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Orthorhombic sphere packings. III. Trivariant lattice complexes with mirror symmetry

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All homogeneous sphere packings and all interpenetrating layers of spheres were derived that refer to the 18 orthorhombic trivariant lattice complexes with mirror symmetry. In total, sphere packings of 51 different types have been found. Only for 28 of these types is the maximal inherent symmetry of their sphere packings orthorhombic. Some crystal structures that can be described by means of sphere packings are listed.

1. Introduction

The present paper is the third part of a series of publications on homogeneous sphere packings with orthorhombic symmetry (*cf.* Fischer *et al.*, 2006; Sowa *et al.*, 2007). It presents a complete table of all sphere-packing types that refer to the 18 trivariant orthorhombic lattice complexes belonging to space groups with mirror symmetry. Part of the sphere packings with symmetry *Pnma* 8*d* have already been derived[1] (Sowa, 2005).

All definitions are given in the first paper on orthorhombic sphere packings (Fischer *et al.*, 2006). The derivation of the sphere packings closely follows the procedure used before for trigonal and hexagonal (Sowa *et al.*, 2003; Sowa & Koch, 2004, 2005, 2006) and for orthorhombic sphere packings (Fischer *et al.*, 2006; Sowa *et al.*, 2007). The range of the lattice parameters that has to be investigated could be reduced for those lattice complexes where for a space group of the characteristic type the affine normalizer interchanges two or three lattice directions (Fischer *et al.*, 2006).

The results were checked for completeness by means of two methods that might also have been used to derive these sphere packings:

(i) In the orthorhombic space groups with mirror reflections there exists a one-to-one correspondence between the sphere packings of the bivariant and those of the trivariant lattice complexes: One can replace each sphere of a sphere packing that belongs to an orthorhombic bivariant lattice complex by a dumb-bell of spheres with orientation perpendicular to the mirror planes. If the new spheres have the original size and the distances between all neighbouring mirror planes are increased by the diameter of one sphere, the resulting arrangement forms a sphere packing of the corresponding trivariant lattice complex.

(ii) The arrangement of spheres between adjacent mirror planes necessarily forms a sphere packing with layer-group symmetry. Such layer-like sphere packings (*cf.* Koch & Fischer, 1978) can be stacked according to the mirror reflections. If a layer-like sphere packing corresponds to a planar graph, the packing may either be puckered with one contact per sphere through a mirror plane or it may be flat with contacts through both neighbouring mirror planes. Accordingly, the relation between the two-periodic and the three-periodic sphere packings is not biunique. As a layer-like sphere packing can have at least 3 and at most 9 contacts per sphere, no sphere packing with 3, 11 or 12 contacts of spheres is possible for the lattice complexes considered.

Furthermore, it has been assured that the results are consistent with the limiting-complex relations between orthorhombic lattice complexes that may be taken from the tables of non-characteristic orbits by Engel *et al.* (1984).

2. Results

Table 1 gives information on all sphere-packing types that can be realized in the 18 trivariant orthorhombic lattice complexes examined. First, for each lattice complex, the characteristic Wyckoff position and the range of the coordinate parameters investigated are given. If the range of the lattice parameters could be restricted, the corresponding inequalities complete this information. All space groups are treated with origin choice 1.

In the second block of information a capital letter designates the coordinate triplet of each possible neighbouring point, *i.e.* the centre of a sphere that may be in contact with the reference sphere. The same letter may symbolize two or more neighbouring points if they are equidistant for symmetry reasons.

The third block describes the sphere packings that refer to the lattice complex under consideration. In the first column, 0.*i*, 1.*i*, 2.*i* or 3.*i* identify a zero-, a one-, a two- or a three-

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[1] Sphere packing type 7/3/*o*7 has to be replaced by 7/3/*o*3 with highest symmetry *Cmcm* 8*g*.

Table 1
The sphere packings corresponding to the 18 orthorhombic trivariant lattice complexes with mirror symmetry.

Pmmm* 8*a* *x*, *y*, *z			**$0 < x \le \frac{1}{4}$, $0 < y \le \frac{1}{4}$, $0 < z \le \frac{1}{4}$; $a \le b \le c$**			
A	$x, -y, z$		*C*	$x, -y + 1, z$	*E*	$-x + 1, y, z$	
B	$x, y, -z$		*D*	$x, y, -z + 1$	*F*	$-x, y, z$	
0.1	6/4/*c*1	*ABCDEF*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; 1, 1			0.52360
Pccm* 8*r* *x*, *y*, *z			**$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 < z \le \frac{1}{4}$; $a \le b$**			
A	$-x, -y, z$		*E*	$x + 1, y, z$	*H*	$x, -y + 1, -z + \frac{1}{2}$	
B	$-x + 1, -y, z$			$x - 1, y, z$	*I*	$-x, -y + 1, z$	
C	$x, -y, -z + \frac{1}{2}$		*F*	$-x + 1, y, -z + \frac{1}{2}$	*J*	$-x + 1, -y + 1, z$	
D	$-x, y, -z + \frac{1}{2}$		*G*	$x, y, -z + 1$	*K*	$x, y, -z$	
0.1	9/3/*o*1	*ABDEFIJK*		$\frac{1}{4}, \frac{1}{4}, 1 - \frac{1}{2}(3)^{1/2}$; $\frac{1}{3}(3)^{1/2}, 1 + \frac{2}{3}(3)^{1/2}$			0.64801
0.2	9/3/*t*2	*ABCDFHIJK*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}$; 1, $1 + (2)^{1/2}$			0.61343
0.3	6/4/*c*1	*CDFGHK*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; 1, 1			0.52360
1.1	7/4/*o*1	*ABDFIJK*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{24}(7 - 13^{1/2})$; $\frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}, \frac{1}{2}(1 + 13^{1/2})$			0.60210
1.2	6/4/*c*1	*ADEIK*		0, $\frac{1}{4}, \frac{1}{8}, \frac{1}{2}$, 2			0.52360
1.3	5/4/*t*6	*CDFHK*		$\frac{1}{4}, \frac{1}{4}, \frac{3}{16}$, 1, $2^{1/2}$			0.44179
Pmma* 8*l* *x*, *y*, *z			**$0 \le x < \frac{1}{4}$, $0 < y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$**			
A	$-x, y, -z$		*C*	$x, y, z + 1$	*E*	$-x - \frac{1}{2}, y, z$	
B	$-x + \frac{1}{2}, y, z$			$x, y, z - 1$	*F*	$-x, y, -z + 1$	
			D	$x, -y + 1, z$	*G*	$x, -y, z$	
0.1	7/3/*o*1	*ABCDFG*		$\frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{4}, \frac{1}{4}$; $1 + \frac{1}{2}(3)^{1/2}, \frac{1}{2}$			0.56119
0.2	6/4/*c*1	*ABDEFG*		0, $\frac{1}{4}, \frac{1}{4}$, 1, 1			0.52360
1.1	6/4/*c*1	*ABCDG*		$\frac{1}{8}, \frac{1}{4}$, 0; 2, $\frac{1}{2}$			0.52360
1.2	5/4/*h*5	*ABDFG*		$\frac{1}{12}, \frac{1}{4}, \frac{1}{4}, \frac{3}{2}, \frac{1}{2}(3)^{1/2}$			0.40307
Pmna* 8*i* *x*, *y*, *z			**$0 < x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$**			
A	$x, -y, -z$		*E*	$-x + \frac{1}{2}, y, -z - \frac{1}{2}$	*H*	$x, -y, -z + 1$	
B	$-x + 1, y, z$		*F*	$x, -y + 1, -z$	*I*	$-x, y, z$	
C	$x, y, z + 1$		*G*	$x, y + 1, z$	*J*	$x, -y + 1, -z + 1$	
	$x, y, z - 1$			$x, y - 1, z$			
D	$-x + \frac{1}{2}, y, -z + \frac{1}{2}$						
0.1	8/3/*h*4	*ACDFHIJ*		$\frac{1}{8}, \frac{1}{4}, \frac{1}{4}, \frac{4}{3}(3)^{1/2}, \frac{1}{3}(3)^{1/2}$			0.60460
0.2	8/3/*h*4	*ADFGHIJ*		$\frac{1}{8}, \frac{1}{4}, \frac{1}{4}$; 4, $3^{1/2}$			0.60460
0.3	7/3/*o*1	*ACDEFI*		$1 - \frac{1}{2}(3)^{1/2}, \frac{1}{4}$, 0; $1 + \frac{1}{2}(3)^{1/2}, \frac{1}{2}$			0.56119
0.4	7/3/*o*1	*ABDFGI*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}$; 2, $2 + 3^{1/2}$			0.56119
0.5	6/4/*c*1	*ABDEFI*		$\frac{1}{4}, \frac{1}{4}$, 0; 1, 1			0.52360
1.1	6/3/*o*3	*ADFGI*		0.14822, $\frac{1}{4}$, 0.13591; 3.37328, 3.18604			0.38975
1.2	6/4/*o*1	*ACDFI*		0.12854, $\frac{1}{4}$, 0.08637; 1.97462, 0.50763			0.54664
1.3	6/4/*c*1	*ABDGI*		$\frac{1}{4}$, 0, $\frac{1}{8}$, 2, 4			0.52360
1.4	6/4/*c*1	*ADFHIJ*		$\frac{1}{8}, \frac{1}{4}, \frac{1}{4}$; $2(2)^{1/2}$, 1			0.52360
1.5	6/4/*c*1	*ADGHI*		$\frac{1}{8}$, 0, $\frac{1}{4}$; 4, 2			0.52360
1.6	5/4/*h*5	*ABDFI*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{12}$; $\frac{2}{3}(3)^{1/2}$, $3^{1/2}$			0.40307
1.7	5/4/*h*5	*ADEFI*		$\frac{1}{6}, \frac{1}{4}$, 0; $\frac{3}{2}, \frac{1}{2}(3)^{1/2}$			0.40307
2.1	5/4/*t*4	*ADGI*		$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $2 + 2^{1/2}$, $2 + 2^{1/2}$			0.35934
2.2	4/4/*o*1	*ADFI*		$\frac{11}{16} - \frac{1}{16}(73)^{1/2}, \frac{1}{4}$, 0.10233; 1.93348, 1.56301			0.28988
Pbam* 8*i* *x*, *y*, *z			**$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 < z \le \frac{1}{4}$; $a \le b$**			
A	$-x, -y, z$		*D*	$-x + \frac{1}{2}, y + \frac{1}{2}, z$	*F*	$x + \frac{1}{2}, -y + \frac{1}{2}, z$	
B	$-x + 1, -y, z$			$-x + \frac{1}{2}, y - \frac{1}{2}, z$		$x - \frac{1}{2}, -y + \frac{1}{2}, z$	
C	$x, y, -z + 1$		*E*	$x + 1, y, z$	*G*	$-x, -y + 1, z$	
				$x - 1, y, z$	*H*	$x, y, -z$	
0.1	8/3/*h*4	*ABCEFH*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{6}(3)^{1/2}, \frac{1}{3}(3)^{1/2}$			0.60460
0.2	8/3/*h*4	*ABCDFH*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}(3)^{1/2}$, 1			0.60460
1.1	7/3/*o*1	*ACEFH*		0, $1 - \frac{1}{2}(3)^{1/2}, \frac{1}{4}$; $2 - 3^{1/2}$, $4 - 2(3)^{1/2}$			0.56119
1.2	7/3/*t*5	*ACDFH*		$\frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{4}$; 1, $6^{1/2} - 2^{1/2}$			0.56119
1.3	6/4/*c*1	*ABCFH*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}(2)^{1/2}$			0.52360
1.4	6/4/*c*1	*ABCDH*		$\frac{1}{4}$, 0, $\frac{1}{4}$; 1, 1			0.52360

1.4′		*ACFGH*	0, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1	
2.1	6/4/*c*1	*CDFH*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1	0.52360
2.2	5/4/*h*5	*ACFH*	0, $\frac{1}{6}$ $\frac{1}{4}$, $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}$	0.40307
2.2′		*ACDH*	$\frac{1}{6}$, 0, $\frac{1}{4}$; $3^{1/2}$, $\frac{2}{3}(3)^{1/2}$	

Pbcm* 8*e* *x*, *y*, *z **$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 \le z < \frac{1}{4}$**

A	$-x, -y, -z$	*E*	$x, -y + \frac{1}{2}, -z$	*H*	$-x + 1, y + \frac{1}{2}, z$	
B	$-x + 1, -y, -z$	*F*	$x, -y - \frac{1}{2}, -z$		$-x + 1, y - \frac{1}{2}, z$	
C	$x, y, -z - \frac{1}{2}$	*G*	$-x, y + \frac{1}{2}, z$	*I*	$x, y + 1, z$	
D	$x + 1, y, z$		$-x, y - \frac{1}{2}, z$		$x, y - 1, z$	
	$x - 1, y, z$			*J*	$x, y, -z + \frac{1}{2}$	

0.1	10/3/*h*2	*ABDEGHJ*	$\frac{1}{4}$, $\frac{1}{12}$, $\frac{1}{4}(6)^{1/2} - \frac{1}{2}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(2^{1/2} + 3^{1/2})$	0.66568
0.2	9/3/*o*1	*EFGHIJ*	$\frac{1}{4}$, 0, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; $3^{1/2}$, $2 + 3^{1/2}$	0.64801
0.3	9/3/*t*2	*ABEFGHJ*	$\frac{1}{4}$, 0, $\frac{1}{4}(2)^{1/2} - \frac{1}{4}$; 1, $1 + 2^{1/2}$	0.61343
0.4	7/3/*o*1	*ABCDEJ*	$\frac{1}{4}$, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$, 0; $2 - 3^{1/2}$, $4 - 2(3)^{1/2}$	0.56119
0.5	6/4/*c*1	*ABCEFJ*	$\frac{1}{4}$, 0, 0; 1, 1	0.52360
1.1	9/3/*o*1	*ABDGHJ*	$\frac{1}{4}$, 0, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; $\frac{1}{3}(3)^{1/2}$, $1 + \frac{2}{3}(3)^{1/2}$	0.64801
1.2	8/3/*o*2	*ABEGHJ*	$\frac{1}{4}$, $\frac{1}{32}$, $\frac{3}{28}$; $\frac{1}{2}(3)^{1/2}$, $\frac{7}{8}(7)^{1/2}$	0.60460
1.3	8/3/*h*4	*EGHIJ*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; $3^{1/2}$, 4	0.60460
1.4	8/3/*h*4	*DEGHJ*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; $\frac{1}{3}(3)^{1/2}$, $\frac{4}{3}(3)^{1/2}$	0.60460
1.5	7/3/*o*1	*ADEGJ*	0, $\frac{1}{8}$, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; $\frac{1}{4}$, $1 + \frac{1}{2}(3)^{1/2}$	0.56119
1.6	7/4/*o*1	*EFGHJ*	$\frac{1}{4}$, 0, $\frac{1}{24}(13^{1/2} - 1)$; $\frac{1}{6}[30 + 6(13)^{1/2}]^{1/2}$, $(4 + 13^{1/2})^{1/2}$	0.60210
1.7	6/3/*o*2	*ABDEJ*	$\frac{1}{4}$, $\frac{1}{64}(105^{1/2} - 3)$, $\frac{1}{16}(105^{1/2} - 9)$; $\frac{1}{4}(15^{1/2} - 7^{1/2})$, $\frac{1}{16}[3(15)^{1/2} + 7^{1/2}]$	0.44226
1.8	6/4/*c*1	*ACDEJ*	0, $\frac{1}{8}$, 0; $\frac{1}{4}$, $\frac{1}{2}$	0.52360
1.9	5/4/*t*6	*ABEFJ*	$\frac{1}{4}$, 0, $\frac{1}{16}$; 1, $2^{1/2}$	0.44179
1.10	5/4/*h*5	*ABCEJ*	$\frac{1}{4}$, $\frac{1}{12}$, 0; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}$	0.40307
2.1	7/4/*o*1	*ABGHJ*	$\frac{1}{4}$, 0, $\frac{1}{24}(13^{1/2} - 1)$; $\frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}$, $\frac{1}{2}(1 + 13^{1/2})$	0.60210
2.2	6/4/*c*1	*ADGJ*	0, 0, $\frac{1}{8}$; $\frac{1}{2}$, 2	0.52360
2.3	6/4/*c*1	*EGHJ*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, $2(2)^{1/2}$	0.52360
2.4	6/4/*c*1	*DEGJ*	0, $\frac{1}{4}$, $\frac{1}{8}$; $\frac{1}{2}$, 2	0.52360
2.5	5/4/*h*5	*ADEJ*	0, $\frac{1}{8}$, $\frac{1}{12}$; $\frac{1}{6}(3)^{1/2}$, $\frac{1}{2}(3)^{1/2}$	0.40307
2.6	4/6/*h*2	*ABEJ*	$\frac{1}{4}$, $\frac{1}{12}$, $\frac{1}{16}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(2)^{1/2}$	0.34009

Pnnm* 8*h* *x*, *y*, *z **$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 < z \le \frac{1}{4}$; $a \le b$**

A	$-x, -y, z$	*E*	$-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$	*G*	$-x, -y + 1, z$	
B	$x, y, -z + 1$		$-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$	*H*	$-x + 1, -y + 1, z$	
C	$-x + 1, -y, z$	*F*	$x - \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$	*I*	$x, y, -z$	
D	$x + 1, y, z$		$x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$			
	$x - 1, y, z$					

0.1	9/3/*o*1	*ACDFGHI*	$\frac{1}{4}$, $\frac{1}{4}$, $1 - \frac{1}{2}(3)^{1/2}$; $\frac{1}{3}(3)^{1/2}$, $1 + \frac{2}{3}(3)^{1/2}$	0.64801
0.2	9/3/*t*2	*ACEFGHI*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; 1, $1 + 2^{1/2}$	0.61343
0.3	8/3/*h*4	*ABCDFI*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{4}$, $\frac{1}{6}(3)^{1/2}$, $\frac{1}{3}(3)^{1/2}$	0.60460
0.4	8/3/*h*4	*ABCEFI*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{4}$, $\frac{1}{2}(3)^{1/2}$, 1	0.60460
1.1	7/3/*o*1	*ABDFI*	0, $1 - \frac{1}{2}(3)^{1/2}$, $\frac{1}{4}$; $2 - 3^{1/2}$, $4 - 2(3)^{1/2}$	0.56119
1.2	7/3/*o*1	*ADFGI*	0, $\frac{1}{4}$, $1 - \frac{1}{2}(3)^{1/2}$; $\frac{1}{2}$, $1 + \frac{1}{2}(3)^{1/2}$	0.56119
1.3	7/3/*o*2	*ACDFI*	$\frac{1}{4}$, $\frac{1}{64}(15 - 33^{1/2})$, $\frac{1}{8}(7 - 33^{1/2})$; $\frac{1}{16}[5(3)^{1/2} - 11^{1/2}]$, $\frac{1}{8}[3(3)^{1/2} + 11^{1/2}]$	0.43908
1.4	7/3/*o*3	*ACEFI*	$\frac{1}{4}$, $\frac{1}{9}(4 - 7^{1/2})$, $\frac{1}{2}(3 - 7^{1/2})$; $\frac{2}{9}[14(7)^{1/2} - 20]^{1/2}$, $\frac{1}{3}(2 + 7^{1/2})$	0.48680
1.5	7/3/*t*5	*ABEFI*	$\frac{1}{4}(3^{1/2} - 1)$, $\frac{1}{4}(3^{1/2} - 1)$, $\frac{1}{4}$; 1, $6^{1/2} - 2^{1/2}$	0.56119
1.6	7/4/*o*1	*ACFGHI*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{24}(7 - 13^{1/2})$; $\frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}$, $\frac{1}{2}(1 + 13^{1/2})$	0.60210
1.7	6/4/*c*1	*ABCFI*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{1}{2}(2)^{1/2}$	0.52360
1.8	6/4/*c*1	*ABFGI*	0, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1	0.52360
1.8′		*ABCEI*	$\frac{1}{4}$, 0, $\frac{1}{4}$; 1, 1	
2.1	6/3/*t*6	*AEFI*	0.19471, 0.19471, 0.18276; 1, 1.50668	0.46435
2.2	6/3/*t*7	*ADFI*	0, $\frac{1}{10}(4 - 6^{1/2})$, $\frac{1}{10}(4 - 6^{1/2})$; $\frac{1}{5}(4 - 6^{1/2})$, 1	0.40281
2.3	6/4/*c*1	*BEFI*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1	0.52360
2.4	5/4/*o*1	*ACFI*	$\frac{1}{4}$, $\frac{1}{7}$, $\frac{1}{6}$; $\frac{2}{7}(3)^{1/2}$, $\frac{3}{7}(7)^{1/2}$	0.40307
2.5	5/4/*h*5	*ABFI*	0, $\frac{1}{6}$, $\frac{1}{4}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}$	0.40307
2.5′		*ABEI*		
2.6	5/4/*h*5	*AFGI*	0, $\frac{1}{4}$, $\frac{1}{6}$; $\frac{1}{2}(3)^{1/2}$, $\frac{3}{2}$	0.40307
2.6′		*ACEI*		

3.1	5/4/*t*6	*EFI*	$\frac{1}{4}, \frac{1}{4}, \frac{3}{16}; 1, 2^{1/2}$	0.44179
3.2	4/4/*t*5	*AFI*	$0, \frac{1}{8}(5-13^{1/2}), \frac{1}{8}(5-13^{1/2}); \frac{1}{6}(5-13^{1/2})(2+13^{1/2})^{1/2}, 1$	0.32252
3.2′		*AEI*		

Pmmn* 8*g* *x*, *y*, *z **$0 < x \le \frac{1}{4}, 0 < y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b$**

A	$x, -y, z$	*C*	$x, y, z+1$	*E*	$x, -y+1, z$
B	$-x+1, y, z$		$x, y, z-1$	*F*	$-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$
		D	$-x+\frac{1}{2}, -y+\frac{1}{2}, -z$	*G*	$-x, y, z$

0.1	7/3/*o*1	*ABCDFG*	$\frac{1}{4}, 1-\frac{1}{2}(3)^{1/2}, \frac{1}{4}; 4-2(3)^{1/2}, 2-3^{1/2}$	0.56119
0.2	6/4/*c*1	*ABDEFG*	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$	0.52360
1.1	6/3/*t*7	*ACDFG*	$\frac{1}{10}(4-6^{1/2}), \frac{1}{10}(4-6^{1/2}), \frac{1}{4}; 1, \frac{1}{5}(4-6^{1/2})$	0.40281
1.2	6/4/*c*1	*ABCDG*	$\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{4}$	0.52360
1.3	5/4/*h*5	*ABDFG*	$\frac{1}{4}, \frac{1}{6}, \frac{1}{4}; \frac{2}{3}, \frac{1}{3}(3)^{1/2}$	0.40307
2.1	5/4/*t*4	*ACDG*	$\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, 0; 1, 1-\frac{1}{2}(2)^{1/2}$	0.35934
2.2	4/4/*t*5	*ADFG*	$\frac{1}{8}(5-13^{1/2}), \frac{1}{8}(5-13^{1/2}), \frac{1}{4}; 1, \frac{1}{6}(5-13^{1/2})(2+13^{1/2})^{1/2}$	0.32252

Pnma* 8*d* *x*, *y*, *z **$0 \le x \le \frac{1}{4}, 0 \le y < \frac{1}{4}, 0 \le z \le \frac{1}{4}$**

A	$x+\frac{1}{2}, y, -z+\frac{1}{2}$	*D*	$x+1, y, z$	*G*	$-x+1, -y, -z$
	$x-\frac{1}{2}, y, -z+\frac{1}{2}$		$x-1, y, z$	*H*	$x, -y-\frac{1}{2}, z$
B	$x+\frac{1}{2}, y, -z-\frac{1}{2}$	*E*	$-x, -y, -z$	*I*	$-x, -y, -z+1$
	$x-\frac{1}{2}, y, -z-\frac{1}{2}$	*F*	$-x+\frac{1}{2}, -y, z+\frac{1}{2}$	*J*	$x, -y+\frac{1}{2}, z$
C	$x, y, z+1$		$-x+\frac{1}{2}, -y, z-\frac{1}{2}$		
	$x, y, z-1$				

0.1	10/3/*h*2	*ABCEFJ*	$\frac{1}{6}, \frac{1}{4}(6)^{1/2}-\frac{1}{2}, 0; \frac{3}{2}(3^{1/2}-2^{1/2}), \frac{1}{2}(3-6^{1/2})$	0.66568
0.2	9/3/*o*1	*ABDEGJ*	$\frac{1}{4}, \frac{1}{2}(3)^{1/2}-\frac{3}{4}, 0; 2-3^{1/2}, 2(3)^{1/2}-3$	0.64801
0.3	9/3/*t*2	*ABEFGJ*	$\frac{1}{4}, \frac{1}{4}(2^{1/2}-1), 0; 2^{1/2}-1, 2^{1/2}-1$	0.61343
0.4	9/3/*t*2	*ACEFIJ*	$\frac{1}{8}, \frac{1}{4}(2^{1/2}-1), \frac{1}{4}; 2-2^{1/2}, 1-\frac{1}{2}(2)^{1/2}$	0.61343
0.5	8/3/*h*4	*AEFGHJ*	$\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$	0.60460
0.6	8/3/*h*4	*ADEGHJ*	$\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}, 3^{1/2}$	0.60460
0.7	8/3/*h*4	*CEFHIJ*	$\frac{1}{8}, 0, \frac{1}{4}; 3^{1/2}, \frac{1}{2}$	0.60460
0.8	8/3/*h*4	*AEFHIJ*	$\frac{1}{8}, 0, \frac{1}{4}; 1, \frac{1}{2}(3)^{1/2}$	0.60460
1.1	9/3/*o*1	*ABCFJ*	$\frac{1}{4}, \frac{1}{2}(3)^{1/2}-\frac{3}{4}, 0; 2(3)^{1/2}-3, 2-3^{1/2}$	0.64801
1.2	8/3/*o*2	*ABEFJ*	$\frac{7}{32}, \frac{3}{28}, 0; \frac{8}{49}(7)^{1/2}, \frac{4}{49}(21)^{1/2}$	0.60460
1.3	8/3/*o*4	*ACEFJ*	$\frac{9}{64}, \frac{3}{28}, \frac{5}{28}; \frac{16}{49}(3)^{1/2}, \frac{2}{7}$	0.60460
1.4	8/3/*h*4	*ABCEJ*	$0, \frac{1}{8}, 0; \frac{1}{4}(3)^{1/2}, \frac{1}{4}$	0.60460
1.5	8/3/*h*4	*ABDEJ*	$0, \frac{1}{8}, 0; \frac{1}{4}, \frac{1}{4}(3)^{1/2}$	0.60460
1.6	7/3/*o*1	*CEFHJ*	$1-\frac{1}{2}(3)^{1/2}, 0, 0; 1+\frac{1}{2}(3)^{1/2}, \frac{1}{2}$	0.56119
1.7	7/3/*o*1	*ADEHJ*	$0, 0, 1-\frac{1}{2}(3)^{1/2}; \frac{1}{2}, 1+\frac{1}{2}(3)^{1/2}$	0.56119
1.8	7/3/*o*1	*ACEIJ*	$0, \frac{1}{2}(3)^{1/2}-\frac{3}{4}, \frac{1}{4}; 4-2(3)^{1/2}, 2-3^{1/2}$	0.56119
1.9	7/3/*o*2	*ADEGJ*	$\frac{1}{4}, \frac{1}{8}(33^{1/2}-5), \frac{1}{64}(1+33^{1/2}); \frac{1}{4}(7-33^{1/2}), \frac{1}{2}[3(3)^{1/2}-11^{1/2}]$	0.43908
1.10	7/3/*o*3	*AEFGJ*	$\frac{1}{4}, \frac{1}{2}(7)^{1/2}-\frac{5}{4}, \frac{1}{36}[4(7)^{1/2}-7]; \frac{2}{3}[26(7)^{1/2}-68]^{1/2}, 7^{1/2}-2$	0.48680
1.11	7/3/*o*5	*CEFIJ*	$\frac{1}{8}, \frac{1}{2}(7)^{1/2}-\frac{5}{4}, \frac{1}{4}; 2[2(7)^{1/2}-5]^{1/2}, 3-7^{1/2}$	0.48680
1.12	7/3/*o*5	*AEFIJ*	$\frac{1}{8}, \frac{1}{2}(7)^{1/2}-\frac{5}{4}, \frac{1}{4}; 6-2(7)^{1/2}, [2(7)^{1/2}-5]^{1/2}$	0.48680
1.13	7/3/*t*5	*AEFHJ*	$\frac{1}{4}(3^{1/2}-1), 0, \frac{1}{4}(3^{1/2}-1); \frac{1}{4}(2^{1/2}+6^{1/2}), \frac{1}{4}(2^{1/2}+6^{1/2})$	0.56119
1.14	7/4/*o*1	*ABEGJ*	$\frac{1}{4}, \frac{1}{24}(13^{1/2}-1), 0; \frac{1}{3}[12-3(13)^{1/2}]^{1/2}, \frac{1}{6}(13^{1/2}-1)$	0.60210
1.15	6/4/*c*1	*EFGHJ*	$\frac{1}{4}, 0, 0; 1, 1$	0.52360
1.16	6/4/*c*1	*AEGHJ*	$\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, 2^{1/2}$	0.52360
1.17	6/4/*c*1	*EFHIJ*	$\frac{1}{8}, 0, \frac{1}{4}; 2^{1/2}, \frac{1}{2}(2)^{1/2}$	0.52360
1.18	6/4/*c*1	*AEHIJ*	$0, 0, \frac{1}{4}; 1, 1$	0.52360
2.1	7/3/*o*1	*ACFJ*	$\frac{1}{4}, \frac{1}{2}(3)^{1/2}-\frac{3}{4}, \frac{1}{4}; 4-2(3)^{1/2}, 2-3^{1/2}$	0.56119
2.2	7/4/*o*1	*ABFJ*	$\frac{1}{4}, \frac{1}{24}(13^{1/2}-1), 0; \frac{1}{6}(13^{1/2}-1), \frac{1}{3}[12-3(13)^{1/2}]^{1/2}$	0.60210
2.3	6/3/*o*2	*CEFJ*	$\frac{1}{64}(19-105^{1/2}), \frac{1}{16}(105^{1/2}-9), 0; \frac{1}{8}[3(15)^{1/2}-7^{1/2}], \frac{1}{8}(13-105^{1/2})$	0.44226
2.4	6/3/*o*3	*ADEJ*	0, 0.10178, 0.11409; 0.29645, 0.94449	0.38975
2.5	6/3/*o*5	*AEFJ*	$\frac{1}{128}(13+105^{1/2}), \frac{1}{16}(105^{1/2}-9), \frac{1}{32}(105^{1/2}-5); \frac{1}{16}[5(35)^{1/2}-11(3)^{1/2}], \frac{1}{4}(21^{1/2}-5^{1/2})$	0.44226
2.6	6/4/*o*1	*ACEJ*	0, 0.12146, 0.16363; 0.50643, 0.25708	0.54664
2.7	6/4/*c*1	*ABEJ*	$0, \frac{1}{8}, 0; \frac{1}{4}(2)^{1/2}, \frac{1}{4}(2)^{1/2}$	0.52360
2.8	6/4/*c*1	*AFHJ*	$\frac{1}{4}, 0, \frac{1}{4}; 1, 1$	0.52360
2.9	5/4/*o*1	*AEGJ*	$\frac{1}{4}, \frac{1}{12}, \frac{3}{28}; \frac{2}{21}(21)^{1/2}, \frac{1}{3}(7)^{1/2}$	0.40307
2.10	5/4/*t*6	*EFGJ*	$\frac{1}{4}, \frac{1}{16}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$	0.44179
2.11	5/4/*t*6	*EFIJ*	$\frac{1}{8}, \frac{1}{16}, \frac{1}{4}; 1, \frac{1}{2}$	0.44179

2.12	5/4/*h*5	*EFHJ*	$\frac{1}{6}$, 0, 0; $\frac{3}{2}$, $\frac{1}{2}(3)^{1/2}$	0.40307
2.13	5/4/*h*5	*AEHJ*	0, 0, $\frac{1}{6}$, $\frac{1}{2}(3)^{1/2}$, $\frac{3}{2}$	0.40307
2.14	5/4/*h*5	*AEIJ*	0, $\frac{1}{12}$, $\frac{1}{4}$, $\frac{2}{3}$, $\frac{1}{3}(3)^{1/2}$	0.40307
3.1	5/4/*h*5	*AFJ*	$\frac{1}{4}$, $\frac{1}{12}$, $\frac{1}{4}$, $\frac{2}{3}$, $\frac{1}{3}(3)^{1/2}$	0.40307
3.2	4/4/*o*1	*AEJ*	0, $\frac{1}{16}(73^{1/2} - 7)$, 0.14767; 0.51720, 0.80839	0.28988
3.3	4/6/*h*2	*EFJ*	$\frac{1}{6}$, $\frac{1}{16}$, 0; $\frac{3}{4}(2)^{1/2}$, $\frac{1}{4}(6)^{1/2}$	0.34009

Cmcm* 16*h* *x*, *y*, *z **$0 < x \leq \frac{1}{4}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z < \frac{1}{4}$**

A	$-x, y, z$	*D*	$-x + \frac{1}{2}, y + \frac{1}{2}, z$	*F*	$x, y, -z - \frac{1}{2}$	
B	$x, -y, -z$		$-x + \frac{1}{2}, y - \frac{1}{2}, z$	*G*	$-x + \frac{1}{2}, -y + \frac{1}{2}, -z$	
C	$1 - x, y, z$	*E*	$x, y + 1, z$	*H*	$x, -y + 1, -z$	
			$x, y - 1, z$	*I*	$x, y, -z + \frac{1}{2}$	
0.1	8/3/*t*5	*ABDEHI*	$1 - \frac{1}{2}(3)^{1/2}$, $\frac{1}{4}$, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; $2 + 3^{1/2}$, $2 + 3^{1/2}$			0.60148
0.2	7/3/*o*1	*ABCDGI*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; 1, $1 + \frac{1}{2}(3)^{1/2}$			0.56119
0.3	7/3/*t*7	*ABDGHI*	$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{4}$, $\frac{1}{4}(2^{1/2} - 1)$; $1 + 2^{1/2}$, $1 + 2^{1/2}$			0.50819
0.4	6/4/*c*1	*ABCFGI*	$\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{2}$			0.52360
0.5	6/4/*c*1	*ABFGHI*	$\frac{1}{8}$, $\frac{1}{4}$, 0; 2, 1			0.52360
1.1	7/3/*o*1	*ABDEI*	$1 - \frac{1}{2}(3)^{1/2}$, 0, $\frac{1}{8}$; $2 + 3^{1/2}$, 4			0.56119
1.2	6/3/*o*6	*ABDGI*	$\frac{1}{16}(13 - 105^{1/2})$, $\frac{1}{256}[71 - 3(105)^{1/2}]$, $\frac{1}{64}(105^{1/2} - 3)$; $\frac{1}{4}(15^{1/2} + 7^{1/2})$, $\frac{1}{64}[25(15)^{1/2} + 13(7)^{1/2}]$			0.44226
1.3	6/4/*t*7	*ABDHI*	[0.145, $\frac{1}{4}$, 0.105; 2.5, 2.5]			>0.50819
1.4	6/4/*c*1	*ABCDI*	$\frac{1}{4}$, 0, $\frac{1}{8}$; 1, 2			0.52360
1.5	6/4/*c*1	*ACDGI*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, 2			0.52360
1.6	5/4/*o*9	*ABGHI*	0.13055, $\frac{1}{4}$, 0.07188; 2.09297, 1.53407			0.42583
1.7	5/4/*t*4	*ABFGI*	$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0; 1, $2 - 2^{1/2}$			0.35934
1.8	5/4/*h*5	*ABCGI*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{12}$, $\frac{1}{3}(3)^{1/2}$, $\frac{1}{2}(3)^{1/2}$			0.40307
2.1	5/4/*o*9	*ADGI*	0.17812, $\frac{1}{4}$, 0.11945; 1.53407, 2.09297			0.42583
2.2	5/4/*h*5	*ABDI*	$\frac{1}{6}$, 0, $\frac{1}{8}$; $3^{1/2}$, $\frac{4}{3}(3)^{1/2}$			0.40307
2.3	4/4/*o*3	*ABGI*	0.15350, 0.14522, 0.07383; 1.04201, 0.90793			0.28988

Cmce* 16*g* *x*, *y*, *z **$0 < x \leq \frac{1}{4}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$**

A	$x, -y, -z$	*F*	$x, y, z + 1$	*J*	$x, y + \frac{1}{2}, -z + \frac{1}{2}$	
B	$-x + \frac{1}{2}, y, -z + \frac{1}{2}$		$x, y, z - 1$		$x, y - \frac{1}{2}, -z + \frac{1}{2}$	
C	$-x + \frac{1}{2}, y, -z - \frac{1}{2}$	*G*	$-x + 1, y, z$	*K*	$x, y - 1, z$	
D	$x, -y + \frac{1}{2}, z + \frac{1}{2}$	*H*	$x, -y + 1, -z$	*L*	$x, -y, -z + 1$	
	$x, -y + \frac{1}{2}, z - \frac{1}{2}$	*I*	$-x + \frac{1}{2}, y + \frac{1}{2}, z$	*M*	$-x, y, z$	
E	$-x + \frac{1}{2}, -y + \frac{1}{2}, -z$		$-x + \frac{1}{2}, y - \frac{1}{2}, z$			
0.1	9/3/*o*1	*ABDEHJM*	$1 - \frac{1}{2}(3)^{1/2}$, $\frac{1}{4}$, $\frac{1}{8}$; $1 + \frac{2}{3}(3)^{1/2}$, $\frac{2}{3}(3)^{1/2}$			0.64801
0.2	9/3/*o*1	*AHIJKM*	$1 - \frac{1}{2}(3)^{1/2}$, $\frac{1}{4}$, $\frac{1}{8}$; $2 + 3^{1/2}$, $2(3)^{1/2}$			0.64801
0.3	9/3/*t*2	*ABEHIJM*	$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{4}$, $\frac{1}{8}$; $1 + 2^{1/2}$, 2			0.61343
0.4	8/3/*t*5	*ABCDFM*	$1 - \frac{1}{2}(3)^{1/2}$, $1 - \frac{1}{2}(3)^{1/2}$, 0; 1, $2 - 3^{1/2}$			0.60148
0.5	8/3/*h*4	*ABDFLM*	$\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{4}$; $\frac{2}{3}(3)^{1/2}$, $\frac{1}{6}(3)^{1/2}$			0.60460
0.6	8/3/*h*4	*ABDJLM*	$\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{4}$; 2, $\frac{1}{2}(3)^{1/2}$			0.60460
0.7	7/3/*o*1	*ABEGIM*	$\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; 1, $1 + \frac{1}{2}(3)^{1/2}$			0.56119
0.8	7/3/*t*7	*ABCDEM*	$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0; 1, $2^{1/2} - 1$			0.50819
0.9	6/4/*c*1	*ABCEGM*	$\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{2}$			0.52360
1.1	8/3/*t*5	*AIJKM*	$1 - \frac{1}{2}(3)^{1/2}$, 0, $1 - \frac{1}{2}(3)^{1/2}$; $2 + 3^{1/2}$, $2 + 3^{1/2}$			0.60148
1.2	7/3/*o*14	*ABDFM*	0.12715, 0.13210, 0.12100; 1.07071, 0.27229			0.58009
1.3	7/3/*o*15	*ABDJM*	0.12642, 0.17164, 0.19469; 2.02294, 0.97373			0.56906
1.4	7/3/*t*7	*ABIJM*	$\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $1 + 2^{1/2}$, $1 + 2^{1/2}$			0.50819
1.5	7/4/*o*1	*ABEHJM*	$\frac{1}{24}(7 - 13^{1/2})$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{2}(1 + 13^{1/2})$, $[10 - 2(13)^{1/2}]^{1/2}$			0.60210
1.6	7/4/*o*1	*AHIJM*	$\frac{1}{24}(7 - 13^{1/2})$, $\frac{1}{4}$, $\frac{1}{8}$, $(4 + 13^{1/2})^{1/2}$, $\frac{1}{3}[30 + 6(13)^{1/2}]^{1/2}$			0.60210
1.7	6/3/*o*7	*ABDEM*	0.13800, 0.16261, 0.07936; 1.22443, 0.57847			0.45648
1.8	6/3/*o*8	*ABEIM*	0.18276, 0.14457, 0.11889; 1.47113, 1.90673			0.46435
1.9	6/4/*t*7	*ABCDM*	[0.145, 0.145, 0; 1, 0.4]			>0.50819
1.10	6/4/*c*1	*ADEHM*	$\frac{1}{8}$, $\frac{1}{4}$, 0; 2, 1			0.52360
1.11	6/4/*c*1	*BEGIM*	$\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, 2			0.52360
1.12	6/4/*c*1	*ABGIM*	$\frac{1}{4}$, 0, $\frac{1}{8}$; 1, 2			0.52360
1.13	6/4/*c*1	*ABDLM*	$\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{4}$, $2^{1/2}$, $\frac{1}{2}$			0.52360
1.14	6/4/*c*1	*ABJLM*	$\frac{1}{8}$, 0, $\frac{1}{4}$; 2, 1			0.52360
1.15	5/4/*o*9	*ABCEM*	0.17812, 0.13055, 0; 0.73296, 0.47779			0.42583

1.16	5/4/*h*5	*ABEGM*	$\frac{1}{4}, \frac{1}{8}, \frac{1}{12}; \frac{1}{3}(3)^{1/2}, \frac{1}{2}(3)^{1/2}$	0.40307
2.1	6/4/*t*7	*AIJM*	[0.145, 0, 0.145; 2.5, 2.5]	>0.50819
2.2	6/4/*c*1	*BDJM*	$\frac{1}{8}, \frac{1}{4}, \frac{1}{4}$; 2, 1	0.52360
2.3	5/4/*o*9	*ADEM*	0.13055, 0.17812, 0; 1.36432, 0.65186	0.42583
2.4	5/4/*o*9	*ABIM*	0.17812, 0, 0.13055; 1.53407, 2.09297	0.42583
2.5	5/4/*o*9	*ABJM*	0.13055, 0, 0.17812; 2.09297, 1.53407	0.42583
2.6	5/4/*o*12	*ABDM*	0.13204, 0.15467, 0.11297; 1.26111, 0.54613	0.44933
2.7	5/4/*t*6	*BEIM*	$\frac{3}{16}, \frac{1}{4}, \frac{1}{8}; 2^{1/2}$, 2	0.44179
2.8	4/4/*o*4	*ABEM*	$\frac{1}{8}(5 - 13^{1/2})$, 0.13380, 0.08715; 0.87612, 0.84474	0.32252

Cmmm* 16*r* *x*, *y*, *z $\mathbf{0 < x \le \frac{1}{4}, 0 < y \le \frac{1}{4}, 0 < z \le \frac{1}{4}; a \le b}$

A	$x, y, -z$		*C*	$-x + 1, y, z$	*E*	$x, y, -z + 1$	
B	$x, -y, z$		*D*	$-x + \frac{1}{2}, -y + \frac{1}{2}, z$	*F*	$-x, y, z$	
0.1	6/4/*c*1	*ABCDEF*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}$			0.52360
1.1	5/4/*t*4	*ABDEF*		$\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}$; 1, $2 - 2^{1/2}$			0.35934

Cccm* 16*m* *x*, *y*, *z $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 < z \le \frac{1}{4}; a \le b}$

A	$-x, -y, z$		*F*	$-x, y, -z + \frac{1}{2}$	*J*	$-x - \frac{1}{2}, -y + \frac{1}{2}, z$	
B	$x, -y, -z + \frac{1}{2}$		*G*	$x, y, -z + 1$	*K*	$-x, -y + 1, z$	
C	$-x + 1, -y, z$		*H*	$-x + 1, y, -z + \frac{1}{2}$	*L*	$x, y, -z$	
D	$-x + \frac{1}{2}, -y + \frac{1}{2}, z$		*I*	$x + 1, y, z$			
E	$-x + \frac{1}{2}, -y - \frac{1}{2}, z$			$x - 1, y, z$			
0.1	8/3/*t*5	*ACDFHIL*		$\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, 1 - \frac{1}{2}(3)^{1/2}$; $2 - 3^{1/2}$, 1			0.60148
0.2	7/3/*o*1	*ADFIJL*		0, $1 - \frac{1}{2}(3)^{1/2}, \frac{1}{8}$; $2 - 3^{1/2}$, $8 - 4(3)^{1/2}$			0.56119
0.3	7/3/*t*7	*ABCDFHL*		$\frac{1}{4}, \frac{1}{4}(2^{1/2} - 1), \frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $2^{1/2} - 1$, 1			0.50819
0.4	6/4/*c*1	*BDFGHL*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}$			0.52360
0.5	6/4/*c*1	*ABCDEL*		$\frac{1}{4}$, 0, $\frac{1}{8}$; 1, 2			0.52360
0.5′		*ADFJKL*		0, $\frac{1}{4}, \frac{1}{8}$; 1, 2			
1.1	6/4/*o*3	*ADFIL*		0.08644, 0.12759, 0.12595; 0.25908, 1.02851			0.54673
1.2	6/4/*t*7	*ACDFHL*		$[\frac{1}{4}$, 0.105, 0.145; 0.4, 1]			>0.50819
1.3	5/4/*o*9	*ABCDL*		$\frac{1}{4}$, 0.07188, 0.13055; 0.65186, 1.36432			0.42583
1.4	5/4/*o*9	*BDFHL*		$\frac{1}{4}$, 0.11945, 0.17812; 0.47779, 0.73297			0.42583
1.5	5/4/*t*4	*BDFGL*		$\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}$; 1, $2 - 2^{1/2}$			0.35934
1.6	5/4/*h*5	*ADFJL*		0, $\frac{1}{6}, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, \frac{4}{3}$			0.40307
1.7	5/3/*t*2	*ABDFL*		$\frac{1}{8}, \frac{1}{8}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}$; 1, $\frac{1}{2}(1 + 2^{1/2})$			0.30672
2.1	4/4/*o*5	*ADFL*		0..10390, 0.14077, 0.13565; 0.86465, 1.23109			0.29323
2.1′		*ABDL*					
2.2	4/4/*t*4	*BDFL*		0.13865, 0.13865, 0.16959; 1, 0.92853			0.28186

Cmme* 16*o* *x*, *y*, *z $\mathbf{0 < x \le \frac{1}{4}, 0 \le y < \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b}$

A	$x, -y, -z$		*D*	$x, y, z + 1$	*G*	$x, -y, -z + 1$	
B	$-x + \frac{1}{2}, y, -z$			$x, y, z - 1$	*H*	$-x + \frac{1}{2}, y, -z + 1$	
C	$x, -y + \frac{1}{2}, z$		*E*	$-x + \frac{1}{2}, -y, z$	*I*	$-x, y, z$	
			F	$-x + 1, y, z$			
0.1	8/3/*t*5	*ABCDGHI*		$1 - \frac{1}{2}(3)^{1/2}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{4}$; 1, $2 - 3^{1/2}$			0.60148
0.2	7/3/*t*7	*ABCEGHI*		$\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}(2^{1/2} - 1), \frac{1}{4}$; 1, $2^{1/2} - 1$			0.50819
0.3	6/4/*c*1	*BCEFHI*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}$			0.52360
1.1	6/4/*t*7	*ABCGHI*		[0.145, 0.105, $\frac{1}{4}$; 1, 0.4]			>0.50819
1.2	6/4/*c*1	*ABCDI*		$\frac{1}{8}, \frac{1}{8}$, 0; 1, $\frac{1}{4}$			0.52360
1.3	5/4/*o*9	*BCEHI*		0.17812, 0.11945, $\frac{1}{4}$; 0.73297, 0.47779			0.42583

Fmmm* 32*p* *x*, *y*, *z $\mathbf{0 < x \le \frac{1}{4}, 0 < y \le \frac{1}{4}, 0 < z \le \frac{1}{4}; a \le b \le c}$

A	$x, y, -z$		*D*	$-x + \frac{1}{2}, -y + \frac{1}{2}, z$	*F*	$x, -y + \frac{1}{2}, -z + \frac{1}{2}$	
B	$x, -y, z$		*E*	$-x + \frac{1}{2}, y, -z + \frac{1}{2}$	*G*	$-x, y, z$	
C	$-x + 1, y, z$						
0.1	6/3/*c*4	*ABDEFG*		$\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}$; 1, 1			0.42099
0.2	6/4/*c*1	*ABCDEG*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{8}, \frac{1}{2}$, 1			0.52360
1.1	5/4/*t*8	*ABDEG*		0.16442, 0.13485, 0.13485; 0.82019, 1			0.40079

Immm* 16*o* *x*, *y*, *z				**$0 < x \le \frac{1}{4}, 0 < y \le \frac{1}{4}, 0 < z \le \frac{1}{4}; a \le b \le c$**			
A	$x, y, -z$		*C*	$-x+1, y, z$	*E*	$-x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$	
B	$x, -y, z$		*D*	$x, -y+1, z$	*F*	$-x, y, z$	
0.1	6/4/*c*1	*ABCDEF*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2$			0.52360
1.1	5/4/*t*4	*ABCEF*		$\frac{1}{4}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}; 2-2^{1/2}, 1$			0.35934
2.1	4/4/*c*2	*ABEF*		$\frac{1}{8}(3-3^{1/2}), \frac{1}{8}(3-3^{1/2}), \frac{1}{8}(3-3^{1/2}); 1, 1$			0.26684

Ibam* 16*k* *x*, *y*, *z				**$0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 < z \le \frac{1}{4}; a \le b$**			
A	$-x, -y, z$		*E*	$-x, y, -z+\frac{1}{2}$	*I*	$x+\frac{1}{2}, -y+\frac{1}{2}, z$	
B	$x, -y, -z+\frac{1}{2}$		*F*	$-x+1, y, -z+\frac{1}{2}$		$x-\frac{1}{2}, -y+\frac{1}{2}, z$	
C	$-x+1, -y, z$		*G*	$x+1, y, z$	*J*	$-x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$	
D	$-x+\frac{1}{2}, y+\frac{1}{2}, z$			$x-1, y, z$	*K*	$-x, -y+1, z$	
	$-x+\frac{1}{2}, y-\frac{1}{2}, z$		*H*	$x, y, -z+1$	*L*	$x, y, -z$	
0.1	9/3/*o*1	*ABCDIJL*		$\frac{1}{4}, \frac{1}{8}, 1-\frac{1}{2}(3)^{1/2}; \frac{1}{2}(3)^{1/2}, 1+\frac{1}{2}(3)^{1/2}$			0.64801
0.2	9/3/*o*1	*ACEFGIL*		$\frac{1}{4}, \frac{1}{8}, 1-\frac{1}{2}(3)^{1/2}; \frac{1}{6}(3)^{1/2}, \frac{1}{2}+\frac{1}{3}(3)^{1/2}$			0.64801
0.3	9/3/*t*2	*ABCEFIJL*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}; \frac{1}{2}, \frac{1}{2}(1+2^{1/2})$			0.61343
0.4	6/4/*c*1	*BEFHJL*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}$			0.52360
1.1	7/3/*o*1	*AEGIL*		$0, 1-\frac{1}{2}(3)^{1/2}, \frac{1}{8}; 2-3^{1/2}, 4(2-3^{1/2})$			0.56119
1.2	7/4/*o*1	*ACEFIL*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{24}(7-13^{1/2}); \frac{1}{4}[10-2(13)^{1/2}]^{1/2}, \frac{1}{4}(1+13^{1/2})$			0.60210
1.3	7/4/*o*1	*ABCIJL*		$\frac{1}{4}, \frac{1}{8}, \frac{1}{24}(7-13^{1/2}); \frac{1}{12}[30+6(13)^{1/2}]^{1/2}, \frac{1}{2}(4+13^{1/2})^{1/2}$			0.60210
1.4	7/3/*t*11	*ADIJL*		$\frac{1}{4}(3^{1/2}-1), \frac{1}{4}(3^{1/2}-1), 1+\frac{1}{2}(3)^{1/2}-\frac{1}{4}[14(3)^{1/2}+24]^{1/2}; 1, 1.99871$			0.58136
1.5	6/3/*o*9	*AEIJL*		0.15357, 0.16467, 0.13643; 0.71393, 1.45001			0.50126
1.5′		*ABDJL*					
1.6	6/4/*c*1	*ABCDL*		$\frac{1}{4}, 0, \frac{1}{8}; 1, 2$			0.52360
1.6′		*AEIKL*		$0, \frac{1}{4}, \frac{1}{8}; 1, 2$			
1.7	5/3/*t*4	*ABEJL*		$\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}; 1, 2^{1/2}$			0.42099
1.8	5/4/*t*4	*BEHJL*		$\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{4}; 1, 2-2^{1/2}$			0.35934
1.9	5/4/*t*6	*BEFJL*		$\frac{1}{4}, \frac{1}{8}, \frac{3}{16}; \frac{1}{2}, \frac{1}{2}(2)^{1/2}$			0.44179
2.1	6/4/*c*1	*DIJL*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2$			0.52360
2.2	5/4/*o*13	*AIJL*		[0.2, 0.14382, 0.13744; 0.64676, 1.40743]			>0.50126
2.2′		*ADJL*					
2.3	5/4/*h*5	*AEIL*		$0, \frac{1}{6}, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, \frac{4}{3}$			0.40307
2.3′		*ABDL*					
2.4	4/4/*o*6	*AEJL*		[0.18272, 0.13108, 0.14571; 0.7, 1.25689]			>0.42099
2.4′		*ABJL*					
2.5	4/4/*t*8	*BEJL*		$\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{3}{16}; 1, 2(2^{1/2}-1)$			0.30319
*n*3.1	$t[48^2]^2$	*AJL*		[0.16289, 0.16289, 0.1355; 1, 1.7]			>0.42099

Imma* 16*j* *x*, *y*, *z				**$0 < x \le \frac{1}{4}, 0 \le y < \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b$**			
A	$x, -y, -z$		*D*	$x, y, z+1$	*F*	$-x+\frac{1}{2}, y, -z-\frac{1}{2}$	
B	$-x+1, y, z$			$x, y, z-1$	*G*	$x, -y-\frac{1}{2}, z$	
C	$x, -y+\frac{1}{2}, z$		*E*	$-x+\frac{1}{2}, y, -z+\frac{1}{2}$	*H*	$-x, y, z$	
0.1	7/3/*o*1	*ACDEFH*		$1-\frac{1}{2}(3)^{1/2}, \frac{1}{8}, 0; \frac{1}{2}+\frac{1}{4}(3)^{1/2}, \frac{1}{4}$			0.56119
0.2	6/4/*c*1	*ABCEFH*		$\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{2}$			0.52360
0.3	6/4/*c*1	*ABCEGH*		$\frac{1}{4}, 0, \frac{1}{8}; 1, 2$			0.52360
1.1	6/4/*t*4	*ACDEH*		$4-15^{1/2}, 15^{1/2}-\frac{15}{4}, \frac{1}{8}; 1, 2(4-15^{1/2})$			0.54063
1.2	5/4/*t*4	*ABCEH*		$\frac{1}{4}, \frac{1}{4}(2^{1/2}-1), \frac{1}{4}(2^{1/2}-1); 2-2^{1/2}, 1$			0.35934
1.3	5/4/*h*5	*ACEFH*		$\frac{1}{6}, \frac{1}{8}, 0; \frac{3}{4}, \frac{1}{4}(3)^{1/2}$			0.40307
2.1	4/4/*t*3	*ACEH*		$\frac{3}{20}, \frac{1}{10}, \frac{1}{8}; 1, \frac{2}{5}(5)^{1/2}$			0.25289

dimensional parameter range, respectively, *i* being a serial number. In the second column, a symbol *k*/*m*/*fn* (Fischer, 1971) characterizes the sphere-packing type: *k* means the number of contacts per sphere, *m* is the length of the shortest ring of spheres with mutual contact within the sphere packing, *f* indicates the highest crystal family for a sphere packing of that type (*o*: orthorhombic, *t*: tetragonal, *h*: hexagonal, *c*: cubic) and *n* is an arbitrary number.

The string of capital letters in the next column describes the centres of spheres in contact with the original sphere. If the parameter region of the regarded type – owing to the choice of the asymmetric unit – disintegrates into two disconnected parts, then each part refers to another string of capital letters and a symmetry operation of the Euclidean or of the affine normalizer of the space group under consideration transforms both sets of symmetry operations into each other.

In such a case the symbol in the first column is modified by a prime.

The last two columns refer to the sphere packing with minimal density belonging to the regarded type: the fourth column shows the corresponding values of the coordinate parameters x, y, z and of the axial ratios a/b and c/b, and the fifth column shows the value ρ_m of the minimal density. Some types of sphere packing do not include an arrangement with minimal density. In such a case, parameters for any other sphere packing of that type are given in square brackets.

3. Discussion

In total, the orthorhombic trivariant lattice complexes with mirror symmetry give rise to sphere packings of 51 different types with contact numbers 4 to 10. For 28 of them the maximal inherent symmetry is orthorhombic. Owing to limiting-complex relationships between lattice complexes from different crystal systems[2] all other types comprehend at least one sphere packing with tetragonal (17 types), hexagonal (4) or cubic (2) inherent symmetry as indicated in the symbol by the letter *t*, *h*, or *c*, respectively.

Thirteen of the 28 orthorhombic types have already been listed before (*cf.* Fischer *et al.*, 2006; Sowa *et al.*, 2007), whereas sphere packings of the other 15 types exclusively occur in one of the trivariant orthorhombic lattice complexes examined. These are four types with contact number 4 (4/4/*o*3 to 4/4/*o*6), two types with contact number 5 (5/4/*o*12, 5/4/*o*13), six types with contact number 6 (6/3/*o*5 to 6/3/*o*9, 6/4/*o*3), two types with contact number 7 (7/3/*o*14, 7/3/*o*15, *cf.* Figs. 1 and 2, respectively), and one type with contact number 8 (8/3/*o*4). Types 6/3/*o*5 and 8/3/*o*4 with symmetry *Pnma* 8*d* have already been mentioned by Sowa (2005).

Most of the newly described types of sphere packing correspond to nets included in the Reticular Chemistry Structure Resource (RCSR) database (O'Keeffe *et al.*, 2008). Some of them were derived by Blatov (2007) using net–subnet relations. 4/4/*o*3, 4/4/*o*4 and 4/4/*o*5 are described as **pcl**, **cag** and **umc** nets, respectively. 5/4/*o*12 corresponds to **vbk**, 6/3/*o*5 to **osc**, 6/3/*o*6 to **vbx**, 6/3/*o*7 to **vbw**, 6/3/*o*8 to **vbr**, 6/3/*o*9 to **vca**, 6/4/*o*3 to **vbm**, 7/3/*o*14 to **vci**, 7/3/*o*15 to **vcq** and 8/3/*o*4 to **osd**.

The orthorhombic lattice complexes with three degrees of freedom that were investigated are incompatible with interpenetrating sphere packings, but *Ibam* 16*k* enables two sets of interpenetrating 48^2 nets $t[48^2]^2$ (*cf.* Koch *et al.*, 2006).

4. Examples of crystal structures

Sphere packings are useful for the description and the comparison of crystal structures. The following examples show structures with atomic arrangements that correspond to sphere packings in trivariant orthorhombic lattice complexes with mirror symmetry.

(i) The B and Si atoms in strontium danburite $Sr(B_2Si_2O_8)$ (Berger & Range, 1996) together correspond to a heterogeneous sphere packing of type 4/4/*o*3. Both kinds of atoms are located in the general position of space group *Pnma*. Analogous homogeneous packings occur in the general position of the supergroup *Cmcm* of *Pnma*.

(ii) Variscite-type compounds $ABO_4{\cdot}2H_2O$ with A = Al, Ga, In, Fe and B = P, As (*e.g.* variscite $AlPO_4{\cdot}2H_2O$; Kniep *et al.*, 1977) crystallize in space group *Pbca*. The *A* and *B* atoms occupy the general position and together form a heterogeneous sphere packing of type 4/4/*o*4. *Pbca* is a subgroup of *Cmce* where the corresponding homogeneous type of packing can be realized in Wyckoff position 16*g* x, y, z.

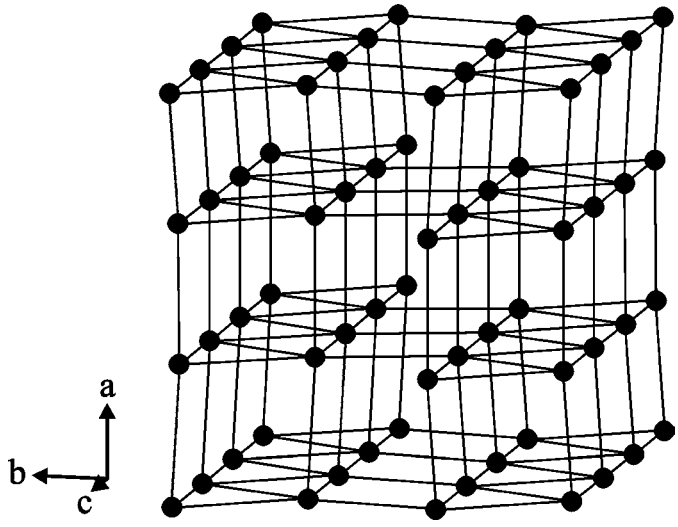

Figure 1
Sphere packing of type 7/3/*o*14 (*Cmce* 16*g*) with flat 3^34^2 nets perpendicular to **a** and flat 4^4 nets perpendicular to **b**.

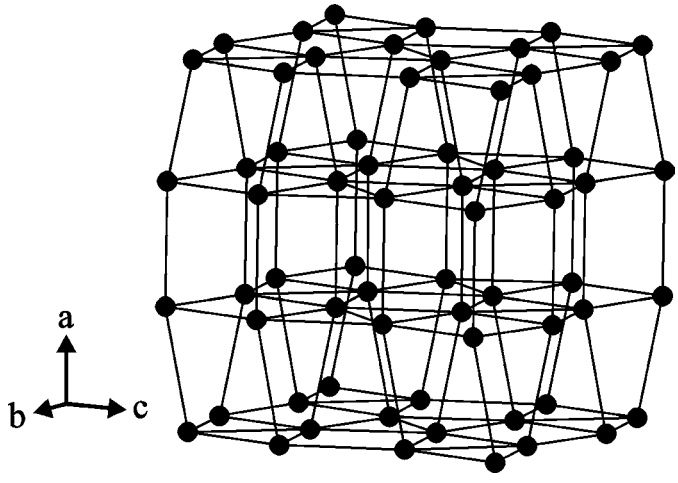

Figure 2
Sphere packing of type 7/3/*o*15 (*Cmce* 16*g*) with flat 3^2434 nets perpendicular to **a**, corrugated 4^4 and 48^2 nets perpendicular to **b** and corrugated square nets 4^4 perpendicular to **c**.

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

(iii) The Pd atoms in YPd_2Si occupy the general position in space group *Pnma* (Moreau *et al.*, 1982). Their arrangement corresponds to a slightly distorted sphere packing of type 4/6/*h*2. The Y and the Si atoms are situated in the trigonal prismatic voids of the packing.

(iv) Many $A_2B_3X_4$ compounds crystallize in *Ibam*. Their anions form distorted sphere packings of type 9/3/*t*2. For instance, in $Cs_2Mn_2Te_4$ (Wu & Ibers, 1997) the arrangement of the Te atoms corresponds to such a sphere packing, while the Mn atoms occupy tetrahedral and the Cs atoms cube-shape voids.

(v) The octahedrally coordinated atoms in orthorhombically distorted perovskite-type structures refer to sphere packings of type 6/4/*c*1. Such compounds are, for instance, $NaNbO_3$ (Xu *et al.*, 2003) that crystallizes in *Pbcm* with Nb atoms within the octahedral voids, and $PbZrO_3$ with symmetry *Pbam* with octahedrally coordinated Zr atoms (Teslic & Egami, 1998).

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