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Orthorhombic sphere packings. I. Invariant and univariant lattice complexes

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All homogeneous sphere packings and all interpenetrating sphere packings were derived that refer to the 6 invariant and the 11 univariant lattice complexes belonging to the orthorhombic crystal system. In total, sphere packings of 38 types have been found. Only for 17 types is the maximal inherent symmetry of their sphere packings orthorhombic. By means of a number of examples, the applicability of sphere packings for the comparison and description of simple crystal structures is demonstrated.

1. Introduction

In the past, homogeneous sphere packings with cubic (Fischer, 1973, 1974, 2004), tetragonal (Fischer, 1991*a*,*b*, 1993, 2005), triclinic (Fischer & Koch, 2002) and hexagonal/trigonal (Sowa *et al.*, 2003; Sowa & Koch, 2004, 2005, 2006) symmetry have been completely derived. Information on orthorhombic sphere packings is limited, however. Niggli & Laves (1930) studied '*homogene systemsymmorphe Baugitter*', *i.e.* homogeneous sphere packings with site symmetry belonging to the regarded crystal system. Within the orthorhombic system, this means that the site symmetry of a sphere has to be *mmm*, 222 or *mm*2, which is the case for five of the six invariant and for ten of the eleven univariant lattice complexes. More recently, Sowa systematically derived sphere packings with symmetry *Cmcm* 4*c* (Sowa, 2000*a*), *Imma* 4*e* (Sowa, 2000*b*), *Cmcm* 8*f* (Sowa, 2001), *Pnna* 8*e* (Sowa & Koch, 2001) and *Pnma* 8*d* (Sowa, 2005) in connection with the interpretation of reconstructive phase transitions. Starting with the six invariant and the eleven univariant lattice complexes, it is the aim of the current series of publications to present all homogeneous sphere packings with orthorhombic symmetry.

2. Definitions

An arrangement of spheres with the symmetry of a space group is called a *sphere packing* if the following conditions hold: (i) each sphere is in contact with at least one other sphere; (ii) no spheres overlap; (iii) any two spheres are connected by a chain of spheres with mutual contact.

A *homogeneous sphere packing* is a sphere packing where all spheres are symmetrically equivalent, *i.e.* form an orbit of spheres with respect to a space group. Otherwise the packing is called *heterogeneous*.

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Two (homogeneous) sphere packings belong to the same *sphere-packing 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*). Each type of sphere packing can be 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, *t*: tetragonal, *o*: orthorhombic) 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. Usually, the density is not constant for an entire type but varies over a certain range. For most sphere-packing types, a minimal density exists (Fischer, 2004, 2005; Koch *et al.*, 2005; Sowa & Koch, 2006).

3. Derivation of sphere packings

The derivation of the orthorhombic sphere packings closely follows the procedure used before (*cf. e.g.* Sowa *et al.*, 2003). For any reference point that refers to the regarded lattice complex and that belongs to the selected asymmetric unit of the Euclidean normalizer of the space group under consideration, all symmetrically equivalent points that might have shortest distances to the first one are determined. The corresponding (sets of) symmetry operations are listed. For all combinations of these, it is checked whether they generate the space group under consideration. Only if this is the case, the set of spheres does not disintegrate into unconnected parts and, therefore, forms a sphere packing. Then, the minimal density ρ_m is calculated by means of the program *EUREKA: THE SOLVER* (1987). The value of ρ_m together with those of k and m facilitates the identification of the sphere-packing type. One specific property of the orthorhombic crystal system

Table 1
The sphere packings corresponding to the six orthorhombic invariant lattice complexes.

***Pmmm* 1*a* *mmm* 0, 0, 0**				***a* ≤ *b* ≤ *c***	
A	1, 0, 0	*B*	0, 1, 0	*C*	0, 0, 1
	−1, 0, 0		0, −1, 0		0, 0, −1
0.1	6/4/*c*1	*ABC*	1, 1		0.52360
***Cmmm* 2*a* *mmm* 0, 0, 0**				***a* ≤ *b***	
A	$\frac{1}{2}, \frac{1}{2}, 0$	*B*	1, 0, 0	*C*	0, 0, 1
	$-\frac{1}{2}, \frac{1}{2}, 0$		−1, 0, 0		0, 0, −1
	$\frac{1}{2}, -\frac{1}{2}, 0$				
	$-\frac{1}{2}, -\frac{1}{2}, 0$				
0.1	8/3/*h*4	*ABC*	$\frac{1}{3}\sqrt{3}, \frac{1}{3}\sqrt{3}$		0.60460
1.1	6/4/*c*1	*AC*	$1, \frac{1}{2}\sqrt{2}$		0.52360
***Fmmm* 4*a* *mmm* 0, 0, 0**				***a* ≤ *b* ≤ *c***	
A	$\frac{1}{2}, 0, \frac{1}{2}$	*B*	$\frac{1}{2}, \frac{1}{2}, 0$	*D*	$0, \frac{1}{2}, \frac{1}{2}$
	$-\frac{1}{2}, 0, \frac{1}{2}$		$-\frac{1}{2}, \frac{1}{2}, 0$		$0, -\frac{1}{2}, \frac{1}{2}$
	$\frac{1}{2}, 0, -\frac{1}{2}$		$\frac{1}{2}, -\frac{1}{2}, 0$		$0, \frac{1}{2}, -\frac{1}{2}$
	$-\frac{1}{2}, 0, -\frac{1}{2}$		$-\frac{1}{2}, -\frac{1}{2}, 0$		$0, -\frac{1}{2}, -\frac{1}{2}$
		C	1, 0, 0		
			−1, 0, 0		
0.1	12/3/*c*1	*ABD*	1, 1		0.74048
0.2	10/3/*t*1	*ABC*	$\frac{1}{3}\sqrt{3}, 1$		0.69813
1.1	8/4/*c*1	*AB*	$\frac{1}{2}\sqrt{2}, 1$		0.68017
***Fddd* 8*a* 222 0, 0, 0**				***a* ≤ *b* ≤ *c***	
A	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	*B*	$\frac{1}{2}, \frac{1}{2}, 0$	*C*	1, 0, 0
	$-\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$		$-\frac{1}{2}, \frac{1}{2}, 0$		−1, 0, 0
	$-\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$		$\frac{1}{2}, -\frac{1}{2}, 0$		
	$\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$		$-\frac{1}{2}, -\frac{1}{2}, 0$		
0.1	10/3/*o*3	*ABC*	$\frac{1}{3}\sqrt{3}, 2$		0.69813
1.1	6/4/*t*2	*AC*	$\frac{1}{15}\sqrt{30}, 1$		0.55851
1.2	8/3/*t*1	*AB*	$1, \sqrt{6}$		0.60460
2.1	4/6/*c*1	*A*	1, 1		0.34009
***Fddd* 16*c* $\bar{1}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$**				***a* ≤ *b* ≤ *c***	
A	$-\frac{1}{8}, \frac{1}{8}, -\frac{1}{8}$	*B*	$\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$	*C*	$\frac{9}{8}, \frac{1}{8}, \frac{1}{8}$
	$-\frac{1}{8}, -\frac{1}{8}, \frac{1}{8}$		$\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$		$-\frac{7}{8}, \frac{1}{8}, \frac{1}{8}$
	$\frac{3}{8}, \frac{1}{8}, \frac{3}{8}$				
	$\frac{3}{8}, \frac{3}{8}, \frac{1}{8}$				
0.1	6/3/*c*2	*AB*	1, 1		0.37024
0.2	6/4/*t*3	*AC*	$\frac{1}{15}\sqrt{15}, 1$		0.55851
1.1	4/4/*t*1	*A*	$\frac{1}{2}\sqrt{2}, 1$		0.34009
***Immm* 2*a* *mmm* 0, 0, 0**				***a* ≤ *b* ≤ *c***	
A	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		$\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}$	*B*	0, 1, 0
	$-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		$-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$		0, −1, 0
	$\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$		$-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$	C	1, 0, 0
	$\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$		$-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}$		−1, 0, 0
0.1	12/3/*c*1	*ABC*	$1, \sqrt{2}$		0.74048
1.1	10/3/*t*1	*AC*	$\frac{1}{3}\sqrt{6}, 1$		0.69813
2.1	8/4/*c*l	*A*	1, 1		0.68017

has to be noted: for space groups of 38 types, the Euclidean normalizers differ from the affine normalizers (*International Tables for Crystallography*, 2002, Vol. A, ch. 15; Koch & Fischer, 2006). In these cases, the affine normalizers are isomorphic either to tetragonal or to cubic space groups. As a consequence, two or three lattice directions may be interchanged giving rise to a further reduction of the parameter region that has to be investigated. Restricting the range either of the lattice parameters or of the coordinate parameters may do this. The possibility mentioned first has been preferred because it is more convenient.

4. Results

The sphere packings corresponding to the six invariant and the eleven univariant lattice complexes are presented in Tables 1 and 2, respectively.

In the first block, its characteristic Wyckoff position, the respective site symmetry and the coordinate triplet of a reference point identify each lattice complex. In the case of a univariant lattice complex, the range of the coordinate parameter that has to be investigated completes this information. In cases where the range of lattice parameters can be restricted, the corresponding inequalities are given. All space groups are treated with origin choice 1.

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

The third block contains information on the types of sphere packings. In the first column, 0.*i*, 1.*i* or 2.*i* designate a zero-, a one- or a two-dimensional parameter range, respectively, *i* being a serial number. The symbol *k*/*m*/*fn* characterizes the sphere-packing type in the second column. The string of capital letters in the next column 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*, *y* or *z* (in the case of a univariant lattice complex) and of *a*/*b* and *c*/*b* are given in the fourth column; the fifth column shows the value ρ_m of the minimal density.

5. Discussion

The orthorhombic invariant lattice complexes give rise to sphere packings belonging to 12 types in total. For only one of these types, *i.e.* 10/3/*o*3 in *Fddd* 8*a*, is the maximal inherent symmetry of all respective sphere packings orthorhombic. These sphere packings may be described as stackings of triangular nets 3^6 with four nets per translation period and two contacts each to spheres from the nets below and above [*cf.* type 11 in Table 9.1.1.2 of *International Tables for Crystallography* (1999), Vol. C; first mentioned by Hellner (1986)]. All other types encompass sphere packings with higher symmetry as may be read from the letter *c*, *h* or *t* in their symbols. In five cases, this enhanced symmetry is cubic, in one case hexagonal, and in five cases tetragonal. This effect reflects limiting-complex relationships due to a specialization of the metrical parameters.[1]

[1] Such relationships were not tabulated as 'non-characteristic orbits' by Engel *et al.* (1984).

Table 2
The sphere packings corresponding to the 11 orthorhombic univariant lattice complexes.

***Pmmm* 2*i* 2*mm* $x, 0, 0$**		**$0 < x \le \frac{1}{4}$; $b \le c$**			
A	$-x, 0, 0$	*C*	$x, 1, 0$	*D*	$x, 0, 1$
B	$1-x, 0, 0$		$x, -1, 0$		$x, 0, -1$
0.1	6/4/*c*1	*ABCD*	$\frac{1}{4}$; 2, 1		0.52360

***Pmma* 2*e* *mm*2 $\frac{1}{4}, 0, z$**		**$0 \le z \le \frac{1}{4}$**			
A	$\frac{3}{4}, 0, -z$	*C*	$\frac{1}{4}, 1, z$	*E*	$\frac{5}{4}, 0, z$
	$-\frac{1}{4}, 0, -z$		$\frac{1}{4}, -1, z$		$-\frac{3}{4}, 0, z$
B	$\frac{3}{4}, 0, 1-z$	*D*	$\frac{1}{4}, 0, 1+z$		
	$-\frac{1}{4}, 0, 1-z$		$\frac{1}{4}, 0, -1+z$		
0.1	8/3/*h*4	*ABCD*	$\frac{1}{4}$; $\sqrt{3}$, 1		0.60460
0.2	8/3/*h*4	*ABCE*	$\frac{1}{4}$; 1, $\sqrt{3}$		0.60460
1.1	6/4/*c*1	*ACD*	0; 2, 1		0.52360
1.2	6/4/*c*1	*ABC*	$\frac{1}{4}$; $\sqrt{2}$, $\sqrt{2}$		0.52360

***Pmmn* 2*a* *mm*2 $0, 0, z$**		**$0 \le z \le \frac{1}{4}$; $a \le b$**			
A	$\frac{1}{2}, \frac{1}{2}, -z$	*B*	$\frac{1}{2}, \frac{1}{2}, 1-z$	*C*	$1, 0, z$
	$-\frac{1}{2}, \frac{1}{2}, -z$		$-\frac{1}{2}, \frac{1}{2}, 1-z$		$-1, 0, z$
	$\frac{1}{2}, -\frac{1}{2}, -z$		$\frac{1}{2}, -\frac{1}{2}, 1-z$	*D*	$0, 1, z$
	$-\frac{1}{2}, -\frac{1}{2}, -z$		$-\frac{1}{2}, -\frac{1}{2}, 1-z$		$0, -1, z$
				E	$0, 0, 1+z$
					$0, 0, -1+z$
0.1	12/3/*c*1	*ABCE*	$\frac{1}{4}$; $\frac{1}{2}\sqrt{2}$, $\frac{1}{2}\sqrt{2}$		0.74048
0.2	12/3/*c*1	*ABCD*	$\frac{1}{4}$; 1, $\sqrt{2}$		0.74048
1.1	8/3/*h*4	*ACE*	0; $\frac{1}{3}\sqrt{3}$, $\frac{1}{3}\sqrt{3}$		0.60460
1.2	10/3/*t*1	*ABE*	$\frac{1}{4}$; 1, $\frac{1}{3}\sqrt{6}$		0.69813
1.3	10/3/*t*1	*ABC*	$\frac{1}{4}$; $\frac{1}{3}\sqrt{6}$, 1		0.69813
2.1	6/4/*c*1	*AE*	0; 1, $\frac{1}{2}\sqrt{2}$		0.52360
2.2	8/4/*c*1	*AB*	$\frac{1}{4}$; 1, 1		0.68017

***Cmcm* 4*c* *m*2*m* $0, y, \frac{1}{4}$**		**$0 \le y \le \frac{1}{4}$**			
A	$0, -y, -\frac{1}{4}$	*D*	$\frac{1}{2}, \frac{1}{2}-y, -\frac{1}{4}$	*F*	$\frac{1}{2}, \frac{1}{2}+y, \frac{1}{4}$
	$0, -y, \frac{3}{4}$		$\frac{1}{2}, \frac{1}{2}-y, \frac{3}{4}$		$\frac{1}{2}, -\frac{1}{2}+y, \frac{1}{4}$
B	$1, y, \frac{1}{4}$		$-\frac{1}{2}, \frac{1}{2}-y, -\frac{1}{4}$		$-\frac{1}{2}, \frac{1}{2}+y, \frac{1}{4}$
	$-1, y, \frac{1}{4}$		$-\frac{1}{2}, \frac{1}{2}-y, \frac{3}{4}$		$-\frac{1}{2}, -\frac{1}{2}+y, \frac{1}{4}$
C	$0, y, \frac{5}{4}$	*E*	$0, 1-y, -\frac{1}{4}$	*G*	$0, 1+y, \frac{1}{4}$
	$0, y, -\frac{3}{4}$		$0, 1-y, \frac{3}{4}$		$0, -1+y, \frac{1}{4}$
0.1	10/3/*o*2	*ABCD*	$\frac{3}{4}-\frac{1}{4}\sqrt{6}$; $\sqrt{3}-\sqrt{2}$, $\sqrt{3}-\sqrt{2}$		0.66568
0.2	10/3/*t*1	*ACDE*	$\frac{1}{4}$; 1, $\frac{1}{3}\sqrt{3}$		0.69813
0.3	12/3/*h*1	*ABDF*	$\frac{1}{6}$; $\frac{1}{3}\sqrt{3}$, $\frac{2}{3}\sqrt{2}$		0.74048
0.4	12/3/*c*l	*ADEF*	$\frac{1}{4}$; 1, 1		0.74048
0.5	10/3/*t*1	*AEFG*	$\frac{1}{4}$; $\sqrt{3}$, $\sqrt{3}$		0.69813
1.1	8/3/*o*1	*ABD*	$\frac{1}{7}$; $\frac{1}{7}\sqrt{7}$, $\frac{2}{7}\sqrt{3}$		0.60460
1.2	8/3/*h*3	*ACD*	$\frac{1}{6}$; $\frac{1}{3}\sqrt{3}$, $\frac{2}{9}\sqrt{3}$		0.53742
1.3	8/4/*c*1	*ADE*	$\frac{1}{4}$; 1, $\frac{1}{2}\sqrt{2}$		0.68017
1.4	8/3/*h*4	*ABF*	0; $\frac{1}{3}\sqrt{3}$, $\frac{2}{3}\sqrt{3}$		0.60460
1.5	10/3/*t*1	*BDF*	$\frac{1}{4}$; $\frac{1}{3}\sqrt{3}$, 1		0.69813
1.6	10/3/*o*1	*ADF*	$\frac{1}{5}$; $\frac{1}{5}\sqrt{15}$, $\frac{2}{5}\sqrt{6}$		0.69813
1.7	8/4/*c*1	*AEF*	$\frac{1}{4}$; $\sqrt{2}$, $\sqrt{2}$		0.68017
1.8	8/3/*h*4	*AFG*	0; $\sqrt{3}$, 2		0.60460
2.1	6/4/*h*2	*AD*	$\frac{1}{6}$; $\frac{1}{3}\sqrt{3}$, $\frac{1}{3}\sqrt{2}$		0.52360
2.2	6/4/*c*1	*AF*	0; 1, $\sqrt{2}$		0.52360
2.3	8/4/*c*1	*DF*	$\frac{1}{4}$; $\frac{1}{2}\sqrt{2}$, 1		0.68017

***Cmmm* 4*g* 2*mm* $x, 0, 0$**		**$0 < x \le \frac{1}{4}$**			
A	$-x, 0, 0$	*C*	$1-x, 0, 0$	*E*	$x, 1, 0$
B	$\frac{1}{2}-x, \frac{1}{2}, 0$	*D*	$x, 0, 1$		$x, -1, 0$
	$\frac{1}{2}-x, -\frac{1}{2}, 0$		$x, 0, -1$		
0.1	6/4/*c*1	*ABCD*	$\frac{1}{4}$; 1, $\frac{1}{2}$		0.52360
0.2	7/3/*o*1	*ABDE*	$1-\frac{1}{2}\sqrt{3}$; $2+\sqrt{3}$, 1		0.56119
1.1	5/4/*h*5	*ABD*	$\frac{1}{6}$; $\sqrt{3}$, $\frac{1}{3}\sqrt{3}$		0.40307

Table 2 (continued)

***Cmmm* 4*k* *mm*2 $0, 0, z$**		**$0 < z \le \frac{1}{4}$; $a \le b$**			
A	$\frac{1}{2}, \frac{1}{2}, z$	*B*	$1, 0, z$	*C*	$0, 0, -z$
	$-\frac{1}{2}, \frac{1}{2}, z$		$-1, 0, z$	*D*	$0, 0, 1-z$
	$\frac{1}{2}, -\frac{1}{2}, z$				
	$-\frac{1}{2}, -\frac{1}{2}, z$				
0.1	8/3/*h*4	*ABCD*	$\frac{1}{4}$; $\frac{1}{3}\sqrt{3}$, $\frac{2}{3}\sqrt{3}$		0.60460
1.1	6/4/*c*1	*ACD*	$\frac{1}{4}$; 1, $\sqrt{2}$		0.52360

***Cmme* 4*g* *mm*2 $0, \frac{1}{4}, z$**		**$0 \le z \le \frac{1}{4}$; $a \le b$**			
A	$\frac{1}{2}, \frac{1}{4}, -z$	*D*	$\frac{1}{2}, \frac{1}{4}, 1-z$	*G*	$\frac{1}{2}, \frac{3}{4}, z$
	$-\frac{1}{2}, \frac{1}{4}, -z$		$-\frac{1}{2}, \frac{1}{4}, 1-z$		$-\frac{1}{2}, \frac{3}{4}, z$
B	$0, \frac{3}{4}, -z$	*E*	$0, \frac{3}{4}, 1-z$		$\frac{1}{2}, -\frac{1}{4}, z$
	$0, -\frac{1}{4}, -z$		$0, -\frac{1}{4}, 1-z$		$-\frac{1}{2}, -\frac{1}{4}, z$
C	$0, \frac{1}{4}, 1+z$	*F*	$1, \frac{1}{4}, z$		
	$0, \frac{1}{4}, -1+z$		$-1, \frac{1}{4}, z$		
0.1	10/3/*t*1	*ABCDE*	$\frac{1}{4}$; 1, $\frac{1}{3}\sqrt{3}$		0.69813
0.2	12/3/*c*1	*ABDEG*	$\frac{1}{4}$; 1, 1		0.74048
0.3	10/3/*t*1	*ADFG*	$\frac{1}{4}$; $\frac{1}{3}\sqrt{3}$, 1		0.69813
1.1	6/4/*c*1	*ABC*	0; 1, $\frac{1}{2}$		0.52360
1.2	8/4/*c*1	*ABDE*	$\frac{1}{4}$; 1, $\frac{1}{2}\sqrt{2}$		0.68017
1.3	8/4/*c*1	*ADG*	$\frac{1}{4}$; $\frac{1}{2}\sqrt{2}$, 1		0.68017

***Fmmm* 8*g* 2*mm* $x, 0, 0$**		**$0 < x \le \frac{1}{4}$; $b \le c$**			
A	$\frac{1}{2}-x, \frac{1}{2}, 0$	*C*	$-x, 0, 0$	*F*	$x, \frac{1}{2}, \frac{1}{2}$
	$\frac{1}{2}-x, -\frac{1}{2}, 0$	*D*	$1-x, 0, 0$		$x, \frac{1}{2}, -\frac{1}{2}$
B	$\frac{1}{2}-x, 0, \frac{1}{2}$	*E*	$x, 1, 0$		$x, -\frac{1}{2}, \frac{1}{2}$
	$\frac{1}{2}-x, 0, -\frac{1}{2}$		$x, -1, 0$		$x, -\frac{1}{2}, -\frac{1}{2}$
0.1	6/4/*c*1	*ABCD*	$\frac{1}{4}$; 1, 1		0.52360
0.2	9/3/*t*2	*ABCF*	$\frac{1}{2}-\frac{1}{4}\sqrt{2}$; $1+\sqrt{2}$, 1		0.61343
0.3	9/3/*o*1	*ACEF*	$1-\frac{1}{2}\sqrt{3}$; $2+\sqrt{3}$, $\sqrt{3}$		0.64801
1.1	5/4/*t*6	*ABC*	$\frac{3}{16}$; $\sqrt{2}$, 1		0.44179
1.2	7/4/*o*1	*ACF*	$\frac{1}{24}(7-\sqrt{13})$; $(4+\sqrt{13})^{1/2}$, $\frac{1}{6}(30+6\sqrt{13})^{1/2}$		0.60210

***Fddd* 16*e* 2.. $x, 0, 0$**		**$0 < x \le \frac{1}{4}$; $b \le c$**			
A	$\frac{1}{4}-x, \frac{1}{4}, \frac{1}{4}$	*D*	$-x, 0, 0$	*H*	$\frac{1}{2}-x, 0, \frac{1}{2}$
	$\frac{1}{4}-x, -\frac{1}{4}, -\frac{1}{4}$	*E*	$1-x, 0, 0$		$\frac{1}{2}-x, 0, -\frac{1}{2}$
B	$-\frac{1}{4}+x, \frac{1}{4}, -\frac{1}{4}$	*F*	$x, \frac{1}{2}, \frac{1}{2}$	*I*	$x, 1, 0$
	$-\frac{1}{4}+x, -\frac{1}{4}, \frac{1}{4}$		$x, \frac{1}{2}, -\frac{1}{2}$		$x, -1, 0$
	$\frac{1}{4}+x, \frac{1}{4}, \frac{1}{4}$		$x, -\frac{1}{2}, \frac{1}{2}$		
	$\frac{1}{4}+x, -\frac{1}{4}, -\frac{1}{4}$		$x, -\frac{1}{2}, -\frac{1}{2}$		
C	$\frac{3}{4}-x, \frac{1}{4}, -\frac{1}{4}$	*G*	$\frac{1}{2}-x, \frac{1}{2}, 0$		
	$\frac{3}{4}-x, -\frac{1}{4}, \frac{1}{4}$		$\frac{1}{2}-x, -\frac{1}{2}, 0$		
0.1	12/3/*c*1	*ABCDEG*	$\frac{1}{4}$; 1, $\sqrt{2}$		0.74048
0.2	12/3/*c*1	*ABCGH*	$\frac{1}{4}$; $\sqrt{2}$, 1		0.74048
0.3	10/3/*t*3	*AFGH*	$\frac{1}{2}-\frac{1}{8}\sqrt{6}$; $2+\sqrt{6}$, 1		0.66568
0.4	9/3/*o*2	*ADFI*	$\frac{1}{2}-\frac{1}{4}\sqrt{3}$; $4+2\sqrt{3}$, $\sqrt{3}$		0.64801
0.5	7/3/*o*6	*ADGI*	$1-\frac{1}{2}\sqrt{3}$; $2+\sqrt{3}$, $\sqrt{2}+\sqrt{6}$		0.58099
0.6	10/3/*o*4	*AFGI*	$\frac{3}{16}$; $4\sqrt{3}$, $\sqrt{3}$		0.69813
1.1	10/3/*t*1	*ABCDE*	$\frac{1}{4}$; $\frac{1}{3}\sqrt{6}$, 1		0.69813
1.2	10/3/*t*1	*ABCG*	$\frac{1}{4}$; $\frac{1}{2}\sqrt{6}$, $\frac{1}{2}\sqrt{6}$		0.69813
1.3	6/4/*t*10	*AGH*	0.20505; 2.66891, 1		0.53543
1.4	7/3/*t*22	*ADF*	$\frac{1}{2}-\frac{1}{4}\sqrt{3}$; $2\sqrt{2}+\sqrt{6}$, 1		0.56119
1.5	5/4/*o*4	*ADG*	$\frac{5}{32}$; 2, $\sqrt{5}$		0.45734
1.6	5/4/*o*5	*ADI*	$3-\frac{1}{2}\sqrt{34}$; $3+\frac{1}{2}\sqrt{34}$, $(\frac{11}{2}+\sqrt{34})^{1/2}$		0.42072
1.7	8/3/*o*3	*AFG*	0.19110; 5.14860, 1.21292		0.65142
1.8	6/3/*o*4	*AGI*	$1-\frac{1}{4}\sqrt{11}$; $\frac{3}{2}\sqrt{3}+\frac{1}{2}\sqrt{33}$, $\frac{1}{2}(24+6\sqrt{11})^{1/2}$		0.46228
2.1	8/4/*c*1	*ABC*	$\frac{1}{4}$; 1, 1		0.68017
2.2	3/10/*t*4	*AD*	$\frac{3}{32}$; 2, 1		0.22089
2.3	4/6/*o*1	*AG*	0.17995; 3.06796, 2.03407		0.38484

Table 2 (continued)

***Immm* 4*e* 2*mm* x, 0, 0**			**$0 < x \leq \frac{1}{4}$; $b \leq c$**		
A	$\frac{1}{2}-x, \frac{1}{2}, \frac{1}{2}$	*B*	$-x, 0, 0$	*E*	$x, 0, 1$
	$\frac{1}{2}-x, \frac{1}{2}, -\frac{1}{2}$	*C*	$1-x, 0, 0$		$x, 0, -1$
	$\frac{1}{2}-x, -\frac{1}{2}, \frac{1}{2}$	*D*	$x, 1, 0$		
	$\frac{1}{2}-x, -\frac{1}{2}, -\frac{1}{2}$		$x, -1, 0$		
0.1	8/3/*h*4	*ABCD*	$\frac{1}{4}$; $2, \sqrt{3}$		0.60460
0.2	9/3/*t*2	*ABDE*	$\frac{1}{2}-\frac{1}{4}\sqrt{2}$; $3+\sqrt{2}, 1$		0.61343
1.1	6/4/*c*1	*ABC*	$\frac{1}{4}$; $\sqrt{2}, 1$		0.52360
1.2	7/3/*o*5	*ABD*	$\frac{1}{2}(3-\sqrt{7})$; $2\sqrt{2}, (1+\frac{1}{2}\sqrt{7})^{1/2}$		0.48680
2.1	5/4/*t*6	*AB*	$\frac{3}{16}$; $2, 1$		0.44179
***Imma* 4*e* *mm*2 0, $\frac{1}{4}$, z**			**$0 \leq z \leq \frac{1}{8}$; $a \leq b$**		
A	$1, \frac{1}{4}, z$	*C*	$0, \frac{1}{4}, 1+z$	*E*	$0, -\frac{1}{4}, -z$
	$-1, \frac{1}{4}, z$		$0, \frac{1}{4}, -1+z$		$0, \frac{3}{4}, -z$
B	$\frac{1}{2}, \frac{1}{4}, \frac{1}{2}-z$	*D*	$\frac{1}{2}, \frac{1}{4}, -\frac{1}{2}-z$	*F*	$0, \frac{5}{4}, z$
	$-\frac{1}{2}, \frac{1}{4}, \frac{1}{2}-z$		$-\frac{1}{2}, \frac{1}{4}, -\frac{1}{2}-z$		$0, -\frac{3}{4}, z$
0.1	8/3/*h*4	*BCDE*	0; $\frac{1}{2}\sqrt{3}, \frac{1}{2}$		0.60460
0.2	8/3/*h*4	*ABDE*	0; $\frac{1}{2}, \frac{1}{2}\sqrt{3}$		0.60460
0.3	8/3/*t*1	*ABEF*	$\frac{1}{8}$; $1, 2\sqrt{3}$		0.60460
1.1	6/4/*c*1	*BDE*	0; $\frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$		0.52360
1.2	6/4/*t*2	*BCE*	$\frac{1}{8}$; $1, \frac{2}{15}\sqrt{15}$		0.55851
1.3	6/3/*o*1	*ABE*	$\frac{1}{8}(11-\sqrt{105})$; $\frac{1}{4}(26-2\sqrt{105})^{1/2}$, $\frac{1}{4}(22+2\sqrt{105})^{1/2}$		0.44226
2.1	4/6/*c*1	*BE*	$\frac{1}{8}$; $1, \sqrt{2}$		0.34009

The orthorhombic univariant lattice complexes yield sphere packings of 34 different types in total. For 16 of them, the maximal symmetry of a sphere packing is orthorhombic, for 4 cubic, for 5 hexagonal and for 9 tetragonal. Some of the types occur more than once; the most frequent type 6/4/*c*1 was found 11 times. It corresponds to the cubic primitive lattice. Owing to limiting-complex relationships, 8 of the 12 sphere-packing types referring to the orthorhombic invariant lattice complexes occur again in univariant lattice complexes. The sphere packings of types 10/3/*o*l, 10/3/*o*2 (both in *Cmcm* 4*c*) and 10/3/*o*4 (*Fddd* 16*e*) have been tabulated before as types 13, 17 and 12, respectively, in Table 9.1.1.2 of *International Tables for Crystallography* (1999), Vol. C. 10/3/*o*1 and 10/3/*o*2 were first derived by Wells & Chamberland (1987), 10/3/*o*4 by O'Keeffe (1998). Sphere packings of types 10/3/*o*1 and 10/3/*o*2 may be described as stacking of square nets 4^4 with two and four nets per translation period, respectively. In 10/3/*o*1, each sphere has three contacts to spheres from both neighbouring nets, whereas in 10/3/*o*2 (*cf.* Fig. 1) each sphere shows four contacts to one net and two to the other net. Similarly to 10/3/*o*3, a sphere packing of type 10/3/*o*4 may be looked at as stacking of triangular nets 3^6 with two contacts per sphere to both neighbouring nets, but with eight nets per translation period. Triangular nets with two contacts per sphere to the first and one contact to the second neighbouring net give rise to sphere packings of types 9/3/*o*1 (*Fmmm* 8*g*) and 9/3/*o*2 (*Fddd* 16*e*). Sphere packings of types 8/3/*o*3 (*Fddd* 16*e*), 7/3/*o*1 (*Cmmm* 4*g*, *cf.* Coutanceau Clarke, 1972) and 7/4/*o*1 (*Fmmm*

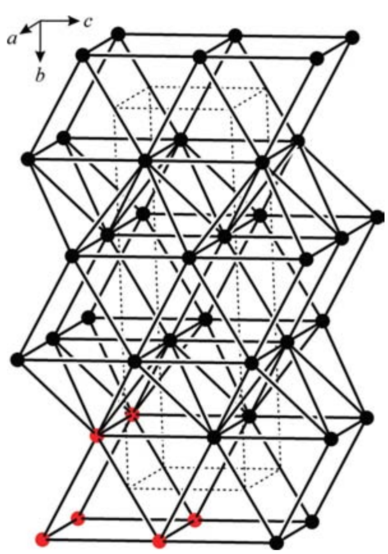

Figure 1
Sphere packing of type 10/3/*o*2 (*Cmcm* 4*c*): stacking of square nets 4^4 with four nets per translation period. Each sphere has four contacts to one neighbouring net and two contacts to the other net. The vertices of one trigonal prismatic void are emphasized in red.

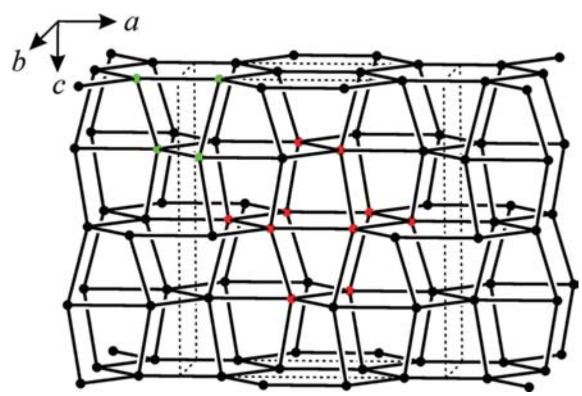

Figure 2
Sphere packing of type 5/4/*o*4 (*Fddd* 16*e*) with minimal density: stacking of flat honeycomb nets 6^3 with four nets per translation period. Each sphere has contacts to one sphere from each neighbouring net. The vertices of one void with 6 + 4 neighbours are emphasized in red, those of one distorted tetrahedral void are marked in green.

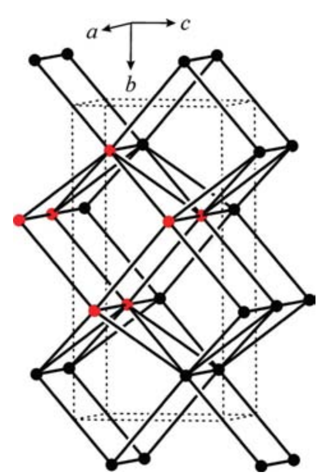

Figure 3
Sphere packing of type 8/3/*o*1 (*Cmcm* 4*c*) that cannot be subdivided into flat nets of spheres with mutual contact. The vertices of one seven-coordinated void are marked in red.

8*g*, *cf.* Wells & Chamberland, 1987) consist of square nets. In the first case, the spheres have two contacts to each of the neighbouring nets; in the other cases, the numbers of contacts to spheres from neighbouring nets are two and one. Sphere packings of type 7/3/*o*6 (*Fddd* 16*e*) can be subdivided into flat nets of triangles and squares $3^3 4^2$, those of type 5/4/*o*4 (*Fddd* 16*e*, *cf.* Fig. 2) into flat honeycomb nets 6^3. The packings of the other six types cannot be subdivided into a flat arrangement of spheres with mutual contact (*cf. e.g.* Fig. 3).

The results presented here were derived without making use of the earlier results by Niggli & Laves (1930). A subsequent comparison shows a large amount of consistency and a few differences: Niggli & Laves did not study the invariant lattice complex *Fddd* 16*c* and the univariant lattice complex *Fddd* 16*e* because of their non-orthorhombic site symmetry; for unknown reasons, they skipped in addition the univariant lattice complexes *Pmmm* 2*i* and *Cmmm* 4*k*; their results for the lattice complex *Cmcm* 4*c* are incomplete: 12/3/*h*1 (h.c.p.), 8/3/*h*3 and 6/4/*h*2 are missing.

6. Examples of crystal structures

Atomic arrangements within inorganic crystal structures may frequently be interpreted as sphere packings. In such a case, the shortest distances between the atoms have to be (approximately) equal. This does not mean, however, that the corresponding atoms are spheres with mutual contact. Some examples will illustrate this. Following Koch & Sowa (2004), the standard deviation s of the normalized distances that correspond to sphere contacts is used as a measure for the agreement between the atomic arrangement and the ideal sphere packing:

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

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

In the following, some orthorhombic crystal structures are given in which the arrangement of some kinds of atom resembles a sphere packing. In all cases, the regarded atomic position corresponds to an invariant or univariant orthorhombic lattice complex. The examples are arbitrarily chosen and the authors do not lay claim to completeness.

(i) A sphere packing of type 5/4/*o*4 with symmetry *Fddd* 16*e* and minimal density (*cf.* Fig. 2) contains two kinds of voids. The centres of the large voids with 6 + 4 neighbours form a distorted diamond packing (4/6/*c*1, *cf.* Table 1), those of the small four-coordinated voids a sphere packing of type 3/10/*t*4 (*cf.* Table 2). In the crystal structure of $TiSi_2$ (Tanaka *et al.*, 2001), the arrangement of the Si atoms is closely related to a sphere packing of type 5/4/*o*4 (s = 0.045), with the Ti atoms occupying the large ten-coordinated voids therein. The B configurations in $CeIr_2B_2$ (*cf.* Jung, 1991; s = 0.015) as well as in LiIrB (*cf.* Klünter *et al.*, 1994; s = 0.022) also form sphere packings of that type to a good approximation. In both structures, the Ir atoms are located in the small distorted tetrahedral voids. The large ten-coordinated voids contain the Ce atoms, whereas the Li atoms have an almost square surrounding and form a sphere packing of type 4/4/*t*1 (*cf.* Table 1).

(ii) The Cl ions in the crystal structure of the high-pressure modification of silver chloride AgCl-III with symmetry *Cmcm* (Hull & Keen, 1999) correspond to a sphere packing of type 8/3/*o*1 (*cf.* Fig. 3 and Table 2) in good approximation (s = 0.01). The cations are located in channels parallel to **a** and are coordinated by seven anions each.

(iii) The Cr arrangement in the crystal structure of CrB with symmetry *Cmcm* (Okada *et al.*, 1987) resembles a sphere packing of type 10/3/*o*2 (s = 0.049) with the B atoms in the trigonal prismatic voids (*cf.* Fig. 1 and Table 2).

(iv) In the average structure of the low-temperature phase obtained from α-PbO (*Cmma*, *cf.* Boher *et al.*, 1985), the Pb atoms form a distorted cubic closest packing 12/3/*c*1 (*cf.* Table 2) that is compressed in the direction of **c** (s = 0.033). The O atoms occupy layers of tetrahedral voids perpendicular to **c**.

(v) $ReSi_2$ (*cf.* Siegrist *et al.*, 1983) crystallizes with symmetry *Immm*. The Si arrangement corresponds well (s = 0.021) to a sphere packing of the tetragonal type 5/4/*t*6 (*cf.* Table 2) with large ten-coordinated and small tetrahedral voids. The Re atoms are surrounded by ten Si atoms forming cubes with two opposite faces capped.

(vi) The Se atoms in the crystal structure of KCu_2Se_2 (*cf.* Tiedje *et al.*, 2003) with symmetry *Fmmm* correspond in good approximation (s = 0.014) to a tetragonal sphere packing of type 9/3/*t*2 (*cf.* Table 2). Within the Se configuration, layers perpendicular to **c** containing K atoms in cubic voids alternate with layers consisting of tetrahedrally coordinated Cu atoms and empty tetragonal pyramids.

(vii) The arrangement of the Pu atoms in the high-temperature phase γ-Pu (Zachariasen & Ellinger, 1955) corresponds to a slightly distorted sphere packing of type 10/3/*o*3 (*cf.* O'Keeffe, 1998).

References

Boher, P., Garnier, P., Gavarri, J. R. & Hewat, A. W. (1985). *J. Solid State Chem.* **57**, 343–350.

Coutanceau Clarke, J. A. R. (1972). *Nature (London)*, **240**, 408–410.

Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *Z Kristallogr.* Suppl. Issue 1.

EUREKA: THE SOLVER (1987). Borland International, Inc., Scotts Valley, USA.

Fischer, W. (1971). *Z. Kristallogr.* **133**, 18–42.

Fischer, W. (1973). *Z. Kristallogr.* **138**, 129–146.

Fischer, W. (1974). *Z. Kristallogr.* **140**, 50–74.

Fischer, W. (1991*a*). *Z. Kristallogr.* **194**, 67–85.

Fischer, W. (1991*b*). *Z. Kristallogr.* **194**, 87–110.

Fischer, W. (1993). *Z. Kristallogr.* **205**, 9–26.

Fischer, W. (2004). *Acta Cryst.* A**60**, 246–249.

Fischer, W. (2005). *Acta Cryst.* A**61**, 435–444.

Fischer, W. & Koch, E. (2002). *Acta Cryst.* A**58**, 509–513.

Hellner, E. (1986) *Z. Kristallogr.* **175**, 227–248.

Hull, S. & Keen, D. A. (1999). *Phys. Rev. B*, **59**, 750–761.

International Tables for Crystallography (1999). Vol. C, 2nd ed., edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.
International Tables for Crystallography (2002). Vol. A, 5th ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.
Jung, W. (1991). *J. Less Common Met.* **171**, 119–125.
Klünter, W., Schmidt, B. & Jung, W. (1994). *J. Alloys Compd*, **205**, 93–100.
Koch, E. & Fischer, W. (2006). *Z. Kristallogr.* **221**, 1–14.
Koch, E. & Sowa, H. (2004). *Eur. J. Mineral.* **16**, 255–260.
Koch, E., Sowa, H. & Fischer, W. (2005). *Acta Cryst.* A**61**, 426–434.
Niggli, P. & Laves, F. (1930). *Z. Kristallogr.* **73**, 381–427.
Okada, S., Atoda, T. & Higashi, I. (1987). *Solid State Chem.* **68**, 61–67.
O'Keeffe, M. (1998). *Acta Cryst.* A**54**, 320–329.
Siegrist, T., Hullinger, F. & Travaglini, G. (1983). *J. Less Common Met.* **92**, 119–129.
Sowa, H. (2000*a*). *Acta Cryst.* A**56**, 288–299.
Sowa, H. (2000*b*). *Z. Kristallogr.* **215**, 335–342.
Sowa, H. (2001). *Acta Cryst.* A**57**, 176–182.
Sowa, H. (2005). *Acta Cryst.* A**61**, 325–330.
Sowa, H. & Koch, E. (2001). *Acta Cryst.* A**57**, 406–413.
Sowa, H. & Koch, E. (2004). *Acta Cryst.* A**60**, 158–166.
Sowa, H. & Koch, E. (2005). *Acta Cryst.* A**61**, 331–342.
Sowa, H. & Koch, E. (2006). *Acta Cryst.* A**62**, 379–399.
Sowa, H., Koch, E. & Fischer, W. (2003). *Acta Cryst.* A**59**, 317–326.
Tanaka, K., Nawata, K., lnui, H., Yamaguchi, M. & Koiwa, M. (2001). *Mater. Res. Soc. Symp. Proc.* **646**, N4.3.1–N4.3.5.
Tiedje, O., Krasovskii, E. E., Schattke, W., Stoll, P., Naether, C. & Bensch, W. (2003). *Phys. Rev. B*, **67**, 134105-1–134105-8.
Wells, A. F. & Chamberland, B. L. (1987). *J. Solid State Chem.* **66**, 26–39.
Zachariasen, W. H. & Ellinger, F. H. (1955). *Acta Cryst.* **8**, 431–433.