

parallel to the (110) plane in the structures. Nevertheless, structural control by electron concentration of necessity involves some geometrical feature, since it results from the action of planes of energy discontinuity in reciprocal space. The one constant geometrical feature common to all of these 40 tetragonal structures is the  $\beta$ -Sn like pseudo-cell of T metal atoms with  $c/na/2 \approx 0.577 = 1/\sqrt{3}$  (the value for equilateral triangles in the nets of T atoms), so it would seem that structural stability must result from the achievement of some constant electron concentration within this pseudo-cell. This conclusion is entirely consistent with the observed fact that (at least for  $V_T \geq 7$ ) the controlling feature is a constant electron concentration *per T atom* or *per  $\beta$ -Sn like pseudo-cell*, and not as in all other recognized cases of 'electron' phases, a controlling electron concentration *per atom* in the structure. Whether the 14 electrons per T atom represent 10 in inner filled energy bands and 4 in outer bands as in  $\beta$ -Sn itself, is an interesting speculation that magnetic measurements might solve.

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**Revised values of effective ionic radii.\*** By R. D. SHANNON and C. T. PREWITT,† *Central Research Department, E. I. du Pont de Nemours & Co., Experimental Station, Wilmington, Delaware 19898, U.S.A.*

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Corrections resulting from an  $r^3$  vs.  $a^3$  replot of earlier data are presented for the ionic radii of rock salt, C rare earth, and fluorite oxides.

The non-equivalence of  $r^3$  vs.  $a^3$  and  $r$  vs.  $a$  plots for isotopic series of compounds was recently pointed out by

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Donnay (1969). We confirmed this non-equivalence empirically for the cubic series of rocksalt, C rare earth, and fluorite oxides by comparing both types of plot. Probably neither type is precisely linear. Thus, the choice of either  $r^3$  vs.  $V$  or  $r$  vs.  $V^{1/3}$  for derivation and comparison of ionic radii is arbitrary. Brisse & Knop (1968) used  $r$  vs.  $V^{1/3}$  plots

Table 1(a). Revised effective radii†

EC, electron configuration; CN, coordination number; SP, electron spin; CR, crystal radii based on  $r(V^{VI}F^-) = 1.19 \text{ \AA}$ ; 'IR', effective ionic radii based on  $r(V^{VI}O^{2-}) = 1.40 \text{ \AA}$ . Values of radii taken from radii vs. volume plots are marked by R, doubtful values by ? and values for which at least 5 structural determinations resulted in radii differing by no more than  $\pm 0.01 \text{ \AA}$  are marked with an asterisk.

Ion	EC	CN	SP	Shannon & Prewitt (1969)	
				CR	'IR'
Am <sup>3+</sup>	5f <sup>6</sup>	VI		1.14	1.00 R
Br <sup>7+</sup>	3d <sup>10</sup>	IV		0.40	0.26
Cd <sup>2+</sup>	4d <sup>10</sup>	IV		0.94	0.80
Ce <sup>3+</sup>	6s <sup>1</sup>	VI		1.15	1.01 R
		IX		1.29	1.15
Co <sup>2+</sup>	3d <sup>7</sup>	IV	HS	0.71	0.57
		VI	HS	0.885	0.745 R*
Cs <sup>1+</sup>	5p <sup>6</sup>	VIII		1.96	1.82 ?
D <sup>1+</sup>	1s <sup>0</sup>	II		0.04	-0.10 ?
Dy <sup>3+</sup>	4f <sup>9</sup>	VI		1.052	0.912 R
Er <sup>3+</sup>	4f <sup>11</sup>	VI		1.030	0.890 R
Eu <sup>3+</sup>	4f <sup>6</sup>	VI		1.087	0.947 R
		VII		1.17	1.03
Fe <sup>2+</sup>	3d <sup>6</sup>	VI	HS	0.920	0.780 R*
Gd <sup>3+</sup>	4f <sup>7</sup>	VII		1.18	1.04
Ho <sup>3+</sup>	4f <sup>10</sup>	VI		1.041	0.901 R
In <sup>3+</sup>	4d <sup>10</sup>	VI		0.940	0.800 R*
La <sup>3+</sup>	4d <sup>10</sup>	VI		1.185	1.045 R
Lu <sup>3+</sup>	4f <sup>14</sup>	VI		1.001	0.861 R
Mg <sup>2+</sup>	2p <sup>6</sup>	IV		0.72	0.58
		V		0.81	0.67
Mn <sup>2+</sup>	3d <sup>5</sup>	VI	HS	0.970	0.830 R*
Mn <sup>3+</sup>	3d <sup>4</sup>	VI	HS	0.785	0.645 R*
Nd <sup>3+</sup>	4f <sup>3</sup>	VI		1.123	0.983 R

Table 1(a) (cont.)

Ion	EC	CN	Shannon & Prewitt (1969)	
			CR	'IR'
Ni <sup>2+</sup>	3d <sup>8</sup>	VI	0.830	0.690R*
Np <sup>3+</sup>	5f <sup>4</sup>	VI	1.16	1.02R
Pa <sup>5+</sup>	6p <sup>6</sup>	VIII	1.05	0.91
Pm <sup>3+</sup>	4f <sup>4</sup>	VI	1.11	0.97 R
Pr <sup>3+</sup>	4f <sup>2</sup>	VI	1.137	0.997R
Po <sup>4+</sup>	6s <sup>2</sup>	VIII	1.22	1.08 R
Pr <sup>4+</sup>	4f <sup>1</sup>	VIII	1.10	0.96 R
Pt <sup>2+</sup>	5d <sup>8</sup>	IVSQ	0.74	0.60
Pu <sup>3+</sup>	5f <sup>5</sup>	VI	1.15	1.01 R
Ra <sup>2+</sup>	6p <sup>6</sup>	VIII	1.62	1.48
		XII	1.78	1.64
Rb <sup>1+</sup>	4p <sup>6</sup>	X	1.80	1.66
Sc <sup>3+</sup>	3p <sup>6</sup>	VI	0.885	0.745R*
Sm <sup>3+</sup>	4f <sup>5</sup>	VI	1.098	0.958R
Sr <sup>2+</sup>	4p <sup>6</sup>	VI	1.27	1.13 R
		XII	1.54	1.40
Tb <sup>3+</sup>	4f <sup>8</sup>	VII	1.16	1.02
Th <sup>4+</sup>	6p <sup>6</sup>	VIII	1.18	1.04 R
Tl <sup>3+</sup>	5d <sup>10</sup>	VI	1.025	0.885R
Tm <sup>3+</sup>	4f <sup>12</sup>	VI	1.020	0.880R
U <sup>3+</sup>	5f <sup>3</sup>	VI	1.18	1.04 R
U <sup>6+</sup>	6p <sup>6</sup>	VI	0.87	0.73
W <sup>6+</sup>	5p <sup>6</sup>	IV	0.56	0.42*
		VI	0.74	0.60*
Y <sup>3+</sup>	4p <sup>6</sup>	VI	1.040	0.900R*
Yb <sup>3+</sup>	4f <sup>13</sup>	VI	1.008	0.868
Zn <sup>2+</sup>	3d <sup>10</sup>	VI	0.890	0.750R*
		VIII	1.04	0.90

† Reference should be made to Shannon & Prewitt (1969) regarding the applicability of these values.

Table 1(b). References for radii revisions

Br <sup>7+</sup>	IV Siegel, S. <i>et al.</i> (1969). <i>Inorg. Chem.</i> <b>8</b> , 1190 (KBrO <sub>4</sub> )
Cd <sup>2+</sup>	IV Reuter, B. <i>et al.</i> (1969). <i>Z. anorg. allgem. Chem.</i> <b>369</b> , 306. (CdV <sub>2</sub> O <sub>4</sub> )
Ce <sup>3+</sup>	IX Brunton, G. (1969). <i>Acta Cryst.</i> <b>B25</b> , 600. (KCeF <sub>4</sub> )
Co <sup>2+</sup>	IVHS Knop, O. <i>et al.</i> (1968). <i>Canad. J. Chem.</i> <b>46</b> , 3472. (Co <sub>3</sub> O <sub>4</sub> )
Cs <sup>1+</sup>	VIII Steinfink, H. & Brunton, G. (1968). <i>Acta Cryst.</i> <b>B24</b> , 807. (CsBeF <sub>3</sub> )
D <sup>1+</sup>	II Delaplane, R. G. <i>et al.</i> (1969). <i>J. Chem. Phys.</i> <b>50</b> , 1920. (DCoO <sub>2</sub> ) Hamilton, W. C. & Ibers, J. A. (1963). <i>Acta Cryst.</i> <b>16</b> , 1209. (DCrO <sub>2</sub> )
Eu <sup>3+</sup>	VII Brandle, C. D. & Steinfink, H. (1968). <i>Proc. 7th Rare Earth Conf.</i> (Eu <sub>4</sub> Al <sub>2</sub> O <sub>4</sub> )
Gd <sup>3+</sup>	VII Smolin, Y. I. <i>et al.</i> (1967). <i>Izv. Akad. Nauk SSR, Neorg. Mat.</i> <b>3</b> , 1034. (Gd <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> )
Mg <sup>2+</sup>	IV Reuter, B. <i>et al.</i> (1969). <i>Z. anorg. allgem. Chem.</i> <b>369</b> , 306. (MgV <sub>2</sub> O <sub>4</sub> ) Zorina, N. G. & Kvitka, S. S. (1969). <i>Sov. Phys. Cryst.</i> <b>13</b> , 599. (MgAl <sub>2</sub> O <sub>4</sub> )
Mg <sup>2+</sup>	V Stephenson, D. A. & Moore, P. B. (1968). <i>Acta Cryst.</i> <b>B24</b> , 1518. (Mg <sub>0.9</sub> Fe <sub>0.1</sub> Al <sub>3</sub> SiBO <sub>9</sub> )
Pa <sup>5+</sup>	VIII Burns, J. H. <i>et al.</i> (1968). <i>Acta Cryst.</i> <b>B24</b> , 1675. (RbPaF <sub>6</sub> ) Brown, D. <i>et al.</i> (1969). <i>J. Chem. Soc. A</i> , p. 1161. (Na <sub>3</sub> PaF <sub>8</sub> )
Rb <sup>1+</sup>	X Burns, J. H. <i>et al.</i> (1968). <i>Acta Cryst.</i> <b>B24</b> , 1675. (RbPaF <sub>6</sub> )
Sr <sup>2+</sup>	XII Jamieson, P. B. <i>et al.</i> (1968). <i>J. Chem. Phys.</i> <b>48</b> , 5048. (Ba <sub>0.27</sub> Sr <sub>0.73</sub> Nb <sub>2</sub> O <sub>5.70</sub> )
Tb <sup>3+</sup>	VII Hubbert-Paletta, E. <i>et al.</i> (1968). <i>Z. anorg. allgem. Chem.</i> <b>363</b> , 145. (Tb <sub>2</sub> O <sub>3</sub> )
U <sup>6+</sup>	VI Loopstra, B. O. <i>et al.</i> (1969). <i>Acta Cryst.</i> <b>B25</b> , 787. (AUO <sub>4</sub> , A <sub>2</sub> UO <sub>5</sub> , A <sub>3</sub> UO <sub>6</sub> )
W <sup>6+</sup>	VI Filipenko, O. <i>et al.</i> (1968). <i>Sov. Phys.-Cryst.</i> <b>13</b> , 127. (ZnWO <sub>4</sub> ) Chichagov, A. <i>et al.</i> (1966). <i>Sov. Phys.-Dokl.</i> <b>11</b> , 11. (CdWO <sub>4</sub> ) Borisev, S. & Klevtsova, R. (1968). <i>Sov. Phys.-Cryst.</i> <b>13</b> , 420. (KYW <sub>2</sub> O <sub>8</sub> ) Gebert, E. & Kihlberg, L. (1969). <i>Acta Chem. Scand.</i> <b>23</b> , 221. (Cu <sub>3</sub> WO <sub>6</sub> )

to compare the radii of trivalent rare earth ions in several series of oxides. In their derivation of effective ionic radii, Shannon & Prewitt (1969) used both  $r^3$  vs.  $V$  plots for non-cubic compounds and  $r$  vs.  $a$  plots for the cubic series (rocksalt,  $C$  rare earth, and fluorite); consequently, radii derived from the  $r$  vs.  $a$  plots were not consistent with those derived from the  $r^3$  vs.  $V$  plots. In this note we present the radii corrections resulting from replotting  $r^3$  vs.  $a^3$  for the rocksalt,  $C$  rare earth, and fluorite series of oxides and fluorides. These corrections, listed in Table 1(a), are thus limited to six-coordinated divalent ions, six-coordinated rare earth ions, and eight-coordinated tetravalent ions. In most cases the corrections are less than 0.02 Å.

In addition to the above corrections, we have also included both new and corrected values of radii derived from crystal structure determinations published in 1968 and early 1969. Examples of these new additions are four-coordinated  $\text{Br}^{7+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Co}^{2+}\text{HS}$ ; five-coordinated  $\text{Mg}^{2+}$ ; seven-coordinated  $\text{Eu}^{3+}$ ,  $\text{Gd}^{3+}$ , and  $\text{Tb}^{3+}$ ; and nine-coordinated  $\text{Ce}^{3+}$ . In addition, an accurate determination of cell volumes of  $\text{ABO}_4$  molybdates and tungstates carried out by

Sleight (1969) led us to conclude that the radii of  $\text{Mo}^{6+}$  and  $\text{W}^{6+}$  do not differ significantly despite the apparent differences in certain interatomic distances derived from structure refinements. Consequently, the radii of both four- and six-coordinated  $\text{Mo}^{6+}$  and  $\text{W}^{6+}$  were made equal. Table 1(b) lists the references upon which the radii changes were based.

*Note added in proof:* – We would like to thank Dr Y. Matsui for pointing out that plots of rare earth radii versus atomic number lead to  $r(\text{VI}\text{Pm}^{3+}) = 0.97$  Å and Dr K. Geschneidner, Jr, for informing us that the cell dimensions given for  $\text{PrO}_2$  by Wyckoff and therefore the radius of  $\text{VIII}\text{Pr}^{4+}$  were in error.

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## International Union of Crystallography

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The Executive Committee of the I.U.Cr. is anxious to promote an increase in the number of Inter-Congress meetings in order to avoid future Triennial Congresses becoming excessively large and cumbersome to handle. A Sub-Committee on the Union Calendar has therefore been set up [see *Acta Cryst.* (1969) **A25**, 719] to implement this policy. Its function is to gather information on proposed or prospective meetings, coordinate the long-term planning of meetings which the Union organizes or co-sponsors, and actively to encourage the initiation of small or intermediate-sized meetings in fields where development is significant.

Since it is the aim of the Sub-Committee to plan at least three, and preferably more, years ahead, it is advisable to have early advice of meetings being planned or in prospect which might appropriately come within the category of Union sponsorship or co-sponsorship in terms of their content, location, size and date. It would therefore be appreciated if bodies such as Commissions of the Union, National Committees for crystallography, regional

associations and other bodies which are contemplating or have begun the planning of a future international meeting on crystallography or with a major content of crystallography would contact the Sub-Committee Chairman:

Dr. A. Líněk  
 Czechoslovak Academy of Sciences  
 Institute of Solid State Physics  
 Cukrovarnická 10  
 PRAHA 6, Czechoslovakia.

The Sub-Committee would be pleased to receive advice of provisional details of proposed Inter-Congress meetings as soon as possible and it will also consider requests for Union co-sponsorship of these meetings. Nominal financial support could be available in some cases.

Contact with the Sub-Committee should assist prospective organizers of meetings to disseminate preliminary information in a convenient manner since lists of meetings of interest to crystallographers will be published in the Journals of the Union from time to time. The Sub-Committee will also be glad to be informed of local or national crystallographic meetings.

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*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).*

### Professor A. V. Shubnikov 1887–1970

Professor Alexey Vasilyevich Shubnikov died on 27 April, 1970. Professor Shubnikov was Head of the Laboratory at the Institute of Crystallography, Academy of Sciences

of the USSR. He was best known internationally as the first editor of *Kristallografiia*, by his participation in the founding of the International Union of Crystallography and by his discussion of the rôle of antisymmetry elements in structure theory ('Shubnikov groups').

A full obituary will be published in the *Journal of Applied Crystallography* in due course.