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.*

Acta Cryst. (1991). A47, 851

The densest packing of equal circles on a sphere. Erratum.

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(*Received* 29 *August* 1991)

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.*

Acta Cryst. (1991). A47, 851-852

Madelung numbers for the theoretical structure type with mutual trigonal prismatic coordination.

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(*Received* 11 *April* 1991; *accepted* 11 *June* 1991)

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 α(NaCl) and its maximum value is also slightly smaller than the maximum value of α(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 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. *Theoretical AB structure type with mutual trigonal prismatic coordination*

Space group: $P\bar{6}m2 - D^1_{3h}$ (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).

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 [α = 1·7226 (1)] occurs at $\mu = 51{\cdot}8\,(1)°$. This μ value is clearly different from that at which the cell volume reaches its maximum ($\mu = 54{\cdot}74°$), but very close to the value at which

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an isolated AB_6 complex with symmetry $\bar{6}2m$ has its electrostatic optimum [$\mu = 51{\cdot}6\,(1)°$].

The maximum α value of the structure type under consideration is not only definitely smaller than that of the NaCl type ($\alpha = 1{\cdot}7476$), but also slightly smaller than the maximum value for the NiAs type, *i.e.* $\alpha = 1{\cdot}733\,(1)$ as derived from the values given by Zemann (1958). It is, therefore, no surprise that the AB structure type with mutual trigonal prismatic coordination has no representatives among ionic structures.

I thank Dr R. Fischer for technical help with the computation of the Madelung numbers.

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Acta Cryst. (1991). A**47**, 852

Quasiperiodic tilings with low-order rotational symmetry. Erratum.

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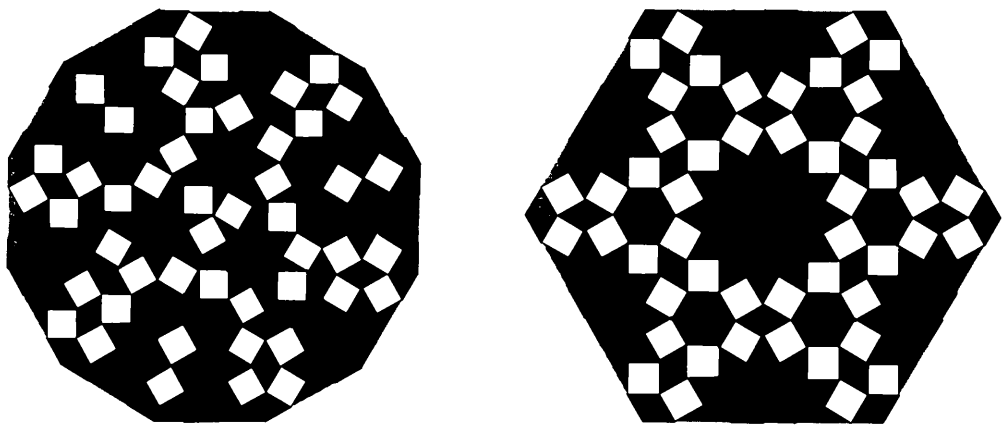
(*Received* 20 *September* 1991)

Abstract

Figs. 10(*a*), (*b*) of the paper by Clark & Suryanarayan [*Acta Cryst.* (1991), A**47**, 498–502] reproduced poorly. Revised figures with better contrast are here published.



(*a*) (*b*)

Fig. 10. (*a*) 3-fold rotational symmetry, 2nd generation. (*b*) 6-fold rotational symmetry, 2nd generation.

International Union of Crystallography

Acta Cryst. (1991). A**47**, 852–853

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