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Hexagonal and trigonal sphere packings. I. Invariant and univariant lattice complexes

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All homogeneous sphere packings and all interpenetrating sphere packings have been derived that refer to the seven invariant and the 23 univariant lattice complexes belonging to the hexagonal crystal family. The respective sphere packings may be assigned to 66 types. In addition, one case of interpenetrating sphere packings was found. For five types, the inherent symmetry of some sphere packings with specialized metrical and coordinate parameters may become cubic. For two further types, namely 8/4/*c*1 (body-centered cubic lattice) and 12/3/*c*1 (face-centered cubic lattice), the inherent symmetry is cubic for all corresponding sphere packings. By means of a large number of examples, the applicability of sphere packings for the comparison and description of simple crystal structures is demonstrated.

1. Introduction

In many cases, sphere packings are a useful tool for the description, interpretation, comparison and classification of crystal structures (*cf. e.g.* Hellner *et al.*, 1981; Koch, 1985; O'Keeffe & Hyde, 1996) and they can help to recognize interrelationships between different structure types. Moreover, structural changes depending *e.g.* on temperature, pressure or chemical composition can be characterized by sphere-packing deformations (*cf. e.g.* Koch & Hellner, 1981; Sowa, 1988, 1997; Sowa & Ahsbahs, 1998; O'Keeffe & Hyde, 1996). Interpenetrating sphere packings may be seen in relation to certain crystal structures consisting of partial structures that are not connected to each other by chemical bonds but interpenetrate each other (*cf. e.g.* Ermer, 1988).

Until now, complete information on homogeneous sphere packings is available only for the cubic (Fischer, 1973, 1974), the tetragonal (Fischer, 1991*a*,*b*, 1993) and the triclinic (Fischer & Koch, 2002) crystal systems. Beyond that, all sphere packings with three contacts per sphere (Koch & Fischer, 1995) and some with ten or more contacts are known (*cf. e.g.* O'Keeffe & Hyde, 1996; *International Tables for Crystallography*, 1999, Vol. C, ch. 9). Only sporadic information has been published on other sphere packings (*cf. e.g.* Zobetz, 1983; O'Keeffe & Hyde, 1996; Sowa, 2000*a*,*b*, 2001; Sowa & Koch, 1999, 2001, 2002). The interpenetrating sphere packings with cubic symmetry have been tabulated by Fischer & Koch (1976), those with tetragonal symmetry have been presented by Fischer & Koch (1990).

The aim of the ongoing research is the complete derivation of all sphere packings and interpenetrating sphere packings that may be generated in space groups of the hexagonal crystal family. To this end, it is not necessary to regard all Wyckoff positions of trigonal and hexagonal space groups, but it is sufficient to investigate the characteristic Wyckoff positions of the lattice complexes (*cf. e.g. International Tables for Crystallography*, 2002, Vol. A, ch. 14). The present paper gives information on all those sphere packings and interpenetrating sphere packings that correspond to point configurations from the seven invariant or the 23 univariant lattice complexes belonging to the hexagonal crystal family.

2. Definitions

Each point configuration (*i.e.* set of points that are symmetrically equivalent with respect to some space group) can be uniquely assigned to a set of spheres, called *sphere configuration* in the following way: (i) each point is the centre of a sphere; (ii) all spheres are equal in size; (iii) each sphere is in contact with at least one other sphere; (iv) no spheres overlap.

A *homogeneous sphere packing* is a sphere configuration that satisfies the following additional condition: (v) any two spheres are connected by a chain of spheres with mutual contact.

As there exist infinitely many such sphere packings, it is necessary to assign them to *sphere-packing types*: Two sphere packings belong to the same type if the spheres of one sphere packing can be mapped onto the spheres of the other one and *vice versa* under preservation of all contact relationships between the spheres (*cf. e.g.* Fischer, 1991*a*). Sphere packings of the same type may be generated by different symmetry, *i.e.* their sphere centres may correspond to point configurations from different Wyckoff positions. These Wyckoff positions can belong to the same space group or to different space groups of the same type or even to space groups of different types. Each

Table 1
The sphere packings corresponding to the seven invariant hexagonal lattice complexes.

$\boldsymbol{R\bar{3}m}$	**3*a***	$\boldsymbol{\bar{3}m}$	**0, 0, 0**	
A	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$	$-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$-\frac{1}{3}, -\frac{2}{3}, \frac{1}{3}$	
	$\frac{1}{3}, \frac{2}{3}, -\frac{1}{3}$	$\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$	$-\frac{2}{3}, -\frac{1}{3}, -\frac{1}{3}$	
B	0, 0, 1	0, 0, −1		
C	1, 0, 0	0, 1, 0	1, 1, 0	
	−1, 0, 0	0, −1, 0	−1, −1, 0	
0.1	8/4/*c*1	*AB*	$c/a = \frac{1}{4}\sqrt{6}$	$\rho_m = 0.68017$
1.1	6/4/*c*1	*A*	$c/a = \frac{1}{2}\sqrt{6}$	$\rho_m = 0.52360$
0.2	12/3/*c*1	*AC*	$c/a = \sqrt{6}$	$\rho_m = 0.74048$
$\boldsymbol{R\bar{3}m}$	**9*e***	**.2/*m***	$\boldsymbol{\frac{1}{2}, 0, 0}$	
A	$\frac{1}{6}, -\frac{1}{6}, \frac{1}{3}$	$\frac{2}{3}, -\frac{1}{6}, \frac{1}{3}$	$\frac{1}{3}, \frac{1}{6}, -\frac{1}{3}$	$\frac{5}{6}, \frac{1}{6}, -\frac{1}{3}$
B	0, 0, 1	0, 0, −1		
C	$\frac{1}{2}, \frac{1}{2}, 0$	$1, \frac{1}{2}, 0$	$0, -\frac{1}{2}, 0$	$\frac{1}{2}, -\frac{1}{2}, 0$
0.1	6/4/*h*1	*AB*	$c/a = \frac{1}{8}\sqrt{6}$	$\rho_m = 0.51013$
1.1	4/6/*c*2	*A*	$c/a = \frac{1}{4}\sqrt{6}$	$\rho_m = 0.39270$
0.2	8/3/*c*2	*AC*	$c/a = \frac{1}{2}\sqrt{6}$	$\rho_m = 0.55536$
$\boldsymbol{P6_222}$	**3*c***	**222**	$\boldsymbol{\frac{1}{2}, 0, 0}$	
A	$\frac{1}{2}, \frac{1}{2}, \frac{1}{3}$	$\frac{1}{2}, -\frac{1}{2}, \frac{1}{3}$	$0, -\frac{1}{2}, -\frac{1}{3}$	$1, \frac{1}{2}, -\frac{1}{3}$
B	$\frac{1}{2}, 0, 1$	$\frac{1}{2}, 0, -1$		
C	$\frac{3}{2}, 0, 0$	$\frac{1}{2}, 1, 0$	$\frac{3}{2}, 1, 0$	
	$-\frac{1}{2}, 0, 0$	$\frac{1}{2}, -1, 0$	$-\frac{1}{2}, -1, 0$	
0.1	6/4/*h*3	*AB*	$c/a = \frac{3}{8}\sqrt{2}$	$\rho_m = 0.51013$
1.1	4/6/*h*1	*A*	$c/a = \frac{3}{4}\sqrt{2}$	$\rho_m = 0.39270$
0.2	10/3/*h*3	*AC*	$c/a = \frac{3}{2}\sqrt{3}$	$\rho_m = 0.69813$
$\boldsymbol{P6/mmm}$	**1*a***	$\boldsymbol{6/mmm}$	**0, 0, 0**	
A	0, 0, 1	0, 0, −1		
B	1, 0, 0	0, 1, 0	1, 1, 0	
	−1, 0, 0	0, −1, 0	−1, −1, 0	
0.1	8/3/*h*4	*AB*	$c/a = 1$	$\rho_m = 0.60460$
$\boldsymbol{P6/mmm}$	**2*c***	$\boldsymbol{\bar{6}m2}$	$\boldsymbol{\frac{1}{3}, \frac{2}{3}, 0}$	
A	$\frac{1}{3}, \frac{2}{3}, 1$	$\frac{1}{3}, \frac{2}{3}, -1$		
B	$\frac{2}{3}, \frac{1}{3}, 0$	$\frac{2}{3}, \frac{4}{3}, 0$	$-\frac{1}{3}, \frac{1}{3}, 0$	
0.1	5/4/*h*5	*AB*	$c/a = \frac{1}{3}\sqrt{3}$	$\rho_m = 0.40307$
$\boldsymbol{P6/mmm}$	**3*f***	$\boldsymbol{mmm}$	$\boldsymbol{\frac{1}{2}, 0, 0}$	
A	$\frac{1}{2}, 0, 1$	$\frac{1}{2}, 0, -1$		
B	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, -\frac{1}{2}, 0$	$0, -\frac{1}{2}, 0$	$1, \frac{1}{2}, 0$
0.1	6/3/*h*13	*AB*	$c/a = \frac{1}{2}$	$\rho_m = 0.45345$
$\boldsymbol{P6_3/mmc}$	**2*c***	$\boldsymbol{\bar{6}m2}$	$\boldsymbol{\frac{1}{3}, \frac{2}{3}, \frac{1}{4}}$	
A	$\frac{2}{3}, \frac{1}{3}, \frac{3}{4}$	$\frac{2}{3}, \frac{4}{3}, \frac{3}{4}$	$-\frac{1}{3}, \frac{1}{3}, \frac{3}{4}$	
	$\frac{2}{3}, \frac{1}{3}, -\frac{1}{4}$	$\frac{2}{3}, \frac{4}{3}, -\frac{1}{4}$	$-\frac{1}{3}, \frac{1}{3}, -\frac{1}{4}$	
B	$\frac{1}{3}, \frac{2}{3}, \frac{5}{4}$	$\frac{1}{3}, \frac{2}{3}, -\frac{3}{4}$		
C	$\frac{4}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{1}{3}, \frac{5}{3}, \frac{1}{4}$	$\frac{4}{3}, \frac{5}{3}, \frac{1}{4}$	
	$-\frac{2}{3}, \frac{2}{3}, \frac{1}{4}$	$\frac{1}{3}, -\frac{1}{3}, \frac{1}{4}$	$-\frac{2}{3}, -\frac{1}{3}, \frac{1}{4}$	
0.1	8/3/*h*3	*AB*	$c/a = \frac{2}{3}$	$\rho_m = 0.53742$
1.1	6/4/*h*2	*A*	$c/a = \frac{1}{3}\sqrt{6}$	$\rho_m = 0.52359$
0.2	12/3/*h*1	*AC*	$c/a = \frac{2}{3}\sqrt{6}$	$\rho_m = 0.74048$

sphere-packing type is designated by a symbol *k*/*m*/*fn*, as was first introduced by Fischer (1971): *k* is the number of contacts per sphere, *m* is the length of the shortest mesh within the sphere packing, *f* indicates the highest crystal family for a sphere packing of that type (*c*: cubic, *h*: hexagonal) and *n* is an arbitrary number.

The *density* ρ *of a sphere packing* is defined as the volume of all spheres within one unit cell divided by the unit-cell volume. If the parameter region of a certain sphere-packing type has degrees of freedom, ρ depends on the choice of the variable parameters. With the exception of a few cases, a minimal density ρ_m can be calculated for each sphere-packing type.

A sphere configuration that is not a sphere packing disintegrates into *partial configurations*. The symmetry group of such a partial configuration may be a point group, a rod group, a layer group or again a space group. In the latter case, the sphere configuration consists of finitely many partial configurations that interpenetrate each other without mutual contact. As each such partial configuration forms a sphere packing by itself, the entire arrangement may be designated as *interpenetrating sphere packings*. It may be described by a symbol $h[k/m/fn]^l$, where *k*/*m*/*fn* symbolizes the type of partial configuration, *l* is their number and the preceeding *h* (or *c*) indicates that the highest possible symmetry of interpenetrating sphere packings of that type is hexagonal (or cubic).

3. Derivation of sphere packings

For the complete derivation of all types of sphere packings, it is sufficient to investigate the characteristic Wyckoff position of each lattice complex. Moreover, only a parameter region, which corresponds to one asymmetric unit of the Euclidean normalizer (*cf. e.g. International Tables for Crystallography*, 2002, Vol. A, ch. 15) of the characteristic space group, has to be regarded. In the case of an invariant trigonal or hexagonal lattice complex, all coordinate parameters are fixed and only the axial ratio *c*/*a* can be varied. A univariant lattice complex has in addition one free positional parameter (*x* or *z*).

For any reference point lying in such an asymmetric unit, all symmetrically equivalent points with shortest distances to the first one can be determined. The parameter region that has to be investigated accordingly disintegrates into two-dimensional, one-dimensional and zero-dimensional subregions. All point configurations of a certain subregion correspond to the same type of sphere configuration or sphere packing. Parameter regions with small values of *c*/*a* give rise to rod-like partial configurations, those with large values of *c*/*a* to layer-like partial configurations. Sphere packings can only occur in parameter regions with intermediate values of *c*/*a*.

In order to prove whether or not a certain sphere configuration is a sphere packing, one may regard the set of symmetry operations that consists of (i) the site-symmetry group of the reference point and (ii) all those symmetry operations that map that point onto its neighbouring points. If this set generates the space group under consideration, a sphere packing is formed. Interpenetrating sphere packings occur if a space group is generated that is a non-trivial subgroup of the original group. In all other cases, the sphere configuration disintegrates into partial configurations with lower periodicity.

Each sphere packing has to be assigned to a sphere-packing type. For a rough classification, the number *k* of the neighbouring spheres and the size *m* of the smallest mesh within the sphere-packing graph can be used. Furthermore, the minimal

Table 2
The sphere packings corresponding to the 23 univariant hexagonal lattice complexes.

$P3_212$	**$3a$**	**..2**	**$x, -x, \frac{2}{3}$**	**$0 \le x \le \frac{1}{6}$**
A	$x, 2x, \frac{1}{3}$		$-2x, -x, 1$	
B	$x, -1+2x, \frac{1}{3}$		$1-2x, -x, 1$	
C	$x, -x, \frac{5}{3}$		$x, -x, -\frac{1}{3}$	
D	$1+x, -x, \frac{2}{3}$		$x, 1-x, \frac{2}{3}$	$1+x, 1-x, \frac{2}{3}$
	$-1+x, -x, \frac{2}{3}$		$x, -1-x, \frac{2}{3}$	$-1+x, -1-x, \frac{2}{3}$
0.1	6/4/*h*3	*ABC*	$\frac{1}{6}; \frac{3}{8}\sqrt{2}$	0.51013
0.2	10/3/*h*3	*ABD*	$\frac{1}{6}; \frac{3}{2}\sqrt{3}$	0.69813
1.1	4/6/*h*1	*AB*	$\frac{1}{6}; \frac{3}{4}\sqrt{2}$	0.39270
1.2	8/3/*h*4	*AD*	0; 3	0.60460
$P3_221$	**$3a$**	**.2.**	**$x, 0, \frac{2}{3}$**	**$0 \le x \le \frac{1}{2}$**
A	$0, x, \frac{1}{3}$		$-x, -x, 1$	
B	$1, x, \frac{1}{3}$		$1-x, -x, 1$	
	$0, -1+x, \frac{1}{3}$		$1-x, 1-x, 1$	
C	$x, 0, \frac{5}{3}$		$x, 0, -\frac{1}{3}$	
D	$1+x, 0, \frac{2}{3}$		$x, 1, \frac{2}{3}$	$1+x, 1, \frac{2}{3}$
	$-1+x, 0, \frac{2}{3}$		$x, -1, \frac{2}{3}$	$-1+x, -1, \frac{2}{3}$
0.1	8/4/*c*1	*ABC*	$\frac{1}{3}; \frac{1}{4}\sqrt{6}$	0.68017
0.2	12/3/*c*1	*ABD*	$\frac{1}{3}; \sqrt{6}$	0.74048
1.1	6/4/*c*1	*AB*	$\frac{1}{3}; \frac{1}{2}\sqrt{6}$	0.52360
1.2	6/4/*h*3	*BC*	$\frac{1}{2}; \frac{3}{8}\sqrt{2}$	0.51013
1.3	10/3/*h*3	*BD*	$\frac{1}{2}; \frac{3}{2}\sqrt{3}$	0.69813
1.4	8/3/*h*4	*AD*	0; 3	0.60460
2.1	4/6/*h*1	*B*	$\frac{1}{2}; \frac{3}{4}\sqrt{2}$	0.39270
$R32$	**$9d$**	**.2**	**$x, 0, 0$**	**$0 < x \le \frac{1}{2}$**
A	$0, x, 0$		$-x, -x, 0$	
B	$\frac{2}{3}-x, \frac{1}{3}-x, \frac{1}{3}$		$\frac{1}{3}, -\frac{1}{3}+x, -\frac{1}{3}$	
C	$x, 0, 1$		$x, 0, -1$	
D	$1, x, 0$		$1-x, -x, 0$	
	$0, -1+x, 0$		$1-x, 1-x, 0$	
E	$\frac{2}{3}, -\frac{2}{3}+x, \frac{1}{3}$		$\frac{4}{3}-x, \frac{2}{3}-x, -\frac{1}{3}$	
0.1	6/4/*h*7	*ABC*	$3-2\sqrt{2}; 3\sqrt{3}-2\sqrt{6}$	0.48054
0.2	8/3/*h*4	*ABD*	$\frac{1}{3}; \sqrt{3}$	0.60460
0.3	8/3/*c*2	*BDE*	$\frac{1}{2}; \frac{1}{2}\sqrt{6}$	0.55536
0.4	6/4/*h*1	*BCE*	$\frac{1}{2}; \frac{1}{8}\sqrt{6}$	0.51013
1.1	4/3/*h*1	*AB*	$\frac{1}{5}; \frac{1}{5}\sqrt{15}$	0.29202
1.2	6/3/*h*18	*BD*	$\frac{3}{5}-\frac{1}{15}\sqrt{6}$; $\frac{1}{5}(15+15\sqrt{6})^{1/2}$	0.50729
1.3	4/6/*c*2	*BE*	$\frac{1}{2}; \frac{1}{4}\sqrt{6}$	0.39270
$R3m$	**$9b$**	**.m**	**$x, -x, z$**	**$0 < x \le \frac{1}{6}, z = 0$**
A	$x, 2x, 0$		$-2x, -x, 0$	
B	$\frac{2}{3}-2x, \frac{1}{3}-x, \frac{1}{3}$		$\frac{1}{3}-2x, -\frac{1}{3}-x, -\frac{1}{3}$	
	$-\frac{1}{3}+x, -\frac{2}{3}+2x, \frac{1}{3}$		$\frac{1}{3}+x, -\frac{1}{3}+2x, -\frac{1}{3}$	
C	$x, -x, 1$		$x, -x, -1$	
D	$x, -1+2x, 0$		$1-2x, -x, 0$	
0.1	8/3/*h*7	*ABC*	$\frac{3}{2}-\frac{1}{6}\sqrt{69}; \frac{9}{2}-\frac{1}{2}\sqrt{69}$	0.65402
0.2	8/3/*c*2	*ABD*	$\frac{1}{6}; \frac{1}{2}\sqrt{6}$	0.55536
1.1	6/3/*h*14	*AB*	$\frac{2}{15}; \frac{1}{5}\sqrt{15}$	0.44959
1.2	6/4/*h*1	*BC*	$\frac{1}{6}; \frac{1}{8}\sqrt{6}$	0.51013
2.1	4/6/*c*2	*B*	$\frac{1}{6}; \frac{1}{4}\sqrt{6}$	0.39270
$P\bar{3}m1$	**$2d$**	**3m.**	**$\frac{1}{3}, \frac{2}{3}, z$**	**$0 \le z \le \frac{1}{4}$**
A	$\frac{2}{3}, \frac{1}{3}, -z$		$-\frac{1}{3}, \frac{1}{3}, -z$	$\frac{2}{3}, \frac{4}{3}, -z$
B	$\frac{2}{3}, \frac{1}{3}, 1-z$		$-\frac{1}{3}, \frac{1}{3}, 1-z$	$\frac{2}{3}, \frac{4}{3}, 1-z$
C	$\frac{1}{3}, \frac{2}{3}, 1+z$		$\frac{1}{3}, \frac{2}{3}, -1+z$	
D	$\frac{4}{3}, \frac{2}{3}, z$		$\frac{1}{3}, \frac{5}{3}, z$	$\frac{4}{3}, \frac{5}{3}, z$
	$-\frac{2}{3}, \frac{2}{3}, z$		$\frac{1}{3}, -\frac{1}{3}, z$	$-\frac{2}{3}, -\frac{1}{3}, z$
0.1	8/3/*h*3	*ABC*	$\frac{1}{4}; \frac{2}{3}$	0.53742
0.2	12/3/*h*1	*ABD*	$\frac{1}{4}; \frac{2}{3}\sqrt{6}$	0.74048
1.1	5/4/*h*5	*AC*	$0; \frac{1}{3}\sqrt{3}$	0.40307
1.2	6/4/*h*2	*AB*	$\frac{1}{4}; \frac{1}{3}\sqrt{6}$	0.52360

Table 2 (continued)

$R\bar{3}m$	**$6c$**	**3m**	**$0, 0, z$**	**$0 < z \le \frac{1}{4}$**
A	$0, 0, -z$			
B	$0, 0, 1-z$			
C	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3}-z$		$-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}-z$	$-\frac{1}{3}, -\frac{2}{3}, \frac{1}{3}-z$
D	$\frac{1}{3}, \frac{2}{3}, \frac{2}{3}-z$		$\frac{2}{3}, -\frac{1}{3}, \frac{2}{3}-z$	$\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}-z$
E	$1, 0, z$		$0, 1, z$	$1, 1, z$
	$-1, 0, z$		$0, -1, z$	$-1, -1, z$
0.1	8/4/*c*1	*ABCD*	$\frac{1}{4}; \frac{1}{2}\sqrt{6}$	0.68017
0.2	10/3/*h*4	*ACE*	$\frac{1}{2}-\frac{1}{6}\sqrt{6}; 3+\sqrt{6}$	0.66568
0.3	12/3/*c*1	*CDE*	$\frac{1}{4}; 2\sqrt{6}$	0.74048
1.1	4/6/*c*1	*AC*	$\frac{1}{8}; \sqrt{6}$	0.34009
1.2	6/4/*c*1	*CD*	$\frac{1}{4}; \sqrt{6}$	0.52360
$R\bar{3}m$	**$18f$**	**.2**	**$x, 0, 0$**	**$0 < x < \frac{1}{2}$**
A	$x, x, 0$		$0, -x, 0$	
B	$\frac{1}{3}, -\frac{1}{3}+x, -\frac{1}{3}$		$\frac{2}{3}-x, \frac{1}{3}-x, \frac{1}{3}$	
C	$x, 0, 1$		$x, 0, -1$	
D	$1-x, 0, 0$			
0.1	6/4/*h*9	*ABC*	$\frac{9}{19}-\frac{2}{19}\sqrt{6}; \frac{9}{19}-\frac{2}{19}\sqrt{6}$	0.50701
0.2	5/4/*h*5	*ABD*	$\frac{1}{3}; 1$	0.40307
0.3	5/4/*h*14	*BCD*	$\frac{7}{5}-\frac{2}{5}\sqrt{6}; \frac{4}{5}\sqrt{6}-\frac{9}{5}$	0.27718
1.1	4/4/*c*1	*AB*	$\frac{1}{4}; \frac{1}{4}\sqrt{6}$	0.27768
1.2	3/8/*h*1	*BD*	$\frac{9}{8}-\frac{1}{8}\sqrt{33}; \frac{9}{8}-\frac{1}{8}\sqrt{33}$	0.17248
$R\bar{3}c$	**$18e$**	**.2**	**$x, 0, \frac{1}{4}$**	**$0 < x \le \frac{1}{2}$**
A	$0, x, \frac{1}{4}$		$-x, -x, \frac{1}{4}$	
B	$\frac{2}{3}-x, \frac{1}{3}, \frac{1}{12}$		$\frac{1}{3}-x, -\frac{1}{3}, \frac{5}{12}$	
C	$\frac{1}{3}, -\frac{1}{3}+x, -\frac{1}{12}$		$\frac{2}{3}-x, \frac{1}{3}-x, \frac{7}{12}$	
D	$\frac{2}{3}, \frac{1}{3}-x, \frac{1}{12}$		$\frac{1}{3}+x, -\frac{1}{3}+x, \frac{5}{12}$	
	$-\frac{1}{3}+x, -\frac{2}{3}+x, \frac{1}{12}$		$\frac{1}{3}, \frac{2}{3}-x, \frac{5}{12}$	
E	$1-x, 0, \frac{3}{4}$		$1-x, 0, -\frac{1}{4}$	
F	$0, -x, \frac{3}{4}$		$0, -x, -\frac{1}{4}$	
	$x, x, \frac{3}{4}$		$x, x, -\frac{1}{4}$	
G	$0, -1+x, \frac{1}{4}$		$1-x, -x, \frac{1}{4}$	
	$1, x, \frac{1}{4}$		$1-x, 1-x, \frac{1}{4}$	
H	$x, 0, \frac{5}{4}$		$x, 0, -\frac{3}{4}$	
0.1	8/3/*h*8	*CFH*	$\frac{27}{49}-\frac{12}{49}\sqrt{2}$; $\frac{2}{49}(339-216\sqrt{2})^{1/2}$	0.60791
0.2	8/3/*h*9	*ACF*	$\frac{9}{8}-\frac{1}{8}\sqrt{57}; \frac{1}{2}(69-9\sqrt{57})^{1/2}$	0.65695
0.3	6/3/*h*19	*ABC*	$\frac{3}{4}-\frac{1}{4}\sqrt{5}; \frac{1}{2}(42-18\sqrt{5})^{1/2}$	0.59542
0.4	8/3/*h*3	*BCD*	$\frac{1}{3}; \frac{2}{3}\sqrt{3}$	0.53742
0.5	8/3/*h*2	*CDE*	$\frac{1}{14}\sqrt{57}-\frac{1}{14}$; $\frac{1}{7}(54\sqrt{57}-390)^{1/2}$	0.52528
0.6	6/3/*h*15	*CEH*	$\frac{37}{47}-\frac{12}{47}\sqrt{2}$; $\frac{2}{47}(627-432\sqrt{2})^{1/2}$	0.31648
0.7	12/3/*h*1	*ABDG*	$\frac{1}{3}; 2\sqrt{2}$	0.74048
1.1	6/4/*h*8	*CF*	0.19854; 0.32962	0.56721
1.2	4/5/*h*2	*BC*	0.26212; 0.90800	0.41845
1.3	6/3/*h*16	*CD*	0.42154; 0.89096	0.45502
1.4	4/5/*h*1	*CE*	0.43053; 0.25508	0.28622
1.5	4/3/*h*2	*AB*	$\frac{5}{4}-\frac{1}{4}\sqrt{17}$; $\frac{1}{2}(18\sqrt{17}-66)^{1/2}$	0.41571
1.6	6/4/*h*2	*BD*	$\frac{1}{3}; \sqrt{2}$	0.52360
1.7	6/4/*h*1	*DE*	$\frac{1}{2}; \frac{1}{4}\sqrt{6}$	0.51013
1.8	8/3/*c*2	*DG*	$\frac{1}{2}; \sqrt{6}$	0.55536
*i*1.1	$h[4/3/h1]^2$	*AC*	–; –	>0.59542
2.1	4/6/*c*2	*D*	$\frac{1}{2}; \frac{1}{2}\sqrt{6}$	0.39270

Table 2 (continued)

$P6_122$	**$6a$ $.2.$**		**$x, 0, 0$**	**$0 \le x \le \frac{1}{2}$**
A	$x, x, \frac{1}{6}$		$0, -x, -\frac{1}{6}$	
B	$1{+}x, 0, 0$		$x, 1, 0$	$1{+}x, 1, 0$
	$-1{+}x, 0, 0$		$x, -1, 0$	$-1{+}x, -1, 0$
C	$x, 0, 1$		$x, 0, -1$	
D	$1{-}x, 0, \frac{1}{2}$		$1{-}x, 0, -\frac{1}{2}$	
E	$x, -1{+}x, \frac{1}{6}$		$1, 1{-}x, -\frac{1}{6}$	
0.1	6/3/*h*17	*ACD*	$\frac{70}{113}-\frac{3}{113}\sqrt{105}$; $\frac{6}{113}(167-12\sqrt{105})^{1/2}$	0.45038
0.2	6/4/*h*3	*ADE*	$\frac{1}{2}$; $\frac{3}{4}\sqrt{2}$	0.51013
0.3	10/3/*h*3	*ABE*	$\frac{1}{2}$; $3\sqrt{3}$	0.69813
1.1	4/6/*h*3	*AD*	0.38285; 0.64227	0.35482
1.2	4/6/*h*1	*AE*	$\frac{1}{2}$; $\frac{3}{2}\sqrt{2}$	0.39270
1.3	8/3/*h*4	*AB*	0; 6	0.60460

$P6_122$	**$6b$ $..2$**		**$x, 2x, \frac{1}{4}$**	**$0 \le x \le \frac{1}{2}$**
A	$2x, x, \frac{1}{12}$		$-x, x, \frac{5}{12}$	
B	$1{+}x, 2x, \frac{1}{4}$		$x, 1{+}2x, \frac{1}{4}$	$1{+}x, 1{+}2x, \frac{1}{4}$
	$-1{+}x, 2x, \frac{1}{4}$		$x, -1{+}2x, \frac{1}{4}$	$-1{+}x, -1{+}2x, \frac{1}{4}$
C	$x, 1{-}x, -\frac{1}{12}$		$1{-}2x, 1{-}x, \frac{7}{12}$	
D	$-1{+}2x, x, \frac{1}{12}$		$1{-}x, x, \frac{5}{12}$	
	$2x, 1{+}x, \frac{1}{12}$		$1{-}x, 1{+}x, \frac{5}{12}$	
E	$1{-}x, 2{-}2x, \frac{3}{4}$		$1{-}x, 2{-}2x, -\frac{1}{4}$	
F	$x, 2x, \frac{5}{4}$		$x, 2x, -\frac{3}{4}$	
0.1	6/4/*h*6	*ACF*	$\frac{35}{73}-\frac{4}{219}\sqrt{210}$; $\frac{6}{73}\sqrt{105}-\frac{24}{73}\sqrt{2}$	0.51632
0.2	8/3/*h*3	*ACD*	$\frac{1}{3}$; 2	0.53742
0.3	12/3/*h*1	*ABD*	$\frac{1}{3}$; $2\sqrt{6}$	0.74048
0.4	6/3/*h*12	*CEF*	$\frac{37}{47}-\frac{12}{47}\sqrt{2}$; $\frac{48}{47}\sqrt{2}-\frac{54}{47}$	0.31648
0.5	8/3/*h*6	*CDE*	$\frac{1}{14}\sqrt{57}-\frac{1}{14}$; $\frac{3}{7}(18\sqrt{57}-130)^{1/2}$	0.52528
1.1	4/5/*h*3	*AC*	0.23648; 1.00012	0.31367
1.2	6/4/*h*2	*AD*	$\frac{1}{3}$; $\sqrt{6}$	0.52360
1.3	8/3/*h*4	*AB*	0; 6	0.60460
1.4	4/5/*h*4	*CE*	0.43053; 0.44182	0.28622
1.5	6/3/*h*10	*CD*	0.42154; 1.54319	0.45502
1.6	6/4/*h*3	*DE*	$\frac{1}{2}$; $\frac{3}{4}\sqrt{2}$	0.51013
1.7	10/3/*h*3	*BD*	$\frac{1}{2}$; $3\sqrt{3}$	0.69813
2.1	4/6/*h*1	*D*	$\frac{1}{2}$; $\frac{3}{2}\sqrt{2}$	0.39270

$P6_222$	**$6f$ $2..$**		**$\frac{1}{2}, 0, z$**	**$0 < z \le \frac{1}{4}$**
A	$\frac{1}{2}, 0, -z$			
B	$\frac{1}{2}, \frac{1}{2}, \frac{1}{3}{-}z$		$\frac{1}{2}, -\frac{1}{2}, \frac{1}{3}{-}z$	
C	$\frac{1}{2}, 0, 1{-}z$			
D	$1, \frac{1}{2}, \frac{2}{3}{-}z$		$0, -\frac{1}{2}, \frac{2}{3}{-}z$	
E	$\frac{3}{2}, 0, z$		$\frac{1}{2}, 1, z$	$\frac{3}{2}, 1, z$
	$-\frac{1}{2}, 0, z$		$\frac{1}{2}, -1, z$	$-\frac{1}{2}, -1, z$
0.1	6/4/*h*3	*ABCD*	$\frac{1}{4}$; $\frac{3}{4}\sqrt{2}$	0.51013
0.2	9/3/*h*3	*ABE*	$\frac{2}{3}-\frac{1}{3}\sqrt{3}$; $3+\frac{3}{2}\sqrt{3}$	0.64801
0.3	10/3/*h*3	*BDE*	$\frac{1}{4}$; $3\sqrt{3}$	0.69813
1.1	3/10/*h*1	*AB*	$\frac{1}{8}$; $\frac{3}{2}\sqrt{2}$	0.25507
1.2	4/6/*h*1	*BD*	$\frac{1}{4}$; $\frac{3}{2}\sqrt{2}$	0.39270

$P6_222$	**$6g$ $.2.$**		**$x, 0, 0$**	**$0 < x < \frac{1}{2}$**
A	$x, x, \frac{1}{3}$		$0, -x, -\frac{1}{3}$	
B	$x, 0, 1$		$x, 0, -1$	
C	$1{-}x, 0, 0$			
D	$-x, 0, 0$			
0.1	5/4/*h*15	*ABC*	$\frac{16}{23}-\frac{6}{23}\sqrt{2}$; $\frac{12}{23}\sqrt{2}-\frac{9}{23}$	0.43565
0.2	4/4/*h*1	*ACD*	$\frac{1}{4}$; $\frac{3}{4}\sqrt{3}$	0.34907
1.1	3/12/*h*1	*AC*	$\frac{17}{24}-\frac{1}{24}\sqrt{97}$; $\frac{1}{8}(102-6\sqrt{97})^{1/2}$	0.29229

Table 2 (continued)

$P6_222$	**$6i$ $..2$**		**$x, 2x, 0$**	**$0 < x < \frac{1}{2}$**
A	$2x, x, -\frac{1}{3}$		$-x, x, \frac{1}{3}$	
B	$x, 2x, 1$		$x, 2x, -1$	
C	$1{-}2x, 1{-}x, -\frac{1}{3}$		$x, 1{-}x, \frac{1}{3}$	
D	$1{-}x, 2{-}2x, 0$			
E	$-x, -2x, 0$			
F	$-x, 1{-}2x, 0$		$1{-}x, 1{-}2x, 0$	
0.1	6/4/*h*5	*ABC*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}$; $\frac{3}{8}\sqrt{6}-\frac{3}{8}\sqrt{2}$	0.54676
0.2	5/4/*h*13	*BCD*	$\frac{7}{5}-\frac{2}{5}\sqrt{6}$; $\frac{12}{5}\sqrt{2}-\frac{9}{5}\sqrt{3}$	0.27718
0.3	6/3/*h*3	*ACF*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}$; $\frac{3}{2}\sqrt{3}-\frac{3}{2}$	0.45821
0.4	5/4/*h*11	*AEF*	$\frac{1}{6}$; $\frac{3}{2}$	0.46542
0.5	5/4/*h*5	*CDF*	$\frac{1}{3}$; $\sqrt{3}$	0.40307
1.1	4/4/*h*2	*AC*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}$; $\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$	0.42089
1.2	3/8/*h*2	*CD*	$\frac{9}{8}-\frac{1}{8}\sqrt{33}$; $\frac{9}{8}\sqrt{3}-\frac{3}{8}\sqrt{11}$	0.17248
1.3	4/4/*h*3	*AF*	$\frac{5}{16}-\frac{1}{48}\sqrt{33}$; $\frac{3}{16}+\frac{3}{16}\sqrt{33}$	0.44621
1.4	4/4/*h*4	*CF*	$\frac{1}{16}+\frac{1}{48}\sqrt{105}$; $\frac{3}{16}\sqrt{3}+\frac{3}{16}\sqrt{35}$	0.33170

$P\bar{6}m2$	**$3j$ $mm2$**		**$x, -x, 0$**	**$0 < x \le \frac{1}{6}$**
A	$x, 2x, 0$		$-2x, -x, 0$	
B	$x, -1{+}2x, 0$		$1{-}2x, -x, 0$	
C	$x, -x, 1$		$x, -x, -1$	
0.1	6/3/*h*13	*ABC*	$\frac{1}{6}$; $\frac{1}{2}$	0.45345

$P\bar{6}2m$	**$3f$ $m2m$**		**$x, 0, 0$**	**$0 < x \le {}^{1}/_{2}$**
A	$0, x, 0$		$-x, -x, 0$	
B	$1, x, 0$		$1{-}x, -x, 0$	
	$0, -1{+}x, 0$		$1{-}x, 1{-}x, 0$	
C	$x, 0, 1$		$x, 0, -1$	
0.1	8/3/*h*4	*ABC*	$\frac{1}{3}$; $\frac{1}{3}\sqrt{3}$	0.60460
1.1	6/3/*h*13	*BC*	$\frac{1}{2}$; $\frac{1}{2}$	0.45345

$P6/mmm$	**$2e$ $6mm$**		**$0, 0, z$**	**$0 < z \le \frac{1}{4}$**
A	$0, 0, -z$			
B	$0, 0, 1{-}z$			
C	$1, 0, z$		$0, 1, z$	$1, 1, z$
	$-1, 0, z$		$0, -1, z$	$-1, -1, z$
0.1	8/3/*h*4	*ABC*	$\frac{1}{4}$; 2	0.60460

$P6/mmm$	**$4h$ $3m.$**		**$\frac{1}{3}, \frac{2}{3}, z$**	**$0 < z \le \frac{1}{4}$**
A	$\frac{1}{3}, \frac{2}{3}, -z$			
B	$\frac{1}{3}, \frac{2}{3}, 1{-}z$			
C	$\frac{2}{3}, \frac{1}{3}, z$		$\frac{2}{3}, \frac{4}{3}, z$	$-\frac{1}{3}, \frac{1}{3}, z$
0.1	5/4/*h*5	*ABC*	$\frac{1}{4}$; $\frac{2}{3}\sqrt{3}$	0.40307

$P6/mmm$	**$6i$ $2mm$**		**$\frac{1}{2}, 0, z$**	**$0 < z \le \frac{1}{4}$**
A	$\frac{1}{2}, 0, -z$			
B	$\frac{1}{2}, 0, 1{-}z$			
C	$\frac{1}{2}, \frac{1}{2}, z$		$1, \frac{1}{2}, z$	
	$\frac{1}{2}, -\frac{1}{2}, z$		$0, -\frac{1}{2}, z$	
0.1	6/3/*h*13	*ABC*	$\frac{1}{4}$; 1	0.45345

$P6/mmm$	**$6j$ $m2m$**		**$x, 0, 0$**	**$0 < x < \frac{1}{2}$**
A	$x, x, 0$		$0, -x, 0$	
B	$1{-}x, 0, 0$			
C	$x, 0, 1$		$x, 0, -1$	
0.1	5/4/*h*5	*ABC*	$\frac{1}{3}$; $\frac{1}{3}$	0.40307

$P6/mmm$	**$6l$ $mm2$**		**$x, 2x, 0$**	**$0 < x < \frac{1}{3}$; $\frac{1}{3} < x < \frac{1}{2}$**
A	$2x, x, 0$		$-x, x, 0$	
B	$x, 2x, 1$		$x, 2x, -1$	
C	$1{-}2x, 1{-}x, 0$		$x, 1{-}x, 0$	
D	$1{-}x, 2{-}2x, 0$			
0.1	6/3/*h*20	*ABC*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}$; $\frac{1}{2}\sqrt{3}-\frac{1}{2}$	0.48601
0.2	5/3/*h*5	*BCD*	$1-\frac{1}{3}\sqrt{3}$; $2-\sqrt{3}$	0.26045

Table 2 (continued)

P*6$_3$/*mcm	***6g***	***m*2*m***	$\mathbf{x, 0, \frac{1}{4}}$	$\mathbf{0 < x \le \frac{1}{2}}$
A	$-x, -x, \frac{1}{4}$		$0, x, \frac{1}{4}$	
B	$x, x, \frac{3}{4}$		$0, -x, \frac{3}{4}$	
	$x, x, -\frac{1}{4}$		$0, -x, -\frac{1}{4}$	
C	$x, 0, \frac{5}{4}$		$x, 0, -\frac{3}{4}$	
D	$1-x, -x, \frac{1}{4}$		$1, x, \frac{1}{4}$	
	$1-x, 1-x, \frac{1}{4}$		$0, -1+x, \frac{1}{4}$	
E	$1-x, 0, \frac{3}{4}$		$1-x, 0, -\frac{1}{4}$	
0.1	8/3/*h*3	*BCE*	$\frac{1}{3}; \frac{2}{9}\sqrt{3}$	0.53742
0.2	12/3/*h*1	*ABDE*	$\frac{1}{3}; \frac{2}{3}\sqrt{2}$	0.74048
1.1	6/4/*h*2	*BE*	$\frac{1}{3}; \frac{1}{3}\sqrt{2}$	0.52360
1.2	6/3/*h*13	*DE*	$\frac{1}{2}; 1$	0.45345
P*6$_3$/*mmc	***4f***	**3*m*.**	$\mathbf{\frac{1}{3}, \frac{2}{3}, z}$	$\mathbf{0 \le z < \frac{1}{4}}$
A	$\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z$			
B	$\frac{1}{3}, \frac{2}{3}, -\frac{1}{2}-z$			
C	$\frac{2}{3}, \frac{1}{3}, -z$		$-\frac{1}{3}, \frac{1}{3}, -z$	$\frac{2}{3}, \frac{4}{3}, -z$
D	$\frac{4}{3}, \frac{2}{3}, z$		$\frac{1}{3}, \frac{5}{3}, z$	$\frac{4}{3}, \frac{5}{3}, z$
	$-\frac{2}{3}, \frac{2}{3}, z$		$\frac{1}{3}, -\frac{1}{3}, z$	$-\frac{2}{3}, -\frac{1}{3}, z$
0.1	5/4/*h*5	*ABC*	$0; \frac{2}{3}\sqrt{3}$	0.40307
0.2	10/3/*h*2	*ACD*	$\frac{1}{4}\sqrt{6}-\frac{1}{2}; 2+\frac{2}{3}\sqrt{6}$	0.66568
1.1	4/6/*h*2	*AC*	$\frac{1}{16}; \frac{2}{3}\sqrt{6}$	0.34009
P*6$_3$/*mmc	***6h***	***mm*2**	$\mathbf{x, 2x, \frac{1}{4}}$	$\mathbf{0 < x < \frac{1}{3}; \frac{1}{3} < x \le \frac{1}{2}}$
A	$-2x, -x, \frac{1}{4}$		$x, -x, \frac{1}{4}$	
B	$2x, x, \frac{3}{4}$		$-x, x, \frac{3}{4}$	
	$2x, x, -\frac{1}{4}$		$-x, x, -\frac{1}{4}$	
C	$x, 2x, \frac{5}{4}$		$x, 2x, -\frac{3}{4}$	
D	$1-2x, 1-x, \frac{1}{4}$		$x, 1-x, \frac{1}{4}$	
E	$1-x, 2-2x, \frac{3}{4}$		$1-x, 2-2x, -\frac{1}{4}$	
F	$2-2x, 2-x, \frac{1}{4}$		$x, 2-x, \frac{1}{4}$	
0.1	8/3/*h*10	*ABD*	$\frac{1}{6}; \frac{1}{3}\sqrt{6}$	0.55536
0.2	8/3/*h*11	*BCD*	$\frac{1}{5}; \frac{2}{5}$	0.58042
0.3	6/3/*h*21	*CDE*	$\frac{3}{7}; \frac{2}{7}$	0.29613
0.4	6/3/*h*13	*DEF*	$\frac{1}{2}; 1$	0.45345
1.1	6/3/*h*22	*BD*	$\frac{13}{24}-\frac{1}{24}\sqrt{73}$; $\frac{1}{6}(39-3\sqrt{73})^{1/2}$	0.51755
1.2	4/3/*h*3	*DE*	$\frac{7}{6}-\frac{1}{6}\sqrt{19}; \frac{1}{3}(6\sqrt{19}-24)^{1/2}$	0.24427

density ρ_m is helpful for the assignment to a sphere-packing type. The values of ρ_m and of the corresponding parameters were determined with the aid of the PC program *EUREKA: THE SOLVER* (1987).

4. Results

Data on all sphere packings and all interpenetrating sphere packings that correspond to the seven invariant and the 23 univariant lattice complexes of the hexagonal crystal family are summarized in Tables 1 and 2. First, each lattice complex is identified by its characteristic Wyckoff position, the respective site symmetry and the coordinate triplet of a reference point. In the case of a univariant lattice complex, this information is completed by the range of the coordinate parameter that has to be investigated.

All possible *neighbouring points*, *i.e.* the centres of all those spheres that may have contact with the sphere with centre at the reference point, are listed in a second block of information. For symmetry reasons, sets with two or more equidistant neighbouring points may be formed, irrespective of the choice of the free coordinate or metrical parameters. Each such (set of) neighbouring point(s) is designated by a capital letter.

The third block lists the types of (interpenetrating) sphere packings together with their parameter regions: In the first column, 0.*i*, 1.*i* or 2.*i* designate a zero-, a one- or a two-dimensional range, respectively, with *i* being a serial number. The sphere-packing type is shown in the second column. A string of capital letters symbolizes all neighbouring points that give rise to sphere contacts. The last two columns are related to those special sphere packings that show minimal density: the corresponding values of *x* or *z* (in the case of a univariant lattice complex) and of *c*/*a* are given in the fourth column; the fifth column displays the value ρ_m of the minimal density.

For each univariant lattice complex, the parameter region that has to be investigated is represented in Fig. 1. Each two-dimensional subregion corresponds to exactly one (set of) neighbouring point(s) with shortest distance to the original point and, therefore, can be labelled by the corresponding capital letter. The borders between these subregions form one-dimensional subregions, *i.e.* lines, and zero-dimensional subregions, *i.e.* points. Each subregion refers to a certain type of sphere configuration. Sphere packings are distinguished by their symbols 0.*i*, 1.*i* or 2.*i* (*cf*. Table 2).

5. Discussion

The hexagonal invariant lattice complexes lead to sphere packings of altogether 15 types. Owing to limiting-complex relationships, however, in five cases the inherent symmetry of the sphere packings with minimal density is cubic: lattice complexes $Pm\bar{3}m$ 1*a*, $Im\bar{3}m$ 2*a* and $Fm\bar{3}m$ 4*a* form limiting complexes of $R\bar{3}m$ 3*a*; lattice complexes $Im\bar{3}m$ 6*b* and $Pm\bar{3}m$ 3*c* form limiting complexes of $R\bar{3}m$ 9*e*.[1] This may be read from the letter *c* in the symbols of the sphere-packing types.

The hexagonal univariant lattice complexes yield sphere packings of 66 different types in total. Owing to limiting-complex relationships, the 15 sphere-packing types referring to the invariant lattice complexes occur again between two and seven times. All other sphere-packing types appear only once. Two further types are found, the maximal inherent symmetry of which is cubic ($Im\bar{3}m$ 12*d* forms a limiting complex of $R\bar{3}m$ 18*f*, $Fd\bar{3}m$ 8*a* a limiting complex of $R\bar{3}m$ 6*c*). None of the sphere packings has contact number seven or eleven.

Interpenetrating sphere packings are found only once, namely with site symmetry .2 for lattice complex $R\bar{3}m$ 18*e* (*cf*. Fig. 2). The corresponding sphere configurations $h[4/3/h1]^2$ disintegrate into two partial configurations, each of which forms a hexagonal sphere packing with symmetry *R*32 9*d* .2 and belongs to type 4/3/*h*1. *R*32 is a subgroup of $R\bar{3}m$ with index 2, and each symmetry operation of $R\bar{3}m$ that does not belong to *R*32 maps one of the two sphere packings onto the

[1] As these limiting complexes are connected not only with specialized coordinates but also with specialized metrical parameters, they have not been tabulated as 'non-characteristic orbits' by Engel *et al.* (1984).

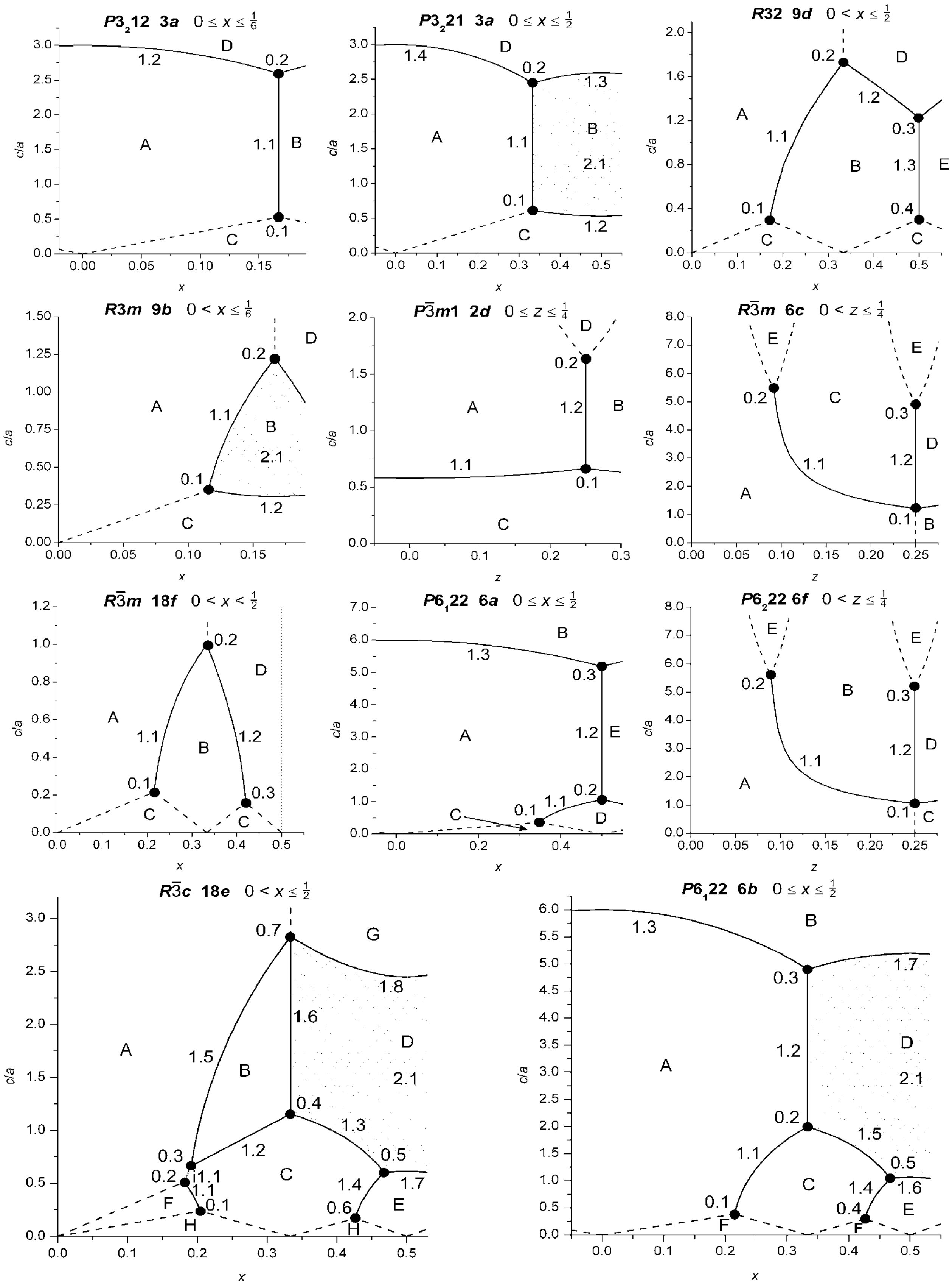

Figure 1
Parameter regions of the sphere configurations belonging to the hexagonal univariant lattice complexes: sphere packings are identified by solid lines (one degree of freedom) or solid circles (no degree of freedom); two-dimensional parameter regions of sphere packings are hatched. The dotted line *i*1.1 in $R\bar{3}c$ 18*e* corresponds to interpenetrating sphere packings $h[4/3/h1]^2$.

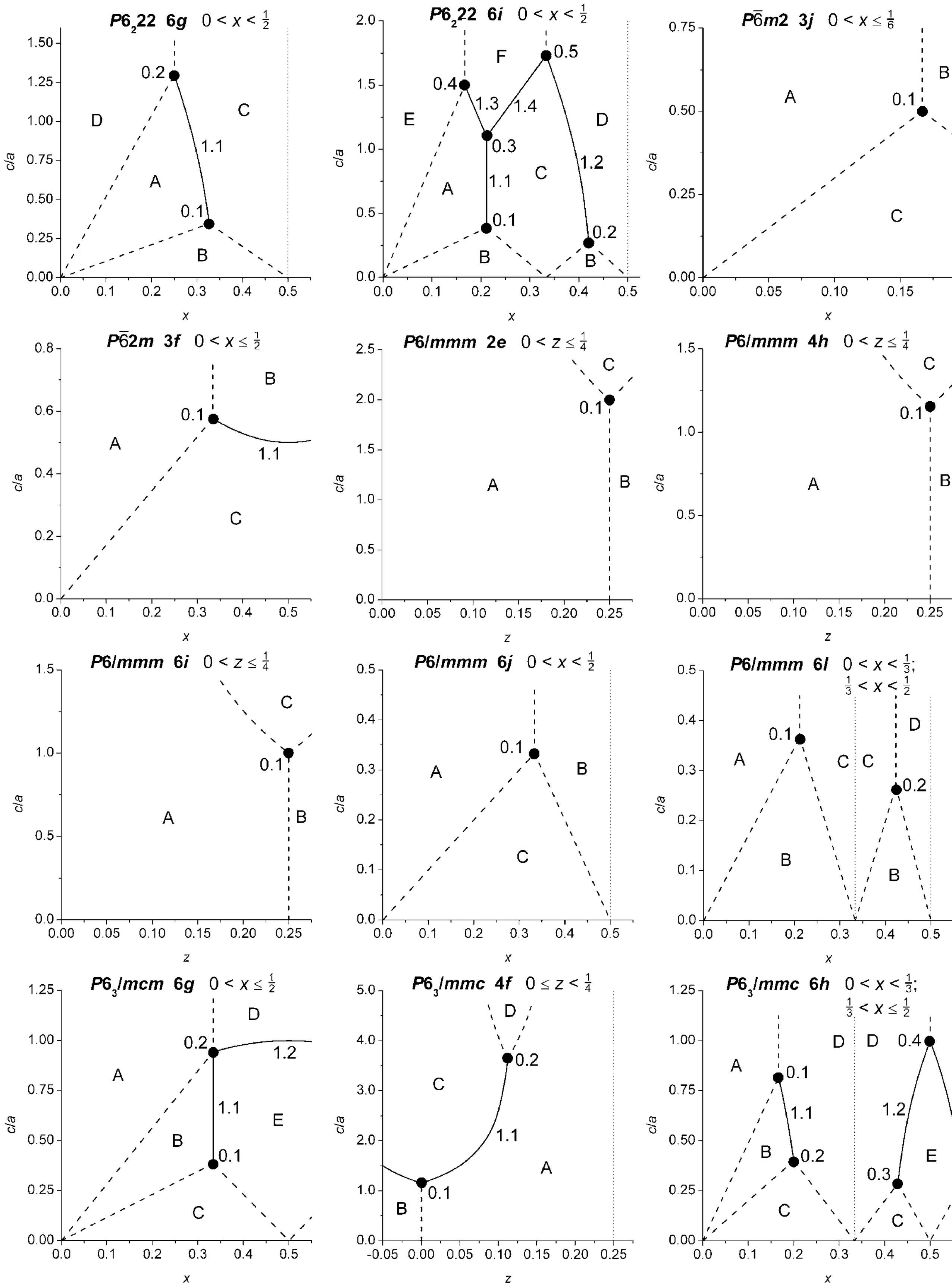

Figure 1 (continued)

Table 3
Examples of crystal structures corresponding to hexagonal sphere packings.

Substance	Symmetry	Sphere-packing type	*c*/*a*	*c*/*a* (ideal)	*x* or *z*	*x* or *z* (ideal)	*s* (%)	References
$\mathbf{Ge}\mathrm{Te}$	$R3m$ 3*a*	12/3/*c*1	2.5672	2.4495			1.6	Goldak *et al.* (1966)
$\mathrm{Ge}\mathbf{Te}$	$R3m$ 3*a*		2.5672	2.4495			1.6	Goldak *et al.* (1966)
$\mathrm{Mn}\mathbf{Cl_2}$	$R\bar{3}m$ 6*c*		4.7400	4.8990	0.2545	$\frac{1}{4}$	2.7	Tornero & Fayos (1990)
$\mathrm{Li_{0.9}(Y_{0.9}Zr_{0.1})}\mathbf{S_2}$	$R\bar{3}m$† 6*c*		4.7613	4.8990	0.249	$\frac{1}{4}$	1.1	Abou Ghaloun *et al.* (1980)
$\mathbf{He}$	$P6_3/mmc$ 2*c*	12/3/*h*1	1.6288	1.6330			0.1	Schuch & Mills (1962)
$\mathrm{Mn}\mathbf{Te}$	$P6_3/mmc$ 2*c*		1.6297	1.6330			0.1	Makovetskii *et al.* (1996)
$\mathrm{Zr}\mathbf{Br_3}$	$P6_3/mcm$ 6*g*		0.9362	0.9428	0.3211	$\frac{1}{3}$	2.2	Larsen *et al.* (1982)
$\mathbf{Zr_3}\mathrm{O}$	$P6_322$ 6*g*		0.9231	0.9428	0.3333	$\frac{1}{3}$	0.7	Riabov *et al.* (1999)
$\mathrm{Re_{1.16}}\mathbf{O_3}$	$P6_322$ 6*g*		0.9380	0.9428	0.359	$\frac{1}{3}$	4.5	Jeitschko & Sleight (1972)
$\mathrm{Zn}\mathbf{S}$	$P6_3mc$ 2*b*		1.6378	1.6330			0.1	Kisi & Elcombe (1989)
$\mathbf{Zn}\mathrm{S}$	$P6_3mc$ 2*b*		1.6378	1.6330			0.1	Kisi & Elcombe (1989)
$\mathrm{Mg}\mathbf{Cl_2}$	$P\bar{3}m1$ 2*d*		1.6278	1.6330	0.23	$\frac{1}{4}$	3.8	Bassi *et al.* (1982)
$\mathrm{Cu_2Er_{0.667}}\mathbf{S_2}$	$P\bar{3}m1$† 2*d*		1.6249	1.6330	0.2457		0.8	Guymont *et al.* (1990)
$\mathrm{V_2}\mathbf{O_3}$	$R\bar{3}c$ 18*e*		2.8252	2.8284	0.3114	$\frac{1}{3}$	3.5	Chen *et al.* (1982)
$\mathrm{Rh}\mathbf{F_3}$	$R\bar{3}c$ 18*e*		2.7806	2.8284	0.6518	$\frac{2}{3}$	2.4	Grosse & Hoppe (1987)
$\mathrm{Nb}\mathbf{Se_2}$	$P6_3/mmc$ 4*f*	10/3/*h*2	3.6418	3.6330	0.1172	0.1124	1.9	Marezio *et al.* (1972)
$\mathbf{Ti}\mathrm{P}$	$P6_3/mmc$ 4*f*		3.3438	3.6330	0.1170	0.1124	3.3	Snell (1967)
$\mathrm{HCr}\mathbf{O_2}$	$R\bar{3}m$ 6*c*	10/3/*h*4	4.4887	5.4495	0.4075	0.4082	7.0	Ichikawa *et al.* (1999)
$\mathrm{Sc}\mathbf{F_3}$	$R32$ 9*e*	8/3/*c*2	1.2289	1.2247	0.487	$\frac{1}{2}$	1.8	Loesch *et al.* (1982)
$\mathrm{Ti}\mathbf{F_3}$	$R\bar{3}c$ 18*e*		2.5106		0.5603		0.1	Hoppe & Becker (1989)
$\mathrm{V}\mathbf{F_3}$	$R\bar{3}c$ 18*e*		2.6002		0.4001		0.1	Daniel *et al.* (1990)
$\mathbf{Al}\mathrm{B_2}$	$P6/mmm$ 1*a*	8/3/*h*4	1.0841	1			3.6	Felten (1956)
$\mathbf{Cs}\mathrm{Cu_3S_2}$	$P\bar{3}m1$ 1*b*		1.1618	1			6.7	Burschka (1980)
$\mathrm{Ni}\mathbf{S}$	$R3m$ 9*b*	8/3/*h*7	0.3275	0.3467	0.1124	0.1156	2.6	Rajamani & Prewitt (1974)
$\mathrm{CsSc}\mathbf{Cl_3}$	$P6_3/mmc$ 6*h*	8/3/*h*10	0.8224	0.8165	0.1611	$\frac{1}{6}$	2.4	Poeppelmeier *et al.* (1980)
$\mathrm{Ni_3}\mathbf{S_2}$	$R32$ 6*c*	8/4/*c*1	1.2416	1.2247	0.2475	$\frac{1}{4}$	0.8	Metcalf *et al.* (1993)
β-$\mathrm{Si}\mathbf{O_2}$	$P6_222$ 6*j*	6/3/*h*3	1.0922	1.0981	0.2076	0.2113	1.0	Kihara (1990)
$\mathrm{Ce}\mathbf{Rh_3}\mathrm{B_2}$	$P6/mmm$ 3*g*	6/3/*h*13	0.5629	$\frac{1}{2}$			5.7	Kasaya *et al.* (1987)
$\mathrm{Na}\mathbf{Pt_3}\mathrm{B}$	$P6/mmm$ 6*i*		0.9922	1	0.2422	$\frac{1}{4}$	1.8	Mirgel & Jung (1988)
$\mathrm{Ta}\mathbf{N}$	$P\bar{6}2m$ 3*f*		0.5602		0.3928		2.3	Christensen & Lebech (1978)
$\mathrm{RbH}\mathbf{S}$	$R\bar{3}m$ 3*b*	6/4/*c*1	1.9855				–	Jacobs *et al.* (1991)
$\mathbf{Rb}\mathrm{HS}$	$R\bar{3}m$ 3*a*		1.9855				–	Jacobs *et al.* (1991)
$\mathrm{H_3Br}\mathbf{O}$	$R3m$ 3*a*		1.7608				–	Lundgren (1970)
$\mathrm{H_3}\mathbf{Br}\mathrm{O}$	$R3m$ 3*a*		1.7608				–	Lundgren (1970)
$\mathbf{Sc}\mathrm{F_3}$	$R32$ 3*a*		1.2289				–	Loesch *et al.* (1982)
$\mathbf{Ti}\mathrm{F_3}$	$R\bar{3}c$ 6*b*		2.5106				–	Hoppe & Becker (1989)
$\mathbf{V}\mathrm{F_3}$	$R\bar{3}c$ 6*b*		2.6002				–	Daniel *et al.* (1990)
$\mathbf{Rh}\mathrm{F_3}$	$R\bar{3}c$ 6*b*		2.7806				–	Grosse & Hoppe (1987)
$\mathbf{Ag_3}\mathrm{BO_3}$	$R32$ 9*d*	6/4/*h*1	0.3424	0.3062	0.5005	$\frac{1}{2}$	4.7	Jansen & Scheld (1981)
$\mathrm{Ni}\mathbf{As}$	$P6_3/mmc$ 2*c*	6/4/*h*2	1.3885				–	Yund (1962)
$\mathbf{Cs}\mathrm{ScCl_3}$	$P6_3/mmc$ 2*d*		0.8224				–	Poeppelmeier *et al.* (1980)
$\mathrm{CsCu_3}\mathbf{S_2}$	$P\bar{3}m1$ 2*d*		1.1618		0.2326	$\frac{1}{4}$	3.5	Burschka (1980)
$\mathrm{Ca}(\mathbf{OH})_2$	$P\bar{3}m1$ 2*d*		1.3683		0.7663	$\frac{3}{4}$	3.8	Desgranges *et al.* (1993)
$\mathrm{CeRh_3}\mathbf{B_2}$	$P6/mmm$ 2*c*	5/4*h*5	0.5629	0.5774			1.2	Kasaya *et al.* (1987)
$\mathrm{Nb}\mathbf{Ge_2}$	$P6_222$ 6*j*	5/4*h*11	1.3656	$\frac{3}{2}$	0.1631	$\frac{1}{6}$	3.8	Kubiak *et al.* (1972)
$\mathrm{Hg_2}\mathbf{O_2}\mathrm{NaI}$	$P6_222$ 6*i*		1.5080	$\frac{3}{2}$	0.1521	$\frac{1}{6}$	5.0	Aurivillius (1964)
$\mathbf{Ni_3}\mathrm{S_2}$	$R32$ 9*e*	4/3/*h*1	1.2416		0.2445		2.1	Metcalf *et al.* (1993)
$\mathrm{In_2}\mathbf{O_3}$	$R\bar{3}c$ 18*e*	4/3/*h*2	2.6444		0.2980		1.8	Prewitt *et al.* (1969)
$\mathbf{In_2}\mathrm{O_3}$	$R\bar{3}c$ 12*c*	4/6/*c*1	2.6444		0.3573		1.7	Prewitt *et al.* (1969)
$\mathbf{V_2}\mathrm{O_3}$	$R\bar{3}c$ 12*c*		2.8252		0.3464		2.8	Chen *et al.* (1982)
β-$\mathbf{Si}\mathrm{O_2}$	$P6_222$ 3*c*	4/6/*h*1	1.0922				–	Kihara (1990)
$\mathbf{Nb}\mathrm{Ge_2}$	$P6_222$ 3*c*		1.3656				–	Kubiak *et al.* (1972)
$\mathrm{Hg_2O_2Na}\mathbf{I}$	$P6_222$ 3*c*		1.5080				–	Aurivillius (1964)
$\mathbf{C}$	$P6_3/mmc$ 4*f*	4/6/*h*2	1.635	1.6330	0.0625	$\frac{1}{16}$	0.0	Bundy & Kasper (1967)
$\mathbf{Hg_2}\mathrm{O_2NaI}$	$P6_222$ 6*f*	3/10/*h*1	1.5080		0.3333		0.3	Aurivillius (1964)

† Wrong space group reported in the literature.

other one. The two interpenetrating sphere packings form an enantiomorphic pair.

6. Examples of crystal structures

Atomic arrangements within crystal structures frequently may be interpreted as sphere packings. That does not mean, however, that indeed the corresponding atoms are spheres in contact. Merely, the shortest distances between the atoms have to be (approximately) equal.

Figs. 3 and 4 illustrate two such sample structures. In both cases, each kind of atom of a binary compound is arranged as a slightly distorted sphere packing. The two sphere packings of one crystal structure belong to different types and are fitted into each other.

Table 3 lists further examples of hexagonal crystal structures. Part of them belong to structure types with a large number of representatives. The chemical composition of each compound is shown in column 1 where the atoms that correspond to a sphere packing are in bold print. The respective symmetry is given in column 2, the sphere-packing type in column 3. If more than one kind of atom can be related to a sphere packing, a certain crystal structure may occur in several lines. The axial ratio *c*/*a* is given in column 4, a variable atomic parameter (x or z) is displayed in column 6. For comparison, the corresponding values of an ideal sphere packing of that type are listed in addition (columns 5 and 7; only given if the sphere-packing type shows no degree of freedom). The standard deviation s (column 8) of the normalized sphere-packing distances can be used as a measure of the agreement between the atomic arrangement and the ideal sphere packing (Koch & Sowa, 2003). The specification of s is left out if it necessarily equals zero for symmetry reasons. s is defined as

$$s = \left[\frac{1}{k}\sum_{j=1}^{k}\left(\frac{d_j}{\bar{d}} - 1\right)^2\right]^{1/2} = \left(\frac{1}{k}\frac{\sum_{j=1}^{k} d_j^2}{\bar{d}^2} - 1\right)^{1/2} \qquad (1)$$

with

$$\bar{d} = \frac{1}{k}\sum_{j=1}^{k} d_j,$$

where k is the number of sphere-packing neighbours, d_j is the distance of the jth neighbour from the reference sphere and $\bar{d}$ is the mean value of the k distances.

The coordinate parameters of some crystal structures listed in Table 3 cannot be directly compared with the sphere-packing parameters shown in Tables 1 and 2. Examples of the necessary coordinate transformations are described in the following:

(i) $Re_{1.16}O_3$ crystallizes in space group $P6_322$ with $c/a = 0.9380$; the oxygen atoms occupy Wyckoff position 6*g* $x00$ with $x = 0.359$. $P6_322$ 6*g* is a non-characteristic Wyckoff position of lattice complex $P6_3/mcm$ 6*g* $x0\frac{1}{4}$ (*cf. International Tables for Crystallography*, 2002, Vol. A, ch. 14). As can be read from Table 2, $x = \frac{1}{3}$ and $c/a = \frac{2}{3}\sqrt{2} = 0.9428$ are the ideal parameters for a sphere packing of type 12/3/*c*1 (cubic closest packings) in $P6_3/mcm$ 6*g* and also in $P6_322$ 6*g*. The oxygen

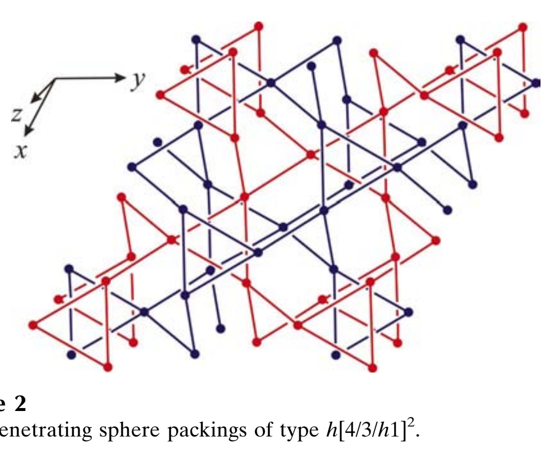

Figure 2
Interpenetrating sphere packings of type $h[4/3/h1]^2$.

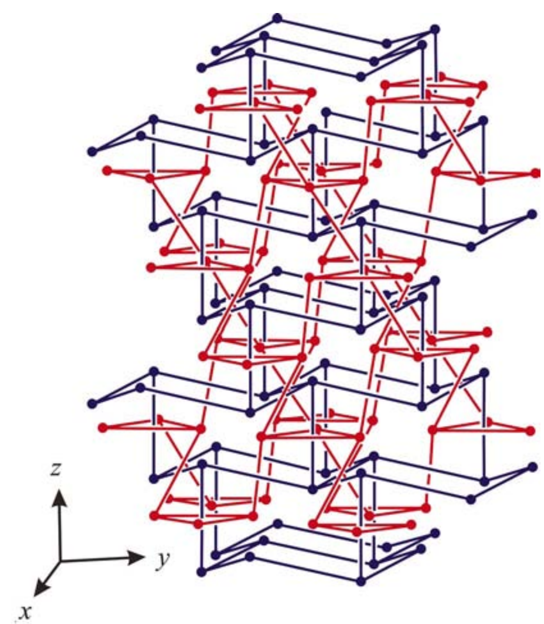

Figure 3
Sphere packings characterizing the crystal structure of In_2O_3 ($R\bar{3}c$): 4/6/*c*1 in blue (In), 4/3/*h*2 in red (O).

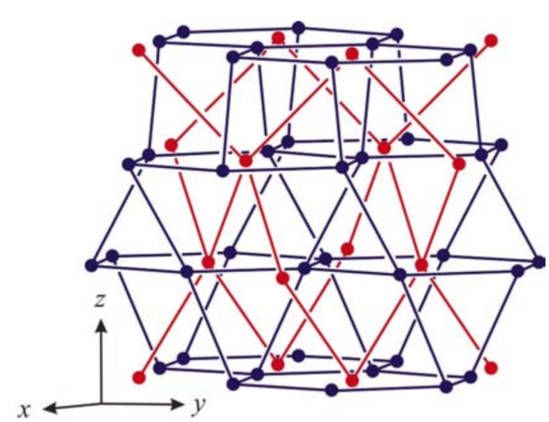

Figure 4
Sphere packings characterizing the crystal structure of $NbGe_2$ ($P6_222$): 5/4/*h*11 in blue (Ge), 4/6/*h*1 in red (Nb).

atoms in $Re_{1.16}O_3$ form, therefore, a slightly distorted cubic closest packing. The standard deviation s of the distances of the 12 nearest neighbours amounts to 4.5% of the mean distance of these neighbours.

(ii) The symmetry group of $Ca(OH)_2$ is $P\bar{3}m1$; the oxygen atoms are located at Wyckoff position $2d\,\frac{1}{3}\frac{2}{3}z$ with $z = 0.7663$. In Table 2, however, only the parameter region $0 \leq z \leq \frac{1}{4}$ (*cf.* also Fig. 1) is described. Reflection at a mirror plane at $xy\frac{1}{2}$ maps the region $0 \leq z \leq \frac{1}{4}$ onto $1 \geq z \geq \frac{3}{4}$. This reflection does not belong to $P\bar{3}m1$ itself but it is part of the Euclidean normalizer $P6/mmm(\mathbf{c}' = \frac{1}{2}\mathbf{c})$ of $P\bar{3}m1$ (*cf. International Tables for Crystallography*, 2002, Vol. A, ch. 15). The oxygen coordinate $z = 0.7663$ approximates $\frac{3}{4}$ and the axial ratio 1.3683 of $Ca(OH)_2$ falls into the parameter range $\frac{2}{3} \leq c/a \leq \frac{2}{3}\sqrt{6} = 1.6330$ of 1.2 (*cf.* Table 2 and Fig. 1). Therefore, the oxygen arrangement may be described as a sphere packing of type 6/4/*h*2. The standard deviation s of the six shortest distances amounts to 3.8%.

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