SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

The densest packing of equal circles on a sphere. Erratum. By D. A. KOTTWITZ, 2152 *Hudson Ave., Richland, WA* 99352, *USA*

Abstract

Two of the literature references for the paper by Kottwitz [*Acta Cryst.* (1991). A47, 158-165] are corrected. In Table 1 (p. 161), the entry for $n = 19$ should read Lazić, Šenk & Šeškar (1987), while that for $n = 23$ should read Tarnai & Gáspár (1990).

All relevant information is given in the *Abstract.*

Madelung numbers for the theoretical structure type with mutual trigonal prismatic coordination. By J. ZEMANN, *Institut für Mineralogie und Kristallographie, Universität Wien, Dr-Karl-Lueger-Ring* 1, *A*-1010 *Wien, Austria*

Abstract

Madelung numbers α are presented for the theoretical AB structure type with mutual trigonal prismatic coordination as a function of the deformation leaving the lengths of the AB distances in the AB_6 ($=BA_6$) prism equal. α is always smaller than $\alpha(NaCl)$ and its maximum value is also slightly smaller than the maximum value of $\alpha(NiAs)$.

The Madelung numbers α for the NaCl structure type and for the NiAs structure type have been known for a long time (see *e.g.* Emersleben, 1953/54; Zemann, 1958). The NaCl type has a mutual octahedral six coordination, while in the NiAs type the Ni atoms are coordinated to six As atoms in the form of an elongated or compressed octahedron and the As atoms to six Ni atoms in the form of a trigonal prism. Theoretically, there also exists an AB structure type with mutual trigonal prismatic coordination. Its Madelung numbers α seem not to have been published as yet.

The crystallographic description of this structure type may be seen in Table 1. The atomic arrangement is closely related to the hexagonal closest packing of spheres: consecutive layers parallel to (00.1) are occupied by A and B ions, respectively, and a deformation along the z axis is allowed. With $A - B = 1$ there is one degree of freedom, for which the angle μ between the AB direction in the trigonal prism and the z axis was chosen. From the point of view of the stereochemistry of ionic compounds only the region of μ with $\arcsin(1/3^{1/2}) \simeq 35 \cdot 26° \le \mu \le \arccos(1/2) = 60°$ is of interest. Outside this range some AA ($=BB$) distances are shorter than the AB distance in the trigonal prismatic coordination. It should be noted that

Table 1. *Theoretical AB structure type with mutual trigonal prismatic coordination*

Space group: $P\bar{6}m2-D_{3h}^1$ (No. 187).
Positions: $1A$ on $1(c)$ 1/3, 2/3, 0; $1B$ on $1(d)$ 2/3, 1/3, 1/2. $A - B = 1$; μ = angle of $A - B$ with the z direction ($\mu < 90°$). $a = 3^{1/2} \sin \mu$, $c = 2\cos \mu$; $V = 3 \times 3^{1/2} \sin^2 \mu \cos \mu$.

μ	a	c	V	α
35·264390*	1·000000	1·632993	1·414214	1·235585
40·000000	1·113341	1·532089	1·644640	1·506440
45·000000	1·224745	1·414214	1·837117	1·656998
49·106605†	1·309307	1·309307	1·943817	1·712437
50·000000	1·326828	1·285575	1·960006	1·717955
51·000000	1·346056	1·258641	1·974963	1·721567
52·000000	1·364875	1·231323	1·986498	1·722523
53·000000	1·383277	1·203630	1·994537	1·720843
54·000000	1·401259	1·175571	1·999014	1·716516
54·735610‡	1·414214	1·154701	2·000000	1·716160
55·000000	1·418813	1·147153	1·999872	1·709493
60·000000§	1·500000	1·000000	1·948557	1·629560

* $\mu = \arcsin(1/3^{1/2})$; ($A + B$) form hexagonal closest packing.
† $\mu = \arctan(2/3^{1/2})$; case for which $a = c$.
‡ $\mu = \arccos(1/3^{1/2})$; case for which V has maximum value.
§ $\mu = \arccos(1/2)$; case for which $A - A$ ($= B - B$) parallel to z equals $A - B$ ($= 1$).

this structure type can also be conveniently described in the black-white space group $P6_3'/mmc'$, No. 267, of the hexagonal system (Shubnikov & Belov, 1964).

Table 1 presents the variation of the lattice parameters, the cell volume and the Madelung number α as a function of μ. The maximum value of the Madelung number [$\alpha = 1·7226$ (1)] occurs at $\mu = 51·8$ (1)°. This μ value is clearly different from that at which the cell volume reaches its maximum ($\mu = 54·74°$), but very close to the value at which