,A., ARKIV KEMI, MINERAL.GEOL. 15B, 3(1942) PB SB2 O6
MOLLER,C.K., ACTA CHEM.SCAND. 8,81(1954) PB (N H4)2 (S O4)2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CS PB F3

PB+2 VIII
FINNEY,J.J., AM.MINERALOGIST 48,1(1963) PB FE2 (AS O4)2 (O H)2
LECIEJEWICZ,J., Z.KRIST. 121,158(1965) PB MO O4
KAY,M.I., ACTA CRYST. 14,80(1961) PB O
QUARENI,S. AND R.DEPIERI, ACTA CRYST. 19,287(1965) PB CR O4
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PB F2

PB+2 IX
COLBY,M.Y. AND L.J.B.LACOSTE, Z.KRIST. 84,299(1932) PB C O3

PB+2 XI
NARAY-SZABO,I. AND G.ARGAY, ACTA CHIM.ACAD.SCI.HUNG. 40,283(1964) PB CR O4

PB+2 XII
HAMILTON,W.C., ACTA CRYST. 10,103(1957) PB (N O)2
SAHL,K., BEITR.MINERAL.PETROG. 9,111(1963) PB S O4

PB+4 VI
BYSTROM,A., ARKIV KEMI,MINERAL.GEOL. 25A,13(1947) PB O2
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) BA PB O3

PB+4 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (FLUORITE)

PD+1 II
ROGERS,D.B. AND R.D.SHANNON, FALL A.C.S. MTG.,ATLANTIC CITY(1968) PD CO O2

PD+2 IVSQ
WASER,J. ET AL., ACTA CRYST. 6,661(1953) PD O

PD+2 VI
BARTLETT,N. AND R.MAITLAND, ACTA CRYST. 11,747(1958) PD F2

PD+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) PD F3

PD+4 VI
SLEIGHT,A.W., TO BE PUBLISHED. R VS A (PYROCHLORE)

PM+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) PM2 O3

PO+4 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (FLUORITE)

PO+6 VI

PR+3 VI
FERT,A., BULL.SOC.FRANC.MINERAL CRIST. 85,267(1962) PR2 O3
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) PR2 O3

PR+3 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

PR+4 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) BA PR O3

PR+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PR O2

PT+2 VI

PT+4 VI
BJORLING,C.O., ARKIV KEMI,MINERAL.GEOL. 15B,2(1942) K2 PT (O H)6
HOEKSTRA,H.R. AND S.SIEGEL, INORG.CHEM. 7,141(1968) TL2 PT2 O7
MELLOR,D.P. AND N.C.STEPHENSON, AUSTR.J.RES. 4A406(1951) K2 PT F6
SHANNON,R.D., SOLID STATE COMM. IN PRESS. R3 VS V (PT O2)

PU+3 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (LA F3)

PU+4 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) BA PU O3

PU+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PU O2

RA+2 VI

RB+1 VI
HOPPE,R. AND H.SABROWSKY, Z.ANORG.ALLGEM.CHEM. 339,144(1965) RB SC O2
PLYUKHIN,V.V. AND N.V.BELOV, SOVIET PHYS.-CRYST. 6,685(1962) RB BE2 F5
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) RB F

RB+1 VII
CORBRIDGE,D.E.C., ACTA CRYST. 9,308(1956) RB P O3
CRUICKSHANK,D.W.J., ACTA CRYST. 17,681(1964) (RB P O3)

RB+1 VIII
ANDERSSON,S. AND A.D.WADSLEY, ACTA CRYST. 15,194(1962) RB2 TI6 O13
BURNS,J.H. AND W.R.BUSING, INORG.CHEM. 4,1310(1965) RB LI F2
CRUICKSHANK,D.W.J., ACTA CRYST. 17,681(1964) (RB P O3)

RB+1 XII
ELLINGER,F.H. AND W.H.ZACHARIASEN, J.PHYS.CHEM. 58,405(1954) RB AM O2 C O3
HOARD,J.L. AND V.BLAIR, J.AM.CHEM.SOC. 57,1985(1935) RB B F4

RE+4 VI
SHANNON, AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)

RE+5 VI
DONOHUE,P.C. ET AL., INORG.CHEM. 4,1152(1965) CD2 RE2 O7

RE+6 VI
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) RE O3

RE+7 IV
KREBS,B. ET AL., CHEM.COMM. (1968)263 RE2 O7
MORROW,J.C., ACTA CRYST. 13,443(1960) K RE O4

RE+7 VI
KREBS,B. ET AL., CHEM.COMM. (1968)263 RE2 O7

RH+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) RH F3
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (PEROVSKITE)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (CORUNDUM)

RH+4 VI
SHANNON, AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RH O2)

RU+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) RU F3
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (PEROVSKITE)

RU+4 VI
COTTON,F.A. AND J.T.MAGUE, INORG.CHEM. 5,317(1965) RU O2
DONOHUE,P.C. ET AL., INORG.CHEM. 4,306(1965) BA RU O3
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORES)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)

S -2 VI

S +4 VI

S +6 IV
BAUR,W.H., ACTA CRYST. 17,863(1964) MG S O4,4 H2 O
BAUR,W.H., ACTA CRYST. 17,1167(1964) MG S O4,7 H2 O
BAUR,W.H., ACTA CRYST. 17,1361(1964) FE S O4,7 H2 O
CROMER,D.T. ET AL., ACTA CRYST. 21,383(1966) CS AL (S O4)2,12 H2 O
GRAEBER,E.J. ET AL., AM.MINERALOGIST 50,1929(1965) K FE (S O4)2

Table 1(*b*) (*cont.*)

GRAEBER,E.J. ET AL.; AM.MINERALOGIST 50,1929(1965) MG (N H4)2 (S 04)2.6 H2 0
HOHNE,E., SOVIET PHYS.-CRYST. 7,559(1963) CA S 04
KOKKOROS,P.A. AND P.J.RENTZEPERIS, Z.KRIST. 119,234(1963) MG S 04
LARSON,A.C., ACTA CRYST. 18,717(1965) LI2 S 04.H2 0
O'CONNOR,B.H. AND D.M.DALE, ACTA CRYST. 21,705(1966) NI S 04.6 H2 0
RENTZEPERIS,P.J., Z.KRIST. 117,431(1962) SN S 04
SAHL,K., BEITR.MINERAL.PETROG. 9,111(1963) BA S 04
SAHL,K., BEITR.MINERAL.PETROG. 9,111(1963) PB S 04
ZALKIN,A. ET AL., ACTA CRYST. 15,1219(1962) CO S 04.6 H2 0

S +6 VI

SB+3 IVPY
BYSTROM,A. AND K.WILHELMI, ARKIV KEMI 3,373(1953) CS SB2 F7
ROGERS,D. AND A.C.SKAPSKI, PROC.CHEM.SOC. 12,400(1964) SB2 04
SKAPSKI,A.C. AND D.ROGERS, CHEM.COMM. (1965)611 SR NB 04

SB+3 V
BYSTROM,A. ET AL., ARKIV KEMI 4,175(1952) K SB F4
BYSTROM,A. ET AL., ARKIV KEMI 6,77(1953) NA SB F4

SB+3 VI

SB+5 VI
AURIVILLIUS,B., ARKIV KEMI 3,153(1951) BI SB 04
AURIVILLIUS,B., ARKIV KEMI 25,505(1966) K3 SB5 014
BODE,H. AND E.VOSS, Z.ANORG.ALLGEM.CHEM. 264,144(1951) K SB F6
BURNS,J.H., ACTA CRYST. 15,1098(1962) LI SB F6
BYSTROM,A. ET AL., ARKIV KEMI,MINERAL.GEOL. 15B,#4(1942) ZN SB2 06
MAGNELI,A., ARKIV KEMI,MINERAL.GEOL. 15B,#3(1942) PB SB2 06
ROGERS,D. AND A.C.SKAPSKI, PROC.CHEM.SOC. 12,400 (1964) B SB2 04
SCHREWELIUS,N., ARKIV KEMI,MINERAL.GEOL. 16B,#7(1943) TL SB F6
SPIEGELBERG,P., ARKIV KEMI,MINERAL.GEOL. 14A,#5(1940) K SB 03
TEUFER,G., ACTA CRYST. 9,539(1956) NA SB F6
ZEMANN,J., NEUES JAHRB.MINERAL.MONATSH. 67,(1959) NA SB (O H)6

SC+3 VI
ABRAHAMS,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 45,2745(1966) SC2 (W 04)3
CRUICKSHANK,D.W.J., ACTA CRYST. 15,491(1962) SC2 SI2 07
GELLER,S. ET AL., Z.KRIST. 124,136(1967) SC2 03
HOPPE,R. AND H.SABROWSKY, Z.ANORG,ALLGEM.CHEM. 339,144(1965) K SC 02
HOPPE,R. ET AL., Z.ANORG.ALLGEM.CHEM. 339,130(1965) LI SC 02
HORYN,R., K.LUKASZEWICZ, BULL.ACAD.POL.SCI.,SER.SCI.CHIM. 14,499(1966) CA SC2 04
JACK,K.H. AND V.GUTMANN, ACTA CRYST. 4,246(1951) SC F3
MILLIGAN,W.O. AND J.L.MCATEE, J.PHYS.CHEM. 60,273(1956) SC 0 0 H
MULLER-BUSCHBAUM,H., H.G.SCHNERING, Z.ANORG.ALLGEM.CHEM. 336,295(1965) CA SC2 04
NOWACKI,W., Z.KRIST. 101,273(1939) SC F3
ROTH,R.S. AND S.J.SCHNEIDER, J.RES.NATL.BUR.STD. 64A,309(1960) R3 VS V (MN2 03)
SCHUBERT,K. AND A.SEITZ, Z.ANORG.ALLGEM.CHEM. 256,226(1948) SC (O H)3
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (MN2 03)

SC+3 VIII
MOONEY,R.C.L., ACTA CRYST. 9,677(1956) SC P 04
MILLIGAN,W.O. AND L.W.VERNON, J.PHYS.CHEM. 56,145(1952) SC V 04
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

SE-2 VI

SE+4 VI

SE+6 IV
FUESS,H. AND G.WILL, Z.ANORG,ALLGEM.CHEM. 358,125(1968) M SE 04
NARAY-SZABO,I. AND G.ARGAY, ACTA CHIM.ACAD.SCI.HUNG. 39,85(1963) NA2 SE 04

SE+6 VI

SI+4 IV
ABRAHAMS,S.C. AND S.GELLER, ACTA CRYST. 11,437(1958) GROSSULARITE
BROWN,B.E. AND S.W.BAILEY, ACTA CRYST. 17,1391(1964) K AL SI3 08
BURNHAM,C.W., Z.KRIST. 118,337(1963) AL2 SI 05
CRUICKSHANK,D.W.J., ACTA CRYST. 17,685(1964) SI-0
GIBBS,G.V. AND J.V.SMITH, AM.MINERALOGIST 50,2023(1965) MG3 AL2 SI3 012
GLASSER,L.S.D. AND F.P.GLASSER, ACTA CRYST. 18,453(1965) SR3 SI 05
LIEBAU,F., ACTA CRYST. 14,395(1961) NA2 SI2 05
LIEBAU,F., ACTA CRYST. 14,399(1961) LI AL SIN 010
MROSE,E. AND D.F.APPLEMAN, Z.KRIST. 117,16(1962) AL BE SI 04 O H
PEACOR,D.R. AND M.J.BUERGER, Z.KRIST. 117,331(1962) CA MN SI2 06
PRANDL,W., Z.KRIST. 123,81(1966) AL2 CA3 (SI 04)3
RENTZEPERIS,P.J., Z.KRIST. 119,117(1963) ZN2 MN (O H)2 SI 04
SMITH,D.K. ET AL., ACTA CRYST. 18,787(1965) CA2 SI 04
SMITH,J.V. AND S.W.BAILEY, ACTA CRYST. 16,801(1963) SI-0
WILLIAMS,P.P. AND H.D.MEGAW, ACTA CRYST. 17,882(1964) ALBITES
ZEMANN,A. AND J.ZEMANN, ACTA CRYST. 14,835(1961) MG3 AL2 SI3 012

SI+4 VI
DEADMORE,D.L. AND W.F.BRADLEY, ACTA CRYST. 15,186(1962) K3 SI F7
HAMILTON,W.C., ACTA CRYST. 15,353(1962) FE SI F6.6 H2 0
HOARD,J.L. AND M.B.WILLIAMS, J.AM.CHEM.SOC. 64,633(1942) (N H4)3 SI F7
STANKO,J.A. AND I.C.PAUL, INORG.CHEM. 6,486(1967) (CO (N H3)5 CL) SI F6
STISHOV,S.M. AND N.V.BELOV, DOKL.AKAD.NAUK SSSR 143,951(1962) SI 02
VAINSHTEIN,B.K. AND M.M.STASOVA, SOVJET PHYS.-CRYST. 1,241(1956) (N H4)2 SI F6
ZALKIN,A. ET AL., ACTA CRYST. 17,1408(1964) NA2 SI F6

SM+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) SM2 03

SM+3 VIII
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) SM2 M2 07
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) SM3 FF2 FE3 012
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

SN+2 VI

SN+2 VIII
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) SN2 M2 07

SN+4 VI
BAUR,W.H., ACTA CRYST. 9,515(1956) SN 02
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 SN2 07
HOPPE,R. AND W.DAHNE, NATURWISS. 49,254(1962) SN F4
LARSEN,F.K. ET AL., ACTA CHEM.SCAND. 21,1281(1967) NA8 SN4 GE10 030 (O H)4
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) M SN 03

SR+2 VI
BARTL,H. AND W.SCHUCKMANN, NEUES JAHRB.MINERAL.MONATSH. 1966,253 SR2 B2 05
GLASSER,L.S.D. AND F.P. GLASSER, ACTA CRYST. 18,453(1965) SR3 SI 05
RIETVELD,H.M., ACTA CRYST. 20,508(1966) SR3 U 06
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) SR O

SR+2 VII
BARTL,H. AND W.SCHUCKMANN, NEUES JAHRB.MINERAL.MONATSH. 1966,253 SR2 B2 05
SCHNERING,H.G. AND R.HOPPE, Z.ANORG.ALLGEM.CHEM. 312,87(1961) SR ZN 02

SR+2 VIII
BARNIGHAUSEN,H. AND J.WEIDLEIN, ACTA CRYST. 22,252(1967) SR (O H)2.H2 0
SMITH,H.G., ACTA CRYST. 6,604(1953) SR (O H)2.8 H2 0
VANNERBERG,N., ARKIV KEMI 14,17(1959) SR 02.8 H2 0
WILHELMI,K.A., ARKIV KEMI 26,149(1967) SR CR2 07
WILHELMI,K.A., ARKIV KEMI 26,157(1967) SR2 CR 04
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) SR F2

SR+2 X
CLARK,J.R., AM.MINERALOGIST 49,1549(1964) SR B6 09 (O H)2.3 H2 0
FERRARI,A. ET AL., ACTA CRYST. 21,681(1966) SR (MN 04)2.3 H2 0
ZACHARIASEN,W.H., ACTA CRYST. 1,263(1948) SR3 (P 04)2

SR+2 XII
DONNAY,J.D.H. ET AL., CRYSTAL DATA DETERMINATIVE TABLES(1963) SR TI 03
GARSKE,D. AND D.R.PEACOR, Z.KRIST. 121,294(1965) SR S 04
ZACHARIASEN,W.H., ACTA CRYST. 1,263(1948) SR3 (P 04)2

TA+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) TA F3
JAHNBERG,L., ACTA CHEM.SCAND. 17,2548(1963) CA TA2 06

TA+4 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED R3 VS V (RUTILE)

TA+5 VI
ABRAHAMS,S.C. AND J.L.BERNSTEIN, J.PHYS.CHEM.SOLIDS 28,1685(1967) LI TA 03
ABRAHAMS,S.C. ET AL., J.PHYS.CHEM.SOLIDS 28,1693(1967) LI TA 03
BODE,H. AND H.DOHREN, ACTA CRYST. 11,80(1958) K TA F6
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) CD2 TA2 07
VOUSDEN,P., ACTA CRYST. 4,373(1951) K TA 03
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K TA 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) NA TA 03

TA+5 VIII
HOARD,J.L. ET AL., J.AM.CHEM.SOC. 76,3820(1954) NA3 TA F8

TB+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) TB2 03

TB+3 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

TB+4 VI
SHANNON,R.D. AND C.T.PREWITT, UNPUBLISHED DATA. R3 VS V (LI2 SN 03)

TB+4 VIII
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) TB 02

TC+4 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

TC+7 VI

TE-2 VI

TE+4 III
HANKE,K., NATURWISS. 54,199(1967) ZN TF 03

TE+4 IV

TE+4 VI

TE+6 VI

TH+4 VI
RUH,R. AND A.D.WADSLEY, ACTA CRYST. 21,974(1966) TH TI2 06

TH+4 VIII
LUNDGREN,G., ARKIV KEMI 2,535(1950) TH (O H)2 S 04
LUNDGREN,G. AND L.G.SILLEN, ARKIV KEMI 1,277(1949) TH (O H)2 CR 04 H2 0
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) TH 02

TH+4 IX
ZACHARIASEN,W.H., ACTA CRYST. 2,390(1949) NA TH2 F9

TI+2 VI

TI+3 VI
ABRAHAMS,S.C., PHYS.REV. 130,2230(1963) TI2 03
BERTAUT,E.F. AND P.BLUM, ACTA CRYST. 9,121(1956) CA TI2 04
NEWNHAM,R.E. AND Y.M.DEHAAN, Z.KRIST. 117,235(1963) TI2 03
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (PEROVSKITE)
SIEGEL,S., ACTA CRYST. 9,684(1956) TI F3

TI+4 V
ANDERSSON,S. AND A.D.WADSLEY, ACTA CHEM.SCAND. 15,663(1961) K2 TI2 05
GUILLEN,M. AND E.F.BERTAUT, COMPT.REND.,SER.A-B 262P,962(1966) LI2 TI 05
MOORE,P.B. AND J.LOUISNATHAN, SCIENCE 156,1361(1967) BA2 (TI 0) SI2 07

TI+4 VI
ANDERSSON,S. AND A.D.WADSLEY, ACTA CRYST. 14,1245(1961) NA2 TI3 07
ANDERSSON,S. AND A.D.WADSLEY, ACTA CRYST. 15,194(1962) NA2 TI6 013
BAUR,W.H., ACTA CRYST. 9,515(1956) TI 02
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 TI2 07
EVANS,H.T.,JR., ACTA CRYST. 4,377(1951) BA TI 03
FISCHER,J. ET AL., ACTA CRYST. 22,338(1967) CU TI F6.4 H2 0
KNOP,O. ET AL., CAN.J.CHEM. 43,2812(1965) ER2 TI2 07
RUH,R. AND A.D.WADSLEY, ACTA CRYST. 21,974(1966) TH TI2 06
SHIRANE,G. ET AL., J.PHYS.SOC.JAPAN 14,1352 (1959) M TI 03
SIEGEL,S., ACTA CRYST. 5,683(1952) K2 TI F6
TEMPLETON,D.H. AND C.H.DAUBEN, J.CHEM.PHYS. 32,1515(1960) BA TI4 09
WEISS,R. ET AL., ACTA CRYST. 20,534(1966) NA3 H TI F8
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) SR TI 03

TL+1 VI
SHANNON,R.D. AND C.T.PREWITT, UNPUBLISHED DATA. R VS A (NA SB F6)

TL+1 VIII
BROSSET,C., Z.ANORG.ALLGEM.CHEM. 239,301(1938) TL AL F4
SHANNON,R.D. AND C.T.PREWITT, UNPUBLISHED DATA. R3 VS V (SCHEELITE)

TL+1 XII
SCHREWELIUS,N., ARKIV KEMI MINERAL GEOL. 16B,#7(1943) TL SB F6
SHANNON,R.D. AND C.T.PREWITT, UNPUBLISHED DATA. R3 VS V (TL SB F6)

TL+3 VI
HOPPE,R. AND H.J.ROHRBORN, Z.ANORG.ALLGEM.CHEM. 329,199(1964) NA TL 02
JOHANSSON,G., ACTA CHEM.SCAND. 13,925(1959) TL O H S 04 (H2 O)2.5
MOONEY,R.C.L., ACTA CRYST. 9,113(1956) TL P 04
PAPANANTELLOS,P., Z.KRIST. 126,143(1968) TL2 03
ROTH,R.S., S.J.SCHNEIDER, J.RES.NATL.BUR.STD. 64A,309(1960) R3 VS V (MN2 03)

TL+3 VIII
HOEKSTRA,H.R. AND S.SIEGEL, INORG.CHEM. 7,141(1968) TL2 PT2 07

TM+3 VI
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) TM2 03

TM+3 VIII
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

U +3 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (LA F3)

U +4 VI

U +4 VII
ZACHARIASEN,W.H., ACTA CRYST. 7,792(1954) K3 U F7

Table 1(*b*) (*cont.*)

U +4 VIII
BRUNTON,G., ACTA CRYST. 21,814(1966) LI U F5
BRUNTON,G., J.INORG.NUCL.CHEM. 29,1631(1967) LI4 U F8
DURIF,A., ACTA CRYST. 9,533(1956) U GE O4
LARSON,A.C. ET AL., ACTA CRYST. 17,555(1964) U F4
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) U O2
ZACHARIASEN,W.H., ACTA CRYST. 2,390(1949) NA2 U F6

U +4 IX
ZACHARIASEN,W.H., ACTA CRYST. 2,390(1949) U2 F9

U +5 VI
ROSENZWEIG,A. AND D.T.CROMER, ACTA CRYST. 23,865(1967) CS U F6
ZACHARIASEN,W.H., ACTA CRYST. 2,390(1949) K2 U F6
ZACHARIASEN,W.H., ACTA CRYST. 2,390(1949) NA2 U F6

U +5 VII
LOOPSTRA,B.O., ACTA CRYST. 17,651(1964) U3 O8
ZACHARIASEN,W.H., ACTA CRYST. 2,296(1949) U F5

U +6 II
ZACHARIASEN,W.H., ACTA CRYST. 7,783(1954) K3 U O2 F5

U +6 IV
ROSS,M. ET AL., AM.MINERALOGIST 49,1603(1964) CU (U O2 P O4)2,8 H2 O

U +6 VI
BARTRAM,S.F., INORG.CHEM. 5,749(1966) LU6 U O12
DEBETS,P.C., ACTA CRYST. 21,589(1966) U O3
RIETVELD,H.M., ACTA CRYST. 20,508(1966) M3 U O6
SIEGEL,S., AND H.R. HOEKSTRA, ACTA CRYST. B24,967(1968) CU U O4
STEARNS,M., ACTA CRYST. 23,264(1967) PB3 U O6
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) U O3
ZACHARIASEN,W.H., ACTA CRYST. 7,788(1954) MG U2 O4

U +6 VII
DEBETS,P.C., ACTA CRYST. 21,589(1966) U O3
LOOPSTRA,B.O., ACTA CRYST. 17,651(1964) U3 O8
SIEGEL,S. ET AL., ACTA CRYST. 20,292(1966) U O3

V +2 VI
MONTGOMERY,H. ET AL., ACTA CRYST. 22,775(1967) V (N H4)2 (S O4)2,6 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) V O

V +3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) V F3
NEWNHAM,R.E. AND Y.M.DEHAAN, Z.KRIST. 117,235(1962) V2 O3
SHANNON,R.D., INORG.CHEM. 6,1474(1967) R3 VS V (PEROVSKITE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CE V O3

V +4 VI
ANDERSSON,G., ACTA CHEM.SCAND. 10,623(1956) V O2
KIERKEGAARD,P. AND J.LONGO, UNPUBLISHED DATA, V O2
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CA V O3

V +5 IV
AU,P.K.L. AND C.CALVO, CAN.J.CHEM. 45,2297(1967) CD2 V2 O7
BAGLIO,J.A. AND G.GASHUROV, ACTA CRYST. B24,292(1968) Y V O4
DONALDSON,D.M. AND W.H.BARNES, AM.MINERALOGIST 40,580(1955) PB MN (V O4) (O H)
EVANS,H.T.,JR., Z.KRIST. 114,257(1960) K V O3
EVANS,H.T.,JR., Z.KRIST. 114,257(1960) N H4 V O3
MILLIGAN,W.O. AND L.W.VERNON, J.PHYS.CHEM. 56,145(1952) M V O4
PATSCHEKE,E. ET AL., CHEM.PHYS.LETTERS 2,47(1968) ER V O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (ZIRCON)

V +5 V
CHRIST,C.L. ET AL., ACTA CRYST. 7,801(1954) K V O3.H2 O
EVANS,H.T.,JR., AND S.BLOCK, INORG.CHEM. 5,1808(1966) K V3 O8
GALT,J. AND A.HARDY, ACTA CRYST. 19,432(1965) LI V2 O5

V +5 VI
CAUGHLAN,C.N. ET AL., INORG.CHEM. 5,2131(1966) V O (O C H3)3
EVANS,H.T.,JR., AND S.BLOCK, INORG.CHEM. 5,1408(1966) K V3 O8
EVANS,H.T.,JR., AND S.BLOCK, INORG.CHEM. 5,1808(1966) CS V3 O8
SWALLOW,A.G., ET AL., ACTA CRYST. 21,397(1966) CA3 V10 O28.17 H2 O

W +4 VI
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)

W +6 IV
ABRAHAMS,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 45,2745(1966) SC2 (W O4)3
BURBANK,R.D., ACTA CRYST. 18,88(1965) CA W O4
TEMPLETON,D.H. AND A.ZALKIN, ACTA CRYST. 16,762(1963) FU2 (W O4)3
ZACHARIASEN,W.H. AND H.A.PLETTINGER, ACTA CRYST. 14,229(1961) LI2 W O4
ZALKIN,A. AND D.H.TEMPLETON, J.CHEM.PHYS. 40,501(1964) CA W O4

W +6 VI
KEELING,R.O.,JR., ACTA CRYST. 10,209(1957) NI W O4
KIERKEGAARD,P., ACTA CHEM.SCAND. 12,1715(1958) W O P2 O7
LOOPSTRA,B.O. AND P.BOLDRINI, ACTA CRYST. 21,158(1966) W O3
ULKU,D., Z.KRIST. 124,192(1967) FE W O4

Y +3 VI
BARTRAM,S.F., INORG.CHEM. 5,749(1966) Y6 U O12.LU6 U O12
BERTAUT,F. AND J.MARESCHAL, COMPT.REND. 257,867(1963) Y AL O3
FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85,267(1962) Y2 O3
HARRIS,L.A. AND H.L.YAKEL, ACTA CRYST. 22,354(1967) Y2 BE O4
MULLER-BUSCHBAUM,H., Z.ANORG.ALLGEM.CHEM. 358,138(1968) SR Y2 O4
PATON,M.G. AND E.N.MASLEN, ACTA CRYST. 19,307(1965) Y2 O3
SHANNON,R.D. AND C.T. PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

Y +3 VIII
BAGLIO,J.A. AND G.GASHUROV, ACTA CRYST. B24,292(1968) Y V O4
BATT,A. AND B.POST, ACTA CRYST. 15,1268(1962) Y3 FE5 O12
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) Y2 M2 O7
CUNNINGHAM,J.A. ET AL., INORG.CHEM. 6,499(1967) Y (C5 H7 O2)3.3 H2 O
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) Y3 M5 O12
GELLER,S. AND M.A.GILLEO, ACTA CRYST. 10,239(1957) Y3 FE5 O12
KRSTANOVIC,I., Z.KRIST. 121,315(1965) Y P O4
MILLIGAN,W.O. AND L.W.VERNON, J.PHYS.CHEM. 56,145(1952) Y V O4
ZALKIN,A. AND D.H.TEMPLETON, J.AM.CHEM.SOC. 75,2453(1953) Y F3

Y +3 IX
FRICKE,R. AND W.DURRWACHTER, Z.ANORG.ALLGEM.CHEM. 259,305(1949) Y (O H)3

YB+3 VI
FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85,267(1962) YB2 O3
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) YB2 O3

YB+3 VIII
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) YB3 M5 O12
MILLIGAN,W.O. AND L.W.VERNON, J.PHYS.CHEM. 56,145(1952) YB V O4
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)

ZN+2 IV
ANSELL,G.B. AND L.KATZ, ACTA CRYST. 21,482(1966) ZN2 M03 O8
CALVO,C., J.PHYS.CHEM.SOLIDS 24,141(1963) ZN3 (P O4)2
COREY,R.B. AND R.W.G.WYCKOFF, Z.KRIST. 86,8(1933) ZN (O H)2
PREWITT,C.T. ET AL., Z.KRIST. 124,115(1967) PB ZN SI O4
RENTZEPERIS,P.J., Z.KRIST. 119,117(1963) ZN2 MN (O H)2 SI O4
SCHNERING,H.G. AND R.HOPPE, Z.ANORG.ALLGEM.CHEM. 312,87(1961) SR ZN O2

SCHNERING,H.G. ET AL., Z.ANORG.ALLGEM.CHEM. 305,241(1960) BA ZN O2
SMITH,P. ET AL., Z.KRIST. 119,375(1964) ZN4 O (B O2)6
SPITSBERGER,U., ACTA CRYST. 13,197(1960) BA ZN O2
STEPHENS,J.S. AND C.CALVO, CAN.J.CHEM. 45,2303(1967) ZN3 (P O4)2

ZN+2 V
ABRAHAMS,S.C., J.CHEM.PHYS. 46,2052(1967) ZN MO O4
COCCO,G. ET AL., Z.KRIST. 123,321(1966) ZN2 (O H) P O4
HANKE,K., NATURWISS. 54,199(1967) ZN TE O3
MONTGOMERY,H. AND E.C.LINGAFELTER, ACTA CRYST. 16,748(1963) ZN (C5 H7 O2)2 H2 O
PLIETH,K. AND G.SANGER, Z.KRIST. 124,91(1967) ZN2 CU AS2 O8
STEPHENS,J.S. AND C.CALVO, CAN.J.CHEM. 45,2303(1967) ZN3 (P O4)2

ZN+2 VI
ABRAHAMS,S.C., J.CHEM.PHYS. 46,2052(1967) ZN MO O4
ANSELL,G.B. AND L.KATZ, ACTA CRYST. 21,482(1966) ZN2 M03 O8
BATES,C.H. ET AL., SCIENCE 137,993(1962) ZN O
BAUR,W.H., ACTA CRYST. 11,488(1958) ZN F2
BYSTROM,A. ET AL., ARKIV KEMI,MINERAL.GEOL. 15B#4(1942) ZN SB2 O6
CALVO,C., CAN.J.CHEM. 43,1147(1965) ZN2 P2 O7
CALVO,C., J.PHYS.CHEM.SOLIDS 24,141(1963) ZN3 (P O4)2
GIGLIO,M., ACTA CRYST. 11,789(1958) NA2 ZN (S O4)2.4 H2 O
SCHNERING,H.G., Z.ANORG.ALLGEM.CHEM. 353,13(1967) BA2 ZN F6
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) AG ZN F3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K ZN F3

ZR+4 VI
BRISSE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) LA2 ZR2 O7
JONA,F. ET AL., PHYS.REV. 105,849(1957) PB ZR O3
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) BA ZR O3
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) SR ZR O3

ZR+4 VII
LUNDGREN,G., ARKIV KEMI 13,59(1958) ZR4 (O H)16 (CR O4)5.2 H2 O
SMITH,D.K. AND H.W.NEWKIRK, ACTA CRYST. 18,983(1965) ZR O2

ZR+4 VIII
BODE,H. AND G.TEUFER, ACTA CRYST. 9,929(1956) K2 ZR F6
BURNS,J.H. ET AL., ACTA CRYST. B24,230(1968) NA7 ZR6 F31
KRSTANOVIC,I.R., ACTA CRYST. 11,896(1958) ZR SI O4
LARSON,A.C. AND D.T. CROMER, ACTA CRYST. 14,128(1961) ZR (I O3)4
SEARS,D.R. AND J.H.BURNS, J.CHEM.PHYS. 41,3478(1964) LI6 BE F4 ZR F8
SINGER,J. AND D.T.CROMER, ACTA CRYST. 12,719(1959) ZR (S O4)2.4 H2 O
TEUFER,G., ACTA CRYST. 15,1187(1962) ZR O2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) ZR O2

* This is not intended to be an exhaustive list of references for each ion. For example, there are many references in the literature to certain ions in the usual coordinations such as $^{VI}Al^{3+}$ and some of these have been omitted to save space. For those ions and coordinations which occur rarely such as $^{IV}Cr^{5+}$ or $^{V}Zn^{2+}$, the list is apt to be more complete.

Table 2. *Anion radii for different coordination numbers*

O^{2-}		F^-	
CN	Radius, Å	CN	Radius, Å
II	1·35 (1·349 ± 5)	II	1·285 (1·285 ± 9)
III	1·36 (1·357 ± 10)	III	1·29 (1·300 ± 12)
IV	1·38 (1·378 ± 4)	IV	1·31
VI	1·40 (1·396 ± 9)	VI	1·33
VIII	1·42		

In the next step appropriate anion radii were subtracted from average distances in cation–anion polyhedra. Approximately 1000 average interatomic distances in oxides and fluorides were taken from more than 700 structure determinations. Values of radii for the trivalent rare-earth ions determined in this way agreed quite well with those of Templeton & Dauben (1954). Since our method was similar to theirs, the Templeton & Dauben values, quoted to three decimal places, were used without revision. Since anion coordination is frequently not discussed in structure papers, the following system (see also Holser, 1959) was used to determine the proper values for a compound $^{P}A_p{}^{Q}B_q{}^{R}X_r$: $pP+qQ=rR$, where P and Q are the CN's of the cations and R is the CN of the anion.

Table 1(*b*) lists, by ion according to CN and spin, (where applicable) all the references from which data were taken to construct Table 1. With most references, the source of data is indicated by a chemical formula, compound type, or radius plot (see below). Structure determinations from 1930 through early 1968 were covered in the literature search. In general, many qualitative judgements were made as to the weight given to a particular interatomic distance. More recent structure determinations not involving film methods, those reporting low R values, and those made on well-characterized crystals were given the most weight. The set of values thus obtained was considered to be a first approximation.

The next step was to plot ionic volume, r^3, *vs.* unit cell volume, V, for more than 60 isotypic series. According to assumption 6 these plots should be linear. Fig. 1 shows the plot for the rutile MO_2 structure (Shannon, 1968). This example is chosen because the rutile structure covers a wide range of cation radii, 0·39–0·78 Å, and unit-cell volumes are accurately known. The radii were adjusted to provide linearity and consistency with crystal structure data. The radii were further adjusted to be consistent with both crystallographic data and unit-cell volume data over those structures containing common ions. A severe limitation, however, was found to be the accuracy of many reported cell dimensions. Numerous examples which first appeared to deviate from linearity were found to fall in line with other data after cell dimensions were redetermined with least-squares refinement using Guinier camera data.

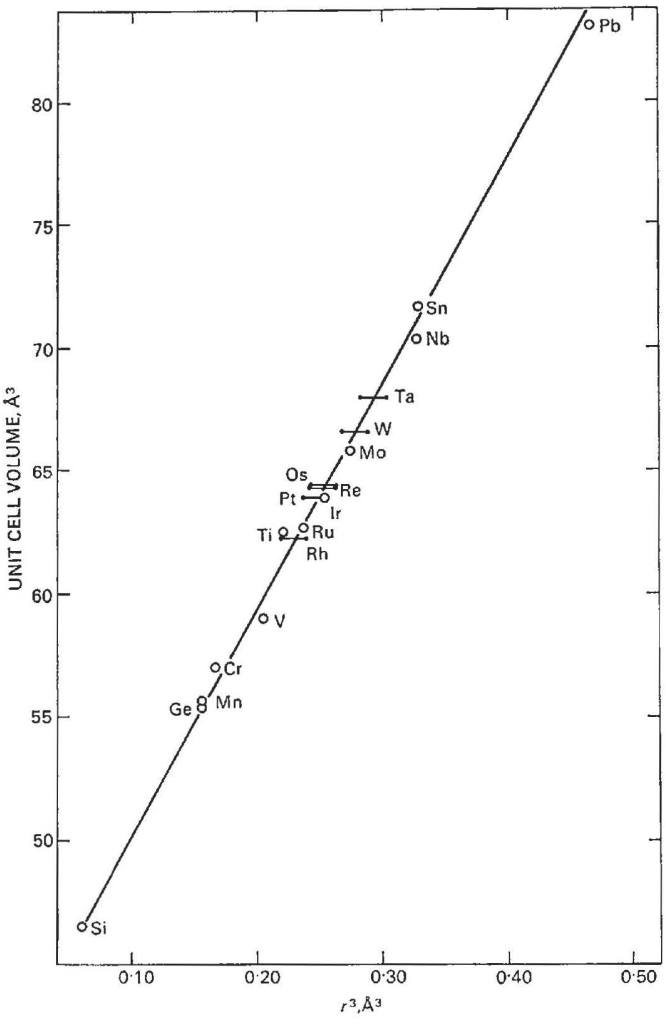


Fig. 1. Cell volume *vs.* r^3 for compounds with the rutile structure. Circles represent data from structure refinements, and the horizontal lines are for compositions where only the cell volumes are known (after Shannon, 1968).

No structure data are available for many ions. In such cases, a reliable estimated value can often be obtained from plots of radii *vs.* cell volume (Fig. 1), radii *vs.* oxidation state, and radii *vs.* electron configuration (Figs. 3 & 4). Examples of radii determined by radii-volume plots are Ni^{3+} and Co^{3+} LS [perovskite (Shannon, 1967)], Rh^{4+}, Pt^{4+}, Re^{4+}, Os^{4+}, W^{4+}, and Ta^{4+} [rutile (Rogers, Shannon, Sleight & Gillson, 1969)] (Fig. 1), and Rh^{3+} [perovskites (Shannon, 1967) and corundum (Prewitt, Shannon, Rogers & Sleight, to be published)]. The accuracy of these values depends on the accuracy of the cell dimensions and on the linearity of the plot.

Plots of radii *vs.* CN (Fig. 2) and radii *vs.* oxidation state are generally found to be regular. This is consistent with the equations given by Zachariasen (1931) and Pauling (1927). Consequently, when the values of radii as determined by structural data appeared to be inconsistent with these regular curves, the sources of data were investigated; if these appeared questionable, the value of the radius was made consistent with the radii plots and marked in Table 1(*a*) with an *E*, *e.g.* Nb^{3+}.

The variation in radii of the first-row transition metal ions with the number of e_g and t_{2g} electrons has been discussed qualitatively by van Santen & van Wieringen (1952), calculated theoretically by Hush & Pryce (1958), and plotted experimentally by Liehr (1960), Knox (1961), Blasse (1965), and Pearson (1968). Similar plots were made for our data, Figs. 3 and 4. By use of these plots, hypothetical values of radii were determined for the low spin ions, Mn^{2+}, Ni^{3+}, Fe^{3+}, Mn^{3+} and Co^{3+}. Low-spin radii for Fe^{2+} and Co^{2+} were taken from radii *vs.* volume plots for the pyrite structure; these radii were consistent with the above electron configuration plots.

As a final step, the anion radii with CN II, III, IV, VI, and VIII were recalculated using interatomic distances from the simple oxide structures and the final refined set of cation radii. These values, given in parentheses in Table 2 with their estimated standard deviations do not differ significantly from the original values. It was not possible to calculate average values for $^{VIII}O^{2-}$ because of the lack of examples. No calculations for $^{IV}F^-$ or $^{VI}F^-$ were made because of a problem with highly symmetric structures discussed in another section.

Results

Table 1(*a*) presents three sets of radii. The first is that of Ahrens (A–IR). The second column contains crystal radii as defined by Fumi & Tosi (CR). This column was derived from column three but it is based on $r(^{VI}F^-) = 1{\cdot}19$ Å and an assumed difference between six-coordinated oxygen and fluorine radii of 0·07 Å as was found for the ionic radii. The third column contains the radii obtained in this work for various coordination numbers and spin states. Except for the radii of S^{2-}, Se^{2-}, and Te^{2-}, which are included in column one and marked with *P*, Pauling's radii are omitted because Ahrens' radii are taken from revised values of Pauling. Each row in Table 1 (*a*) contains the ion, the electron configuration (EC), coordination number (Roman nume-

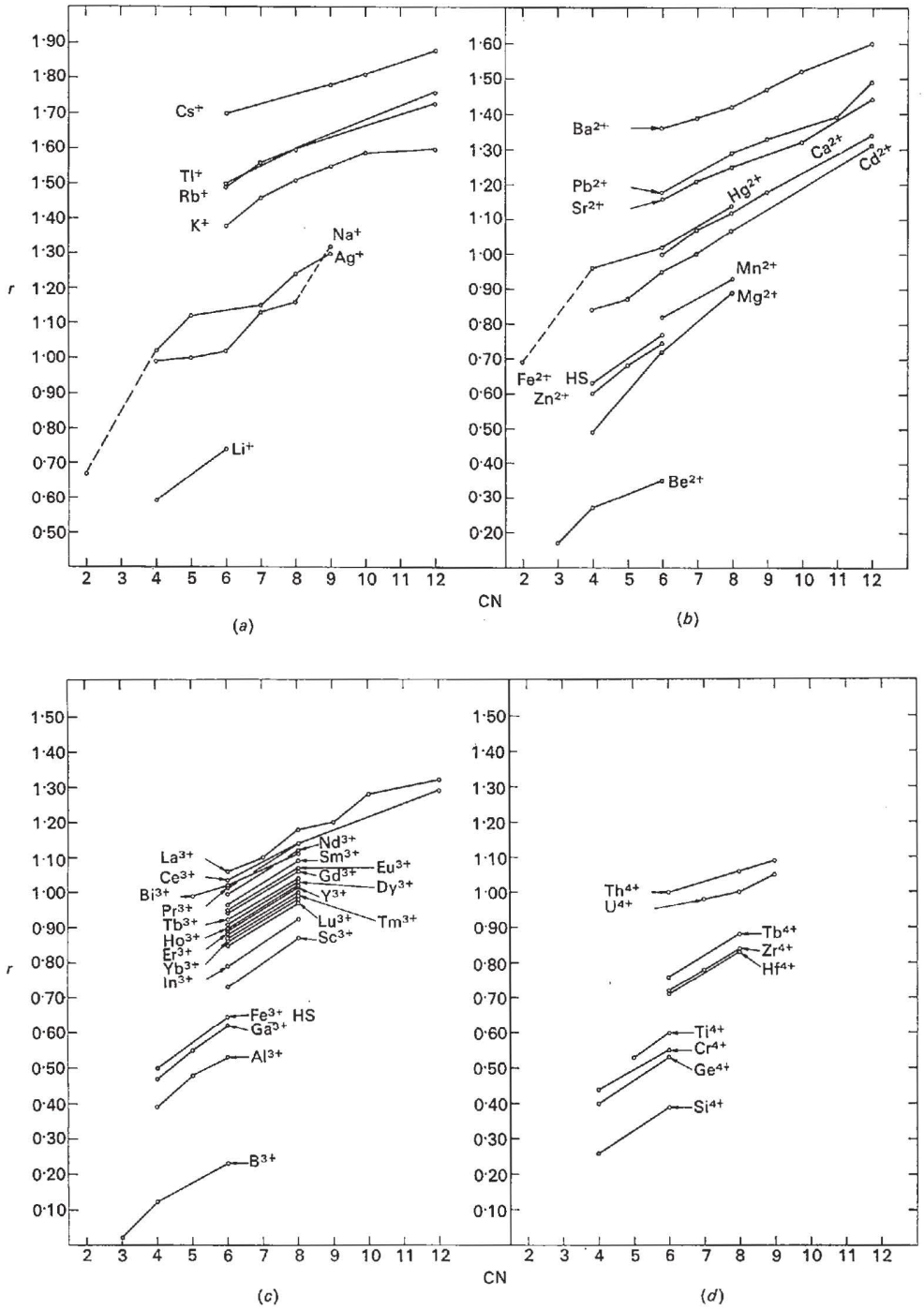


Fig. 2. 'Effective' ionic radius *vs.* CN for some common cations.

ral), spin state (HS or LS), three values of ionic radii, and finally a symbol giving some indication of the reliability (?, *E*, *R*, *, or no symbol). The values indicated by a question mark are considered doubtful because of one or more reasons: uncertainty as to oxidation state, CN, or composition of the compounds studied, or deviation from radii *vs.* CN, or radii *vs.* valence plots. The values estimated from radii *vs.* CN, radii *vs.* oxidation state, or radii *vs.* electron configuration plots are followed by the letter *E*. Values of radii taken from radii *vs.* volume plots are marked by *R*. Finally, those values for which at least 5 structural determinations resulted in radii differing by no more than ±0·01 Å are marked with an asterisk.

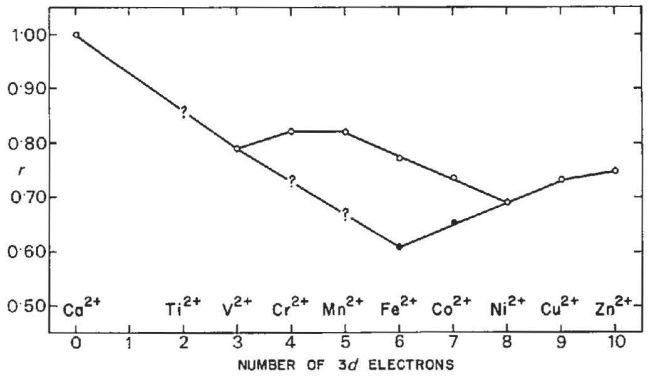


Fig. 3. 'Effective' ionic radius *vs.* number of 3*d* electrons for divalent transition-metal ions.

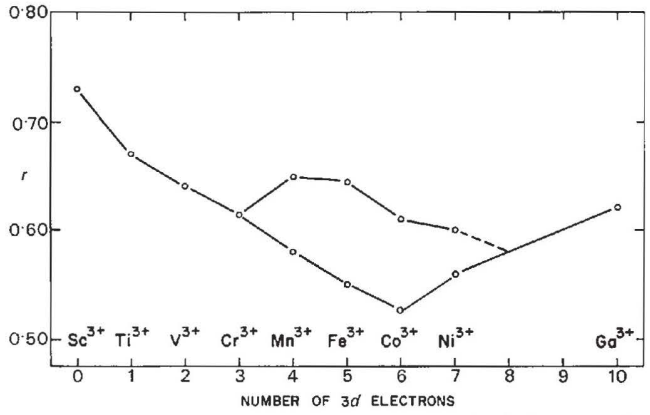


Fig. 4. 'Effective' ionic radius *vs.* number of 3*d* electrons for trivalent transition-metal ions.

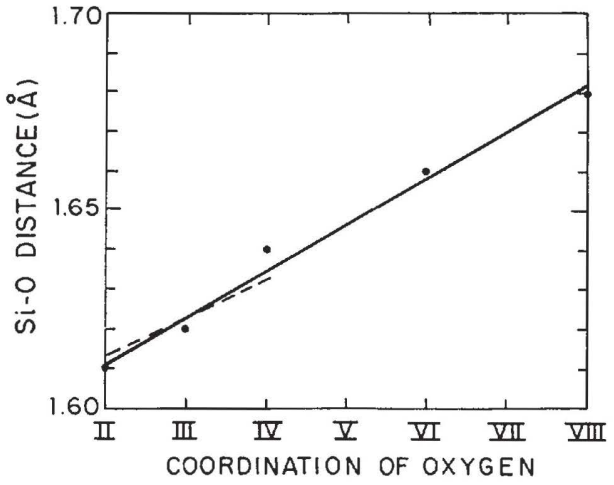


Fig. 5. Si–O distance *vs.* oxygen coordination. The dashed line represents the variation of Si–O distances reported by Smith & Bailey (1963).

Although many different types of coordination exist for a given CN, for simplicity we have chosen to differentiate only the common types of four coordination: square planar (IVSQ), square pyramidal (IVPY), and tetrahedral (IV).

Table 3 compares observed and calculated interatomic distances in more than 100 compounds with the use of radii from Zachariasen, Pauling, Ahrens, and Table 1(*a*). The first three columns in Table 3 contain calculated interatomic distances of Zachariasen, Pauling, and Ahrens corrected for cation coordination using the correction factors listed by Pauling (1960) and Zachariasen (1931). The agreement between observed and calculated distances is seen to be much improved in most cases where CN of the cation and/or anion is different from VI.

When the distances calculated from Table 1(*a*) differ significantly from the observed distances, a reason for the discrepancy can usually be found. One of these reasons is that interatomic distances in highly symmetric structures are generally shorter than expected and another is that it is often difficult to establish exact coordination numbers for some ions. These effects are discussed further in later sections of this paper. Other reasons are that some radii are based on insufficient data and/or that a structure solution and refinement may be, to some degree, in error. In addition there are undoubtedly some unexplained departures from additivity which are reflected in deviations of the order of ±0·01 Å.

Discussion

Change of anion radius with CN

Although the dependence of interatomic distance on CN was noted by Goldschmidt (1927) and the idea of increases of cation radii with CN has been mentioned by several investigators (Pauling, 1927; Zachariasen, 1931; Geller, 1957; Sasvári, 1960), the possibility that anion radii may also depend upon CN appears to have been considered by only a few authors (Slaughter, 1966; Jeffrey & Slaughter, 1963). The effect of CN on anion radii is not great, but it is noticeable when comparing interatomic distances in structures containing a series of *M*–O distances where the CN of O^{2-} varies (Tables 3 and 4). This is probably the principal cause of the variations in Si–O distances noted by Smith & Bailey (1963) in their survey of silicate structures.*

* This effect was recently discovered independently by Gibbs & Brown (1968).

Table 3. *Comparison of observed and calculated interatomic distances in oxides and fluorides*

Compound	Distance	R_{Calc} Zach.	Pauling	Ahrens	S & P	R_{Obs}	Year
$AgFeO_2$	$^{II}Ag\text{-}^{IV}O$	--	2.36	2.40	2.05	2.06	68
Al_2SiO_5	$^{IV}Al\text{-}^{III}O$	1.78	1.78	1.81	1.75	1.77	63
$AlPO_4$	$^{IV}Al\text{-}^{II}O$	1.78	1.78	1.81	1.74	1.74	66
Al_2O_3	$^{VI}Al\text{-}^{IV}O$	1.90	1.90	1.91	1.91	1.91	62
$LiAlO_2$	$^{IV}Al\text{-}^{IV}O$	1.78	1.78	1.81	1.77	1.76	65
$LiAlO_2$	$^{VI}Al\text{-}^{VI}O$	1.90	1.90	1.91	1.93	1.90	66
$BeAl_2O_4$	$^{VI}Al\text{-}^{IV}O$	1.90	1.90	1.91	1.91	1.914	63
AlF_3	$^{VI}Al\text{-}^{II}F$	1.77	1.86	1.84	1.815	1.80	51
$As_2O_5 \cdot 5/3H_2O$	$^{IV}As\text{-}^{II}O$	--	1.78	1.75	1.685	1.69	66
CdB_4O_7	$^{III}B\text{-}^{III}O$	1.35	1.38	1.40	1.38	1.37	66
CaB_2O_4	$^{III}B\text{-}^{II}O$	1.35	1.38	1.40	1.37	1.37	63
$LiBO_2$	$^{IV}B\text{-}^{IV}O$	1.42	1.47	1.50	1.50	1.47	65
$\gamma\text{-}HBO_2$	$^{IV}B\text{-}^{II}O$	1.42	1.47	1.50	1.47	1.47	63
KB_5O_8	$^{IV}B\text{-}^{III}O$	1.42	1.47	1.40	1.48	1.46	65
BaO	$^{VI}Ba\text{-}^{VI}O$	2.76	2.75	2.74	2.76	2.76	63
$BaGeO_3$	$^{VIII}Ba\text{-}^{IV}O$	2.84	2.82	2.80	2.80	2.785	62
BaF_2	$^{VIII}Ba\text{-}^{IV}F$	2.68	2.79	2.74	2.73	2.69	63
$Ba(OH)_2 \cdot 8H_2O$	$^{VIII}Ba\text{-}^{IV}O$	2.84	2.82	2.80	2.80	2.74	64
$BaGe_4O_9$	$^{X}Ba\text{-}^{III}O$	2.90	2.88	2.84	2.88	2.96	66
$BaSO_4$	$^{XII}Ba\text{-}^{IV}O$	2.96	2.94	2.89	2.98	2.95	63
$Ba_3(PO_4)_2$	$^{XII}Ba\text{-}^{V}O$	2.96	2.94	2.89	2.99	3.01	48
Y_2BeO_4	$^{III}Be\text{-}^{IV}O$	1.55	1.47	1.51	1.55	1.55	67
BeO	$^{IV}Be\text{-}^{IV}O$	1.63	1.57	1.61	1.65	1.649	64
Li_2BeF_4	$^{IV}Be\text{-}^{III}F$	1.53	1.53	1.54	1.57	1.554	66
$Bi_4Si_3O_{12}$	$^{VI}Bi\text{-}^{III}O$	--		2.36	2.38	2.385	66
Bi_2GeO_5	$^{VI}Bi\text{-}^{III}O$	--		2.36	2.38	2.35	64
Ca_2SiO_4	$^{VIII}Ca\text{-}^{IV}O$	2.50	2.47	2.48	2.50	2.515	64
$CaWO_4$	$^{VIII}Ca\text{-}^{III}O$	2.50	2.47	2.48	2.48	2.461	65
CaB_2O_4	$^{VIII}Ca\text{-}^{III}O$	2.50	2.47	2.48	2.48	2.505	63
CaF_2	$^{VIII}Ca\text{-}^{IV}F$	2.34	2.43	2.40	2.43	2.37	63
$CaSO_4$	$^{VIII}Ca\text{-}^{III}O$	2.50	2.48	2.48	2.48	2.46	63
$CdSO_4$	$^{IV}Cd\text{-}^{II}O$	--	2.28	2.28	2.19	2.168	63
CdO	$^{VI}Cd\text{-}^{VI}O$	--	2.37	2.37	2.35	2.348	63
$Cd_2V_2O_7$	$^{VI}Cd\text{-}^{III}O$	--	2.37	2.37	2.31	2.31	67
$CePO_4$	$^{VIII}Ce\text{-}^{III}O$	--	2.57	2.53	2.50	2.50	50
CoF_2	$^{VI\ HS}Co\text{-}^{III}F$	--	2.10	2.05	2.035	2.04	58
$CoMoO_4$	$^{VI\ HS}Co\text{-}^{III}O$	--	2.14	2.12	2.095	2.08	65
CoO	$^{VI\ HS}Co\text{-}^{VI}O$	--	2.14	2.12	2.135	2.133	63
Cr_2O_3	$^{VI}Cr\text{-}^{IV}O$	--	2.09	2.03	1.995	1.99	62
Cr_5O_{12}	$^{VI}Cr\text{-}^{II}O$	--	2.09	2.03	1.965	1.97	65
CrF_3	$^{VI}Cr\text{-}^{II}F$	--	2.05	1.96	1.90	1.90	60
$PbCrO_4$	$^{IV}Cr\text{-}^{III}O$	1.65	1.82	1.82	1.66	1.65	65
$LiCr_3O_8$	$^{IV}Cr\text{-}^{III}O$	1.65	1.82	1.82	1.66	1.65	67
$CuFeO_2$	$^{II}Cu\text{-}^{IV}O$	--	2.01	2.10	1.84	1.83	68
$Dy_3Fe_5O_{12}$	$^{VIII}Dy\text{-}^{IV}O$	--		2.38	2.40	2.40	65
Eu_3O_4	$^{VI}Eu\text{-}^{VI}O$	--	2.43	2.38	2.35	2.340	66
FeO	$^{VI}Fe\text{-}^{VI}O$	--	2.16	2.14	2.17	2.155	63
$FeWO_4$	$^{VI}Fe\text{-}^{III}O$	--	2.16	2.14	2.13	2.104	67
Fe_2SiO_4	$^{VI}Fe\text{-}^{IV}O$	--	2.16	2.14	2.15	2.172	65
$FeGe(OH)_6$	$^{VI}Fe\text{-}^{III}O$	--	2.16	2.14	2.12	2.13	61
$Y_3Fe_5O_{12}$	$^{IV}Fe\text{-}^{IV}O$	--	1.94	1.94	1.88	1.88	62
$Na_3Fe_5O_9$	$^{IV}Fe\text{-}^{IV}O$	--	1.94	1.94	1.88	1.867	67
Fe_2O_3	$^{VI}Fe\text{-}^{IV}O$	--	2.04	2.04	2.025	2.030	66
FeF_3	$^{VI}Fe\text{-}^{II}F$	--	2.00	1.97	1.93	1.92	57
$GaNbO_4$	$^{VI}Ga\text{-}^{III}O$	--	2.02	2.02	1.98	1.996	65
$\alpha\text{-}Ga_2O_3$	$^{VI}Ga\text{-}^{IV}O$	--	2.02	2.02	2.00	2.00	65
$Y_3Ga_5O_{12}$	$^{VI}Ga\text{-}^{IV}O$	--	2.02	2.02	1.980	1.995	65
GaF_3	$^{VI}Ga\text{-}^{II}F$	--	1.98	1.95	1.905	1.89	59
$BaGe_4O_9$	$^{VI}Ge\text{-}^{III}O$	--	1.93	1.93	1.900	1.877	66
$Na_4Ge_9O_{20}$	$^{VI}Ge\text{-}^{III}O$	--	1.93	1.93	1.910	1.907	63
In_2O_3	$^{VI}In\text{-}^{IV}O$	--	2.21	2.21	2.17	2.18	66
$CaIn_2O_4$	$^{VI}In\text{-}^{V}O$	--	2.21	2.21	2.18	2.157	67
$InPO_4 \cdot 2H_2O$	$^{VI}In\text{-}^{II}O$	--	2.21	2.21	2.14	2.16	61
Ca_2IrO_4	$^{VI}Ir\text{-}^{IV}O$	--	2.04	2.08	2.01	2.01	66
KF	$^{VI}K\text{-}^{VI}F$	2.66	2.69	2.66	2.71	2.673	63
$KMnO_4$	$^{VIII}K\text{-}^{III}O$	2.90	2.83	2.82	2.82	2.86	67
Li_2WO_4	$^{IV}Li\text{-}^{III}O$	1.99	1.84	1.91	1.95	1.96	61
$LiAlO_2$	$^{IV}Li\text{-}^{IV}O$	1.99	1.84	1.91	1.97	2.00	65
$LiGaO_2$	$^{IV}Li\text{-}^{IV}O$	1.99	1.84	1.91	1.97	1.98	65
$Li_2Si_2O_5$	$^{IV}Li\text{-}^{III}O$	1.99	1.84	1.91	1.95	1.94	61
$LiAlO_2$	$^{VI}Li\text{-}^{VI}O$	2.12	2.00	2.08	2.14	2.12	66
$LiGaO_2$	$^{VI}Li\text{-}^{VI}O$	2.12	2.00	2.08	2.14	2.14	65
LiF	$^{VI}Li\text{-}^{VI}F$	2.01	1.96	2.01	2.07	2.008	63
Li_4UF_8	$^{VI}Li\text{-}^{II}F$	2.01	1.96	2.01	2.025	2.08	67
$LiUF_5$	$^{VI}Li\text{-}^{III}F$	2.01	1.96	2.01	2.04	2.055	66
MgO	$^{VI}Mg\text{-}^{VI}O$	2.10	2.05	2.06	2.12	2.105	63
$MgSO_4 \cdot 4H_2O$	$^{VI}Mg\text{-}^{IV}O$	2.10	2.05	2.06	2.10	2.076	62
MgF_2	$^{VI}Mg\text{-}^{III}F$	1.98	2.01	1.99	2.02	1.992	56
$MgHPO_4 \cdot 3H_2O$	$^{VI}Mg\text{-}^{III}O$	2.10	2.05	2.06	2.08	2.084	67
$MnMoO_4$	$^{VI\ HS}Mn\text{-}^{III}O$	--	2.20	2.20	2.18	2.164	65
Mg_6MnO_8	$^{VI}Mn\text{-}^{V}O$	--	1.94	2.20	1.93	1.928	54
$DyMn_2O_5$	$^{VI}Mn\text{-}^{IV}O$	--	1.94	2.20	1.92	1.92	67
MoO_2	$^{VI}Mo\text{-}^{III}O$	--	2.06	2.10	2.01	2.011	67
$Zn_2Mo_3O_8$	$^{VI}Mo\text{-}^{III}O$	--	2.06	2.10	2.02	2.02	66
$MnMoO_4$	$^{IV}Mo\text{-}^{III}O$	1.82	1.94	1.92	1.78	1.763	65
$PbMoO_4$	$^{IV}Mo\text{-}^{III}O$	1.82	1.94	1.92	1.78	1.772	65
NaF	$^{VI}Na\text{-}^{VI}F$	2.31	2.31	2.30	2.35	2.31	63
Na_2SiF_6	$^{VI}Na\text{-}^{III}F$	2.31	2.31	2.30	2.32	2.32	64
$NaHCO_3$	$^{VI}Na\text{-}^{IV}O$	2.44	2.35	2.37	2.40	2.44	65
Nb_2O_5	$^{VI}Nb\text{-}^{II}O$	2.00	2.10	2.09	1.99	1.99	64
$GaNbO_4$	$^{VI}Nb\text{-}^{III}O$	2.00	2.10	2.09	2.00	2.031	65
$LiNbO_3$	$^{VI}Nb\text{-}^{IV}O$	2.00	2.10	2.09	2.02	2.00	66
NiF_2	$^{VI}Ni\text{-}^{III}F$	--	2.08	2.02	2.00	2.00	58
$NiSO_4 \cdot 6H_2O$	$^{VI}Ni\text{-}^{III}O$	--	2.12	2.09	2.06	2.06	66
Ba_2NiF_6	$^{VI}Ni\text{-}^{V}F$	--	2.08	2.02	2.02	2.01	67
PbO_2	$^{VI}Pb\text{-}^{III}O$	--	2.24	2.24	2.135	2.16	47
RuO_2	$^{VI}Ru\text{-}^{III}O$	--	2.03	2.07	1.98	1.971	66
$LiSbF_6$	$^{VI}Sb\text{-}^{II}F$	--	1.98	1.95	1.895	1.88	62
Sb_2O_4	$^{VI}Sb\text{-}^{II}O$	--	2.02	2.02	1.96	1.97	64
$K_3Sb_5O_{14}$	$^{VI}Sb\text{-}^{IV}O$	--	2.02	2.02	1.99	1.984	66
Sc_2O_3	$^{VI}Sc\text{-}^{IV}O$	2.16	2.21	2.21	2.11	2.11	67
$Sc_2(WO_4)_3$	$^{VI}Sc\text{-}^{II}O$	2.16	2.21	2.21	2.08	2.063	66
$CaSc_2O_4$	$^{VI}Sc\text{-}^{V}O$	2.16	2.21	2.21	2.12	2.12	65
ScF_3	$^{VI}Sc\text{-}^{II}F$	2.02	2.17	2.14	2.015	2.01	51
$ScPO_4$	$^{VIII}Sc\text{-}^{III}O$	2.24	2.28	2.29	2.23	2.23	56
SiO_2	$^{IV}Si\text{-}^{II}O$	1.63	1.71	1.72	1.61	1.607	66
$KAlSi_3O_8$	$^{IV}Si\text{-}^{III}O$	1.63	1.71	1.72	1.62	1.61	64
Ca_2SiO_4	$^{IV}Si\text{-}^{IV}O$	1.63	1.71	1.72	1.64	1.644	65
SiO_2	$^{VI}Si\text{-}^{III}O$	1.73	1.81	1.82	1.75	1.768	66
K_3SiF_7	$^{VI}Si\text{-}^{IV}F$	1.60	1.77	1.75	1.71	1.70	62
Na_2SiF_6	$^{VI}Si\text{-}^{III}F$	1.60	1.77	1.75	1.70	1.695	64
$(NH_4)_2SiF_6$	$^{VI}Si\text{-}^{II}F$	1.60	1.77	1.75	1.685	1.674	56
SnO_2	$^{VI}Sn\text{-}^{III}O$	--	2.11	2.11	2.05	2.053	56
SnF_4	$^{VI}Sn\text{-}^{II}F$	--	2.07	2.04	1.975	2.14	62
SrF_2	$^{VIII}Sr\text{-}^{IV}F$	2.54	2.56	2.52	2.56	2.51	63
Ti_2O_3	$^{VI}Ti\text{-}^{IV}O$	--	2.16	2.16	2.05	2.040	62
TiF_3	$^{VI}Ti\text{-}^{II}F$	--	2.12	2.09	1.955	1.97	56
TiO_2	$^{VI}Ti\text{-}^{III}O$	1.96	2.08	2.08	1.965	1.959	56
$Er_2Ti_2O_7$	$^{VI}Ti\text{-}^{IV}O$	1.96	2.08	2.08	1.985	1.955	65
$Na_2Ti_3O_7$	$^{VI}Ti\text{-}^{V}O$	1.96	2.08	2.08	1.995	1.99	61
V_2O_3	$^{VI}V\text{-}^{IV}O$	--	2.14	2.14	2.02	2.01	62
VO_2	$^{VI}V\text{-}^{III}O$	--	2.00	2.03	1.95	1.937	56
$Cd_2V_2O_7$	$^{IV}V\text{-}^{III}O$	1.77	1.89	1.89	1.715	1.717	67
$FeWO_4$	$^{VI}W\text{-}^{III}O$	--		2.02	1.94	1.94	67
WO_3	$^{VI}W\text{-}^{II}O$	--		2.02	1.93	1.927	66
Y_2O_3	$^{VI}Y\text{-}^{IV}O$	2.32	2.33	2.32	2.272	2.27	62
ZnF_2	$^{VI}Zn\text{-}^{III}F$	--	2.10	2.07	2.045	2.03	58
ZrO_2	$^{VIII}Zr\text{-}^{IV}O$	2.21	2.26	2.26	2.22	2.26	62

Fig. 5 shows how the average Si-O distance would vary with average oxygen coordination in silicates although most silicates fall in the range ^{II}O–^{IV}O as indicated by the dashed line which is taken from the Smith & Bailey work.

The change in anion radii with CN is much smaller in magnitude [$r(^{VI}O^{2-}) - r(^{II}O^{2-}) = 0{\cdot}05$ Å] than the change in radii with cation CN [$r(^{VIII}Cd^{2+}) - r(^{IV}Cd^{2+}) = 0{\cdot}26$ Å; $r(^{VIII}Mg^{2+}) - r(^{IV}Mg^{2+}) = 0{\cdot}41$ Å]. One explanation for this effect involves electronic polarizabilities of cations and anions. Intuitively, one might expect the change in radius of an ion with CN to be roughly proportional to its electronic polarizability. A comparison of cation and anion polarizabilities from various sources made by Tessman, Kahn & Shockley (1953) shows generally that polarizabilities of

Table 4. *Comparison of observed and calculated interatomic distances in oxides and fluorides with varying coordination*

Distance	CN of O^{2-}	Compound	$R_{obs.}$	$R_{calc.}$
^{IV}Al-O	II	$LiAlSi_4O_{10}$	1.720	1.74
		$AlPO_4$	1.739	"
	III	$KAlSi_3O_8$ (microcline)	1.741	1.75
		$NaAlSi_3O_8$ (low albite)	1.737	"
		Al_2SiO_5 (sillimanite)	1.770	"
	IV	$LiAlO_2$	1.761	1.77
^{VI}Al-O	II	$NaAl(SO_4)_2 \cdot 12H_2O$	1.881	1.88
		$CsAl(SO_4)_2 \cdot 12H_2O$	1.882	"
	III	Al_2SiO_5 (kyanite)	1.906	1.89
	IV	$Mg_3Al_2Si_3O_{12}$	1.886	1.91
		Al_2O_3	1.91	1.91
	VI	$LiAlO_2$	1.90	1.93
^{VI}Cd-O	II	$3CdSO_4 \cdot 8H_2O$	2.30	2.30
	III	$Cd_2V_2O_7$	2.31	2.31
	VI	CdO	2.348	2.35
$^{VI}Co^{2+}$-O	II	$CoSO_4$	2.07	2.085
	III	$CoMoO_4$	2.082	2.095
		$Co(NH_2)_2(SO_4)_2 \cdot 6H_2O$	2.094	"
	VI	CoO	2.133	2.135
$^{VI}Cr^{3+}$-O	II	Cr_5O_{12}	1.972	1.965
	III	KCr_3O_{12}	1.97	1.975
		$HCrO_2$	1.979	"
	IV	Cr_2O_3	1.99	1.995
$^{VI}Fe^{2+}$-O	III	$FeWO_4$	2.104	2.13
		$FeGe(OH)_6$	2.14	"
	IV	$FeSiF_6 \cdot 6H_2O$	2.140	2.15
		Fe_2SiO_4	2.172	"
	VI	FeO	2.155	2.170
$^{VI}Ga^{3+}$-O	III	$GaNbO_4$	1.997	1.98
		β-Ga_2O_3	2.00	"
	IV	α-Ga_2O_3	2.00	2.00
	VI	$LiGaO_2$	2.00	2.02
^{IV}Ge-O	II	GeO_2	1.739	1.75
	III	$BaGe_4O_9$	1.740	1.76
		$Na_2O \cdot GeO_2 \cdot 6H_2O$	1.769	"
		$Na_8Sn_4Ge_{10}O_{30}(OH)_4$	1.752	"
	IV	$BaGeO_3$	1.785	1.78
$^{VI}Ni^{2+}$-O	III	$NiSO_4 \cdot 6H_2O$	2.063	2.06
		$NiWO_4$	2.08	"
	VI	NiO	2.084	2.08
$^{IV}P^{5+}$-O	II	$MoPO_4$	1.528	1.52
		$AlPO_4$	1.515	"
		P_2O_5	1.54	"
	III	$Na_2H_2P_4O_{12}$	1.542	1.53
		$NaPO_3NH_3$	1.528	"
^{VI}Sc-O	II	$Sc_2(WO_4)_3$	2.063	2.08
	III	γ-ScOOH	2.10	2.09
		$Sc(OH)_3$	2.08	"
	IV	Sc_2O_3	2.11	2.11
	V	$CaSc_2O_4$	2.122	2.12
	VI	$KScO_2$	2.12	2.13
		$LiScO_2$	2.11	"
		$RbScO_2$	2.12	"
^{IV}Si-O	II	SiO_2 (quartz)	1.607	1.610
		SiO_2 (low cristobalite)	1.605	"
		SiO_2 (coesite)	1.613	"
		Al_2SiO_5 (sillimanite)	1.615	"
		$LiAlSi_4O_{10}$	1.609	"
	III	$Sc_2Si_2O_7$	1.622	1.620
		$ZrSiO_4$	1.612	"
		Al_2SiO_5 (kyanite)	1.628	"
		Al_2SiO_5 (andalusite)	1.629	"
		$Zn_2Mn(OH)_2SiO_4$	1.626	"
		$AlBeSiO_4OH$	1.625	"
		$NaAlSi_3O_8$	1.618	"
		$KAlSi_3O_8$	1.612	"
		$Li_2Si_2O_5$	1.631	"
		$Ca_2NaHSi_3O_9$	1.630	"
		$CaMnSi_2O_6$	1.623	"
	IV	γ-Ca_2SiO_4	1.644	1.640
		Mg_2SiO_4	1.625	"
		$MgFeSiO_4$	1.638	"
		Fe_2SiO_4	1.634	"
		$Ca_3Al_2(SiO_4)_3$	1.649	"
		$Mg_3Al_2Si_3O_{12}$	1.635	"
^{VI}Si-F	II	$(NH_4)_2SiF_6$	1.674	1.685
		$[Co(NH_3)_5Cl]SiF_6$	1.664	"
	III	Na_2SiF_6	1.695	1.700
	IV	K_3SiF_7	1.70	1.710
		$(NH_4)_3SiF_7$	1.71	"
$^{VI}Ti^{4+}$-O	II	$Na_2Ti_6O_{13}$	1.957	1.955
		$Rb_2Ti_6O_{13}$	1.983	"
	III	$ThTi_2O_6$	1.970	1.965
		TiO_2	1.959	"
	IV	$NiTiO_3$	1.99	1.985
		$MnTiO_3$	1.99	"
		$BaTi_4O_9$	1.98	"
	V	$Na_2Ti_3O_7$	1.992	1.995

anions are larger than those of most cations, in distinct contrast to the relative change in anion and cation radii with CN. However, Ruffa (1964) has shown in TiO_2 and other compounds with high Madelung potentials that the polarizability of the cation may be considerably greater than that of the anion. Thus, the possibility still exists that there may be some correlation between change in radius with CN and polarizability.

An alternative explanation for this effect depends on the anion–anion repulsive forces described by Pauling (1928). In most of the oxides for which reliable radii have been determined, the cation/anion radius ratio, ϱ, is considerably less than 1. When this condition holds, anion–anion forces can be large. As ϱ becomes small and as the anion CN diminishes from VI to II, the nearest neighbor anion interactions become more important. The increase in anion–anion forces prevents the anion from deforming as much as might be expected from polarizability considerations. The *cations* in such structures, however, cannot approach each other closely and cation–cation repulsion is probably less than anion–anion forces. Consequently, the cation is easily able to expand into the void between the anions – thus shortening considerably the cation–anion distance.

Absolute values of radii

The question of absolute values for anion and cation radii is still not resolved. Although it has been possible to devise sets of radii which are almost additive, the values of anionic radii have been determined by approximate methods. This question of the relative sizes of anion and cation radii is very important because it determines the physical picture we have of ionic solids. Traditionally this has been a picture of anion-close-packed solids.

Values of anion radii have been chosen from: (1) molar refractivities of salts in solution (Wasastjerna, 1923); (2) anion–anion distances in close-packed solids (Bragg & West, 1927); (3) Born repulsive coefficients determined from isothermal compressibilities and thermal expansion coefficients (Fumi & Tosi, 1964) and (4) electron density distribution in alkali halides (Witte & Wölfel, 1955; Schoknecht, 1957; and Meisalo & Inkinen, 1967). The traditional sets of radii were based on (1) and (2). The first values of ionic radii were determined by Wasastjerna who used the ratio of the cube root of the molar refractivities of the free ions to determine $r_c:r_a$ in the alkali halides. He arrived at $r(^{VI}F^-)=1{\cdot}33$ Å and $r(^{VI}O^{2-})=1{\cdot}32$ Å. Bragg & West noted that observed O–O distances in silicates were roughly 2·7 Å and concluded that $r(O^{2-})=1{\cdot}35$ Å. Used with available sets of interatomic distances in common oxides, these values led to small $r_c:r_a$ and resulted in the concept of anion close-packed oxides. Many solid state phenomena such as diffusion, mechanical deformation, kinetics of transformations, and solid state reactions have been interpreted on this basis.

More recent evidence, however, indicates that the ratio $r_c:r_a$ may be considerably larger than indicated by the traditional sets of radii. Comparative calculations of wave functions of free ions and ions in a crystal by Petrashen, Abarenkov & Kristofel (1960) showed a tightening of electron clouds in anions and a relaxation of cation electrons in solids. Analysis of electron density distributions in NaCl (Witte & Wölfel, 1955), LiF (Krug, Witte & Wölfel, 1955) and KBr (Meisalo & Inkinen, 1967), indicated anion radii and cation radii smaller and larger respectively than traditional ionic radii. Fumi & Tosi on the basis of calculations of Born repulsive parameters from compressibility and thermal expansion data present convincing evidence that $r_c:r_a$ is larger than in the traditional sets of radii. They found $r(^{VI}F^-)=1{\cdot}15$–$1{\cdot}20$ Å with an estimated error of 0·05 Å. Assuming a constant difference of $r(^{VI}O^{2-})-r(^{VI}F^-)=0{\cdot}07$ Å, then $r(^{VI}O^{2-})=1{\cdot}22$–$1{\cdot}27$ Å. These values are more in agreement with the shortest nonbonding O–O distances in many oxides. As shown in Table 5 these range from 2·15 Å in the $NaNO_3$ structure to greater than 3 Å in the antifluorite structures. Perhaps the most surprising distance in this group is that of the 2·16 Å shared edges of the SiO_6 octahedra in the rutile form of SiO_2 (stishovite). Although extremely high pressure must be used to synthesize stishovite, it is difficult to reconcile this short O–O distance with an $r(^{III}O^{2-})=1{\cdot}36$ Å, especially since Fig. 1 shows there is nothing unusual about the cell volume of stishovite. Furthermore, with smaller anions one is not forced to assume negative radii for $^{III}C^{4+}$ in the carbonate ion and $^{III}N^{5+}$ in the nitrate ion. Although there is intrinsically no objection to negative radii so long as one does not assume a hard sphere model, it is esthetically more pleasing to have positive radii. However, even with Fumi & Tosi's crystal radii it is not possible to achieve a complete set of positive radii. The O–H and F–H distances in hydrogen-bonded compounds result in negative radii of $-0{\cdot}04$ and $-0{\cdot}24$ Å for $^{II}H^+$ and $^{I}H^+$. Although the value for $r(^{II}H^+)$ falls within the estimated error of the crystal radii and would still allow a completely positive set of radii, this is not possible for $^{I}H^+$. One is forced to the interpretation that an $^{I}H^+$–O bond results in a highly deformed oxygen ion in which the proton penetrates the electron cloud of the oxygen ion. On the basis of the above considerations, the

Table 5. *Shortest oxygen–oxygen distances in some simple oxides*

Compound	Structure type	O–O
$NaNO_3$	calcite	2·15 Å
SiO_2	rutile	2·16
$CaCO_3$	calcite	2·22
Al_2SiO_5	andalusite	2·25
B_2O_3(II)	B_2O_3(II)	2·36
S_3O_9	S_3O_9	2·37
B_2O_3(I)	B_2O_3(I)	2·38
Al_2O_3	corundum	2·52
SiO_2	quartz	2·60
BeO	wurtzite	2·70
MgO	rocksalt	2·98
Li_2O	antifluorite	3·27

Fumi & Tosi crystal radii (CR) are probably more satisfactory than the traditional sets of radii.

Pauling (1928) noted a correlation between radius ratios and the relative stability of certain structures. Values of ϱ for structures with tetrahedral cation coordination were generally of the order of 0·2–0·4 whereas values of ϱ for octahedral cation coordination were of the order of 0·4–0·7. There were exceptions, but in general the radius ratio was found to provide some indication of the type of prevalent coordination of anions about the cation in ionic crystals. Phillips & Williams (1965) noted that the critical radius ratios were not satisfactory in predicting CN changes but their analysis involved highly covalent rather than ionic crystals.

It is clear that any new set of radii should provide a correlation between radius ratios and CN at least as satisfactory as Pauling's table of ionic radii. Table 6 gives values of ϱ calculated by means of an average radius of 1·38 Å for oxygen for numerous cations with CN III, IV, VI, and VIII. As long as ϱ falls within $\pm 0{\cdot}02$ of the limits defined by Pauling (1960) the radius ratio is in boldface. It will be noted that values of ϱ calculated from ionic radii (IR) do not fall within the expected limits for most of the small ions, *e.g.* $^{VI}Al^{3+}$, $^{VI}As^{5+}$, $^{III}B^{3+}$, $^{IV}B^{3+}$, $^{IV}S^{6+}$, $^{IV}Si^{4+}$, and $^{VI}Si^{4+}$, whereas values of ϱ calculated from crystal radii (CR) give poor agreement for $^{IV}Ga^{3+}$, $^{IV}Li^{+}$, $^{VI}Mn^{2+}$, $^{IV}Zn^{2+}$, and $^{IV}Mo^{6+}$. Since ions with strong covalent mixing (Ga^{3+} and Zn^{2+}) prefer four coordination *via* sp^3 hybridization, even though $\varrho > 0{\cdot}414$, it is felt that crystal radii predicts CN on the basis of radius ratio as well as effective ionic radii.

Perhaps the most important conclusion to be drawn from the above arguments is that specific values from this or any other set of radii should not be used too rigidly to derive a physical picture of ionic solids. Currently available information on electron density distributions in solids is not sufficient to establish absolute values of radii. Furthermore, if one assumes that the radius of an ion, say oxygen, is the distance from the oxygen nucleus to the minimum in electron density between the oxygen ion and a cation, this radius may vary depending on the type of cation, *i.e.* on the covalency of the bond. If, however, the crystal radii in Table 1(*a*) are more accurate than the ionic radii, certain concepts of the structures of ionic solids are no longer valid. For example, oxides should not be thought of as close-packed arrangements of anion spheres whose interstices are partly filled with cations. Instead, the cation–anion bonds should be considered as the important factors determining crystal structure and close-packed anion arrangements as merely the result of the structure attaining a lowest-energy configuration.

Interatomic distances in highly symmetric oxides and fluorides

Agreement between observed and calculated distances from Table 1(*a*) over a wide variety of compounds with varying cation and anion coordination was shown to be quite good. However, the compounds with rock-salt, fluorite, and perovskite structures show rather poor agreement (Table 7). A possible source of error could be the cation radii. However, the value of $r(^{VIII}Ca^{2+})$ taken from more than 15 Ca–O distances which agree to within 0·02 Å results in $R_{calc} - R_{obs} = 0{\cdot}06$ Å for CaF_2. Therefore, it is felt that the lack of agreement of interatomic distances between symmetric and unsymmetric structures is significant. The effect appears to be greater for the fluorides than for oxides and greater for smaller cations than for larger cations. The smaller observed interatomic distances are qualitatively explained by minimization of anion–anion repulsive forces. The regular polyhedra result in the maximum distances between all cations and anions and,

Table 6. *Radius ratios for oxides*

Ion	CN	IR	CR	Ion	CN	IR	CR
Al^{3+}	IV	**0·28**	**0·42**	Mg^{2+}	VI	**0·52**	**0·69**
	VI	0·38	**0·54**	Mn^{2+}	VI	**0·59**	0·79
As^{5+}	IV	**0·24**	**0·38**	Mo^{6+}	IV	**0·30**	0·45
	VI	0·36	**0·52**		VI	**0·43**	**0·60**
B^{3+}	III	0·02	**0·12**	Ni^{2+}	VI	**0·51**	**0·66**
	IV	0·09	**0·21**	P^{5+}	IV	0·12	**0·25**
Be^{2+}	III	**0·12**	**0·25**	S^{6+}	IV	0·09	**0·21**
	IV	**0·20**	**0·33**	Sc^{3+}	VI	**0·53**	**0·70**
Ca^{2+}	VIII	**0·81**	**1·01**	Si^{4+}	IV	0·19	**0·32**
Ce^{4+}	VIII	0·70	**0·90**		VI	0·30	**0·43**
Co^{2+}	VI	**0·53**	**0·71**	Sn^{4+}	VI	**0·50**	**0·67**
Cr^{3+}	VI	**0·44**	**0·61**	Ti^{4+}	VI	**0·44**	**0·60**
Fe^{2+}	VI	**0·56**	**0·73**	W^{6+}	IV	**0·30**	**0·44**
Fe^{3+}	IV	**0·36**	0·52		VI	**0·42**	**0·58**
	VI	**0·47**	**0·63**	Y^{3+}	VI	**0·65**	**0·83**
Ga^{3+}	IV	**0·34**	0·49		VIII	**0·74**	**0·93**
	VI	**0·45**	**0·61**	Zn^{2+}	IV	**0·43**	0·60
Ge^{4+}	IV	**0·29**	**0·44**		VI	**0·54**	**0·71**
	VI	**0·39**	**0·55**	Zr^{4+}	VI	**0·52**	**0·69**
In^{3+}	VI	**0·57**	**0·75**				
Li^{+}	IV	**0·43**	0·59				
	VI	**0·54**	**0·71**				

therefore, the least repulsion interactions. The greater polarizabilities of the oxide ion and larger cations result in deformation of these ions into voids and consequent reductions in repulsive effects.

Table 7. *Calculated and observed interatomic distances in highly symmetric oxides and fluorides*

	R_{Calc}^{M-O}	R_{Obs}^{M-O}	ΔR
Rocksalt			
MO			
VI–VI			
NiO	2·10	2·084	0·016
MgO	2·12	2·105	0·015
CoO	2·135	2·133	0·002
FeO	2·17	2·155	0·015
MnO	2·22	2·222	−0·002
CdO	2·35	2·348	+0·002
CaO	2·40	2·405	−0·005
SrO	2·56	2·58	−0·02
BaO	2·76	2·762	−0·002
MF			
VI–VI			
LiF	2·07	2·008	0·062
NaF	2·35	2·31	0·04
AgF	2·48	2·46	0·02
KF	2·71	2·673	0·037
CsF	3·03	3·00	0·03
Fluorite			
MO_2			
VIII–IV			
CeO_2	2·35	2·34	0·01
UO_2	2·38	2·37	0·01
ThO_2	2·44	2·42	0·02
MF_2			
VIII–IV			
CdF_2	2·38	2·333	0·053
CaF_2	2·43	2·37	0·06
HgF_2	2·45	2·40	0·05
SrF_2	2·56	2·51	0·05
BaF_2	2·73	2·69	0·04
Perovskite			
MBO_3			
VI–VI orX II–VI			
$BaCeO_3$	2·25	2·198	0·052
$SrCeO_3$	2·25	2·135	0·115
$CeCrO_3$	2·015	1·933	0·082
$KNbO_3$	3·00	2·84	0·16
$KNbO_3$	2·04	2·011	0·029
$BaMoO_3$	2·05	2·02	0·03
$SrMoO_3$	2·05	1·987	0·063
$BaPbO_3$	2·175	2·136	0·039
$BaSnO_3$	2·09	2·058	0·032
$CaSnO_3$	2·09	1·96	0·13
$SrSnO_3$	2·09	2·016	0·074
$BaZrO_3$	2·12	2·096	0·024
$SrZrO_3$	2·12	2·05	0·07
MBF_3			
VI–VI or XII–VI			
$KCoF_3$	2·065	2·035	0·030
$RbCoF_3$	2·065	2·03	0·035
$TlCoF_3$	2·065	2·064	0·001
$CsMnF_3$	2·15	2·13	0·02
$CsMnF_3$	3·25	3·13	0·12
$KFeF_3$	2·10	2·06	0·04
$RbFeF_3$	2·10	2·087	0·013
$KMgF_3$	2·05	1·986	0·064
$KMnF_3$	2·15	2·095	0·055
$KNiF_3$	2·03	2·006	0·024
$CsPbF_3$	2·51	2·405	0·105
$KZnF_3$	2·075	2·027	0·048
$AgZnF_3$	2·075	1·99	0·085

Unusual and irregular coordination

When the distances in polyhedra are almost equal, it is easy to determine the coordination. In this case there is usually a clear cut-off point for which peripheral anions may be considered as bonded to the central atom. However, in many cases there is a gradual increase in near-neighbor distances up to very large interatomic distances for the large alkali and alkaline earth ions in network structures such as silicates; consequently, the CN of these ions is frequently uncertain. The curves of radii *vs.* CN reflect this uncertainty [Figs. 2(*a*) and 2(*b*)]. For the purposes of this paper a break of 0·02–0·05 Å was sought as the cut-off point in the interatomic distances. When there was no such break, the distances were tabulated as questionable values. It seems likely that the slopes of radii *vs.* CN plots should be regular. The deviation from regularity is particularly noticeable for Na^+, Ag^+, K^+, Cs^+, Pb^{2+}, Sr^{2+}, and Ba^{2+}. The lack of regularity is attributed either to an insufficient number of examples of a particular coordination and/or to the difficulty in determining the CN.

Several other groups of ions exhibit irregular coordination which frequently does not result in consistent interatomic distances. Also, the radii derived from these distances do not fall on the regular curves of radii *vs.* CN. These are the ions with the following electron configurations:

d^4 – Mn^{3+}HS, Cr^{2+}HS
d^8 – Ag^{3+}, Au^{3+}, Pd^{2+}, Pt^{2+}
d^9 – Cu^{2+}, Ag^{2+}
d^{10} – Ag^+, Au^+, Hg^{2+}, Cu^+
s^2 – As^{3+}, Sb^{3+}, Bi^{3+}, Pb^{2+}, Te^{4+}

A detailed discussion of the stereochemistry of d^4, d^8, d^9, and d^{10} ions is given by Orgel (1960). Ions with d^8 configuration frequently occur in square planar coordination. This coordination is usually clearly recognized, *e.g.* PdO, AuF_3. The ions with d^4 and d^9 configurations have the familiar Jahn–Teller distortion exemplified by Cu^{2+}. These ions are characterized by four ligands at one distance and two ligands at a different distance, either closer or further away. When the difference is slight, the coordination is pseudo-octahedral; when the difference is large, square-planar or two-coordinated structures result. In the cupric oxides and fluorides the distances of the fifth and sixth neighbors range from just slightly larger than the other four

to distances almost outside the bonding sphere. In the case of cupric compounds we have calculated the average distance of all six neighbors for octahedral coordination and the four near neighbors for square-planar coordination and have listed the radii in Table 1 as both IVSQ and VI.

Ions with the d^{10} configuration have been observed with linear two coordination. Orgel has related this behavior to the small separation in energy of the d^{10} and d^9s states and predicts linear coordination of Cu^+, Ag^+, Au^+, and Hg^{2+}. Two-coordinated radii are tabulated for Cu^+, Ag^+, and Hg^{2+}.

Another group represents the ions with a lone pair of electrons: As^{3+}, Sb^{3+}, Bi^{3+}, Pb^{2+}, and Te^{4+}. The oxides formed with these ions are considered to be highly covalent. For example in PbO the lone pair acts as a ligand and results in a coordination of four neighbors in a plane on one side of the Pb^{2+} ion and the lone pair on the other side at the apex of the pyramid. This configuration has been designated in Table 1(*a*) as IVPY.

Summary

The goal of this work has been to provide radii which will be *useful* to anyone interested in the structures of oxides and fluorides. The set of empirical radii derived here is primarily intended to be used in calculating expected interatomic distances in oxide and fluoride crystal structures. Although the absolute values of radii were considered, one cannot reliably assign specific numbers to specific ions. Certain effects such as anion–anion repulsion, irregular coordination, and metal–metal bonding cause deviations from predicted interatomic distances wich have been largely ignored because these effects are difficult to include in a simple table of radii. These 'high-order' effects probably are of greater importance in structures with larger anions than in those containing oxide or fluoride ions and must be left to future work.

Note added in proof: – Prof. B. Reuter, who has just completed a refinement of the structure of the ordered spinel, MgV_2O_4, has suggested a value of $r(^{IV}Mg^{2+}) = 0{\cdot}58$ Å. Because the original value of 0·49 Å came from a single structure refinement and because this new value is more consistent with Fig. 2(*b*), the new value is preferred.

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Stereochemistry and Crystal Structure of a Cobalt(III) Sulphito Complex: *trans*-Sulphiteisothiocyanate-bis(ethylenediamine)cobalt(III) Dihydrate

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The crystal structure of $Co(en)_2SO_3NCS.2H_2O$ has been determined from three-dimensional X-ray data and refined by the full-matrix least-squares method to a residual of 0·078. The compound crystallizes in the monoclinic system, space group $P2_1/c$ with four molecules in the unit cell of dimensions $a=9·13\pm0·02$, $b=6·59\pm0·02$, $c=22·88\pm0·06$ Å, $\beta=95·5\pm0·5°$. The coordination around the metal atom is octahedral, the sulphito group being bonded through sulphur to the metal and in *trans* configuration. The Co–N(NCS) distance is not significantly different from the Co–N(en) distances. Some important dimensions are: Co–S, $2·203\pm0·006$ Å; mean Co–N(en), $1·962\pm0·010$ Å; mean S–O, $1·485\pm0·012$ Å; mean O–S–O, $110·3\pm0·7°$; Co–N(NCS), $1·974\pm0·018$ Å.

Introduction

Recently, the infrared and visible absorption spectra of a series of sulphito-bis(ethylenediamine)cobalt(III) complexes were measured by Baldwin (1961). These spectra, together with measurements of conductivity in aqueous solution and a study of chemical reactions, were interpreted by Baldwin in terms of possible structures for these complexes. For $Co(en)_2SO_3NCS.2H_2O$ it was postulated that the sulphito group is bonded through sulphur, the bond possibly involving $d\pi$–$d\pi$ bonding, and that the compound had the *cis* configuration. Kinetic studies of sulphito complexes of Co^{III} have also been made recently, indicating that the sulphito group has a marked *trans* labilizing effect (Tewari, Gaver, Wilcox & Wilmarth, 1967).

We undertook the structure determination of this compound in order to establish whether the postulated structure was correct, and, if so, to compare the dimensions of the sulphito group coordinated to Co^{III}, with the dimensions found for this group in $PdSO_3(NH_3)_3$ (Spinnler & Becka, 1967). Furthermore, we considered that a comparison between the different Co–N distances in this compound would be of interest in relation to the kinetics of reaction of sulphito complexes. In an earlier communication (Baggio & Becka, 1967) we described the main features of the structure as obtained from least-squares refinement with individual isotropic temperature factors. In this paper we give the details of the structure and structure determination with individual anisotropic temperature factors for Co, the atoms of SO_3, and the atoms of NCS.

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Experimental

Preparation

$Co(en)_2SO_3NCS.2H_2O$ was prepared by the method reported by Baldwin (1961), and crystals suitable for X-ray studies were obtained by recrystallization. The chemical and physical properties of the sample were in good agreement with those reported previously. Chemical analysis of a sample gave the following percentage composition for C, N and H: C, 17·37; N, 19·21; H, 5·75, the theoretical composition being: C, 16·59; N, 19·83; H, 5·66.

Crystal data

Name of substance: *trans*-sulphiteisothiocyanate-bis(ethylenediamine)cobalt(III) dihydrate. Chemical formulae: structural, $Co(en)_2SO_3NCS.2H_2O$; alpha-