

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 $\overline{1}$ } – 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

* Goldschmidt's & Pauling's radii and correction factors for coordination number ($CN \neq VI$) 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 isotopic 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 $r(O^{2-}) = 1.32 \text{ \AA}$.* Bragg & West arrived at a value of $r(O^{2-}) = 1.35 \text{ \AA}$ 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 $r(O^{2-}) = 1.32 \text{ \AA}$ and $r(F^-) = 1.33 \text{ \AA}$. Because structural data were scarce, Goldschmidt's table was necessarily limited. However he was able to extend the table to cover radii for which there were no experimental interatomic distances by interpolation or extrapolation of unit-cell dimensions of isotopic series *e.g.* In^{3+} , Y^{3+} , and Tl^{3+} from the C rare earth oxide structure type. If his radii are based on $r(O^{2-}) = 1.40 \text{ \AA}$, 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.

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

Pauling (1927) calculated a set of radii based on an inverse variation with effective nuclear charge in iso-electronic series of the alkali ions. The radii of the alkali ions were determined from interatomic distances in alkali halides assuming $r(O^{2-}) = 1.40 \text{ \AA}$ and $r(F^-) = 1.36 \text{ \AA}$. 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 $r(K^+) = 1.33 \text{ \AA}$ and $r(Cl^-) = 1.81 \text{ \AA}$. 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 $r(O^{2-}) = 1.40 \text{ \AA}$. 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 $r(\text{VI}O^{2-}) = 0.60 \text{ \AA}$, which reproduced interatomic distances in 1200 metallic, covalent, and ionic solids to a deviation of $\pm 0.12 \text{ \AA}$. 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

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 $r(\text{VI O}_2^-) = 1.40$ Å and $r(\text{VII F}^-) = 1.33$ 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 co-ordination 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, $r(\text{II O}_2^-) = R_{\text{av}}(\text{Si}-\text{O}) - r(\text{IV Si}^{4+}) = 1.607 - 0.26 = 1.347$ Å. The consistency of these values can be taken as a measure of their validity.

* The approximate linearity of radii-volume plots has been shown by Bertaut & Forrat (1957) for $A_3B_5\text{O}_{12}$ garnets, by Whinfrey, Eckart & Tauber (1960), and Brisse & Knop (1968) for $A_2B_2\text{O}_7$ pyrochlores, by Gattow (1963, 1964) for A_2BX_4 compounds, by Pannetier & Courtine (1966) for $AB\text{O}_4$, by Giglio (1963) for ABX_6 , by Sasvári (1960) for AX_2 and by Roth & Schneider (1960) for $A_2\text{O}_3$. 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'	ION	EC	CN	SP	A-IR	CR	'IR'	
AC+3	6P	6	VI		1.18		CS+1	5P	6	XII		2.02	1.88	
AG+1	4D10	II			.81	.67	CU+1	3D10	II	VI		.60	.46	
	IVSQ				1.16	1.02	CU+2	3D	9	IVSQ		.76	.62	
	V				1.26	1.12		V		VI	(.72)	.87	.73	
	VI				1.26	1.29		VII		VII				
	VII				1.38	1.24	DY+3	4F	9	VI		1.048	.908 R	
	VIII				1.44	1.30		VIII		VIII				
AG+2	4D	9	VI		.89		ER+3	4F11	VI			1.17	1.03	
AG+3	4D	8	IVSQ		.79	.65	EU+2	4F	7	VI		1.021	.881 R	
AL+3	2P	6	IV		.53	.39 *		VIII		VIII				
	V				.62	.48	EU+3	4F	6	VI		1.39	1.25	
	VI				.51	.670	F -1	2P	6	II		1.090	.950 R	
AM+3	5F	6	VI		1.07	1.15		VIII		VIII				
AM+4	5F	5	VI		.92	1.01	R*	F -1	2P	6	II		1.21	1.07 R
	VIII							VIII		VIII				
AS+3	4S	2	VI	(.58)		1.09	.95	F +7	1S	2	VI		1.16	1.30
AS+5	3D10	IV					FE+2	3D	6	IV	HS			
	VI							VI		VI				
AT+7	5D10	VI			.46	.64		VI		LS				
AU+1	5D10	VI			.62			VI		HS				
AU+3	5D	8	IVSQ		1.37			VI		VI				
	VI							VI		LS				
B +3	1S	2	III					VI		HS				
	IV							VI		HS				
	VI													
BA+2	5P	6	VI		1.34	1.50	1.36	FR+1	6P	6	VI			
	VII					1.53	1.39	GA+3	3D10	IV				
	VIII					1.56	1.42		V					
	IX					1.61	1.47		VI					
	X					1.66	1.52	GD+3	4F	7	VI			
	XII					1.74	1.60		VIII					
BE+2	1S	2	III			.31	.17	GE+2	4S	2	VI	(.73)	1.20	1.06 R
	IV					.41	.27	GE+4	3D10	IV				
	VI							VI						
BI+3	6S	2	V		.35			H +1	1S	0	I			
	VI							VI		VI				
	VIII			(.96)		1.13	.99	H +1	1S	0	I			
BI+5	5D10	VI			.74	1.25	1.11	R	II					
BK+3	5F	8	VI					HF+4	4F14	VI				
BK+4	5F	7	VIII						VI					
BR+1	4P	6	VI		1.96	1.07	.93	R						
BR+7	3D10	VI			.39									
C +4	1S	2	III											
	IV													
	VI													
CA+2	3P	6	VI		.99	1.14	1.00	HO+3	4F10	VI				
	VII					1.21	1.07		VIII					
	VIII					1.26	1.12	*	I -1	5P	6	VI		
	IX							I +5	5S	2	VI			
	X							I +7	4D10	VI				
	XII							IN+3	4D10	VI				
CD+2	4D10	IV							VIII					
	V													
	VI													
	VII													
	VIII													
	XII													
CE+3	6S	1	VI	1.07	1.174	1.034	R	IR+3	5G	6	VI			
	VIII					1.28	1.14	R	I +4	5G	5	VI		
	XII					1.43	1.29		K +1	3P	6	VI		
CE+4	5P	6	VI		.9	.94	.80	P	VII					
	VIII													
CF+3	6D	1	VI											
CL-1	3P	6	VI		1.81	1.09	.95	R						
CL+5	3S	2	III											
CL+7	2P	6	IV											
	VI													
CM+3	5F	7	VI											
CM+4	5F	6	VIII											
CO+2	3D	7	VI	LS										
	HS													
CO+3	3D	6	VI	LS										
	HS													
CR+2	3D	4	VI	LS										
	HS													
CR+3	3D	3	VI		.63	.755	.615	R*	MN+2	3D	5	VI		
CR+4	3D	2	IV			.58	.44		LS					
	VI					.69	.55	R	HS					
CR+5	3D	1	IV			.490	.350	R						
	VIII					.71	.57							
CR+6	3P	6	IV			.44	.30							
	VI													
CS+1	5P	6	VI		.52	1.84	1.70		MN+3	3D	3	VI		
	IX					1.92	1.78		VI					
	X					1.95	1.81		HS					

Table 1(a) (cont.)

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

EC - electron configuration, CN - coordination number, SP - electronic spin, A-IR - Ahrens ionic radii (CN=VI) (Ahrens, 1952), CR - crystal radii based on $r(V^{\text{IF}}^-)=1.19 \text{ \AA}$, 'IR' - effective ionic radii based on $r(V^{\text{IO}_2^-})=1.40 \text{ \AA}$.

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

- AC+3 VI**
- AG+1 VII**
PREWITT,C.T., AND R.D.SHANNON, TO BE PUBLISHED. AG FF 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AG2 0
- AG+1 IVSO**
BYSTRÖM,A., AND L.EVERES, ACTA CHEM.ScAND. 4,613(1960) AG2 PR 02
DONDUE,J., AND L.ELMHOLZ,J., ACTA CHEM.SOC. 66,295(1964) K AG 2 OX
SCATTURINI,V., AND P.L.BELLONI, J.ELFCRÖCHM.SOC. 10A,191(1961) AG 0
- AG+1 V**
JOST,K.H., ACTA CRYST. 14,770(1961) AG P 03 X
- AG+1 VI**
RODEH,M., Z.ANORG.ALLGEM.CHEM. 267,62(1951) AG SR F6
KIERKEGAARD,P., AND S.HOLMEN, ARKIV KEMI 23,213(1965) AG MN P 06
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AG F
ZACHARIASEN,W.H., Z.KRIST. 82,161(1952) AG2 S 04
- AG+1 VII**
KIERKEGAARD,P., AND S. HOLMEN, ARKIV KEMI 23,213(1965) AG MN P 06
- AG+1 VIII**
KROGH-MOE,J., ACTA CRYST. 18,771(1965) AG2 RR 013
WELLS,A.F., Z.KRIST. 95,74(1956) AR CO (N H3)2 (N 02)4
- AG+2 VI**
- AG+3 IVSO**
SCATTURINI,V., AND P.L.BELLONI, J.ELFCRÖCHM.SOC. 10A,191(1961) AG+1 AG+3 02
- AL+3 IV**
BROWN,F.E., AND S.W.BAILEY, ACTA CRYST. 17,1301(1964) K AL CI3 08
BURNHAM,C.W., Z.KRIST. 118,127(1963) AL2 ST 05
EULER,F., AND J.A.BRUCE, ACTA CRYST. 19,971(1965) M3 ALF 01P
MICHALSCHIK,F., Z.KRIST. 94,22(1956) AL AS 04
MOONEY,R.C., AND J.P.REMEKIJA, ACTA CRYST. 17,729(1964) AL 04
SCHWARZENBACH,O., Z.KRIST. 129,151(1966) AL P 04
SMITH,J.V., AND S.W.BAILEY, ACTA CRYST. 18,801(1963) AL-O
WILLIAMS,P.P., AND H.D.MEGAW, ACTA CRYST. 17,782(1965) ALRTTYES
LIEBAU,F., ACTA CRYST. 14,398(1961) LI AL SI4 O10
MAREZIO,M., ACTA CRYST. 19,396(1965) LT AL 02
- AL+3 V**
BERTAUT,F., AND J.MARESCHALI, COMPT.REND. 257,867(1963) Y AL 03
BURNHAM,C.W., AND K.J.BUERGER, Z.KRIST. 115,269(1961) AL2 ST 05
- AL+3 VI**
BURNHAM,C.W., Z.KRIST. 118,77(1963) AL2 ST 05
CROMERO,D.T., ET AL., ACTA CRYST. 22,182(1967) N AL (S H4)2,12 H2 O
CROMERO,D.T., ET AL., ACTA CRYST. 21,389(1966) CS2 H2 O
EULER,F., AND J.A.BRUCE, ACTA CRYST. 19,971(1965) M3 ALF 01P
FARRELL,E.F., ET AL., AM. MINERALOGIST 48,804(1963) RE AL2 08
GIBBS,G.V., AND J.V.SMITH, AM. MINERALOGIST 50,203(1965) M3 AL2 ST3 01P
JACK,K.H., AND V.GUTTMANN, ACTA CRYST. 4,296(1951) AL F3
MAREZIO,M., AND J.P.REMEKIJA, J.CHEM. 44,5143(1966) LT AL 02
NARAY-SZABÓ,S.T.V., AND K.SASVÁRI, Z.KRIST. 99,27(1959) N3 AL F6
NEGRONI,E., AND V.M.BURNHAM, Z.KRIST. 117,2551(1962) AL2 03
PDEFEREND,J., ACTA CHEM.SCAN. 16,421(1952) AR NR 04
PRANDLY,J., Z.KRIST. 123,811(1960) AL2 CAS (S) 043
SADANAGAI,T., ET AL., ACTA CRYST. 15,68(1962) AL4 SI 06
- AM+3 VI**
SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (LA F3)
- AM+4 VI**
- AM+5 VIII**
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) AM 02
- AS+3 VI**
- AS+5 IV**
FINNEY,J.J., AM. MINERALOGIST 48,1(1963) PR FP2 (AS 04)2 (O H2)
FINNEY,J.J., ACTA CRYST. 21,37(1966) CU2 (AS 04) (O H)3 H2 O
HILMER,W., ACTA CRYST. 9,67(1956) (LI AS 03)X
JOEST,K.H., ET AL., ACTA CRYST. 21,408(1966) AG2 05,5/3 H2 O
LIEBAU,F., ACTA CRYST. 9,411(1956) (NA AS 03)X
LUKASZEWSKI,Z., BULL. ACADEMIA POLONICA SCI.SCI.CHEM. 11,361(1963) MG2 AS2 07
MAREZIO,M., AND J.P.REMEKIJA, ACTA CRYST. 19,971(1965) M3 AL 02
MOONEY,R.C., ACTA CRYST. 14,311(1961) SI AS 06
MORIH., AND T.ITO, ACTA CRYST. 5,116(1950) FE3 AS 08,8 H2 O
PLIETH,K., AND G.SANGER, Z.KRIST. 126,91(1967) ZN2 CU AS2 O4
POULSEN,S.J., AND C.CALVO, CAN.J.CHEM. 46,917(1968) CU5 AS2 O8
SCHULZE-G.E.R., Z.PHYSIK CHEM. 24A,215(1954) B AS 09
SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (ZIRCON)
- AS+5 VI**
THERS,J.A., ACTA CRYST. 9,967(1956) K AS F6
JOST,K.H., ET AL., ACTA CRYST. 21,808(1964) AG2 05,5/3 H2 O
- AT+7 VI**
- AU+1 VI**
- AU+3 IVSO**
EINSTEIN,F.W.B., ET AL., J.CHEM.SOC. A1967,678 AU F3
- AU+3 VI**
- B+3 III**
BLOCK,S., AND A.PERLOFF, ACTA CRYST. 19,297(1965) RA RA 07
IMARA,M., AND J.KROGH-MOE, ACTA CRYST. 20,132(1964) CO 9B 07
KROGH-MOE,J., ACTA CRYST. 13,889(1964) CS2 BG 018
KROGH-MOE,J., ACTA CRYST. 15,190(1964) LT2 9B 07
KROGH-MOE,J., ACTA CRYST. 16,771(1965) AG2 RR 01X
MAREZIO,M., ET AL., ACTA CRYST. 16,974(1963) K2 RR 07,4 H2 O
MAREZIO,M., ET AL., ACTA CRYST. 16,974(1963) K2 RR 07,4 H2 O
ZACHARIASEN,W.H., ET AL., ACTA CRYST. 16,1144(1964) RE2 R 0X (O H)
- B+3 IV**
BLOCK,S., AND A.PERLOFF, ACTA CRYST. 19,297(1965) RA RA 07
CLARK,J.R., AND V.R.LAIR, J.AM.CHEM.SOC. 57,1945(1935) CO R 04
HOARD,J.R., AND V.R.LAIR, J.AM.CHEM.SOC. 57,1945(1935) CO R 04
IMARA,M., AND J.KROGH-MOE, ACTA CRYST. 20,132(1964) CO 9B 07
KROGH-MOE,J., ACTA CRYST. 16,205(1964) SR RR 07
KROGH-MOE,J., ACTA CRYST. 13,889(1964) CS2 BG 018
KROGH-MOE,J., ACTA CRYST. 15,190(1964) LT2 9B 07
KROGH-MOE,J., ACTA CRYST. 16,771(1965) AG2 RR 01X
MAREZIO,M., ET AL., ACTA CRYST. 16,974(1963) K2 RR 07,4 H2 O
MAREZIO,M., ET AL., ACTA CRYST. 16,974(1963) K2 RR 07,4 H2 O
PANT,A.K., AND J.P.REMEKIJA, J.CHEM.PHYS. 48,3348(1966) LT R 02
PERLOFF,A., AND S.BLOCK, ACTA CRYST. 20,278(1966) SR RR 07
PREWITT,C.T., AND R.D.SHANNON, ACTA CRYST. R24,B66(1968) R2 03
PEMEKIJA,J.P., AND M.MAREZIO, J.PHYS.CHEM.SOLIDOS 26,2083(1965) LT R 02
ZACHARIASEN,W.H., ACTA CRYST. 16,340(1963) H B 02
ZACHARIASEN,W.H., ACTA CRYST. 16,345(1963) H B 02
- B+3 VI**
HILMER,W., ACTA CRYST. 15,1101(1962) RA GE 03
SCHNERING,H.G., ET AL., Z.ANORG.ALLGEM.CHEM. 314,154(1962) RA ZN 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) BA 0
ZACHARIASEN,W.H., Z.KRIST. 7a,139(1950) BA TI ST3 09
- BA+2 VII**
HILMER,W., ACTA CRYST. 15,1101(1962) RA GE 03
SCHNERING,H.G., Z.ANORG.ALLGEM.CHEM. 314,154(1962) RA CR 09
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 3,(1965) RA NT 04
- BA+2 VIII**
BLAND,J.A., ACTA CRYST. 14,875(1961) RA2 TI 04
HILMER,W., ACTA CRYST. 15,1101(1962) BA GE 03
LANDER,J., ACTA CRYST. 16,180(1965) RA2 TI 04
MANOHAR,H., AND J.RAMASESHAN, Z.KRIST. 119,35(1964) BA (O H)2,8 H2 O
NARDELLI,D.H., AND G.FAVA, ACTA CRYST. 15,477(1962) BA S2 03, H2 O
RAO,R.V.G.S., ET AL., Z.KRIST. 110,231(1958) CU BA2 (C O H)2,6 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) RA BN 07
BURLEY,J.S., J.RES.NATL.BUR.STD. 60,231(1958) RA H P 09
NEWNHAM,R.E., AND H.D.MEGAW, ACTA CRYST. 20,133(1960) RA AL2 ST2 08
ROBBINS,C., ET AL., J.RES.NATL.BUR.STD. 70A,345(1966) RA GE 09
TEMPLETON,D.H., AND C.H.DAUBEN, J.CHEM.PHYS. 32,1515(1960) RA TI 04
ZACHARIASEN,W.H., ACTA CRYST. 1,263(1948) RA3 (P 04)2
- BA+2 X**
BLOCK,S., AND A.PERLOFF, ACTA CRYST. 19,297(1965) RA BN 07
BURLEY,J.S., J.RES.NATL.BUR.STD. 60,231(1958) RA H P 09
NEWNHAM,R.E., AND H.D.MEGAW, ACTA CRYST. 20,133(1960) RA AL2 ST2 08
ROBBINS,C., ET AL., J.RES.NATL.BUR.STD. 70A,345(1966) RA GE 09
ZACHARIASEN,W.H., ACTA CRYST. 1,263(1948) RA3 (P 04)2
- BA+2 XI**
EVANS,H.T., JR., ACTA CRYST. 4,377(1951) RA TI 03
HOARD,J.L., AND W.VINCENT, J.AM.CHEM.SOC. 62,3126(1940) BA SI F6,BA GE F6
SAHLIK,J., BEITR.MINERAL.PETROG. 9,111(1963) BA S 04
SCHNERING,H.G., Z.ANORG.ALLGEM.CHEM. 353,13(1967) BA2 M F6
SHIRANE,G., ET AL., PHYS.REV. 105,856(1957) BA TI 03
ZACHARIASEN,W.H., ACTA CRYST. 1,263(1948) RA3 (P 04)2
- BA+2 XII**
HARRIS,L.A., AND H.L.YAKEL, ACTA CRYST. 22,354(1967) Y2 BE 04
- BE+2 IV**
BEEVERS,C.A., AND H.LIPSON, Z.KRIST. 82,297(1932) BE S ON,4 H2 O
BUSSJÖH.J.H., AND E.K.GORDON, ACTA CRYST. 20,133(1960) LT2 BE 04
FARNELL,E.F., AND J.M.SLATER, Z.KRIST. 117,371(1962) BE P 04
GOLOVATSKOV,N.I., SOVIET PHYS.-CRYST. 6,733(1962) NA RE P 04
HARRIS,L.A., AND H.L.TAKEL, Z.KRIST. 117,16(1962) AL RE ST 04 O H
NORSEIM,E., AND D.EAPPLEMAN, Z.KRIST. 117,16(1962) LT6 BE F4 ZR F8
SEARS,I.R., AND J.H.BURNS, J.CHEM.PHYS. 41,3478(1964) LT6 BE F4 ZR F8
SMITH,D.K., ET AL., J.ELECTROCHEM.SOC. 111,18(1964) RE 0
ZACHARIASEN,W.H., ET AL., ACTA CRYST. 16,1144(1963) RE2 B 03 (O H)
- BE+2 VI**
- BI+3 V**
ABRAHAMS,S.C., ET AL., J.CHEM.PHYS. 47,4036(1967) BI2 RE 09
AURIVILLIUS,B., ACTA CHEM.SCAN. 18,2375(1964) BI2 OZ S 04,H2 O
- BI+3 VI**
AURIVILLIUS,B., ACTA CHEM.SCAN. 18,375(1964) BI2 OZ 5 O H2 O
AURIVILLIUS,B., AND T.JOHNSON, ARKIV KEMI 19,271(1962) RI O H CR 04
AURIVILLIUS,B., ET AL., ACTA CHEM.SCAN. 18,1555(1964) BI2 GE 05
SEGAL,D.J., ET AL., Z.KRIST. 123,711(1966) BI4 ST3 O12
ZEMANNI,J., HEIDELBERGER BEITR.MINERAL.PETROG.WITT. 5,139(1956) BI2 MO 06
- BI+3 VIII**
AURIVILLIUS,B., ARKIV KEMI 3,153(1951) BI SB 04
MOONEY,R.C., ACTA CRYST. 1,163(1954) BI AS 04
MOONEY-SLATER,R.C.L., Z.KRIST. 117,371(1962) BI P 04
GURASHI,M.M., AND W.H.BARNES, AM.MINERALOGIST 38,489(1953) BI V 04
SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (ZIRCON)
TOMASHPOL'SKII,Y., ET AL., SOVIET PHYS.-CRYST. 9,715(1965) BI FE 03
- BI+5 VI**
- BK+3 V**
PETTERSON,J.R., AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967) BK2 O3
- BK+6 VIII**
PETTERSON,J.R., AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967) BK 02
- BR-1 VI**
- BR+7 VI**
- C+4 III**
CHESSIN,H.W.C., HAMILTON, AND B.POSS, ACTA CRYST. 18,689(1965) CA C 03
- C+4 IV**
- C+4 VI**
- CA+2 VI**
BUERGER,M.J., Z.KRIST. 109,248(1956) CA2 NA H SI3 09
CLARK,J.R., ET AL., ACTA CRYST. 15,207(1962) CA B3 O 0 H
CRUICKSHANK,D.W.J., ACTA CRYST. 17,685(1961) CA2 SI 04
GARD,J.A., AND H.F.W.TAYLOR, ACTA CRYST. 13,785(1960) CA4 (SI3 09) (O H)2
KITA,T., ET AL., ACTA CRYST. 5,209(1952) K2 CA4 RE2 AL2 S12,060, H2 O
KLEINVELD,H., ET AL., ACTA CRYST. 16,180(1965) CA3 S 06
SMITH,D.K., ET AL., ACTA CRYST. 18,1555(1964) CA2 ST 04
STEINIMK,H., AND F.J.SANS, AM.MINERALOGIST 44,679(1959) CA MG (C O3)2
TAKUECHI,Y., AND G.DONNAY, ACTA CRYST. 12,465(1959) CA AL2 SI2 08
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**
BAKATIN,V.V., AND N.V.BELOV, DOKL.AKADEM.NAUK SSSR 135,587(1960) CA BE2 (P 04)2
CHRIST,L., ET AL., ACTA CRYST. 11,761(1958) CA B3 O4 (O H)3, H2 O
MEGAN,H.D., ACTA CRYST. 5,477(1952) CA3 (SI 03) O H2,2 H2 O
POSNER,A.S., ET AL., ACTA CRYST. 11,308(1958) CA10 (P 04)6 F2
PRANDLY,J., Z.KRIST. 123,811(1966) AL2 CA3 (SI 04)3
ROUSSEAU,B., ET AL., Z.KRIST. 123,811(1966) AL2 CA3 (SI 04)3
SWALLOW,J.S., ET AL., ACTA CRYST. 21,597(1966) CA3 V10 028,17 H2 O
WEBB,N.C., ACTA CRYST. 21,942(1966) CA2 P2 07
ZACHARIASEN,W.H., Z.KRIST. 73,7(1950) CA TI ST 05
- CA+2 VIII**
BERGNER,E.F., AND P.BLUM, ACTA CRYST. 9,121(1956) CA TI2 04
BURLEY,J.R., AND V.R.LAIR, J.AM.CHEM.SOC. 57,1945(1935) CA W 04
CLARK,J.R., AND C.L.CHRIST, Z.KRIST. 112,213(1968) CA B3 O3,(O H)5,2 H2 O
CRUICKSHANK,D.W.J., ACTA CRYST. 17,685(1961) CA2 SI 04
DECKER,B.F., AND J.S.KASPER, ACTA CRYST. 10,332(1957) CA FE2 04

Table 1(b) (cont.)

HARRIS,L.A. AND H.L.YANKEL, ACTA CRYST., 20,295(1966)	CA12 BF17 029
MILL,P.M. ET AL., ACTA CRYST., 9,961(1956)	CA FE2 CR 04
MOHNE,F., SOVIET PHYS.-CRYST., 7,559(1963)	CA 5 04
JAHNBERGL,L., ACTA CHEM,SCAND., 17,258(1963)	CA TA2 06
MAREZIO,M. ET AL., ACTA CRYST., 16,390(1963)	CA 2B 09
MULER-BUSCHBAUM,H., H.G.SCHNERING, J,ANORG,ALLGEM,CHEM., 336,295(1965)	CA SC2 04
PAVLOV,P.V. AND N.V.BELOV, SOVIET PHYS.-CRYST., 10,300(1965)	CA RE P 04 F
PETERSON,D.H. AND J.W.BARTH, Z.KRIST., 80,331(1962)	CA MN S12 06
PRANDI,L. Z.KRIST., 123,81(1962)	CA AL2 C43 ISI 04 03
WEBB,N.C., ACTA CRYST., 21,982(1963)	CA P2 07
WILHELMIK,A. AND O.JONSSON, ACTA CHIM,SCAND., 19,177(1965)	CA5 0 H (CR 04)3
ZALKINIA,I. AND O.H.TEPLITZON, J.CHEM,PHYS., 46,501(1964)	CA W 04
CA+2 IX JOHANSSON,G., ACTA CRYST., 12,522(1959)	CA R2 S12 08
POSNER,A.S. ET AL., ACTA CRYST., 11,308(1958)	CA10 (P 0416 F2
RODI,F. AND D.BABEL, Z.ANORG,ALLGEM,CHEM., 336,17(1965)	CA IR 03
CA+2 X MAREZIO,M. ET AL., TO BE PUBLISHED	CA R2 04
CA+2 XII MAREZIO,M. ET AL., TO BE PUBLISHED	CA R2 04
CD+2 IV KOKKROS,P.A. AND P.J.RENTZEPERIS, Z.KRIST., 119,234(1963)	CD 5 04
SCHNERING,H.G. Z.ANORG,ALLGEM,CHEM., 314,144(1962)	CA CO 03
CO+2 W CALVO,C. AND J.S.STEVENS, CAN.J.CHEM., 46,903(1968)	CD 2N2 (P 04)2
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM., 46,903(1968)	CD 2 N 7 (P 04)2
CD+2 VI AU,P.K.L. AND C.CALVO, CAN.J.CHEM., 46,227(1967)	CD2 V2 07
DEHOFF,R.P.M. ACTA CRYST., 11,432(1966)	CD (O H2
LIPSON,H. PROC.ROY.SOC.(LONDON)SER.A 156,446(1963)	3CD S 04, R H2 O
POSNIKAE,E. AND T.F.W.BARTH, Z.KRIST., 86,271(1963)	CA TT 03
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	CD 0
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	K CR F3
CO+2 VIII CALVO,C. AND J.S.STEVENS, CAN.J.CHEM., 46,903(1968)	CD 2N2 (P 04)2
CALVO,C. AND J.S.STEVENS, CAN.J.CHEM., 46,903(1968)	CD 2 N 7 (P 04)2
CD+2 VIII BRISSEAU, PH.D.THESES DALHOUSIE UNIV., HALIFAX,N.S.,(1967)	CD2 TA2 07
DOOLITTLE,P.C. ET AL., INORG.CHEM., 4,1152(1965)	CD2 RE2 07
HAKVOOT,C. ET AL., ACTA CRYST., 21,719(1966)	CD IN 03)2,4 H2O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	CD F2
CO+2 XII POSNIKAE,E. AND T.F.W.BARTH, Z.KRIST., 86,265(1964)	CD TT 03
CE+3 VI SLEIGHT,A.W. TO BE PUBLISHED (RF)2 S3	
TEMPLETON,D.H. AND C.H.DAUBEN, J.AMER.CHEM.SOC., 76,5237(1954)	
CE+3 VIII HODNEY,R.C., ACTA CRYST., 3,337(1958)	CE R 04
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R3 VS V (ZIRCON)
CE+3 XII ZALKINIA, ET AL., J.CHEM,PHYS., 39,281(1963)	CF2 M63 (N 03)12,24 H2 O
CE+4 VI WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	BA CE 03
CE+4 VIII WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	SR CF 03
CF+3 VI GREEN,J.L. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,345(1967)	CF2 03
PETERSON,J.R. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967)	CF2 03
CL+1 VI	
CL+5 III ZACHARIASEN,W.H., Z.KRIST., 71,517(1929)	K CL 03
CL+7 IV GOTTFRIED,C. AND C.SCHUSTERIUS, Z.KRIST., 84,65(1952)	K CL 04
ZACHARIASEN,W.H., Z.KRIST., 73,141(1950)	NA CL 04
CL+7 VI	
CM+3 VI PETERSON,J.R. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967)	CM2 03
CM+4 VIII PETERSON,J.R. AND B.B.CUNNINGHAM, INORG.NUCL.CHEM.LETTERS 3,327(1967)	CM 02
CO+2 VI LS	
CO+2 VI HS BAUR,W.H. ACTA CRYST., 11,486(1958)	CO F2
IBERS,J.A. AND G.W.SMITH, ACTA CRYST., 11,487(1964)	MA CO2.3 MO3 012
MONTGOMERY, E. ET AL., CAN.J.CHEM., 22,775(1967)	CO (M H4)2.15 042.6 H2 O
REINHOLDIS,P.J. NEUES JAHRZ.MINERAL.ROHSTOFF., 226(1958)	CO S 04
SCHNERING,H.G., Z.ANORG,ALLGEM.CHEM., 355,13(1967)	RA2 CO F6
SMITH,G.W. AND J.A.IBERS, ACTA CRYST., 19,269(1965)	CO MO 04
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	CO F2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	CO F3
ZALKINIA, ET AL., ACTA CRYST., 19,210(1962)	CO S 04.6 H2 O
CO+3 VI LS BLASSE,G. J.INORG. NUCL. CHEM. 27,748(1965)	LT CO 02
SHANNON,R.D., INORG.CHEM., 6,1474(1967)	R3 VS V (PROVOSKITE)
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,X.H. AND R. WAITLAND, PROC.CHEM.SOC.LONDON 212(1957)	CR F2
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R3 VS V (RUTILE)
STEINFINK,H. AND J.H.BURNS, ACTA CRYST., 17,823(1964)	CR2 F5
CR+3 VI HS DOUGLASS,R.M. ACTA CRYST., 10,423(1967)	H CR 02
KNOPEK,O. ET AL., J.CHEM., 43,281(1965)	FR2 F3
SHANNON,R.D. AND Y.E.DEHMAN, Z.KRIST., 117,235(1962)	CR2 03
SHANNON,R.D. AND J.H.BURNS, ACTA CRYST., 17,821(1964)	CR2 F5
STEINFINK,H. AND J.H.BURNS, ACTA CRYST., 17,821(1964)	K CR (CR 04)2
WILHELMIK,A. ACTA CHEM,SCAND., 12,1965(1958)	K CR (CR 04)2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	CE CR 03
CR+4 IV DOUGLASS,R.M. ACTA CRYST., 10,423(1967)	H CR 02
KNOPEK,O. ET AL., J.CHEM., 43,281(1965)	FR2 F3
SHANNON,R.D. AND Y.E.DEHMAN, Z.KRIST., 117,235(1962)	CR2 03
SHANNON,R.D. AND J.H.BURNS, ACTA CRYST., 17,821(1964)	CR2 F5
STEINFINK,H. AND J.H.BURNS, ACTA CRYST., 17,821(1964)	K CR (CR 04)2
WILHELMIK,A. ACTA CHEM,SCAND., 12,1965(1958)	K CR (CR 04)2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	CE CR 03
CR+4 IV WILHELMIK,A. ET AL., ARKIV KEMI 26,157(1967)	SR2 CR 04
CR+4 VI CHAMBERLAND,B.L., SOLID STATE COMMUN. 5,663(1967)	SP CR 03
CLOUD,W.H. ET AL., J.APPL.PHYS., SUPPL., 35,1149(1962)	CR 02
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R3 VS V (RUTILE)
CR+4 IV GREENBLATT,M. ET AL., ACTA CRYST., 23,166(1967)	CA2 CR 04 CL
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R3 VS V (ZIRCON)
WILHELMIK,A. AND O.JONSSON, ACTA CHEM,SCAND., 19,177(1964)	CA5 0 H (CR 04)5
CR+5 VIII STROMBERG,R. AND C.BROSSET, ACTA CHEM,SCAND., 14,441(1960)	K3 CR 08
CR+6 IV AURIVILLIUS,B. AND I.JONSSON, ARKIV KEMI 19,271(1962)	91 0 H CP 04
BYSTROM,G. AND K.WILHELMIK, ACTA CHEM,SCAND., 4,151(1959)	CP 03
COLLODING, ET AL., ACTA CRYST., 12,414(1959)	CD CR 04
LUVINSKJAER, AND S.ETELIN, ARKIV KEMI 1,277(1960)	TH,10,HI2 CR 04 H2 O
LUNDENGREN,G. ARKIV KEMI 13,159(1958)	ZRH (O H16 (CR 04)2, H2 O
MILLER,J.J. Z.KRIST., 99,32(1938)	C52 CR 04
NARAY-SZABO,I. AND GARGATTA, ACTA CHIM,ACAD,SCI,HUNG., 40,243(1964)	PR CR 04
QUARENIG,S. AND R.DEPIERRE, ACTA CRYST., 19,287(1965)	PRB CR 04
WILHELMIK,A. ACTA CHEM,SCAND., 19,165(1965)	CP 03
WILHELMIK,A. ARKIV KEMI 26,131(1967)	LI CR3 08
WILHELMIK,A. ARKIV KEMI 26,111(1967)	CS CR3 08
ZACHARISSEN,W.H. AND G.E.ZIEGLER, Z.KRIST., 80,164(1931)	K2 CR 04
ZHUKOVA,L.A. AND Z.G.PISKER, SOVIET PHYS.-CRYST., 9,31(1964)	K2 CRP 07
CR+6 VI	
CS+1 VI BURNS,H. AND W.R.BUSING, INORG.CHEM., 4,1510(1965)	CS LT F2
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	CS F
CS+1 IX MILLER,J.J. Z.KRIST., 99,32(1938)	C52 CR 04
CS+1 X BYSTROM,D.T. ET AL., ACTA CRYST., 21,343(1966)	CS 582 F7
KROGH-MOE,J. AND H.IIHARA, ACTA CRYST., 23,427(1967)	CS 59 014
MILLER,J.J. Z.KRIST., 99,32(1938)	C52 CR 04
CS+1 XI CROMER,D.T. ET AL., ACTA CRYST., 21,343(1966)	CS AL (S 04)2,12 H2 O
EVANS,N.T.,JR. AND S.BLOCK, INORG.CHEM., 5,180(1966)	CS V3 08
ROSENZWEIG,A. AND D.T.CROMER, ACTA CRYST., 23,465(1967)	CS U F6
ZALKINIA, ET AL., J.CHEM,PHYS., 37,697(1962)	CS MN F3
CU+1 II PASTS,A. AM,MINERALOGIST 31,539(1961)	CU FE 02
PREWITT,C.T. AND R.D.SHANNON, TO BE PUBLISHED.	CU FE 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	CU2 O
CU+1 VI	
CU+2 IVS0 BACHMANN,H.G. AND J.ZEMANN, ACTA CRYST., 19,747(1961)	PR CU S 04 (O H)2
BRUNTON,G. ET AL., ACTA CRYST., 11,169(1961)	CUR MGR (C 03)4 (O H)24, H2 O
BUKOWSKA-STREYZENSKA,M., ACTA CRYST., 19,357(1965)	CU (H C O)2,2 H2 O
FLUGEL-KAHLER,E. ET AL., ACTA CRYST., 16,1009(1963)	CU3 (S 04) 0 H4
GATTOW,G. ACTA CRYST., 11,377(1958)	CU SE 03,2 H2 O
GATTOW,G. AND J.ZEMANN, ACTA CRYST., 11,466(1958)	CU3 (O H)2 (C 03)2
GHOSE,S. ACTA CRYST., 15,1105(1962)	CU I 03 0 H
GHOSE,S. ACTA CRYST., 16,124(1963)	CUS (P 04)2 (O H)4
JAGGI,H. AND H.R.OSWALD, ACTA CRYST., 18,137(1961)	CU 10 H2
KIRIATI,Y. ET AL., ACTA CRYST., 16,1009(1963)	CU2 (O H)2,2 H2 O
PLATNER,R. AND B.SANGIOR,Z.KRIST., 12,203(1967)	ZNH CU (AS 04)2
RAO,B.RAMA, ACTA CRYST., 14,738(1961)	NA2 CU (S 04)2,2 H2 O
TUNELL,E. ET AL., Z.KRIST., 90,120(1955)	CU O
VAN NIJKERK,J.N. F.R.SCHOENING, ACTA CRYST., 6,227(1953)	CU P (C H C O)4,2 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	CU3 AS2 08
CU+2 V BACHMANN,H.G. ET AL., ACTA CRYST., 19,747(1961)	PR CU S 04 (O H)2
FLUGEL-KAHLER,E. ET AL., ACTA CRYST., 16,1009(1963)	CU2 (O H)2 (O H)2
HERITS,H. Z.KRIST., 99,466(1958)	CU2 O H AS 04
HERITS,H. Z.KRIST., 102,1(1959)	CU2 O H (P 04)
POULSEN,S. AND C.CALVO, CAN.J.CHEM., 46,917(1968)	CU3 AS2 08
CU+2 VI BACHMANN,H.G. AND J.ZEMANN, ACTA CRYST., 14,747(1961)	PR CU S 04 (O H)2
BILLY,C. AND H.M.KAENDLER, J.AM.CHEM.SOC., 50,719(1928)	CU F2
BUKOWSKA-STREYZENSKA,M., ACTA CRYST., 19,357(1965)	CU (H C O)2,2 H2 O
FINNEY,J.J. ACTA CRYST., 21,347(1966)	CU2 (AS 04) (O H)2,2 H2 O
FLUGEL-KAHLER,E. ACTA CRYST., 16,1009(1963)	CU2 O H AS 04
GINETTI,Y. BULL.SOC.ROM.RELIEF, 63,229(1953)	CU (C H)2,2 H2 O
HEPPELL,H. ACTA CRYST., 19,104(1962)	CU2 (O H)2 (AS 04)
HERITS,H. Z.KRIST., 102,1(1959)	CU2 (O H)2 (P 04)
JAGGI,H. AND H.R.OSWALD, ACTA CRYST., 14,104(1961)	CU (O H)2
KNOX,K. J.CHEM.PHYS. 30,991(1959)	K2 CU F6
NOVACKI,W. AND R.SCHEIDERER, HELV.CHEM.ACTA 35,375(1952)	CU2 (O H)3 N 03
RAO,R.V.G. SONDRA, ET AL., Z.KRIST., 110,230(1958)	CU2P (C O O)2 H6,4 H2 O
RAO,B.RAMA, ACTA CRYST., 14,738(1961)	NA2 CU (S 04)2,2 H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964)	K CU F3
DT+3 VI TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC., 76,5237(1954)	DY2 O3
DT+3 VIII ADRAGAMS,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS., 46,3776(1967)	DY MN2 05
EULER,E. AND BRUCE,J.A. ACTA CRYST., 19,971(1965)	DY3 FF2 F3 012
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R VS A (PYROCHLORITE)
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)	FR2 TI2 07
PATSCHEKE,E. ET AL., CHEM.PHYS.LETTERS 2,47(1968)	PP H 04
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R VS A (PYROCHLORITE)
EU+2 VI WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	EU 0
EU+2 VII RAU,R.C. ACTA CRYST., 20,716(1966)	EU3 ON
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963)	EU F2
EU+3 VI RAU,R.C. ACTA CRYST., 20,716(1966)	FU3 ON
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(1964)	FU3 FE2 GA3 012
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED.	R VS A (PYROCHLORITE)
TEMPLETON,D.H. AND A.ZALKIN, ACTA CRYST., 16,762(1963)	FU2 (O 04)3

Table 1(b) (cont.)

F -1 II	
F -1 III	
F -1 IV	
F -1 VI	
F +7 VII	
FE+2 IV HS HANISCH,K.,NEUES JAHRB.MINERAL.MONATSH., 128,362(1956) FE FE2 ALB SI4 O24	
FE+6 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 ON8 H2 O BURNHAM,C.W., CARNEGIE INST.WASH.YEAR BOOK 65,285(1966) FE SI O3 GIBBS,G.V., ET AL., AM.MINERALOGIST, IN PRESS. FE2 SI O4 HAMILTON,W.C., ACTA CRYST., 15,353(1962) FE SI F6 H2 O KROPP,F., ET AL., INORG.CHEM., 5,1682(1966) RA FF F3 RUMANOVIĆ,I.-M., MATER.ZINKEVICH, A.YA. SOVIET CRYST., 5,651(1961) CA2 FE (P O4)2 H2 O SMITH,D.K., ET AL., ACTA CRYST., 19,497(1965) FE2 SI O4 STRUNZ,H. AND M.GIGLIOLI, ACTA CRYST., 14,205(1961) FE GE (O H16) ULKUD, Z.KRIST., 124,192(1967) FE W O4 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) FE O WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) K FE F3 ZEIMANN,J., NEUES JAHRB. MINERAL.MONATSH., 67(1959) FE GF (O H16)	
Fe+3 IV HS BATTIA, AND B.POSET, ACTA CRYST., 15,1268(1962) Y3 FE5 O12 BERTAUT,E.F., ET AL., ACTA CRYST., 12,149(1959) CA2 FE2 O5 BERTAUT,F., ET AL., COMPT.REND., 257,421(1963) NA FF O2 EULER,F. AND J.A.BRUCE, ACTA CRYST., 19,971(1965) MS FE5 O12 ELLER,F. AND M.A.GILLEO, ACTA CRYST., 10,239(1957) Y3 FE5 O12 FELLER,S., ET AL., INORG.CHEM., 22,768(1967) NAS FE5 O9 RODRIGUEZ, ET AL., ACTA CRYST., 22,768(1967) NAS FE5 O9 WEIDENBORNER,J.E., ACTA CRYST., 14,1051(1961) 603 FE5 O12	
FE+6 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 MIIT (CN)6)	
FE+3 VI HS ABRAHAMS,S.C., ET AL., J.CHEM.PHYS., 42,3957(1965) GA FE O3 BATTIA, AND B.POSET, ACTA CRYST., 15,1268(1962) Y3 FE5 O12 BERTAUT,E.F., ET AL., ACTA CRYST., 12,149(1959) CA2 FE2 O5 BLAKER,R.L., ET AL., AM.MINERALOGIST, 51,123(1966) FF2 O3 BLASSE,G., J.INORG.NUCL.CHEM., 27,748(1965) COPPENS,P. AND M.EIBSCHUTZ, ACTA CRYST., 19,524(1965) GD FE O3 EULER,F. AND J.A.BRUCE, ACTA CRYST., 19,971(1965) MS FE5 O12 FELLER,S., J.CHEM.PHYS., 33,676(1960) GAO2 O3 MAREZIO,M., ET AL., INORG.CHEM., 16,119(1967) FE2 O4 (O H12) HEPWORTH,M.A., ET AL., ACTA CRYST., 19,63(1965) FE F2 SHANNON,R.D., INORG.CHEM., 6,176(1967) R3 VS V (PEROVSKITE) TOMASHARIAN,SKIIYI, ET AL., SOVIET PHYS.-CRYST., 9,715(1965) RT FE O3 WEIDENBORNER,J.E., ACTA CRYST., 14,1051(1961) 603 FE5 O12	
FR+1 VI	
GA+3 IV ABRAHAMS,S.C., ET AL., J.CHEM.PHYS., 42,3957(1965) GA FE O3 EULER,F. AND J.A.BRUCE, ACTA CRYST., 19,971(1965) MS GA5 O12 SELLER,S., J.CHEM.PHYS., 33,676(1960) GAO2 O3 MAREZIO,M., ACTA CRYST., 18,481(1965) LI GA O2 MOONEY,R.C.L., ACTA CRYST., 9,728(1956) GA O4	
GA+3 V SHANNON,R.D. AND C.T.PREWITT, J.INORG.NUCL.CHEM. IN PRESS. IN GA O3	
GA+6 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) MS GA5 O12 GODDARD,J., AND P.REINHOLD, INORG.CHEM., 10,505(1965) 26,127(1965) GA2 O3 MOONEY-SLATER,R.C.L., ACTA CRYST., 20,526(1964) GA O4 H2 O MOROSINI,B. AND A.ROSENZWEIG, ACTA CRYST., 18,879(1965) GA NR O4 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CE DA O3	
GD+3 VI TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC., 76,5237(1954) GD2 O3	
GD+3 VII BRISSE,F., PH.D.THESES/DALHOUSIE UNIV.,HALIFAX,N.S.(1967) GD2 TI2 O7 EULER,F. AND J.A.BRUCE, ACTA CRYST., 19,971(1965) 603 AL2 AL3 O12 SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE) WEIDENBORNER,J.E., ACTA CRYST., 14,1051(1961) 603 FE5 O12	
GE+2 VI	
GE+4 IV ABRAHAMS,S.C., ET AL., J.CHEM.PHYS., 47,4036(1967) BI12 GE O20 DURIF,A., ACTA CRYST., 9,515(1956) GE U O6 GENNARO,T., BULL.SOC.CHEM. ITALIES 63,209(1958) CU GE O3 HILMER,W., INORG.CHEM., 18,111(1969) GE O3 HILMER,W., INORG.CHEM., 18,111(1969) SR GE O3 INGRIN,A. AND G.LUNDGREN, ACTA CHEM.SCAND., 17,617(1963) NAS GE9 O20 JAMIESON,P.B. AND L.S.D.GLAESER, ACTA CRYST., 21,1281(1967) NA2 FE3 O3.6 H2 O LARSEN,F.K., ET AL., ACTA CHEM.SCAND., 21,1281(1967) NAs SN8 GE10 O30 (O H4) ROBBINS,C., ET AL., J.RES.NATL.BUR.STD., 70A,35(1966) BA3 GE4 O9 SMITH,S.W. AND P.B.ISABA, ACTA CRYST., 17,842(1964) GE O2	
GE+4 VI HOARD,W.H., ACTA CRYST., 9,515(1956) GE O2 HOARD,J.L. AND W.B.VINCENT, J.AM.CHEM.SOC., 61,2049(1939) K2 BE F6 INGRIN,A. AND G.LUNDGREN, ACTA CHEM.SCAND., 17,617(1963) NAS GE9 O20 ROBBINS,C., ET AL., J.RES.NATL.BUR.STD., 70A,35(1966) BA3 GE4 O9 SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS V (RUTILE) STRUNZ,H. AND M.GIGLIOLI, ACTA CRYST., 14,205(1961) FE GE (O H16) ZEIMANN,J., NEUES JAHRB.MINERAL.MONATSH., 67(1959) FE GE (O H16)	
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 CRERAR,D., ET AL., ACTA CRYST., 24,172(1966) ALUM KOPIERSY, ET AL., J.CHEM.PHYS., 25,727(1956) HF PIMENTEL,S.C. AND A.L.MCLELLAN, 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 04 CL) HAMILTON,W.C. AND J.A.IBERS, ACTA CRYST., 16,1209(1963) H CR O2 MC DONALD,T.R.R., ACTA CRYST., 13,131(1960) IN H H F2 MC DONALD,T.R.R., ACTA CRYST., 19,260(1965) H CR O2 PETTERSON,S.W. AND H.A.LEVY, J.CHEM.PHYS., 20,704(1952) K H F2 PETTERSON,S.W. AND H.A.LEVY, J.CHEM.PHYS., 29,948(1958) K H IC2 H2 O4	
HF+6 VI BRISSE,F., PH.D.THESES/DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 HF2 O7 SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)	
HF+6 VIII WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) HF O2	
H6+1 III GROENIG,D., J.CHEM.SOC., 1312(1956) H62 (N O3)2.2H2 O	
H6+2 II AURIVILLIUS,K., ACTA CRYST., 9,685(1956) HG O AURIVILLIUS,K., ACTA CHEM.SCAND., 10,1305(1964) HG O ROTH,W.L., ACTA CRYST., 9,277(1956) HG O	
H6+2 IV BONEFACI,C.A., ACTA CRYST., 14,116(1961) HG S O4,H2 O KOKKOROS,P.A. AND P.J.RENTZEPERTS, Z.KRIST., 119,234(1963) HG S O4	
H6+2 VI BONEFACI,C.A., ACTA CRYST., 14,116(1961) HG S O4,H2 O	
H6+2 VII SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE) SLEIGHT,A.W., TO BE PUBLISHED. H62 H2 O7 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) HG F2	
H6+3 VI FERTA,L., BULL.SO.FRANC.MINERAL.CRYST., 85,667(1962) H62 O3 TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC., 76,5237(1956) H62 O5	
H6+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) GS I O3 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) RB I O3	
I +7 VII	
IN4+3 VI BERNHARDT,H. AND H.KASPER, ACTA CRYST., 83,388(1968) CU2 IN2 O5 JOHANSSON,G., ACTA CHEM.SCAND., 15,157(1961) IN O H S O4 (H2 O7) MAREZIO,M., ACTA CRYST., 20,723(1966) IN2 O3 NOONETR,C.L., ACTA CRYST., 9,113(1956) IN P O8 MOONEY-SLATER,R.C.L., ACTA CRYST., 14,118(1961) IN P O4.2 H2 O REIDA,F., INORG.CHEM., 6,631(1967) CA IN2 O4 ROTH,R.S., S.J.SCHNEIDER, J.RES.NATL.BUR.STD., 64A,309(1960) R3 VS V (HN2 O4) SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. IN2 O3	
IN4+3 VII SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)	
IR+3 VI HEPMORTH,M.A. ET AL., ACTA CRYST., 10,45(1957) IR F3	
IR+4 VI BABEL,D. ET AL., Z.INORG.ALLGEM.CHEM., 347,282(1966) CA2 IR O8 BODI,F. AND D.BABEL, Z.INORG.ALLGEM.CHEM., 356,17(1965) CA IR O3 SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)	
K +1 VI BODEH,M. AND E.VOSS, Z.INORG.ALLGEM.CHEM., 266,144(1951) K S6 F6 HOPPE,R. AND E.VOSS, Z.INORG.ALLGEM.CHEM., 339,164(1965) K SC O2 STANLEY,E., ACTA CRYST., 9,897(1956) KS S2 O6 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) K F ZACHARIASEN,W.H., ACTA CRYST., 7,783(1954) K3 U O2 F5 ZACHARIASEN,W.H., ACTA CRYST., 9,792(1954) K3 U F7 ZIEGLER,E., Z.KRIST., 9,491(1956) K N O2	
K +1 VII EAMES,E.D. AND H.MONDOK, ACTA CRYST., 15,1288(1962) LI K2 P3 O9,H2 O FARBER,H., Z.KRIST., 20,103(1961) K N O2 HEPMORTH,M.A. ET AL., ACTA CRYST., 16,975(1963) K2 B8 O7.4 H2 O ZACHARIASEN,W.H., J.CHEM.CHEM., 5,919(1957) K B O2 ZUKHOVKA,L.A. AND Z.B.PISKNER, SOVIET PHYS.-CRYST., 9,31(1964) K2 CR2 O7	
K +1 VIII ANDERSSON,S. AND A.D.WADDELEY, ACTA CHEM.SCAND., 15,663(1961) K2 T12 O5 BELTR,F., AND H.C.BAENZIGER, J.AM.CHEM.SOC., 79,3316(1957) K 5 O3 (N H O H) CHRISTICAL,L. ET AL., ACTA CRYST., 7,801(1958) K V O3 H2 O FORRESTER,J.D. ET AL., ACTA CRYST., 16,558(1963) K H2 F3 LINDGKVIST,I. AND M.MORTSELL, ACTA CRYST., 10,406(1957) K2 S2 O5 MAREZIO,M., ACTA CRYST., 16,975(1963) K2 B8 O7.4 H2 O ZACHARIASEN,W.H., ACTA CRYST., 7,783(1954) K B O2 ZUKHOVKA,L.A. AND Z.B.PISKNER, SOVIET PHYS.-CRYST., 9,31(1964) K2 CR2 O7	
K +1 X ANDERSSON,S. AND A.D.WADDELEY, ACTA CHEM.SCAND., 15,663(1961) K2 T12 O5 BETLER,F., AND H.C.BAENZIGER, J.AM.CHEM.SOC., 79,3316(1957) K 5 O3 (N H O H) CHRISTICAL,L. ET AL., ACTA CRYST., 7,801(1958) K V O3 H2 O FORRESTER,J.D. ET AL., ACTA CRYST., 16,558(1963) K H2 F3 LINDGKVIST,I. AND M.MORTSELL, ACTA CRYST., 10,406(1957) K2 S2 O5 MORROG,K., ACTA CRYST., 13,463(1960) K RE O6 PARKER,K., ACTA CRYST., 16,558(1963) K BR F4 SIEGEL,S., ACTA CRYST., 9,693(1956) K BR F4 SUTOR,D.J. ET AL., ACTA CRYST., 7,145(1958) K2 C H2 N O4 WADDELEY,A.D. AND A.D.CRISTY, 17,623(1964) TI NB O5 ZADLICKY,J. AND A.D.WADDELEY, ACTA CRYST., 16,558(1963) K2 S2 O5 ZACHARIASEN,W.H., ACTA CRYST., 7,783(1954) K3 U F7 ZACHARIASEN,W.H. AND H.A.PLATTINGER, ACTA CRYST., 16+376(1963) K B5 O8.4 H2 O	
K +1 XI ARAVINDAKSHAN,C., Z.KRIST., 11,135(1958) K CL O3 BALZD., K. PLIETH, Z.ELEKTROCHEM., 59,545(1955) K2 NT F4 BODEH,M. AND E.TEUFEL, ACTA CRYST., 9,929(1958) K2 HF F6 BROWN,G.M. AND L.A.WALKER, ACTA CRYST., 20,220(1966) K2 NB F7 DOUGHERY,J. AND L.A.WALKER, ACTA CRYST., 20,220(1966) K2 C G O3 HORNIG,K., J.CHEM.SOC., 6,1282(1939) K2 NB P7 KNODK,X., J.CHEM.PHYS., 30,991(1959) K2 CU F6 KROGH-MOE,H., ACTA CRYST., 18,1088(1955) K2 B18 O16 LOOPSTRA,L.I.H. AND C.H.MACBELLAVRAY, ACTA CRYST., 11,349(1958) K H S O4 PALENIK,G.J., INORG.CHEM., 5,507(1967) K MN O8 RODRIGUEZ,J., ACTA CRYST., 18,784(1961) KAD2 S O4.2% H2 O ZACHARIASEN,W.H., ACTA CRYST., 16,558(1963) K2 C H2 N O4 ZACHARIASEN,W.H., Z.KRIST., 7,501(1959) K CL O3 ZACHARIASEN,W.H., Z.KRIST., 89,252(1954) K2 S3 O6 ZACHARIASEN,W.H. AND G.E.ZIEGLER, Z.KRIST., 50,116(1951) K2 CR O4	
K +1 XII BOSTROM,A. ET AL., ARKIV KEMI 4,175(1952) K SB F4 CAMINOLLO,F. ET AL., ACTA CRYST., 21,200(1966) K N4 F2 T12 (S14 O12) EVANS,H.T., JR., Z.KRIST., 114,257(1958) K V O3 KEEN,R.C., Z.KRIST., 9,129(1957) K2 S2 O8 PALENIK,G.J., INORG.CHEM., 5,507(1967) K MN O8 ZACHARIASEN,W.H. AND G.E.ZIEGLER, Z.KRIST., 50,116(1951) K2 CR O4	
K +1 XIII BOEDDE,H. AND H.V.DOREN, ACTA CRYST., 11,60(1958) K TA F6 BOEDDE,H. AND H.V.DOREN, ACTA CRYST., 11,80(1958) K NB F6 ELLINGER,F.H. AND ZACHARIASEN,W.H., J.PHYS.CHEM., 58,405(1954) K PU P02 C 03 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM., 5,1808(1966) K V3 O8 GOTTFRIED,C. AND C.SCHUSTERUS, Z.KRIST., 84,65(1952) K CL O8 HEPWORTH,M.A., ET AL., J.INORG.NUCL.CHEM., 2,79(1956) K OS F6 HOARD,J.L. AND W.B.VINCENT, J.AM.CHEM.SOC., 71,2849(1949) K2 BE F6 KREFFT,J. AND A.D.CRISTY, 17,623(1964) K2 C H2 N O4 LITOT,T., ET AL., ACTA CRYST., 5,209(1952) K2 CA4 BEN AL2 S12 O6 O2 H2 O KATZL., AND H.D.MEGAW, ACTA CRYST., 22,639(1967) K NB O3 SIEGEL,S., ACTA CRYST., 5,685(1952) K2 TI F6 VOUSDEN,P., ACTA CRYST., 4,373(1951) K TA O3 WILHELMIK,M., ACTA CHEM.SCAND., 12,1965(1958) K CR3 O8 WYCKOFF,R.W.G., CRYSTAL STRUCTURES 3,(1965) K AL3 (O H)6 (S O4)2	
LA+3 VI	

Table 1(b) (cont.)

- SILLEN,L.G. AND K.LUNDBORG, Z.ANORG.ALLGEM.CHEM., 252,2(1943) LA2 MO 06
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) LA2 03
- LA+3 VII
GUILLON,M. AND E.F.BERTAUT, COMPT.REND. SER.A+B 262B,962(1966) LA2 TI 05
- LA+3 VIII
BRISSE,F., PH.D.THESES,DALHOUSTE UNIV.,HALIFAX,N.S.(1967) LA2 M2 07
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
- LA+3 IX
HUNTER,E.B.,JR., ET AL., ACTA CRYST. 7,106(1954) LA2 IS 0413.9 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 REK 019
- LA+3 XII
HUNTER,E.B.,JR., ET AL., ACTA CRYST. 7,106(1954) LA2 IS 0413.9 H2 O
- L1+1 IV
BURNS,J.H. AND W.R.BUSING, INORG.CHEM. 4,1510(1965) RB1 LF2
BURNS,J.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 47,1510(1925) CS 02 F2
BURS,J.H. AND E.W.GORDON, ACTA CRYST. 20,1280(1966) LT2 HF4
FANES,J.D. AND H.M.ONDIKA, ACTA CRYST. 15,1280(1962) LI2 K2 P3 09, H2 O
GALY,J. AND A.HARDY, ACTA CRYST. 19,432(1965) LT V2 05
KEFFER,C. ET AL., INORG.CHEM. 6,119(1967) LT3 F4
LARSON,A.C., ACTA CRYST. 18,717(1965) LT2 S 04,H2 O
LIEBAU,F., ACTA CRYST. 14,389(1961) LT2 S12 05
LIEBAU,F., ACTA CRYST. 14,390(1961) LT2 S14 010
MAREZIO,M., ACTA CRYST. 18,313(1965) LT1 6A 01
MAREZIO,M., ACTA CRYST. 19,396(1965) LT1 AL 02
MAREZIO,M. AND J.P.REMIKA, J.CHEM.PHYS. 44,334(1966) LT R 02
REMEIKA,J.P. AND MAREZIO, J.PHYS.CHEM.SOLIDOS 26,2025(1965) LT B 02
SEARS,D.R. AND J.H.BURNS, J.CHEM.PHYS. 41,347(1964) LT2 BF4 ZR FB
ZACHARIASEN,W.H. AND H.A.PLETTINGER, ACTA CRYST. 14,229(1961) LT2 W 04
ZEMANN,A., ACTA CRYST. 13,463(1960) LT3 P 04
ZINTL,E. ET AL., Z.ELEKTROCHEM. 40,548(1934) LT2 O
- L1+1 VI
ABRAHAM,S.C. AND J.L.BERNSTEIN, J.PHYS.CHEM.SOLIDOS 26,2025(1965) LI TA 03
ABRAHAM,S.C. AND H.J.WILLATZKE, J.CHEM.PHYS. 39,2923(1965) LI CU CL3 H2 O
ABRAHAM,S.C. ET AL., J.PHYS.CHEM.SOLIDOS 27,497(1966) LI NR 03
ABRAHAM,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 40,1693(1967) LI TA 03
BRUNTON,G., ACTA CRYST. 21,814(1966) LI U F5
BRUNTON,G., J.INORG.NUCL.CHEM. 29,1631(1967) LIU U F8
BURNS,J.H., ACTA CRYST. 15,1092(1962) LT SR FG
CANNILLO,F. ET AL., ACTA CRYST. 21,200(1966) K N3 FE2 TI2 (SI4 O12)
GALY,J. AND A.HARDY, ACTA CRYST. 19,432(1965) LT V2 05
GELLER,J. AND J.L.DURAND, ACTA CRYST. 13,325(1960) LT P 04
MAREZIO,M. AND J.P.REMIKA, J.CHEM.PHYS. 40,137(1965) LT1 GA 02
MAREZIO,M. AND J.P.REMIKA, J.CHEM.PHYS. 44,334(1966) LT1 AL 02
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) LT F
- LU+3 VI
BARTRAM,S.F., INORG.CHEM. 5,749(1966) LU6 U 012
TEMPLETON,D.H. AND C.H.DAUBEN, J.AM.CHEM.SOC. 76,5237(1954) LU2 03
- LU+3 VIII
BRISSE,F., PH.D.THESES,DALHOUSTE UNIV.,HALIFAX,N.S.(1967) LU2 TI 07
EULER,F. AND J.A.BRUCE, ACTA CRYST. 19,971(1965) LU3 M5 012
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 07
- MG+2 VI
BAUR,W.H., ACTA CRYST. 9,515(1956) MG F2
BAUR,W.H., ACTA CRYST. 15,815(1962) FE S 04.4 H2 O
BAUR,W.H., ACTA CRYST. 16,104(1961) CUM MO8 (C3)4 (O H2)4.8 H2 O
CALVOY,C. CANAD.MERIT. 45,109(1965) MO8 P2 07
CORBIN,D.E.C., ACTA CRYST. 9,991(1956) MG H P3.6 H2 O
GIBBS,G.V. ET AL., AM.MINERALOGIST, IN PRESS, MO9 ST 04
KASPER,J.S. AND J.S.PRENER, ACTA CRYST. 7,246(1954) MO6 MN 08
LUKASZEWCZK,J., BULL.ACAD.POLON.SCI.SPR.CI.CHEM. 11,361(1961) MO2 AS 07
RENTZEPERIS,P.J. AND C.T.SOLDATOS, ACTA CRYST. 11,686(1959) MG S 04
STEINER,N.K.H. AND F.J.SANS, J.CHEM.SOC. 1967,167(1967) CA MN G (C3)2
SUUTALA,T., ACTA CRYST. 13,418(1967) MG H P 04 SMO 0
TAKEUCHI,Y., ACTA CRYST. 5,574(1952) MG2 B2 05
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. 7,780(1954) MG U 04
ZEMANN,A. AND J.ZEMANN, ACTA CRYST. 10,409(1957) K2 MG2 (S 04)3
- MG+2 VII
GIBBS,G.V. AND J.V.SMITH, AM.MINERALOGIST 50,2023(1965) MG3 AL2 SI2 O12
ZEMANN,A. AND J.ZEMANN, ACTA CRYST. 14,835(1965) MG3 AL2 SI2 O12
- MN+2 VI LS
- MN+2 VI HS
ABRAHAM,S.C. AND J.M.REDDY, J.CHEM.PHYS. 43,2533(1965) MN MO 04
BAUR,W.H., ACTA CRYST. 11,468(1958) MN F2
GELLER,S. AND J.L.DURAND, ACTA CRYST. 13,325(1960) LI MN P 04
MROSE,E.M. AND D.E.APPLEMAN, Z.KRIST. 117,16(1962) (MN,FF) BE (P 04) (O H)
PEACOR,D.R. AND M.J.BUERGER, Z.KRIST. 117,33(1962) CA MN SI2 06
RENTZEPERIS,P.J. AND C.T.SOLDATOS, ACTA CRYST. 11,686(1959) S 04
RENTZEPERIS,P.J. AND C.T.SOLDATOS, ACTA CRYST. 13,418(1967) MN TT 04
SNEDDER,W., ACTA CRYST. 14,764(1961) K2 MN (S 04)2 ST 04
SHIRANE,G. ET AL., J.PHYS.SOC.JAPAN 14,1352(1959) MN TT 03
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
ABRAHAM,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 46,3776(1967) DY MN2 05
YAKEL,I.H. ET AL., ACTA CRYST. 16,957(1963) Y MN 03
- 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 M11 (C N16)
- MN+3 VI HS
COLLINS,R. AND W.N.LIPSCOMB, ACTA CRYST. 2,104(1949) H MN 02
DACK,J.H. Z.KRIST. 116,303(1963) MN O H
FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85,267(1962) MN2 O3
HASIW, ET AL., Z.KRIST. 124,428(1967) MN2 03
HEPWORTH,M.A. AND K.H.JACK, ACTA CRYST. 10,345(1957) MN F3
NORRESTAM,R., ACTA CHEM.SCAN. 21,287(1967) MN2 03
ROTTER,S. AND S.J.SCHNEIDER, J.CHEM.SOC. 1967,603(1967) R3 VS V (MHN2 O5)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (PEROVSKITE)
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (MHN2 O5)
- MN+4 VI
ABRAHAM,S.C. AND J.L.BERNSTEIN, J.CHEM.PHYS. 46,3776(1967) DY MN2 05
BOEHM,H. AND W.WENDT, Z.ANORG.ALGEM.CHEM. 10,103(1952) PB2 MN F6
KASPER,J.S. AND J.S.PRENER, ACTA CRYST. 7,246(1954) MO6 MN 08
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)
WADSLY,A.D., ACTA CRYST. 5,165(1955) ZN MN 07,3 H2 O
- MN+4 IV
ABRAHAM,S.C., INORG.CHEM. 6,507(1967) K2 MN 04
- MN+7 IV
FERRARI,A. ET AL., ACTA CRYST. 21,681(1966) SR (MN 04)2.3 H2 O
JAVANA,A. AND A.ENGELBRECHT, PHYS.REV. 96,649(1956) MN 03 F
MOONEY,R.C.L., PHYS.REV. 37,1306(1951) K MN 04
PALENIK,O.J., INORG.CHEM. 6,503(1967) K MN 04
SASVARI,K., Z.KRIST. 99,9(1958) AG MN 04
- MN+7 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) MO F3
- MO+4 VI
ANGELIG,B. AND L.KATZ, ACTA CRYST. 21,682(1966) ZN2 MO3 OR
BRANDT,B. AND A.C.SKAPULSKI, ACTA CHEM.SCAN. 21,651(1967) MO 02
SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) SR MO 03
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) SR MO 03
- MO+5 VI
EDWARDS,A.J. AND R.D.PEACOCK, J.CHEM.SOC. 1961,1253 NA MO F6
KIERKEGAARD,P. AND M.WESTERLUND, ACTA CHEM.SCAN. 16,227(1964) MO P 05
- MO+6 VI
ABRAHAM,S.C. J.CHEM.PHYS. 46,2052(1967) ZN MO 04
ABRAHAM,S.C. AND J.M.REDDY, J.CHEM.PHYS. 43,2533(1965) MN MO 04
ABRAHAM,S.C. ET AL., J.CHEM.PHYS. 47,1261(1967) MO 04
IDEN, R. AND A.ENGELBRECHT, Z.KRIST. 119,190(1964) NA CO2.3 MO3 012
KIMHLBORG,L., ARKIV KEMI 21,357(1963) MO 03
KIMHLBORG,L., ARKIV KEMI 21,365(1963) MO4 O11 (MON), MO4 O11 (O-RH)
LECIEJEWEJCZJ., Z.KRIST. 121,158(1965) PB MO 04
SELEBORG,M., ACTA CHEM.SCAN. 20,2195(1966) K2 MO3 O10
SELEBORG,M., ACTA CHEM.SCAN. 21,299(1967) NA2 MO2 O7
SILLEN,L.G. AND K.LUNDBORG, Z.ANORG.ALGEM.CHEM. 252,2(1943) LA2 MO 06
- MO+6 V
EICK,H.A. AND L.KIMHLBORG, ACTA CHEM.SCAN. 20,1658(1966) V2 MO 08
GATEHOUSE,B.M. AND P.LEVERETT, CHEM.COMM. 1967,374 K2 MO3 O10
SELEBORG,M., ACTA CHEM.SCAN. 20,2195(1966) K2 MO3 O10
- MO+6 VI
ABRAHAM,S.C. J.CHEM.PHYS. 47,1262(1967) ZN MO 04
ABRAHAM,S.C. AND J.M.REDDY, J.CHEM.PHYS. 43,2533(1965) MN MO 04
ABRAHAM,S.C. ET AL., J.CHEM.PHYS. 47,1261(1967) MO 04
IDEN, R. AND A.ENGELBRECHT, Z.KRIST. 119,190(1964) NA CO2.3 MO3 012
KIMHLBORG,L., ARKIV KEMI 21,357(1963) MO 03
KIMHLBORG,L., ARKIV KEMI 21,365(1963) MO4 O11 (MON), MO4 O11 (O-RH)
KIMHLBORG,L., ARKIV KEMI 21,427(1964) MO5 014
KIMHLBORG,L., ARKIV KEMI 21,435(1964) MO18 052
KIMHLBORG,L., ARKIV KEMI 21,461(1964) MO8 023
SELEBORG,M., ACTA CHEM.SCAN. 20,2195(1966) K2 MO3 O10
SMITH,G.W. AND J.A.IBERS, ACTA CRYST. 19,269(1965) CO MO 04
- MO+6 VII
KIMHLBORG,L., ARKIV KEMI 21,427(1964) MO5 014
- N+3 VI
N+5 III
CHERIN,P. ET AL., ACTA CRYST. 23,455(1967) NA N 05
- N+5 VI
NA+4 IV
CORBRIDGE,D.E.C., ACTA CRYST. 15,263(1960) NA5 P3 010
WUNDERLICH,J.A., ACTA CRYST. 10,462(1957) NA O H2 O
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) NA2 O 0
- NA+4 V
HEMLY,P., ACTA CRYST. 10,37(1958) NA O H2 O H2 O
LARSEN,F.K. ET AL., ACTA CHEM.SCAN. 21,1281(1967) NA3 SWN GE10 O30 (O H4)
MCDONALD,R.S. AND D.W.CRUCKSHANK, Z.KRIST. 22,37(1967) NA2 ST 05
ONDRIK,H., ACTA CRYST. 18,268(1955) MA3 P3 010
ONDRIK,H., ACTA CRYST. 18,269(1955) MA3 P3 010
PANT,A.K. AND D.W.M.CRUCKSHANK, ACTA CRYST. B24,13(1968) NA2 SI2 05
ROMERS,C. ET AL., ACTA CRYST. 22,766(1967) NA3 FE5 09
- NA+4 VI
HEMLY,P., ACTA CRYST. 10,37(1958) NA O H2 O H2 O
LARSEN,F.K. ET AL., ACTA CHEM.SCAN. 21,1281(1967) NA3 SWN GE10 O30 (O H4)
MCDONALD,R.S. AND D.W.CRUCKSHANK, Z.KRIST. 22,37(1967) NA2 ST 05
ONDRIK,H., ACTA CRYST. 18,268(1955) MA3 P3 010
ONDRIK,H., ACTA CRYST. 18,269(1955) MA3 P3 010
PANT,A.K. AND D.W.M.CRUCKSHANK, ACTA CRYST. B24,13(1968) NA2 SI2 05
ROMERS,C. ET AL., ACTA CRYST. 22,766(1967) NA3 FE5 09
- NA+4 VII
HEMLY,P., ACTA CRYST. 10,37(1958) NA O H2 O H2 O
LARSEN,F.K. ET AL., ACTA CHEM.SCAN. 21,1281(1967) NA3 SWN GE10 O30 (O H4)
MCDONALD,R.S. AND D.W.CRUCKSHANK, Z.KRIST. 22,37(1967) NA2 ST 05
ONDRIK,H., ACTA CRYST. 18,268(1955) MA3 P3 010
ONDRIK,H., ACTA CRYST. 18,269(1955) MA3 P3 010
PANT,A.K. AND D.W.M.CRUCKSHANK, ACTA CRYST. B24,13(1968) NA2 SI2 05
ROMERS,C. ET AL., ACTA CRYST. 22,766(1967) NA3 FE5 09
- NA+4 VIII
BURNS,J.H., INORG.CHEM. 4,881(1965) NA MO F8
CORBRIDGE,D.E.C., ACTA CRYST. 15,263(1960) NA P3 D10
CROMER,D.T. ET AL., ACTA CRYST. 21,182(1967) NA AL (S 04)2.12 H2 O
CRUCKSHANK,D.W.J., ACTA CRYST. 17,678(1964) NA P2 07,10 H2 O
DAYER,I.D. ET AL., J.AM.CHEM.SOC. 76,1499(1954) NI NI O2
GIESER,F., JR., SCIENCE 154,1853(1966) NA2 BI 05 (O H2)3 H2 O
KIERKEGAARD,P., ARKIV KEMI 18,353(1962) NA2 BI 05 (O H2)3 H2 O
HOOD, R. AND A.ENGELBRECHT, Z.KRIST. 119,171(1964) NA SHN F5
ONDRIK,H., ET AL., ACTA CRYST. 18,355(1963) NA H C O3
WEISS,R., ET AL., ACTA CRYST. 20,534(1966) NA3 H T1 F8
WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) NA F
ZACHARIASEN,W.H., ACTA CRYST. 23,390(1949) NA TH2 F9
ZACHARIASEN,W.H., ACTA CRYST. 23,391(1949) NA TH3 F6
ZALKIN,A. ET AL., ACTA CRYST. 17,1408(1968) NA2 ST 05
ZALKIN,A. ET AL., ACTA CRYST. 17,1408(1968) NA2 ST 05
- NA+4 I VII
ANDERSSON,S. AND A.D.WADSLY, ACTA CRYST. 14,1245(1961) NA2 TI3 07
CANNIOLI,F. ET AL., ACTA CRYST. 21,200(1965) K N3 FE2 TI2 (SI4 O12)
FANG,S. AND Z.KRIST. 194,1(1958) B 02
KIERKEGAARD,P., ARKIV KEMI 18,353(1962) NA W 02 P 08
KOKOROS,P., Z.KRIST. 99,38(1958) NA AL F AS 06
MAREZIO,M. ET AL., ACTA CRYST. 16,599(1963) NA B 02
RAOB-RAMA, ACTA CRYST. 18,738(1961) NA2 C (S 04)2.2 H2 O
- NA+1 VIII
ANDERSSON,S. AND A.D.WADSLY, ACTA CRYST. 14,1245(1961) NA2 TI3 07
ANDERSSON,S. AND A.MAGNELI, ACTA CHEM.SCAN. 11,1065(1957) NB 0
NB+2 VI
ANDERSSON,S. AND A.MAGNELI, ACTA CRYST. 11,1065(1957) NB 0
- NB+3 VI
HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) NA F3
- NB+4 VI
MARINDER,B. AND C.T.PREWITT, TO BE PUBLISHED. R3 VS V (RUTILE)
- NB+5 IV
GATEHOUSE,B.M. AND A.D.WADSLY, ACTA CRYST. 17,1545(1964) NR2 05
- NB+5 VI
ABRAHAM,S.C. ET AL., J.PHYS.CHEM.SOLIDOS 27,997(1966) LI NR 03

Table 1(b) (cont.)

PB+2 XII	HAMILTON,W.C., ACTA CRYST. 10+103(1957) PB (N 0312)
	SAHLK., BEITR.MINERAL.PETROG. 9+11(1963) PB S 04
PB+4 VI	BYSTROM,A., ARKIV KEMI MINERAL.GEOL. 25+13(1947) PB 02
	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 03
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 02
PD+2 IV/SO	WASER,J. ET AL., ACTA CRYST. 6+61(1953) PD 0
PD+2 VI	BARTLETT,N. AND R.MAITLAND, ACTA CRYST. 11+74(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 03
PO+4 VIII	SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED. R VS A (FLUORITE)
PO+6 VI	
PR+3 VI	FERTA+, BULL.SOC.FRANC.MINERAL.CRIST. 85+267(1962) PR2 03
	TEMPLETON,D.H. AND C.H.DAUBEN. J.AM.CHEM.SOC. 76,5237(1954) PR2 03
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 03
PR+4 VIII	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PR 02
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 07
	HELLER,D.P. AND N.C.STEPHENSON, AUSTR.J.PET. 8A+6(1951) K2 PT F6
	SHANNON,R.D., SOLID STATE COMM. IN PRESS. RS VS V (PT 02)
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 03
PU+4 VIII	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PU 02
RA+2 VI	
RB+1 VI	ROGERS,R. AND H.SABROWSKY, Z.INORG.ALLGEM.CHEM. 339+188(1965) RB SC 02
	PLYAKHIN,V.V. AND N.V.BELOV, SOVIET PHYS.+CRYST. 6+685(1962) RB RE2 F5
	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) RA F
RB+1 VII	CORBRIDGE,O.E.C., ACTA CRYST. 9,308(1956) RB P 03
	CRUICKSHANK,D.W.J., ACTA CRYST. 17,681(1964) (RB P 03)
RB+1 VIII	ANDERSSON,S. AND A.D.MADSEY, ACTA CRYST. 15,194(1962) RB2 TI6 013
	BURNS,J.H. AND W.R.BUSING, INORG.CHEM. 4+1510(1965) RB LI F2
	CRUICKSHANK,D.W.J., ACTA CRYST. 17,681(1964) (RB P 03)
RB+1 XI	ELLINGER,F.H. AND W.H.ZACHARIASEN, J.PHYS.CHEM. 58,405(1954) RB AM 02 C 03
	HOARD,J.L. AND V.BLAIR, J.AM.CHEM.SOC. 57+1945(1935) RA 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) CN2 RE2 07
RE+6 VI	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) RE 03
RE+7 IV	KREBS,B. ET AL., CHEM.COMM. (1968)263 RE2 07
	MORROW,J.C., ACTA CRYST. 13+643(1960) K RE 04
RE+7 VI	KREBS,B. ET AL., CHEM.COMM. (1968)263 RE2 07
RH+3 VIII	HEPWORTH,M.A. ET AL., ACTA CRYST. 10,63(1957) RH F3
	SHANNON,R.D., INORG.CHEM. 6+151(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 02)
RH+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)
RH+4 VI	COTTON,F.A. AND J.T.MAGUE, INORG.CHEM. 5+317(1965) RU 02
	DONOHUE,P.C. ET AL., INORG.CHEM. 4+306(1965) BA RU 03
	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. 17,663(1964) MG 5 04,4 H2 0
	BAUR,W.H., ACTA CRYST. 17,1167(1968) MG 5 04,7 H2 0
	BAUR,W.H., ACTA CRYST. 17,1361(1964) FE 5 04,7 H2 0
	CROWDER,D.T. ET AL., ACTA CRYST. 21+383(1964) CS AL (S 04)2,12 H2 0
	GRAEBER,E.J. ET AL., AM.MINERALOGIST 50,1929(1965) K FF (S 04)2
PB+2 IX	BROWN,D. ET AL., J.CHEM.SOC. 1967A,1429 K2 PA F7
PB+2 IV/PY	BOUCHER,M.L. AND D.R.PEACOR, Z.KRIST. 126,98(1968) PB SI 03
	BYSTROM,A. AND L.LEVERS, ACTA CHEM.SCAND. 4+613(1950) A52 PB 02
	KAT.M.I., ACTA CRYST. 14+80(1961) PB 0
PB+2 VI	MAGNELL,I.A., ARKIV KEMI, MINERAL.GEOL. 15R, 3(1942) PB SB2 06
	HOLLERICK., ACTA CHEM.SCAND. 6+81(1954) PB (N H)2 (S 04)2
	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1964) CS PB F3
PB+2 VIII	MINARSKY,J., AM.MINERALOGIST 46,1(1963) PB FE2 (AS ON)2 (O H)2
	LECIEJEWICZ,J., Z.KRIST. 121,158(1968) PR MO 08
	KAY,M.I., ACTA CRYST. 14+80(1961) PB 0
	QUARENIG, AND R.DEPIERRE, ACTA CRYST. 19,287(1965) PB CR 04
	WYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) PB F2
PB+2 IX	COLBY,M.Y. AND L.J.B.LACOSTE, Z.KRIST. 84+294(1932) PB C 03
PB+2 XI	NARAY-SZABO,I. AND S.ARDAY, ACTA CHIM.ACAD.SCT.HUNG. 40+283(1964) PB CR 04

Table 1(b) (cont.)

- GRAEBER,E.J., ET AL., AM.MINERALOGIST 50:1929(1965) MG (H4)2 (S 04)2.6 H2 O
 HOMME,E., SOVIET PHYS.-CRYST. 7:559(1963) CA S 04
 KOKKOROS,P.A., AND P.J., RENTZEPERIS,Z., KRIST. 16:125(1963) MG S 04
 LARSEN,F.K., ET AL., ACTA CRYST. 16:171(1963) LI2 S 04 H2 O
 CONNELL,J.H., AND J.H., DALE, ACTA CRYST. 21:705(1966) NI S 04.6 H2 O
 RENTZEPERIS,P.J., Z.KRIST. 17:431(1962) SN S 04
 SAHLIK., BEITR.MINERAL.PETROG. 9:111(1963) BA S 04
 SAMLIK., BEITR.MINERAL.PETROG. 9:111(1963) PB S 04
 ZALKIN,A., ET AL., ACTA CRYST. 15:1219(1962) CO S 04.6 H2 O
- S 46 VI
- SB+3 IV/P
 BYSTROM,A. AND K.WILHELMII, ARKIV KEMI 3:373(1953) CS SR2 F7
 ROGERS,D. AND A.C., SKAPSKI, PROC.CHEM.SOC. 12:400(1964) SB2 04
 SKAPSKI,A.C. AND D.ROGERS, CHEM.COMM. (1965) 161 SR NB 04
- SB+3 V
 BYSTROM,A. ET AL., ARKIV KEMI 4:175(1952) X S8 F4
 BYSTROM,A. ET AL., ARKIV KEMI 6:77(1955) NA S8 F4
- SB+3 VI
- AURIVILLIUS,B., ARKIV KEMI 3:153(1951) BI S8 04
 AURIVILLIUS,B., ARKIV KEMI 25:205(1956) X S8 04
 BODDIE,J.D. AND J.VOSS, Z.ANORG.ALLEM.CHEM. 264:149(1951) K S8 F6
 BURNS,J.H., ACTA CRYST. 15:1098(1952) LI S8 F6
 BYSTROM,A. ET AL., ARKIV KEMI,MINERAL.GEOL. 156:84(1942) ZN S82 06
 MAGNELIA,I., ARKIV KEMI,MINERAL.GEOL. 156:83(1942) PB S82 06
 ROGERS,D. AND A.C., SKAPSKI, PROC.CHEM.SOC. 12:401(1964) B S82 04
 SCHREWEILUS,N., ARKIV KEMI,MINERAL.GEOL. 169:87(1943) TL S8 F6
 SPIEGELBERG,P., ARKIV KEMI,MINERAL.GEOL. 164:85(1940) K S8 03
 TEUFER,G., ACTA CRYST. 9:539(1956) NA S8 F6
 ZEMANN,J., NEUES JAHRB.MINERAL.MONATSH. 67:1(1959) NA S8 (H)6
- SC+3 VI
 ABRAHAMS,S.C. AND J.L.,BERNSTEIN, J.CHEM.PHYS. 45:2745(1965) SC2 (W 04)3
 CRUTICKSHANK,D.W.J., ACTA CRYST. 15:442(1962) SC2 S12 07
 GELLER,S. ET AL., Z.KRIST. 124:136(1967) SC2 S12 07
 HOPPER,R. AND H.SABINE, Z.ANORG.ALLEM.CHEM. 279:109(1965) K SC2 02
 HOPPER,R. AND H.SABINE, Z.ANORG.ALLEM.CHEM. 289:130(1965) LT SC2 02
 HORNYKIEWICZ,K., LUKASZEWCZ, BULL.ACAD.POL.SCI.,SER.CHEM. 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.SCHNEIDER, Z.ANORG.ALLEM.CHEM. 336:295(1965) CA SC2 04
 NOWACKI,W., Z.KRIST. 101:273(1939)
 ROTTER,S. AND S.J.,SEITZ, Z.ANORG.ALLEM.CHEM. 256:256(1961) R3 VS V (MN2 03)
 SCHUBERT,K. AND S.J.,SEITZ, Z.ANORG.ALLEM.CHEM. 256:256(1961) SC (H)3
 SHANNON,R.D., INORG.CHEM. 6:1479(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 08
 SHANNON,R.D. AND C.T.,PREWITT, TO BE PUBLISHED. R VS A (PYROCHLORE)
- SE-2 VI
- SE+4 VI
- FUESS,M. AND G.WILL, Z.ANORG.ALLEM.CHEM. 358:125(1968) M SE 04
 NARAY-SZABO,I. AND G.ARDAY, ACTA CHIM.ACAD.SCI.HUNG. 39:5(1963) NA2 SE 04
- SE+6 VI
- ABRAHAMS,S.C. AND S.GELLER, ACTA CRYST. 11:437(1958) GROSSULARITE
 BROWN,L.E. AND S.W.BAILLY, ACTA CRYST. 17:134(1964) K AL S13 08
 BURNS,J.H., ACTA CRYST. 15:1098(1952) AL2 S12 05
 CRUCKSHANK,D.W.J., ACTA CRYST. 17:665(1964) SI=0
 GIBBS,G.V. AND J.V.,SMITH, AM.MINERALOGIST 50:2023(1965) MG3 AL2 S13 012
 GLASSER,L.S.D. AND F.P.,GLASSER, ACTA CRYST. 18:453(1965) SR3 ST 05
 LIEBAU,F., ACTA CRYST. 14:395(1961) LI AL S12 05
 LIEBAU,F., ACTA CRYST. 14:399(1961) LI AL S12 010
 MRSCHEIN,E. AND D.F.,APPLEMAN, Z.KRIST. 17:133(1962) AL RE SI 04 H 0 H
 PEPPER,R. AND W.,PRANDI, Z.KRIST. 125:1(1966) AL2 CA3 (SI 04)
 PRANDI,W., Z.KRIST. 119:117(1963) ZN2 MN (H)2 SI 04
 RENTZEPERIS,P.J., Z.KRIST. 119:117(1963) CA2 SI 04
 SMITH,D.K. ET AL., ACTA CRYST. 16:787(1965) CA2 SI 04
 SMITH,J.V. AND S.W.,BATLEY, ACTA CRYST. 16:801(1965) SI=0
 WILLIAMS,P.P. AND H.D.,MEGAW, ACTA CRYST. 17:682(1964) ALBITES
 ZEMANNIA, AND J.ZEMANN, ACTA CRYST. 14:835(1961) MG3 S13 012
- SI+4 VI
 DEADMORE,D.L. AND W.F.,BRADLEY, ACTA CRYST. 15:106(1962) K3 SI F7
 HAMILTON,W.C., ACTA CRYST. 15:353(1962) FE S8 F6.6 H2 O
 HOARD,J.L. AND M.B.,WILLIAMS, J.AM.CHEM.SOC. 64:633(1942) (H)H13 SI F7
 STANKO,J.A. AND I.C.,PAUL, INORG.CHEM. 6:88(1967) (H)H13 CL SI F6
 STISHOV,S.M. AND N.V.,BELOV, DOKL.AKADEM.NAUK SSSR 143:951(1962) ST 02
 VAISSTEINEN,B.K. AND M.M.,ISTASOVA, SOVIET PHYS.-CRYST. 1:2(1956) (H)H2 ST F6
 ZALKINA,A. ET AL., ACTA CRYST. 17:104(1964) NA2 SI F6
- SI+3 VI
 TEMPLETON,D.H. AND C.H.,DAUBEN, J.AM.CHEM.SOC. 76:5237(1954) SMI 03
- SM+3 VIII
 BRITSEFF., 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
- BRITSEFF., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) SN2 M2 07
- SN+4 VI
 BRISKE,W.H., ACTA CRYST. 9:515(1956) SN 02
 BRISKE,F., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 SN2 07
 HOPPER,R. AND W.D.,NATURWISS. 49:254(1962) SN F6
 LARSEN,F.K. ET AL., ACTA CRYST. 21:1281(1966) NAB SN4 GE10 OS0 (H)H4
 RIEVELD,H.M., ACTA CRYST. 20:508(1966) SR3 U 06
 MYCKOFF,R.W.G., CRYSTAL STRUCTURES 2,(1963) SR O
- SR+2 VI
 BARTL,H. AND W.SCHUCKMANN, NEUES JAHRB.MINERAL.MONATSH. 1966:253 SR2 B2 05
 SCHNERING,H.G. AND R.HOPPE, Z.ANORG.ALLEM.CHEM. 312:87(1961) SR ZN 02
 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.ALLEM.CHEM. 312:87(1961) SR ZN 02
 SR+2 VIII
 BARNIGHAUSEN,M. AND J.WEDELEIN, ACTA CRYST. 23:252(1967) SR (H)2 H2 O
 SMITH,H.G., ACTA CRYST. 6:604(1953) SR (H)2 H2 O
 VANHERREWELD,H., ARKIV KEMI 14:17(1959) SR 02.8 H2 O
 WELHELMI,K.A., ARKIV KEMI 26:149(1967) SR CR 07
 WELHELMI,K.A., ARKIV KEMI 26:157(1967) SR2 CR 04
 MYCKOFF,R.W.G., CRYSTAL STRUCTURES 1,(1963) SR O
- SR+2 X
 CLARK,J.R., AM.MINERALOGIST 49:1549(1964) SR B6 09 (O H12.3 H2 O
 FERRARI,A. ET AL., ACTA CRYST. 21:681(1966) SR (MN 04)2.3 H2 O
 ZACHARIASEN,W.H., ACTA CRYST. 1:263(1948) SR3 IP 0412
- SR+2 XII
 DONNAY,J.D.H. ET AL., CRYSTAL DATA DETERMINATIVE TABLES(1963) SR TT 03
 GARSKO,D. AND D.R.,PEACOR, Z.KRIST. 121:204(1965) SR 5 04
 ZACHARIASEN,W.H., ACTA CRYST. 1:263(1948) SR3 IP 0412
- TA+3 VI
 HEPPNER,H.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.SOLID 28:1645(1967) LI TA 03
 ABRAHAMS,S.C. ET AL., J.PHYS.CHEM.SOLID 28:1693(1967) LI TA 03
 BODE,H. AND H.DOREHN, ACTA CRYST. 11:80(1958) K TA F6
 BRITSEFF., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) C02 TA 07
 VOUDSEN,P., ACTA CRYST. 4:373(1951) TA 03
 MYCKOFF,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 FR
- 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 (L12 SN 03)
- TB+4 VIII
 MYCKOFF,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
 HANKEK., NATURWISS. 54:199(1967) ZN TF 03
- TE+4 IV
- TE+4 VI
- TE+6 VI
- TH+4 VI
 RUHR., AND A.D.,WADSLY, ACTA CRYST. 21:974(1966) TH TIP 06
- TH+4 VIII
 LUNDGREN,G., ARKIV KEMI 2:535(1950) TH (O H12 S 04
 LUNDGREN,G. AND L.G.,SILLEN, ARKIV KEMI 1:277(1949) TH (O H12 CR 04 H2 O
 MYCKOFF,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.P. AND P.BLAU, ACTA CRYST. 9:121(1956) CA TI2 ON
 NEUMAYER,M. AND H.D.,DEDEHAN, 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.,WADSLY, ACTA CRYST. 15:663(1961) K2 TI2 05
 GUILLERM,H. AND E.F.,BERTAUT, COMPT.REND.,SER.AB 262:962(1966) L12 TI 05
 MOORE,P.B. AND J.L.,LOUISIANATH, SCIENCE 156:1361(1967) BA2 (TI O) S12 07
- TI+4 VI
 ANDERSSON,S. AND A.D.,WADSLY, ACTA CRYST. 14:1245(1961) NA2 TI3 07
 BAUDR.,AND A.D.,WADSLY, ACTA CRYST. 15:194(1962) NA2 TI6 D13
 BAUDR.,W.H., ACTA CRYST. 9:515(1956) TI 02
 BRISKI,T., PH.D.THESIS,DALHOUSIE UNIV.,HALIFAX,N.S.(1967) M2 TI2 07
 EVANS,T., J.AM.CHEM.SOC. 37:1(1915) BA TI 02
 FISCHER,J. ET AL., ACTA CRYST. 22:338(1967) CU TI F6,4 H2 O
 KNOPF,O. ET AL., CAN.J.CHEM. 43:281(1965) ER2 TI12 07
 RUHR., AND A.D.,WADSLY, 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) KC TI F6
 TEMPLETON,D.H. AND C.H.,DAUBEN, J.AM.CHEM.SOC. 71:1515(1960) RA TI4 09
 WEISSER,H., ACTA CRYST. 20:53(1966) NA3 H TI F8
 MYCKOFF,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 S8 F6)
- TL+1 VIII
 BROSSAT,C., Z.ANORG.ALLEM.CHEM. 239:301(1958) TL AL F4
 SHANNON,R.D. AND C.T.,PREWITT, UNPUBLISHED DATA. R3 VS V (SCHEELITE)
- TL+1 XII
 SCHREWEILUS,N., ARKIV KEMI MINERAL.GEOL. 168:87(1943) TL SR F6
 SHANNON,R.D. AND C.T.,PREWITT, UNPUBLISHED DATA. R3 VS V (TL S8 F6)
- TL+3 VI
 HOPPER,R. AND H.J.,ROMBORN, Z.ANORG.ALLEM.CHEM. 329:199(1964) NA TL 02
 JOHANSSON,S., 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 06
 PAPAMANTLOS,P., Z.KRIST. 126:143(1968) TL2 03
- TL+3 VIII
 HOEKSTRA,H.R. AND S.SIEGEL, INORG.CHEM. 7:141(1966) TL? PT? 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 +6 VIII
 BRUNTON,G., ACTA CRYST. 21:814(1961) LI U F5
 BRUNTON,G., J.INORG.NUCL.CHEM. 29:1631(1967) L14 U F8
 BRUNTON,G., ACTA CRYST. 9:553(1956) UE 04
 LARSON,A.C., ET AL., ACTA CRYST. 17:555(1964) U F4
 WICKOFF,F.R.W.G., CRYSTAL STRUCTURES 1,(1963) U 02
 ZACHARIASEN,W.H., ACTA CRYST. 2:390(1949) N42 U F6

U +6 IX
 ZACHARIASEN,W.H., ACTA CRYST. 2:390(1949) U2 F9

U +5 VI
 ROSENWEIG,A., AND D.T.CROMER, ACTA CRYST. 23:965(1967) CS U F6
 ZACHARIASEN,W.H., ACTA CRYST. 2:390(1949) K2 U F6
 ZACHARIASEN,W.H., ACTA CRYST. 2:390(1949) N42 U F6

U +5 VII
 LOOPSTRABO,B.O., ACTA CRYST. 17:651(1964) U3 08
 ZACHARIASEN,W.H., ACTA CRYST. 2:296(1949) U F5

U +6 II
 ZACHARIASEN,W.H., ACTA CRYST. 7:783(1954) K3 U 02 F5

U +6 IV
 ROSS,M. ET AL., AM.MINERALOGIST 49:1603(1964) CU (U 02 P 04)2,R H2 O

U +6 VI
 BARTMAN,S.F., INORG.CHEM. 5:789(1966) LU6 U 012
 DEBEITS,P.C., ACTA CRYST. 21:589(1966) U 03
 RIETVELD,H.W., ACTA CRYST. 20:508(1966) M3 U 06
 SIEGEL,S., AND H.R. HOEKSTRA, ACTA CRYST. B24:967(1968) CU U 04
 STEARNS,H., ACTA CRYST. 23:264(1967) P83 U 06
 WICKOFF,F.R.W.G., CRYSTAL STRUCTURES 2,(1964) U 03
 ZACHARIASEN,W.H., ACTA CRYST. 7:783(1954) N6 U2 04

U +6 VII
 DEBEITS,P.C., ACTA CRYST. 21:589(1966) U 03
 LOOPSTRABO,B.O., ACTA CRYST. 17:651(1964) U3 08
 SIEGEL,S. ET AL., ACTA CRYST. 28:292(1966) U 03

V +2 VI
 MONTGOMERY,H., ET AL., ACTA CRYST. 22:775(1967) V (N H4)2 (S 04)2,6 H2 O
 WICKOFF,F.R.W.G., CRYSTAL STRUCTURES 1,(1963) V O

V +3 VI
 HERPOMTH,W.H., ET AL., ACTA CRYST. 10:43(1957) V F3
 NEHMANN,R.E., AND Y.M.DEEHAAN, Z.KRIST. 117:235(1962) V2 03
 SHANNON,R.D., INORG.CHEM. 6:1479(1967) VS V (PE60VSITE)
 WICKOFF,F.R.W.G., CRYSTAL STRUCTURES 2,(1964) CE V3

V +4 VI
 ANDERSON,G., ACTA CHEM.SCAND. 10:623(1956) V 02
 KIERKEGAARD,P., AND J.LONGO, UNPUBLISHED DATA, V 02
 SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED, R3 VS V (RUTILE)
 WICKOFF,F.R.W.G., CRYSTAL STRUCTURES 2,(1964) CA V 03

V +5 IV
 CHRIST,C.L., ET AL., ACTA CRYST. 7:801(1954) K V 03 H2 O
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180(1966) K V 03
 GALY,J., AND A.HARDY, ACTA CRYST. 19:432(1965) LI V2 05'

V +5 VI
 CHRIST,C.L., ET AL., ACTA CRYST. 7:801(1954) K V 03 H2 O
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180(1966) K V 03
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180B(1966) CS VS 03
 SWALLOW,A.G., ET AL., ACTA CRYST. 21:397(1966) CA V10 028,17 H2 O

M +6 VI
 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 03 H2 O
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180B(1966) K V 03
 GALY,J., AND A.HARDY, ACTA CRYST. 19:432(1965) LI V2 05'

V +5 VI
 CHRIST,C.L., ET AL., INORG.CHEM. 5:2131(1966) V O (C H3)3
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180B(1966) K V 03
 EVANS,H.T., JR., AND S.BLOCK, INORG.CHEM. 5:180B(1966) CS VS 03
 SWALLOW,A.G., ET AL., ACTA CRYST. 21:397(1966) CA V10 028,17 H2 O

M +6 VI
 SHANNON,R.D. AND C.T.PREWITT, TO BE PUBLISHED, R3 VS V (IPUTILE)

M +6 IV
 ABRAHAMS,S.C., AND J.L.BERNSTEIN, J.CHEM.PHYS. 45:2745(1966) SC2 (W 08)3
 BURBANK,D.R., ACTA CRYST. 18:BB(1968) WA W 04
 TEMPLETON,D.H., AND A.ZALKIN, ACTA CRYST. 16:762(1963) FU2 (W 04)3
 ZACHARIASEN,W.H., AND H.A.PLETTINGER, ACTA CRYST. 14:229(1961) LI2 W 04
 ZALKIN,A. AND D.H.TEMPLETON, J.CHEM.PHYS. 40:501(1964) CA W 04

M +6 VI
 KEELING,R.O., JR., ACTA CRYST. 10:209(1957) NI W 00
 KIERKEGAARD,P., ACTA CHEM.SCAND. 12:1715(1958) W P 02 07
 LOOPSTRABO,B.O., AND P.BOLDRINI, ACTA CRYST. 21:158(1966) W 03

T +3 VI
 BRISSE,F., INORG.CHEM. 5:749(1966) Y6 U 012;LU6 U 012
 BERTAUT,F., AND J.HARESCHAL, COMPT.REND. 257:867(1963) Y AL 03
 FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85:267(1962) Y2 03
 HARRIS,L.A., AND H.I.YAKEL, ACTA CRYST. 22:354(1967) Y2 BE 08
 MULLER-BUSCHBAUM,H., Z ANORG.ALLOGM.CHEM. 35:13(1968) SR Y2 04
 PATON,M.G., AND E.N.MASLEN, ACTA CRYST. 19:307(1965) Y2 03
 SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED, R VS A (PYROCHLOR)

T +3 VII
 BAGLIO,J.A., AND G.GASHUROV, ACTA CRYST. B29:292(1968) Y V 04
 BATT,A., AND B.PОСT, ACTA CRYST. 15:1268(1962) YF5 012
 BRITSE,F., PH.D.THESES, DALHOUSIE UNIV., HALIFAX,N.S.(1967) Y2 M2 07
 CUNNINGHAM,J.A., ET AL., INORG.CHEM. 6:495(1967) Y (C H7 0213,3 H2 O
 EULER,F., AND J.H.VERNON, J.CHEM.PHYS. 19:117(1963) Y5 M5 012
 GEDDIE,R., AND M.A.GILDED, ACTA CRYST. 10:239(1957) Y P 04
 KRSTANOVIC,I., Z.KRIST. 121:151(1965) Y P 04
 MILLIGAN,W.O., AND L.W.VERNON, J.CHEM.PHYS. 56:145(1962) Y V 04
 ZALKIN,A. AND D.H.TEMPLETON, J.AM.CHEM.SOC. 75:2953(1953) Y F3

T +3 IX
 FRICKE,R., AND W.DURRWACHTER, Z.ANORG.ALLOGM.CHEM. 259:307(1949) Y (O H3)

YB+3 VI
 FERT,A., BULL.SOC.FRANC.MINERAL.CRIST. 85:267(1962) YB2 03
 TEMPLETON,D.H., AND C.H.DAUBEN, J.AM.CHEM.SOC. 76:5237(1954) TB2 03

YB+3 VIII
 EULER,F., AND J.A.BRUCE, ACTA CRYST. 19:971(1965) YB3 M5 012
 MILLIGAN,W.O., AND L.W.VERNON, J.CHEM.PHYS. 56:145(1962) Y V 04
 SHANNON,R.D., AND C.T.PREWITT, TO BE PUBLISHED, R VS A (PYROCHLOR)

Zn+2 IV
 ANSEL,G.B., AND L.KATZ, ACTA CRYST. 21:482(1961) ZN2 H03 08
 CALVO,C., J.CHEM.PHYS. 11:141(1963) ZN2 (P 06)2
 COREY,R.B., AND R.W.G.WICKOFF, Z.KRIST. 86:81(1963) ZN (H)2
 PREWITT,C.T., ET AL., Z.KRIST. 129:115(1967) PB ZN SI 01
 RENTZEPERIS,P.J., Z.KRIST. 119:117(1967) ZN2 MN 10 H2 SI 04
 SCHNEIDER,H.G., AND R.HOPPE, Z.ANORG.ALLOGM.CHEM. 312:87(1961) SR ZN 02
 SCHNEIDER,H.G., ET AL., Z.ANORG.ALLOGM.CHEM. 353:241(1960) RA ZN 02
 SMITH,N.P., ET AL., Z.KRIST. 119:375(1964) ZN0 (R 02)6
 SPITSBERGER,U., ACTA CRYST. 13:197(1960) RA ZN 02
 STEPHENS,J.S., AND C.CALVO, CAN.J.CHEM. 45:2303(1967) ZN3 (P 04)2

Zn+2 V
 ANSEL,G.B., AND L.KATZ, ACTA CRYST. 21:482(1961) ZN H0 04
 COCCO,G., ET AL., Z.KRIST. 123:321(1966) ZN2 IO H1 P 04
 HANKE,K., NATURWISS. 56:199(1967) TE 03
 MONTGOMERY,H., AND E.C.LINGAFELTER, ACTA CRYST. 16:748(1963) ZN (C H7 0212 H2
 PLEITH,K., AND G.SANGER, Z.KRIST. 124:91(1967) ZN2 CU AS2 04
 STEPHENS,J.S., AND C.CALVO, CAN.J.CHEM. 45:2303(1967) ZN3 (P 04)2

Zn+2 VI
 BRAHAMS,S.C., J.CHEM.PHYS. 46:2052(1967) ZN MO 04
 ANSEL,G.B., AND L.KATZ, ACTA CRYST. 21:482(1961) ZN2 H03 08
 BATES,C.H., ET AL., SCIENCE 137:993(1962) ZN 0
 BAUR,H., AND A.ZALKIN, ACTA CRYST. 11:488(1958) ZN F2
 BYSTRÖM,A., ET AL., ARKIV KEMI:MINERAL.GEOL. 15B:64(1942) ZN S82 06
 CALVO,C., J.CHEM.PHYS. 43:1197(1965) ZN2 P2 OT 07
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 CALVO,C., J.CHEM.PHYS. 43:2871(1965) ZN2 (P 04)2
 CALVO,C., J.CHEM.PHYS. 43:2879(1965) ZN2 (P

* 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 VIAl^{3+} and some of these have been omitted to save space. For those ions and coordinations which occur rarely such as IVCr^{5+} or VZn^{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 dis-

tances 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 isotopic 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,

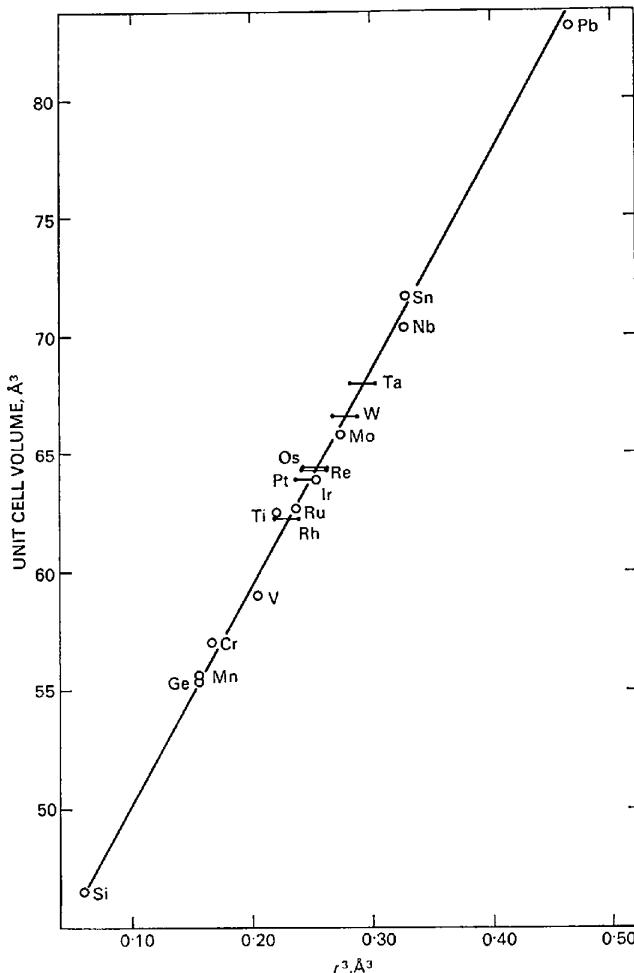


Fig. 1. Cell volume vs. r^3 for compounds with the rutile structure. Circles represent data from structure refinements, and the horizontal lines are for compositions where only the cell volumes are known (after Shannon, 1968).

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.

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 VIIIO_2^- because of the lack of examples. No calculations for IVF^- or VIF^- 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 $r^{(VIF^-)} = 1.19 \text{ \AA}$ and an assumed difference between six-coordinated oxygen and fluorine radii of 0.07 \AA 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 num-

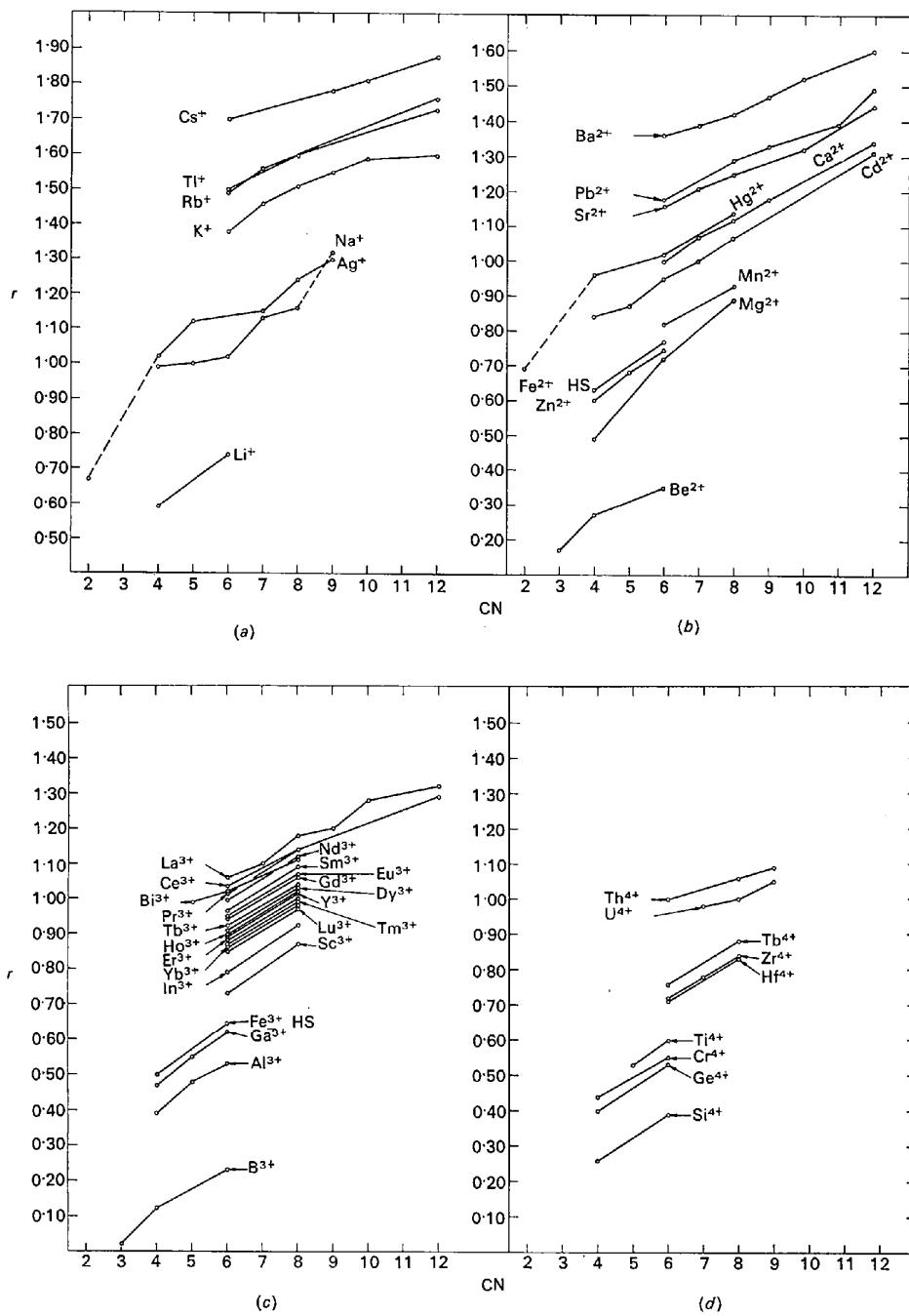


Fig. 2. 'Effective' ionic radius vs. CN for some common cations.

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,

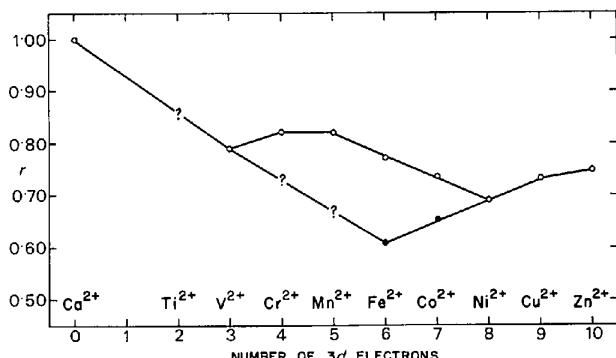


Fig. 3. 'Effective' ionic radius *vs.* number of 3d electrons for divalent transition-metal ions.

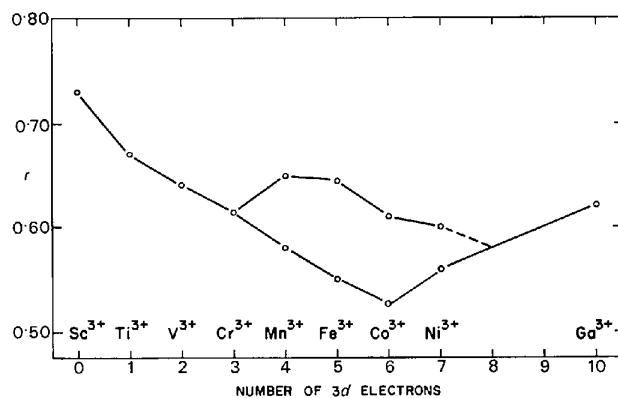


Fig. 4. 'Effective' ionic radius *vs.* number of 3d electrons for trivalent transition-metal ions.

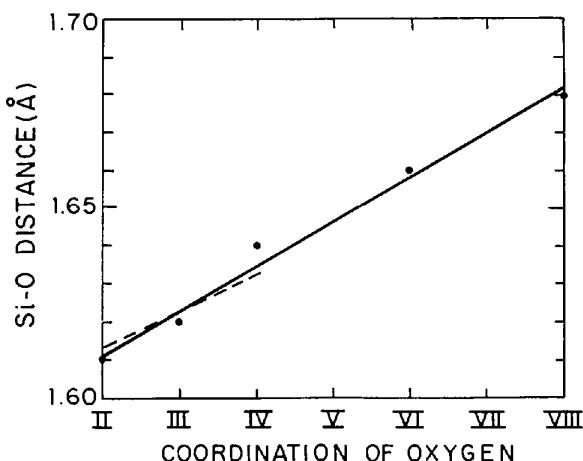


Fig. 5. Si-O distance *vs.* oxygen coordination. The dashed line represents the variation of Si-O distances reported by Smith & Bailey (1963).

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.

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 O²⁻ 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}				R _{Obs}	Year	Compound	Distance	R _{Calc}				R _{Obs}	Year
		Zach.	Pauling	Ahrens	S & P					Zach.	Pauling	Ahrens	S & P		
AgFeO ₂	V _{II} Ag-V _{IV} O	--	2.36	2.40	2.05	2.06	68	KF	V _{II} K-V _{IV} F	2.66	2.69	2.66	2.71	2.673	63
Al ₂ SiO ₅	IV _{Al} -III ₀	1.78	1.78	1.81	1.75	1.77	63	KMnO ₄	V _{II} K-III ₀	2.90	2.83	2.82	2.86	2.89	67
AlPO ₄	IV _{Al} -II ₀	1.78	1.78	1.81	1.74	1.74	66	Li ₂ WO ₄	IV _{L1} -III ₀	1.99	1.84	1.91	1.95	1.96	61
Al ₂ O ₃	VI _{Al} -IV ₀	1.90	1.90	1.91	1.91	1.91	62	LiAlO ₂	IV _{L1} -IV ₀	1.99	1.84	1.91	1.97	2.00	65
LiAlO ₂	IV _{Al} -IV ₀	1.78	1.78	1.81	1.77	1.76	65	Li ₂ SiO ₂	IV _{L1} -IV ₀	1.99	1.84	1.91	1.97	1.98	65
LiAlO ₂	VI _{Al} -V ₀	1.90	1.90	1.91	1.93	1.90	66	Li ₂ Si ₂ O ₅	IV _{L1} -III ₀	1.99	1.84	1.91	1.95	1.94	61
BeAl ₂ O ₄	VI _{Al} -IV ₀	1.90	1.90	1.91	1.91	1.914	63	LiAlO ₂	VI _{L1} -VI ₀	2.12	2.00	2.08	2.14	2.12	66
AlF ₃	VI _{Al} -I ₀ F	1.77	1.86	1.84	1.815	1.80	51	LiGaO ₂	VI _{L1} -VI ₀	2.12	2.00	2.08	2.14	2.14	65
As ₂ O ₅ *5/3H ₂ O	IV _{As} -II ₀	--	1.78	1.75	1.685	1.69	66	LiF	VI _{L1} -VI ₀	2.01	1.96	2.01	2.07	2.008	63
CdF ₄ O ₇	III _B -III ₀	1.35	1.38	1.40	1.38	1.37	66	Li ₄ UF ₈	VI _{L1} -II ₀ F	2.01	1.96	2.01	2.025	2.08	67
CaB ₂ O ₄	III _B -III ₀	1.35	1.38	1.40	1.37	1.37	63	LiUF ₅	VI _{L1} -III ₀ F	2.01	1.96	2.01	2.04	2.055	66
LiBO ₂	IV _B -IV ₀	1.42	1.47	1.50	1.50	1.47	65	MgO	VI _{Mg} -VI ₀	2.10	2.05	2.06	2.12	2.105	63
γ -HBO ₂	IV _B -II ₀	1.42	1.47	1.50	1.47	1.47	63	MgSO ₄ *4H ₂ O	VI _{Mg} -IV ₀	2.10	2.05	2.06	2.10	2.076	62
KB ₂ O ₈	IV _B -III ₀	1.42	1.47	1.40	1.48	1.46	65	MgF ₂	VI _{Mg} -III ₀ F	1.98	2.01	1.99	2.02	1.992	56
BaO	VI _{Ba} -VI ₀	2.76	2.75	2.74	2.76	2.76	63	MgHPO ₄ *3H ₂ O	VI _{Mg} -III ₀	2.10	2.05	2.06	2.08	2.084	67
BaGeO ₃	VIII _{Ba} -IV ₀	2.84	2.82	2.80	2.80	2.785	62	MnMoO ₄	VI _{HS} Mn-III ₀	--	2.20	2.20	2.18	2.164	65
BaF ₂	VIII _{Ba} -IV _F	2.68	2.79	2.74	2.73	2.69	63	Mg ₂ MnO ₈	VI _{Mn} -V ₀	--	1.94	2.20	1.93	1.928	54
Ba(OH) ₂ *8H ₂ O	VIII _{Ba} -IV ₀	2.84	2.82	2.80	2.80	2.74	64	DyMn ₂ O ₅	VI _{Mn} -IV ₀	--	1.94	2.20	1.92	1.92	67
BaGe ₄ O ₉	X _{Ba} -III ₀	2.90	2.88	2.84	2.88	2.96	66	MnO ₂	VI _{Mn} -III ₀	--	2.06	2.10	2.01	2.011	67
BaSO ₄	XII _{Ba} -IV ₀	2.96	2.94	2.89	2.98	2.95	63	Zn ₂ Mo ₃ O ₈	VI _{Mn} -III ₀	--	2.06	2.10	2.02	2.02	66
Ba ₂ (PO ₄) ₂	XII _{Ba} -V ₀	2.96	2.94	2.89	2.99	3.01	48	MnMoO ₄	IV _{Mo} -III ₀	1.82	1.94	1.92	1.78	1.763	65
Y ₂ BeO ₄	III _{Be} -IV ₀	1.55	1.47	1.51	1.55	1.55	67	PbMoO ₄	IV _{Mo} -III ₀	1.82	1.94	1.92	1.78	1.772	65
BeO	IV _{Be} -IV ₀	1.63	1.57	1.61	1.65	1.649	64	NaF	VI _{Na} -VI ₀ F	2.31	2.31	2.30	2.35	2.31	63
Li ₂ BeF ₄	IV _{Be} -III ₀ F	1.53	1.53	1.54	1.57	1.554	66	Na ₂ SiF ₆	VI _{Na} -III ₀ F	2.31	2.31	2.30	2.32	2.32	64
Bi ₄ Si ₃ O ₁₂	V _{II} Bi-III ₀	--	2.36	2.38	2.38	2.385	66	NaHCO ₃	VI _{Na} -IV ₀	2.44	2.35	2.37	2.40	2.44	65
Bi ₂ GeO ₅	V _{II} Bi-III ₀	--	2.36	2.38	2.35	2.36	64	Nb ₂ O ₅	VI _{Nb} -II ₀	2.00	2.10	2.09	1.99	1.99	64
Ca ₂ SiO ₄	VIII _{Ca} -IV ₀	2.50	2.47	2.48	2.50	2.515	64	GaNbO ₄	VI _{Nb} -III ₀	2.00	2.10	2.09	2.00	2.031	65
CaNO ₄	VIII _{Ca} -III ₀	2.50	2.47	2.48	2.48	2.461	65	LiNbO ₃	VI _{Nb} -IV ₀	2.00	2.10	2.09	2.02	2.00	66
CaB ₂ O ₄	VIII _{Ca} -III ₀	2.50	2.47	2.48	2.48	2.505	63	MgF ₂	VI _{Ni} -III ₀ F	--	2.08	2.02	2.00	2.00	58
CaF ₂	VIII _{Ca} -IV _F	2.34	2.43	2.40	2.43	2.37	63	MgSO ₄ *6H ₂ O	VI _{Ni} -III ₀	--	2.12	2.09	2.06	2.06	66
CaSO ₄	VIII _{Ca} -III ₀	2.50	2.48	2.48	2.48	2.46	63	Ba ₂ NiF ₆	VI _{Ni} -V ₀ F	--	2.08	2.02	2.02	2.01	67
CdSO ₄	IV _{Cd} -II ₀	--	2.28	2.28	2.19	2.168	63	PbO ₂	VI _{Pb} -III ₀	--	2.24	2.24	2.135	2.16	47
CdO	VI _{Cd} -VI ₀	--	2.37	2.37	2.35	2.348	63	RuO ₂	VI _{Ru} -III ₀	--	2.03	2.07	1.98	1.971	66
Cd ₂ V ₂ O ₇	VI _{Cd} -III ₀	--	2.37	2.37	2.31	2.31	67	LiSbF ₆	VI _{Sb} -II ₀ F	--	1.98	1.95	1.895	1.88	62
CePO ₄	VIII _{Ce} -III ₀	--	2.57	2.53	2.50	2.50	50	Sb ₂ O ₄	VI _{Sb} -II ₀	--	2.02	2.02	1.96	1.97	64
CoF ₂	VI _{HS} Co-III ₀ F	--	2.10	2.05	2.035	2.04	58	K ₃ Sn ₅ O ₁₄	VI _{Sb} -IV ₀	--	2.02	2.02	1.99	1.984	66
CoMoO ₄	VI _{HS} Co-VI ₀	--	2.14	2.12	2.095	2.08	65	Sc ₂ O ₃	VI _{Sc} -II ₀	2.16	2.21	2.21	2.11	2.11	67
CoO	VI _{HS} Co-VI ₀	--	2.14	2.12	2.135	2.133	63	Sc ₂ (W ₄ O ₁₃) ₃	VI _{Sc} -II ₀	2.16	2.21	2.21	2.08	2.063	66
Cr ₂ O ₃	VI _{Cr} -IV ₀	--	2.09	2.03	1.995	1.99	62	CaSc ₂ O ₄	VI _{Sc} -V ₀	2.16	2.21	2.21	2.12	2.12	65
Cr ₅ ¹²	VI _{Cr} -II ₀	--	2.09	2.03	1.965	1.97	65	ScF ₃	VI _{Sc} -II _F	2.02	2.17	2.14	2.015	2.01	51
CrF ₃	VI _{Cr} -II _F	--	2.05	1.96	1.90	1.90	60	ScPO ₄	VIII _{Sc} -III ₀	2.24	2.28	2.29	2.23	2.23	56
PbCrO ₄	IV _{Cr} -III ₀	1.65	1.82	1.66	1.65	1.65	65	SiO ₂	IV _{Si} -II ₀	1.63	1.71	1.72	1.61	1.607	66
LiCr ₃ O ₈	IV _{Cr} -III ₀	1.65	1.82	1.66	1.65	1.67	67	KAlSi ₃ O ₈	IV _{Si} -III ₀	1.63	1.71	1.72	1.62	1.61	64
CuFeO ₂	II _{Cu} -IV ₀	--	2.01	2.10	1.84	1.83	68	Ca ₂ SiO ₄	IV _{Si} -IV ₀	1.63	1.71	1.72	1.64	1.644	65
Dy ₃ Fe ₅ O ₁₂	VIII _{Dy} -IV ₀	--	2.38	2.40	2.40	2.40	65	SiO ₂	VI _{Si} -III ₀	1.73	1.81	1.82	1.75	1.768	66
Bu ₃ O ₄	VI _{Bu} -VI ₀	--	2.43	2.38	2.35	2.340	66	K ₃ SiF ₇	VI _{Si} -IV ₀	1.60	1.77	1.75	1.71	1.70	62
FeO	VI _{Fe} -VI ₀	--	2.16	2.14	2.17	2.155	63	Na ₂ SiF ₆	VI _{Si} -III _F	1.60	1.77	1.75	1.70	1.695	64
FeWO ₄	VI _{Fe} -III ₀	--	2.16	2.14	2.13	2.104	67	(NH ₄) ₂ SiF ₆	VI _{Si} -II _F	1.60	1.77	1.75	1.685	1.674	56
Fe ₂ SiO ₄	VI _{Fe} -IV ₀	--	2.16	2.14	2.15	2.172	65	SnO ₂	VI _{Sn} -III ₀	--	2.11	2.11	2.05	2.053	56
FeGe(OH) ₆	VI _{Fe} -III ₀	--	2.16	2.14	2.12	2.13	61	SnF ₄	VI _{Tl} -II _F	--	2.07	2.04	1.975	2.14	62
Y ₃ Fe ₅ O ₁₂	IV _{Fe} -IV ₀	--	1.94	1.94	1.88	1.88	62	SrF ₂	VIII _{Sr} -IV _F	2.54	2.56	2.52	2.51	2.51	63
Na ₃ Fe ₅ O ₉	IV _{Fe} -IV ₀	--	1.94	1.94	1.88	1.867	67	Ti ₂ O ₃	VI _{Tl} -IV ₀	--	2.16	2.16	2.05	2.040	62
Fe ₂ O ₃	VI _{Fe} -IV ₀	--	2.04	2.04	2.025	2.030	66	TiF ₃	VI _{Tl} -II _F	--	2.12	2.09	1.955	1.97	56
Fe ₂ P ₃	VI _{Fe} -II _F	--	2.00	1.97	1.93	1.92	57	TiO ₂	VI _{Tl} -III ₀	1.96	2.08	2.08	1.965	1.959	56
Ga ₂ O ₃	VI _{Ga} -III ₀	--	2.02	2.02	1.98	1.996	65	Er ₂ Ti ₂ O ₇	VI _{Tl} -IV ₀	1.96	2.08	2.08	1.985	1.955	65
α -Ga ₂ O ₃	VI _{Ga} -IV ₀	--	2.02	2.02	2.00	2.00	65	Na ₂ Ti ₂ O ₇	VI _{Tl} -V ₀	1.96	2.08	2.08	1.995	1.99	61
Y ₃ Ga ₅ O ₁₂	VI _{Ga} -IV ₀	--	2.02	2.02	1.980	1.995	65	V ₂ O ₃	VI _V -IV ₀	--	2.14	2.14	2.02	2.01	62
Ga ₂ O ₃	VI _{Ga} -II _F	--	1.98	1.95	1.905	1.89	59	V ₂ O ₂	VI _V -III ₀	--	2.00	2.03	1.95	1.937	56
BaGeO ₄	VI _{Ge} -III ₀	--	1.93	1.93	1.900	1.877	66	Ca ₂ V ₂ O ₇	IV _V -III ₀	1.77	1.89	1.89	1.715	1.717	67
Na ₄ Ge ₉ O ₂₀	VI _{Ge} -II ₀	--	1.93	1.93	1.910	1.907	63	FeWO ₄	VI _W -III ₀	--	2.02	1.94	1.94	1.94	67
In ₂ O ₃	VI _{In} -IV ₀	--	2.21	2.21	2.17										

Fig. 5 shows how the average Si-O distance would vary with average oxygen coordination in silicates although most silicates fall in the range $\text{II}^{\text{O}}\text{--IV}^{\text{O}}$ 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 [$r(\text{VI}^{\text{O}}\text{O}^{2-}) - r(\text{II}^{\text{O}}\text{O}^{2-}) = 0.05 \text{ \AA}$] than the change in radii with cation CN [$r(\text{VIII}^{\text{Mg}}\text{Cd}^{2+}) - r(\text{IV}^{\text{Mg}}\text{Cd}^{2+}) = 0.41 \text{ \AA}$]. 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

<u>Distance</u>	<u>CN of O²⁻</u>	<u>Compound</u>	<u>R_{obs.}</u>	<u>R_{calc.}</u>	<u>Distance</u>	<u>CN of O²⁻</u>	<u>Compound</u>	<u>R_{obs.}</u>	<u>R_{calc.}</u>
$\text{IV}_{\text{Al}-0}$	II	$\text{LiAlSi}_4\text{O}_{10}$	1.720	1.74	$\text{VI}_{\text{Sc}-0}$	II	$\text{Sc}_2(\text{WO}_4)_3$	2.063	2.08
		AlPO_4	1.739	"		III	$\gamma\text{-ScOOH}$	2.10	2.09
	III	KAlSi_3O_8 (microcline)	1.741	1.75			Sc(OH)_3	2.08	"
		$\text{NaAlSi}_3\text{O}_8$ (low albite)	1.737	"		IV	Sc_2O_3	2.11	2.11
		Al_2SiO_5 (sillimanite)	1.770	"		V	CaSc_2O_4	2.122	2.12
	IV	LiAlO_2	1.761	1.77		VI	KScO_2	2.12	2.13
$\text{VI}_{\text{Al}-0}$	II	$\text{NaAl}(\text{SO}_4)_2\cdot 12\text{H}_2\text{O}$	1.881	1.88			LiScO_2	2.11	"
		$\text{CsAl}(\text{SO}_4)_2\cdot 12\text{H}_2\text{O}$	1.882	"			RbScO_2	2.12	"
	III	Al_2SiO_5 (kyanite)	1.906	1.89	$\text{IV}_{\text{Si}-0}$	II	SiO_2 (quartz)	1.607	1.610
	IV	$\text{Mg}_2\text{Al}_2\text{Si}_3\text{O}_{12}$	1.886	1.91			SiO_2 (low cristobalite)	1.605	"
		Al_2O_3	1.91	1.91			SiO_2 (coesite)	1.613	"
	VI	LiAlO_2	1.90	1.93			Al_2SiO_5 (sillimanite)	1.615	"
$\text{VI}_{\text{Cd}-0}$	II	$3\text{CdSO}_4\cdot 8\text{H}_2\text{O}$	2.30	2.30		III	$\text{LiAlSi}_4\text{O}_{10}$	1.609	"
	III	$\text{Cd}_2\text{V}_2\text{O}_7$	2.31	2.31			$\text{Sc}_2\text{Si}_2\text{O}_7$	1.622	1.620
	VI	CdO	2.348	2.35			ZrSiO_4	1.612	"
$\text{VI}_{\text{Co}^{2+}-0}$	II	CoSO_4	2.07	2.085			Al_2SiO_5 (kyanite)	1.628	"
	III	CoMoO_4	2.082	2.095			Al_2SiO_5 (andalusite)	1.629	"
		$\text{Co}(\text{NH}_2)_2(\text{SO}_4)_2\cdot 6\text{H}_2\text{O}$	2.094	"			$\text{Zn}_2\text{Mn}(\text{OH})_2\text{SiO}_4$	1.626	"
	VI	CoO	2.133	2.135			$\text{AlBeSiO}_4\text{OH}$	1.625	"
$\text{VI}_{\text{Cr}^{3+}-0}$	II	Cr_5O_{12}	1.972	1.965			$\text{NaAlSi}_3\text{O}_8$	1.618	"
	III	$\text{KCr}_3\text{O}_{12}$	1.97	1.975			KAlSi_3O_8	1.612	"
		HCrO_2	1.979	"			$\text{Li}_2\text{Si}_2\text{O}_5$	1.631	"
	IV	Cr_2O_3	1.99	1.995			$\text{Ca}_2\text{NeHSi}_3\text{O}_9$	1.630	"
							$\text{CaMnSi}_2\text{O}_6$	1.623	"
$\text{VI}_{\text{Fe}^{2+}-0}$	III	FeWO_4	2.104	2.13		IV	$\gamma\text{-Ca}_2\text{SiO}_4$	1.644	1.640
		$\text{FeGe}(\text{OH})_6$	2.14	"			Mg_2SiO_4	1.625	"
	IV	$\text{FeSiF}_6\cdot 6\text{H}_2\text{O}$	2.140	2.15			MgFeSiO_4	1.638	"
		Fe_2SiO_4	2.172	"			Fe_2SiO_4	1.634	"
	VI	FeO	2.155	2.170			$\text{Ca}_3\text{Al}_2(\text{SiO}_4)_3$	1.649	"
$\text{VI}_{\text{Ga}^{3+}-0}$	III	GaNbO_4	1.997	1.98			$\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$	1.635	"
		$\beta\text{-Ga}_2\text{O}_3$	2.00	"					
	IV	$\alpha\text{-Ga}_2\text{O}_3$	2.00	2.00	$\text{VI}_{\text{Si}-\text{F}}$	II	$(\text{NH}_4)_2\text{SiF}_6$	1.674	1.685
	VI	Li_2AO_2	2.00	2.02			$[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{SiF}_6$	1.664	"
$\text{IV}_{\text{Ge}-0}$	II	GeO_2	1.739	1.75			Na_2SiF_6	1.695	1.700
	III	BaGe_4O_9	1.740	1.76			K_3SiF_7	1.70	1.710
		$\text{Na}_2\text{O}\cdot \text{GeO}_2\cdot 6\text{H}_2\text{O}$	1.769	"	$\text{VI}_{\text{Tl}^{4+}-0}$	II	$(\text{NH}_4)_3\text{SiF}_7$	1.71	"
		$\text{Na}_8\text{Sn}_4\text{Ge}_10\text{O}_{30}(\text{OH})_4$	1.752	"			$\text{Na}_2\text{Ti}_6\text{O}_{13}$	1.957	1.955
	IV	BaGeO_3	1.785	1.78			$\text{Rb}_2\text{Ti}_6\text{O}_{13}$	1.983	"
							TlTi_2O_5	1.970	1.965
$\text{VI}_{\text{Ni}^{2+}-0}$	III	$\text{NiSO}_4\cdot 6\text{H}_2\text{O}$	2.063	2.06			TiO_2	1.959	"
		NiWO_4	2.08	"			NiTiO_3	1.99	1.985
	VI	NiO	2.084	2.08			MnTiO_3	1.99	"
$\text{IV}_{\text{P}^{5+}-0}$	II	MoPO_4	1.528	1.52			BaTi_4O_9	1.98	"
		AlPO_4	1.515	"			$\text{Na}_2\text{Ti}_3\text{O}_7$	1.992	1.995
		P_2O_5	1.54	"					
	III	$\text{Na}_2\text{H}_2\text{P}_4\text{O}_{12}$	1.542	1.53					
		$\text{Na}_2\text{PO}_3\text{NH}_3$	1.528	"					

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 $r(\text{VI}F^-)=1.33 \text{ \AA}$ and $r(\text{VI}O^{2-})=1.32 \text{ \AA}$. Bragg & West noted that observed O-O distances in silicates were roughly 2.7 \AA and concluded that $r(O^{2-})=1.35 \text{ \AA}$. 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 $r(\text{VI}F^-)=1.15-1.20 \text{ \AA}$ with an estimated error of 0.05 \AA . Assuming a constant difference of $r(\text{VI}O^{2-})-r(\text{VI}F^-)=0.07 \text{ \AA}$, then $r(\text{VI}O^{2-})=1.22-1.27 \text{ \AA}$. 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 \AA in the NaNO_3 structure to greater than 3 \AA in the antifluorite structures. Perhaps the most surprising distance in this group is that of the 2.16 \AA 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 $r(\text{III}O^{2-})=1.36 \text{ \AA}$, 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 $\text{III}C^{4+}$ in the carbonate ion and $\text{III}N^{5+}$ 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 -0.04 and -0.24 \AA for IIH^+ and IH^+ . Although the value for $r(\text{IIH}^+)$ falls within the estimated error of the crystal radii and would still allow a completely positive set of radii, this is not possible for IH^+ . One is forced to the interpretation that an IH^+-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 \AA
SiO_2	rutile	2.16
CaCO_3	calcite	2.22
Al_2SiO_5	andalusite	2.25
$\text{B}_2\text{O}_3(\text{II})$	$\text{B}_2\text{O}_3(\text{II})$	2.36
S_3O_9	S_3O_9	2.37
$\text{B}_2\text{O}_3(\text{I})$	$\text{B}_2\text{O}_3(\text{I})$	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 ± 0.02 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. VIAl^{3+} , VIAs^{5+} , IIIB^{3+} , IVB^{3+} , IVS^{6+} , IVSi^{4+} , and VISe^{4+} , whereas values of ϱ calculated from crystal radii (CR) give poor agreement for IVGa^{3+} , IVLi^{+} , VIMn^{2+} , IVZn^{2+} , and IVMo^{6+} . Since ions with strong covalent mixing (Ga^{3+} and Zn^{2+}) prefer four coordination via sp^3 hybridization, even though $\varrho > 0.414$, 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 $r(\text{VIII} \text{Ca}^{2+})$ taken from more than 15 Ca-O distances which agree to within 0.02 Å results in $R_{\text{calc}} - R_{\text{obs}} = 0.06$ 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

Rocksalt			
MO	$R_{\text{Calc}}^{\text{M-O}}$	$R_{\text{Obs}}^{\text{M-O}}$	ΔR
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			
MO₂			
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
MF₂			
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
MBO₃			
VI-VI or X 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
MBF₃			
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

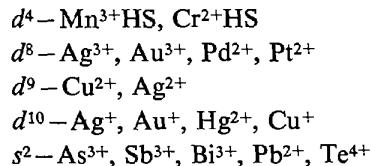
Table 7 (cont.)

	$R_{\text{Calc}}^{\text{M-O}}$	$R_{\text{Obs}}^{\text{M-O}}$	ΔR
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⁺, Pb²⁺, Sr²⁺, and Ba²⁺. 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:



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, AuF₃. The ions with d^4 and d^9 configurations have the familiar Jahn-Teller distortion exemplified by Cu²⁺. 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 I 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 which 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 $r(\text{IVMg}^{2+}) = 0.58 \text{ \AA}$. Because the original value of 0.49 \AA 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 $\text{Co}(\text{en})_2\text{SO}_3\text{NCS} \cdot 2\text{H}_2\text{O}$ 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 $a = 9.13 \pm 0.02$, $b = 6.59 \pm 0.02$, $c = 22.88 \pm 0.06 \text{ \AA}$, $\beta = 95.5 \pm 0.5^\circ$. The coordination around the metal atom is octahedral, the sulphito group being bonded through sulphur to the metal and in *trans* configuration. The $\text{Co}-\text{N}(\text{NCS})$ distance is not significantly different from the $\text{Co}-\text{N}(\text{en})$ distances. Some important dimensions are: $\text{Co}-\text{S}$, $2.203 \pm 0.006 \text{ \AA}$; mean $\text{Co}-\text{N}(\text{en})$, $1.962 \pm 0.010 \text{ \AA}$; mean $\text{S}-\text{O}$, $1.485 \pm 0.012 \text{ \AA}$; mean $\text{O}-\text{S}-\text{O}$, $110.3 \pm 0.7^\circ$; $\text{Co}-\text{N}(\text{NCS})$, $1.974 \pm 0.018 \text{ \AA}$.

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 $\text{Co}(\text{en})_2\text{SO}_3\text{NCS} \cdot 2\text{H}_2\text{O}$ 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 $\text{PdSO}_3(\text{NH}_3)_3$ (Spinnler & Becka, 1967). Furthermore, we considered that a comparison between the different $\text{Co}-\text{N}$ 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.

Experimental

Preparation

$\text{Co}(\text{en})_2\text{SO}_3\text{NCS} \cdot 2\text{H}_2\text{O}$ 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, $\text{Co}(\text{en})_2\text{SO}_3\text{NCS} \cdot 2\text{H}_2\text{O}$; alpha-

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