

Orthorhombic sphere packings. II. Bivariant lattice complexes

Heidrun Sowa,*‡ Elke Koch and Werner Fischer

Institut für Mineralogie, Petrologie und Kristallographie der Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany. Correspondence e-mail: heidrun.sowa@geo.uni-goettingen.de

All homogeneous sphere packings and all interpenetrating layers of spheres were derived that refer to the 22 orthorhombic bivariant lattice complexes. In total, sphere packings of 90 different types have been found. Only for 47 of these types is the maximal inherent symmetry of their sphere packings orthorhombic. Some examples demonstrate the usefulness of sphere packings for the comparison and description of crystal structures.

© 2007 International Union of Crystallography
Printed in Singapore – all rights reserved

1. Introduction

The present paper is the second part of a series of publications on homogeneous sphere packings with orthorhombic symmetry (*cf.* Fischer *et al.*, 2006). It presents a complete table of those sphere packings that refer to the 22 bivariant orthorhombic lattice complexes. In connection with the interpretation of 'reconstructive' phase transitions, Sowa (2001) has already derived the sphere packings with symmetry *Cmcm* 8*f*.

All definitions can be taken from the previous 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).

As described in the previous paper, the region of the lattice parameters that has to be investigated could be reduced for those lattice complexes where the affine normalizer of the characteristic space group interchanges the two lattice directions that run parallel to the mirror plane under consideration.

The results were checked for completeness (except for *Fdd2* 16*b*) by comparison with the two-periodic sphere packings corresponding to the layer complexes (*cf.* Koch & Fischer, 1978). For this purpose, two cases have to be distinguished, namely (i) lattice complexes *Pmmm* 4*u*, *Pmma* 4*i*, *Pbam* 4*g* and *Cmmm* 8*p* and (ii) the other orthorhombic bivariant lattice complexes except *Fdd2* 16*b*.

(i) Each corresponding sphere packing splits up into parallel plane layers of spheres stacked directly above each other. As a consequence, the spheres of each layer form a two-periodic sphere packing that has been tabulated for the respective bivariant complex of a layer group. The sphere

packings of *Pbam* 4*g*, for example, split up into layers with symmetry¹ *Pba(m)* - ..*m*.

(ii) Each corresponding sphere packing may be subdivided into parallel double layers with the symmetry of a general position of a layer group. This layer group is, for example, *P(2)2₁2* for lattice complex *Pmna* 4*c*. As the spheres of the single layers are located at a mirror plane of the space group under consideration, reflection through these planes leads to a three-periodic sphere packing. In some cases, a single layer of spheres contains sufficiently wide openings to enable additional contacts to spheres from the next but one layer. Such contacts are necessarily due to a translation of the space group. All possible double layers are compiled in Table 4 of Koch & Fischer (1978).

2. Results

All sphere packings corresponding to the 22 bivariant lattice complexes are described in Table 1. For each lattice complex, the information is subdivided into three parts. The characteristic Wyckoff position together with its site symmetry, a coordinate triplet of a reference point, *i.e.* the centre of a reference sphere, and the investigated range of the coordinate parameters are given first. If the range of the lattice parameters could be restricted, the corresponding inequalities complete the information. All space groups are treated with origin choice 1.

Each possible neighbouring point, *i.e.* the centre of a sphere that may have contact to the reference sphere, is listed in a second block and is designated by a capital letter. Two or more neighbouring points are symbolized with the same letter if

‡ Present address: GZG Abt. Kristallographie, Georg-August-Universität Göttingen, Goldschmidtstrasse 1, D-37077 Göttingen, Germany.

¹ The layer groups are symbolized following a proposal by Bohm & Dornberger-Schiff (1967).

Table 1

The sphere packings corresponding to the 22 orthorhombic bivalent lattice complexes.

Fdd2 16b x, y, z			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{8}, a \leq b$			
A	$-x, -y, 0$		F	$x+\frac{1}{4}, -y+\frac{1}{4}, \frac{1}{4}$	K	$x+\frac{1}{2}, y, \frac{1}{2}$
B	$x, y, 1$			$x-\frac{1}{4}, -y+\frac{1}{4}, -\frac{1}{4}$		$x+\frac{1}{2}, y, -\frac{1}{2}$
	$x, y, -1$		G	$-x+\frac{3}{4}, y-\frac{1}{4}, \frac{1}{4}$		$x-\frac{1}{2}, y, \frac{1}{2}$
C	$-x+1, -y, 0$			$-x+\frac{3}{4}, y+\frac{1}{4}, -\frac{1}{4}$		$x-\frac{1}{2}, y, -\frac{1}{2}$
D	$-x+\frac{1}{2}, -y, \frac{1}{2}$		H	$x-\frac{1}{4}, -y-\frac{1}{4}, \frac{1}{4}$	L	$x+1, y, 0$
	$-x+\frac{1}{2}, -y, -\frac{1}{2}$			$x+\frac{1}{4}, -y-\frac{1}{4}, -\frac{1}{4}$		$x-1, y, 0$
E	$-x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{4}$		I	$-x+\frac{1}{2}, -y+\frac{1}{2}, 0$		
	$-x+\frac{1}{4}, y-\frac{1}{4}, -\frac{1}{4}$		J	$-x+\frac{1}{2}, -y-\frac{1}{2}, 0$		
0.1	12/3/c1	ACDEFGH		$\frac{1}{4}, 0, z; \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$		0.74048
0.2	12/3/c1	ACEFGHIJ		$\frac{1}{4}, 0, z; 1, \sqrt{2}$		0.74048
0.3	11/3/o1	ABDFK		$\frac{1}{6}, \frac{3}{4}\sqrt{2}-1, z; \frac{9}{2}-3\sqrt{2}, \frac{3}{2}\sqrt{3}-\sqrt{6}$		0.71868
0.4	10/3/o4	ACFKL		$\frac{1}{4}, \frac{1}{16}, z; \frac{1}{12}\sqrt{3}, \frac{1}{4}$		0.69813
0.5	10/3/t3	ACDFK		$\frac{1}{4}, \frac{1}{8}\sqrt{6}-\frac{1}{4}, z; \frac{3}{2}\sqrt{6}-1, \frac{1}{2}\sqrt{6}-1$		0.66568
0.6	9/3/o3	ABDEF		0.13668, 0.05792, z; 0.84749, 0.25901		0.66314
0.7	7/3/o6	ACFIL		$\frac{1}{4}, \frac{1}{2}\sqrt{3}-\frac{3}{4}, z; 2-\sqrt{3}, \sqrt{6}-\sqrt{2}$		0.58099
1.1	10/3/o4	BDFK		$\frac{1}{4}, \frac{1}{16}, z; \frac{1}{4}, \frac{1}{12}\sqrt{3}$		0.69813
1.2	10/3/t1	ACEFGH		$\frac{1}{4}, 0, z; \frac{1}{3}\sqrt{6}, 1$		0.69813
1.3	10/3/t1	DEFGH		$\frac{1}{4}, 0, z; 1, \frac{1}{3}\sqrt{6}$		0.69813
1.4	9/3/o2	AFKL		$0, \frac{1}{2}-\frac{1}{4}\sqrt{3}, z; 1-\frac{1}{2}\sqrt{3}, \sqrt{3}-\frac{3}{2}$		0.64801
1.5	9/3/o2	ABFK		$0, \frac{1}{2}-\frac{1}{4}\sqrt{3}, z; \sqrt{3}-\frac{3}{2}, 1-\frac{1}{2}\sqrt{3}$		0.64801
1.6	9/3/o4	ADFK		0.21713, 0.05810, z; 0.23444, 0.20127		0.65469
1.7	8/3/o3	ACFK		$\frac{1}{4}, 0.05890, z; 0.19423, 0.23558$		0.65141
1.8	8/3/t11	BDEF		$\frac{1}{6}, \frac{1}{12}, z; 1, \frac{1}{27}\sqrt{54}$		0.62056
1.9	7/3/o6	ABDE		$1-\frac{1}{2}\sqrt{3}, 0, z; \frac{1}{4}\sqrt{2+\frac{1}{4}\sqrt{6}}, \frac{1}{4}\sqrt{6}-\frac{1}{4}\sqrt{2}$		0.58099
1.10	7/3/o7	ABDF		0.14226, 0.06002, z; 0.50210, 0.18660		0.58099
1.11	7/3/o8	ADEF		$\frac{1}{6}, \frac{3}{8}-\frac{1}{8}\sqrt{7}, z; \frac{3}{2}(2\sqrt{7}-5)^{1/2}, \frac{1}{2}(6\sqrt{7}-15)^{1/2}$		0.50736
1.12	7/3/t1	ABEF		$\frac{1}{14}\sqrt{11}-\frac{1}{14}, \frac{1}{14}\sqrt{11}-\frac{1}{7}, z; 1, \frac{1}{7}\sqrt{22}-\frac{2}{7}\sqrt{2}$		0.59276
1.13	6/3/o4	ACFL		$\frac{1}{4}, 0.07916, z; 0.18280, 0.60560$		0.46228
1.14	6/4/t10	ACDF		$\frac{1}{4}, 0.04495, z; 0.37468, 0.37468$		0.53543
1.15	6/4/t3	AFIL		$\frac{1}{8}, \frac{1}{8}, z; \frac{1}{15}\sqrt{15}, 1$		0.55851
1.16	6/3/c2	AEFI		$\frac{1}{8}, \frac{1}{8}, z; 1, 1$		0.37024
1.17	5/4/o4	ACFI		$\frac{1}{4}, \frac{3}{32}, z; \frac{1}{2}, \frac{1}{2}\sqrt{5}$		0.45734
2.1	8/3/o3	DFK		$\frac{1}{4}, 0.05890, z; 0.23558, 0.19423$		0.65142
2.2	8/4/c1	EFGH		$\frac{1}{4}, 0, z; 1, 1$		0.68017
2.3	7/3/t22	AFK		$0, \frac{1}{2}-\frac{1}{4}\sqrt{3}, z; \sqrt{2}-\frac{1}{2}\sqrt{6}, \sqrt{2}-\frac{1}{2}\sqrt{6}$		0.56119
2.4	6/3/o4	BDF		$\frac{1}{4}, 0.07916, z; 0.60560, 0.18280$		0.46228
2.4'		BDE				
2.5	6/3/t32	DEF		$\frac{3}{16}, \frac{1}{16}, z; 1, \frac{1}{2}$		0.48096
2.6	6/4/t3	BEF		$\frac{1}{8}, \frac{1}{8}, z; 1, \frac{1}{15}\sqrt{15}$		0.55851
2.7	5/4/o4	ADE		$\frac{5}{32}, 0, z; \frac{2}{5}\sqrt{5}, \frac{1}{5}\sqrt{5}$		0.45734
2.8	5/4/o5	ABF		$0, 3-\frac{1}{2}\sqrt{34}, z; (4\sqrt{34}-23)^{1/2}, 6-\sqrt{34}$		0.42072
2.8'		ABE				
2.9	5/4/o5	AFL		$0, 3-\frac{1}{2}\sqrt{34}, z; 6-\sqrt{34}, (4\sqrt{34}-23)^{1/2}$		0.42072
(2.9)		FIL				
2.10	5/4/o6	ADF		$\frac{5}{28}, \frac{5}{96}, z; \frac{7}{30}\sqrt{5}, \frac{1}{30}\sqrt{105}$		0.45734
2.11	5/3/t1	AEF		0.11075, 0.11075, z; 1, 0.74632		0.34503
2.12	4/6/o1	ACF		$\frac{1}{4}, 0.07005, z; 0.32595, 0.66301$		0.38484
2.13	4/4/t1	AFI		$\frac{1}{8}, \frac{1}{8}, z; \frac{1}{2}\sqrt{2}, 1$		0.34009
3.1	4/6/o1	DF		$\frac{1}{4}, 0.07005, z; 0.66301, 0.32595$		0.38484
3.1'		DE				
3.2	3/10/t4	AF		$0, \frac{3}{32}, z; \frac{1}{2}, \frac{1}{2}$		0.22089
3.2'		AE				
3.3	4/4/t1	EF		$\frac{1}{8}, \frac{1}{8}, z; 1, \frac{1}{2}\sqrt{2}$		0.34009
Pmmm 4u 0, y, z			$0 < y \leq \frac{1}{4}, 0 < z \leq \frac{1}{4}, b \leq c$			
A	$0, -y, z$		C	$0, -y+1, z$	E	$1, y, z$
B	$0, y, -z$		D	$0, y, -z+1$		$-1, y, z$
0.1	6/4/c1	ABCDE		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}, 1$		0.52360
Pccm 4q x, y, 0			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, a \leq b$			
A	$-x, -y, 0$		E	$x+1, y, 0$	H	$x, -y+1, \frac{1}{2}$
B	$-x+1, -y, 0$			$x-1, y, 0$		$x, -y+1, -\frac{1}{2}$
C	$x, -y, \frac{1}{2}$		F	$-x+1, y, \frac{1}{2}$	I	$-x, -y+1, 0$
	$x, -y, -\frac{1}{2}$			$-x+1, y, -\frac{1}{2}$		

Table 1 (continued)

<i>D</i>	$-x, y, \frac{1}{2}$ $-x, y, -\frac{1}{2}$		<i>G</i>	$x, y, 1$ $x, y, -1$	<i>J</i>	$-x+1, -y+1, 0$	
0.1	12/3/ <i>c</i> 1	<i>ABCDFHIJ</i>		$\frac{1}{4}, \frac{1}{4}, 1, 1$			0.74048
0.2	10/3/ <i>t</i> 1	<i>ABDEFIJ</i>		$\frac{1}{4}, \frac{1}{4}, \frac{1}{3}\sqrt{3}, 1$			0.69813
0.3	10/3/ <i>t</i> 1	<i>CDFGH</i>		$\frac{1}{4}, \frac{1}{4}, 1, \frac{1}{3}\sqrt{3}$			0.69813
1.1	8/4/ <i>c</i> 1	<i>ABDFIJ</i>		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\sqrt{2}, 1$			0.68017
1.2	8/4/ <i>c</i> 1	<i>CDFH</i>		$\frac{1}{4}, \frac{1}{4}, 1, \frac{1}{2}\sqrt{2}$			0.68017
1.3	6/4/ <i>c</i> 1	<i>ADEI</i>		$0, \frac{1}{4}, \frac{1}{2}, 1$			0.52360
<i>Pmma</i> 4<i>i</i> <i>x</i>, 0, <i>z</i>			$0 \leq x < \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$				
<i>A</i>	$-x, 0, -z$		<i>C</i>	$x, 0, z+1$	<i>D</i>	$x, 1, z$	
<i>B</i>	$-x+\frac{1}{2}, 0, z$			$x, 0, z-1$		$x, -1, z$	
0.1	7/3/ <i>o</i> 1	<i>ABCDEF</i>	<i>E</i>	$-x-\frac{1}{2}, 0, z$	<i>F</i>	$-x, 0, -z+1$	0.56119
0.2	6/4/ <i>c</i> 1	<i>ABDEF</i>		$\frac{1}{2}\sqrt{3}-\frac{3}{4}, \frac{1}{4}, 2+\sqrt{3}, 1$			0.52360
1.1	6/4/ <i>c</i> 1	<i>ABCD</i>		$0, \frac{1}{4}, 2, 2$			0.52360
1.2	5/4/ <i>h</i> 5	<i>ABDF</i>		$\frac{1}{8}, 0; 4, 1$			0.40307
				$\frac{1}{12}, \frac{1}{4}, 3, \sqrt{3}$			0.40307
<i>Pmma</i> 4<i>k</i> $\frac{1}{4}$, <i>y</i>, <i>z</i>			$0 < y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$				
<i>A</i>	$\frac{1}{4}, -y, z$		<i>C</i>	$\frac{1}{4}, y, z+1$	<i>E</i>	$\frac{3}{4}, y, -z+1$	
<i>B</i>	$\frac{3}{4}, y, -z$ $-\frac{1}{4}, y, -z$		<i>D</i>	$\frac{1}{4}, y, z-1$	<i>F</i>	$-\frac{1}{4}, y, -z+1$	
0.1	8/3/ <i>h</i> 4	<i>ABDEF</i>		$\frac{1}{4}, -y+1, z$		$\frac{5}{4}, y, z$	0.60460
0.2	8/3/ <i>h</i> 4	<i>ABCDE</i>		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}\sqrt{3}$		$-\frac{3}{4}, y, z$	0.60460
1.1	6/4/ <i>c</i> 1	<i>ABDE</i>		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\sqrt{3}, \frac{1}{2}$			0.52360
1.2	6/4/ <i>c</i> 1	<i>ABCD</i>		$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$			0.52360
				$\frac{1}{4}, 0; 1, \frac{1}{2}$			0.52360
<i>Pmma</i> 4<i>h</i> 0, <i>y</i>, <i>z</i>			$0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$				
<i>A</i>	$0, -y, -z$		<i>D</i>	$\frac{1}{2}, y, -z+\frac{1}{2}$	<i>F</i>	$0, -y+1, -z$	
<i>B</i>	$1, y, z$ $-1, y, z$			$-\frac{1}{2}, y, -z+\frac{1}{2}$	<i>G</i>	$0, y+1, z$	
<i>C</i>	$0, y, z+1$ $0, y, z-1$		<i>E</i>	$\frac{1}{2}, y, -z-\frac{1}{2}$	<i>H</i>	$0, y-1, z$	
0.1	8/3/ <i>h</i> 4	<i>ABDEF</i>		$-\frac{1}{2}, y, -z-\frac{1}{2}$		$0, -y, -z+1$	0.60460
0.2	8/3/ <i>h</i> 4	<i>ACDEF</i>		$\frac{1}{4}, 0; \frac{1}{2}, \frac{1}{2}\sqrt{3}$			0.60460
0.3	8/3/ <i>h</i> 4	<i>ACDFH</i>		$\frac{1}{4}, 0; \frac{1}{2}\sqrt{3}, \frac{1}{2}$			0.60460
0.4	8/3/ <i>h</i> 4	<i>ADFGH</i>		$\frac{1}{4}, \frac{1}{4}, \frac{2}{3}\sqrt{3}, \frac{1}{3}\sqrt{3}$			0.60460
0.5	8/3/ <i>t</i> 1	<i>ABDFG</i>		$\frac{1}{4}, \frac{1}{4}, 2, \sqrt{3}$			0.60460
1.1	7/3/ <i>o</i> 1	<i>ABDG</i>		$\frac{1}{4}, \frac{1}{8}, 1, 2\sqrt{3}$			0.56119
1.2	6/3/ <i>o</i> 1	<i>ABDF</i>		$0, 1-\frac{1}{2}\sqrt{3}; 1, 2+\sqrt{3}$			0.44226
1.3	6/3/ <i>o</i> 1	<i>ADFG</i>		$\frac{1}{4}, \frac{11}{8}-\frac{1}{8}\sqrt{105}; \frac{1}{4}\sqrt{21}-\frac{1}{4}\sqrt{5}, \frac{1}{4}\sqrt{7}+\frac{1}{4}\sqrt{15}$			0.44226
1.4	6/4/ <i>t</i> 2	<i>ACDF</i>		$\frac{1}{4}, \frac{1}{8}\sqrt{105}-\frac{3}{8}; \frac{1}{4}\sqrt{5}+\frac{1}{4}\sqrt{21}, \frac{3}{4}\sqrt{3}+\frac{1}{4}\sqrt{35}$			0.55851
1.5	6/4/ <i>c</i> 1	<i>ADEF</i>		$\frac{1}{4}, \frac{1}{8}, 1, \frac{2}{15}\sqrt{15}$			0.52360
1.6	6/4/ <i>c</i> 1	<i>ADFH</i>		$\frac{1}{4}, 0; \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$			0.52360
1.7	6/4/ <i>c</i> 1	<i>ADGH</i>		$\frac{1}{4}, \frac{1}{4}, \sqrt{2}, 1$			0.52360
2.1	5/4/ <i>h</i> 5	<i>ADG</i>		$0, \frac{1}{4}, 2, 2$			0.52360
2.2	4/6/ <i>c</i> 1	<i>ADF</i>		$0, \frac{1}{6}, \sqrt{3}, 3$			0.40307
				$\frac{1}{4}, \frac{1}{8}, 1, \sqrt{2}$			0.34009
<i>Pbam</i> 4<i>g</i> <i>x</i>, <i>y</i>, 0			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, a \leq b$				
<i>A</i>	$-x, -y, 0$		<i>D</i>	$-x+\frac{1}{2}, y+\frac{1}{2}, 0$	<i>F</i>	$x+\frac{1}{2}, -y+\frac{1}{2}, 0$	
<i>B</i>	$-x+1, -y, 0$			$-x+\frac{1}{2}, y-\frac{1}{2}, 0$		$x-\frac{1}{2}, -y+\frac{1}{2}, 0$	
<i>C</i>	$x, y, 1$ $x, y, -1$		<i>E</i>	$x+1, y, 0$	<i>G</i>	$-x, -y+1, 0$	
0.1	8/3/ <i>h</i> 4	<i>ABCEF</i>		$x-1, y, 0$			0.60460
0.2	8/3/ <i>h</i> 4	<i>ABCDF</i>		$\frac{1}{4}, \frac{1}{8}, \frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{3}$			0.60460
1.1	7/3/ <i>o</i> 1	<i>ACEF</i>		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\sqrt{3}, \frac{1}{2}$			0.56119
1.2	7/3/ <i>t</i> 5	<i>ACDF</i>		$0, 1-\frac{1}{2}\sqrt{3}; 2-\sqrt{3}, 2-\sqrt{3}$			0.56119
1.3	6/4/ <i>c</i> 1	<i>ABCF</i>		$\frac{1}{4}\sqrt{3}-\frac{1}{4}, \frac{1}{4}\sqrt{3}-\frac{1}{4}, 1, \frac{1}{2}\sqrt{6}-\frac{1}{2}\sqrt{2}$			0.52360
1.4	6/4/ <i>c</i> 1	<i>ABCD</i>		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}, \frac{1}{4}\sqrt{2}$			0.52360
1.4'		<i>ACFG</i>		$\frac{1}{4}, 0; 1, \frac{1}{2}$			0.52360
2.1	6/4/ <i>c</i> 1	<i>CDF</i>		$0, \frac{1}{4}, 1, \frac{1}{2}$			0.52360
2.2	5/4/ <i>h</i> 5	<i>ACF</i>		$\frac{1}{4}, \frac{1}{4}, 1, \frac{1}{2}$			0.40307
2.2'		<i>ACD</i>		$0, \frac{1}{6}, \frac{1}{3}\sqrt{3}, \frac{1}{3}$			0.40307

Table 1 (continued)

Pbcm 4g x, y, $\frac{1}{4}$			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}$			
A	$-x, -y, \frac{3}{4}$ $-x, -y, -\frac{1}{4}$		D	$x+1, y, \frac{1}{4}$ $x-1, y, \frac{1}{4}$	G	$-x, y+\frac{1}{2}, \frac{1}{4}$ $-x, y-\frac{1}{2}, \frac{1}{4}$
B	$-x+1, -y, \frac{3}{4}$ $-x+1, -y, -\frac{1}{4}$		E	$x, -y+\frac{1}{2}, \frac{3}{4}$ $x, -y+\frac{1}{2}, -\frac{1}{4}$	H	$-x+1, y+\frac{1}{2}, \frac{1}{4}$
C	$x, y, \frac{5}{4}$ $x, y, -\frac{3}{4}$		F	$x, -y-\frac{1}{2}, \frac{3}{4}$ $x, -y-\frac{1}{2}, -\frac{1}{4}$	I	$x, y+1, \frac{1}{4}$ $x, y-1, \frac{1}{4}$
0.1	12/3/h1	ABDEGH		$\frac{1}{4}, \frac{1}{12}, \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{2}$		0.74048
0.2	12/3/c1	ABEFGH		$\frac{1}{4}, 0; 1, 1$		0.74048
0.3	10/3/o2	ABCDE		$\frac{1}{4}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \sqrt{3}-\sqrt{2}, \sqrt{3}-\sqrt{2}$		0.66568
0.4	10/3/t1	ABCEF		$\frac{1}{4}, 0; 1, \frac{1}{3}\sqrt{3}$		0.69813
0.5	10/3/t1	EFGHI		$\frac{1}{4}, 0; \sqrt{3}, \sqrt{3}$		0.69813
1.1	10/3/o1	ABEGH		$\frac{1}{4}, \frac{1}{20}; \frac{1}{5}\sqrt{15}, \frac{2}{5}\sqrt{6}$		0.69813
1.2	10/3/t1	ABDGH		$\frac{1}{4}, 0; \frac{1}{3}\sqrt{3}, 1$		0.69813
1.3	8/3/o1	ABDE		$\frac{1}{4}, \frac{3}{28}; \frac{1}{7}\sqrt{7}, \frac{2}{7}\sqrt{3}$		0.60460
1.4	8/3/h3	ABCE		$\frac{1}{4}, \frac{1}{12}; \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}$		0.53742
1.5	8/3/h4	ACDE		$0, \frac{1}{8}; \frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{3}$		0.60460
1.6	8/3/h4	ADEG		$0, \frac{1}{8}; \frac{1}{2}, \frac{1}{2}\sqrt{3}$		0.60460
1.7	8/3/h4	DEGH		$\frac{1}{4}, \frac{1}{4}; \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}$		0.60460
1.8	8/3/h4	EGHI		$\frac{1}{4}, \frac{1}{4}; \sqrt{3}, 2$		0.60460
1.9	8/4/c1	ABEF		$\frac{1}{4}, 0; 1, \frac{1}{2}\sqrt{2}$		0.68017
1.10	8/4/c1	EFGH		$\frac{1}{4}, 0; \sqrt{2}, \sqrt{2}$		0.68017
2.1	8/4/c1	ABGH		$\frac{1}{4}, 0; \frac{1}{2}\sqrt{2}, 1$		0.68017
2.2	6/4/h2	ABE		$\frac{1}{4}, \frac{1}{12}; \frac{1}{3}\sqrt{3}, \frac{1}{3}\sqrt{2}$		0.52360
2.3	6/4/c1	ADE		$0, \frac{1}{8}; \frac{1}{4}\sqrt{2}, \frac{1}{2}$		0.52360
2.4	6/4/c1	ADG		$0, 0; \frac{1}{2}, 1$		0.52360
2.5	6/4/c1	DEG		$0, \frac{1}{4}; \frac{1}{2}, 1$		0.52360
2.6	6/4/c1	EGH		$\frac{1}{4}, \frac{1}{4}; 1, \sqrt{2}$		0.52360
Pnmm 4g x, y, 0			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, a \leq b$			
A	$-x, -y, 0$		E	$-x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}$ $-x+\frac{1}{2}, y+\frac{1}{2}, -\frac{1}{2}$	F	$x+\frac{1}{2}, -y+\frac{1}{2}, \frac{1}{2}$ $x+\frac{1}{2}, -y+\frac{1}{2}, -\frac{1}{2}$
B	$x, y, 1$ $x, y, -1$			$-x+\frac{1}{2}, y-\frac{1}{2}, \frac{1}{2}$ $-x+\frac{1}{2}, y-\frac{1}{2}, -\frac{1}{2}$	H	$x-\frac{1}{2}, -y+\frac{1}{2}, \frac{1}{2}$ $x-\frac{1}{2}, -y+\frac{1}{2}, -\frac{1}{2}$
C	$-x+1, -y, 0$				G	$-x, -y+1, 0$
D	$x+1, y, 0$ $x-1, y, 0$				H	$-x+1, -y+1, 0$
0.1	12/3/h1	ABCEF		$\frac{1}{4}, \frac{1}{6}; \frac{2}{3}\sqrt{2}, \frac{1}{3}\sqrt{3}$		0.74048
0.2	12/3/c1	ACEFGH		$\frac{1}{4}, \frac{1}{4}; 1, 1$		0.74048
0.3	10/3/o2	ABCDF		$\frac{1}{4}, \frac{3}{4}; \frac{1}{4}\sqrt{6}; \sqrt{3}-\sqrt{2}, \sqrt{3}-\sqrt{2}$		0.66568
0.4	10/3/t1	ACDFGH		$\frac{1}{4}, \frac{1}{4}; \frac{1}{3}\sqrt{3}, 1$		0.69813
1.1	11/3/t1	ABEF		$\frac{1}{2}\sqrt{2}-\frac{1}{2}, \frac{1}{2}\sqrt{2}-\frac{1}{2}, 1, 2-\sqrt{2}$		0.71868
1.2	10/3/o1	ACEF		$\frac{1}{4}, \frac{1}{5}; \frac{2}{5}\sqrt{6}, \frac{1}{5}\sqrt{15}$		0.69813
1.3	9/3/t2	ABDF		$0, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1-\frac{1}{2}\sqrt{2}, 1-\frac{1}{2}\sqrt{2}$		0.61343
1.4	8/3/o1	ABCF		$\frac{1}{4}, \frac{1}{7}; \frac{2}{7}\sqrt{3}, \frac{1}{7}\sqrt{7}$		0.60460
1.5	8/3/h3	ACDF		$\frac{1}{4}, \frac{1}{6}; \frac{2}{9}\sqrt{3}, \frac{1}{3}\sqrt{3}$		0.53742
1.6	8/3/h4	ADFG		$0, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}\sqrt{3}$		0.60460
1.7	8/3/h4	ABFG		$0, \frac{1}{4}; \frac{1}{2}\sqrt{3}, \frac{1}{2}$		0.60460
1.7'		ABCE				
1.8	8/4/c1	ACFGH		$\frac{1}{4}, \frac{1}{4}; \frac{1}{2}\sqrt{2}, 1$		0.68017
2.1	10/3/t1	BEF		$\frac{1}{4}, \frac{1}{4}; 1, \frac{1}{3}\sqrt{3}$		0.69813
2.2	9/3/t1	AEF		0.22150, 0.22150; 1, 0.74632		0.69006
2.3	7/3/o5	ADF		$0, \frac{3}{2}-\frac{1}{2}\sqrt{7}; 3-\sqrt{7}, (2\sqrt{7}-5)^{1/2}$		0.48680
2.4	7/3/o5	ABF		$0, \frac{3}{2}-\frac{1}{2}\sqrt{7}; (2\sqrt{7}-5)^{1/2}, 3-\sqrt{7}$		0.48680
2.4'		ABE				
2.5	6/4/h2	ACF		$\frac{1}{4}, \frac{1}{6}; \frac{1}{3}\sqrt{2}, \frac{1}{3}\sqrt{3}$		0.52360
2.6	6/4/c1	AFG		$0, \frac{1}{4}; \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$		0.52360
2.6'		ACE				
3.1	8/4/c1	EF		$\frac{1}{4}, \frac{1}{4}; 1, \frac{1}{2}\sqrt{2}$		0.68017
3.2	5/4/t6	AF		$0, \frac{3}{16}; \frac{1}{2}, \frac{1}{2}$		0.44179
3.2'		AE				
Pmmm 4e 0, y, z			$0 < y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$			
A	$0, -y, z$		C	$0, y, z+1$ $0, y, z-1$	E	$0, -y+1, z$
B	$1, y, z$ $-1, y, z$		D	$\frac{1}{2}, -y+\frac{1}{2}, -z$ $-\frac{1}{2}, -y+\frac{1}{2}, -z$	F	$\frac{1}{2}, -y+\frac{1}{2}, -z+1$ $-\frac{1}{2}, -y+\frac{1}{2}, -z+1$

Table 1 (continued)

0.1	9/3/t2	ABCDF	$\frac{1}{2}\frac{1}{4}\sqrt{2}, \frac{1}{4}, 1-\frac{1}{2}\sqrt{2}, 1-\frac{1}{2}\sqrt{2}$	0.61343
0.2	8/3/h4	ABDEF	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}\sqrt{3}$	0.60460
0.3	8/3/h4	ACDEF	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\sqrt{3}, \frac{1}{2}$	0.60460
1.1	7/3/o1	ABCD	$1-\frac{1}{2}\sqrt{3}, 0; 2-\sqrt{3}, 2-\sqrt{3}$	0.56119
1.2	7/3/o5	ABDF	$\frac{3}{2}-\frac{1}{2}\sqrt{7}, \frac{1}{4}, 3-\sqrt{7}, (2\sqrt{7}-5)^{1/2}$	0.48680
1.3	7/3/o5	ACDF	$\frac{3}{2}-\frac{1}{2}\sqrt{7}, \frac{1}{4}, (2\sqrt{7}-5)^{1/2}, 3-\sqrt{7}$	0.48680
1.4	6/4/c1	ADEF	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$	0.52360
1.5	6/4/c1	ACDE	$\frac{1}{4}, 0; 1, \frac{1}{2}$	0.52360
2.1	5/4/h5	ACD	$\frac{1}{6}, 0; \frac{1}{3}\sqrt{3}, \frac{1}{3}$	0.40307
2.2	5/4/t6	ADF	$\frac{3}{16}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}$	0.44179

Pnma 4c $x, \frac{1}{4}, z$

		$0 \leq x \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$			
A	$x+\frac{1}{2}, \frac{1}{4}, -z+\frac{1}{2}$	E	$-x, \frac{3}{4}, -z$	G	$-x+1, \frac{3}{4}, -z$
	$x-\frac{1}{2}, \frac{1}{4}, -z+\frac{1}{2}$		$-x, -\frac{1}{4}, -z$		$-x+1, -\frac{1}{4}, -z$
B	$x+\frac{1}{2}, \frac{1}{4}, -z-\frac{1}{2}$	F	$-x+\frac{1}{2}, \frac{3}{4}, z+\frac{1}{2}$	H	$x, \frac{5}{4}, z$
	$x-\frac{1}{2}, \frac{1}{4}, -z-\frac{1}{2}$		$-x+\frac{1}{2}, \frac{3}{4}, z-\frac{1}{2}$		$x, -\frac{3}{4}, z$
C	$x, \frac{1}{4}, z+1$		$-x+\frac{1}{2}, -\frac{1}{4}, z+\frac{1}{2}$	I	$-x, \frac{3}{4}, -z+1$
	$x, \frac{1}{4}, z-1$		$-x+\frac{1}{2}, -\frac{1}{4}, z-\frac{1}{2}$		$-x, -\frac{1}{4}, -z+1$
D	$x+1, \frac{1}{4}, z$				
	$x-1, \frac{1}{4}, z$				
0.1	12/3/h1	ABCEF	$\frac{1}{6}, 0; \frac{3}{4}\sqrt{2}, \frac{1}{4}\sqrt{6}$	0.74048	
0.2	12/3/h1	AEFGH	$\frac{1}{4}, \frac{1}{12}, \frac{2}{3}\sqrt{6}, \sqrt{3}$	0.74048	
0.3	12/3/c1	ABEFG	$\frac{1}{4}, 0; 1, 1$	0.74048	
0.4	12/3/c1	ACEFI	$\frac{1}{8}, \frac{1}{4}, \sqrt{2}, \frac{1}{2}\sqrt{2}$	0.74048	
0.5	12/3/c1	AEFHI	$\frac{1}{8}, \frac{1}{4}, 2, \sqrt{2}$	0.74048	
0.6	12/3/c1	CEFHI	$\frac{1}{8}, \frac{1}{4}, 2\sqrt{2}, 1$	0.74048	
0.7	10/3/o2	ADEGH	$\frac{1}{4}, \frac{1}{4}\sqrt{6}-\frac{1}{2}, 1, \sqrt{2}+\sqrt{3}$	0.66568	
0.8	10/3/t1	ABDEG	$\frac{1}{4}, 0; \frac{1}{3}\sqrt{3}, 1$	0.69813	
1.1	10/3/o1	ABEF	$\frac{1}{5}, 0; \frac{5}{12}\sqrt{6}, \frac{1}{4}\sqrt{10}$	0.69813	
1.2	10/3/o1	AEFG	$\frac{1}{4}, \frac{1}{20}, \frac{2}{5}\sqrt{10}, \frac{1}{3}\sqrt{15}$	0.69813	
1.3	10/3/o2	CEFH	$\frac{3}{4}-\frac{1}{4}\sqrt{6}, 0; \sqrt{2}+\sqrt{3}, 1$	0.66568	
1.4	10/3/o5	ACEF	$\frac{3}{20}, \frac{1}{8}, \frac{5}{6}\sqrt{15}$	0.69813	
1.5	10/3/o6	AEFH	$\frac{1}{8}\sqrt{6}-\frac{1}{8}, \frac{1}{6}\sqrt{6}-\frac{1}{4}, \frac{1}{3}(18+6\sqrt{6})^{1/2}, \frac{1}{2}(6+2\sqrt{6})^{1/2}$	0.66568	
1.6	10/3/t1	ABCF	$\frac{1}{4}, 0; 1, \frac{1}{3}\sqrt{3}$	0.69813	
1.7	10/3/t1	AEFI	$\frac{1}{8}, \frac{1}{4}, \frac{2}{3}\sqrt{6}, 1$	0.69813	
1.8	10/3/t1	EFGH	$\frac{1}{4}, 0; \sqrt{3}, \sqrt{3}$	0.69813	
1.9	10/3/t1	CEFI	$\frac{1}{8}, \frac{1}{4}, 2, \frac{1}{3}\sqrt{6}$	0.69813	
1.10	10/3/t1	EFHI	$\frac{1}{8}, \frac{1}{4}, \sqrt{6}, \frac{1}{2}\sqrt{6}$	0.69813	
1.11	8/3/o1	AEGH	$\frac{1}{4}, \frac{3}{28}, \frac{2}{7}\sqrt{21}, \sqrt{7}$	0.60460	
1.12	8/3/t1	ADEH	$0, \frac{1}{8}, 1, 2\sqrt{3}$	0.60460	
1.13	8/3/h3	ADEG	$\frac{1}{4}, \frac{1}{12}, \frac{2}{3}, \sqrt{3}$	0.53742	
1.14	8/3/h4	ABDE	$0, 0; \frac{1}{2}, \frac{1}{2}\sqrt{3}$	0.60460	
1.15	8/3/h4	ABCE	$0, 0; \frac{1}{2}\sqrt{3}, \frac{1}{2}$	0.60460	
1.16	8/3/h4	ACEI	$0, \frac{1}{4}, \frac{2}{3}\sqrt{3}, \frac{1}{3}\sqrt{3}$	0.60460	
1.17	8/3/h4	AEHI	$0, \frac{1}{4}, 2, \sqrt{3}$	0.60460	
1.18	8/4/c1	ABEG	$\frac{1}{4}, 0; \frac{1}{2}\sqrt{2}, 1$	0.68017	
2.1	8/3/o1	CEF	$\frac{1}{7}, 0; \frac{2}{6}\sqrt{3}, \frac{1}{6}\sqrt{21}$	0.60460	
2.2	8/3/o5	AEF	$\frac{5}{28}, \frac{1}{8}, \frac{7}{12}\sqrt{6}, \frac{1}{6}\sqrt{42}$	0.60460	
2.3	8/3/h3	EFH	$\frac{1}{6}, 0; \frac{3}{2}\sqrt{3}, \frac{3}{2}$	0.53742	
2.4	8/3/h4	ACF	$\frac{1}{4}, \frac{1}{4}, \frac{2}{3}\sqrt{3}, \frac{1}{3}\sqrt{3}$	0.60460	
2.5	8/3/h4	AFH	$\frac{1}{4}, \frac{1}{4}, 2, \sqrt{3}$	0.60460	
2.6	8/4/c1	ABF	$\frac{1}{4}, 0; 1, \frac{1}{2}\sqrt{2}$	0.68017	
2.7	8/4/c1	EFG	$\frac{1}{4}, 0; \sqrt{2}, \sqrt{2}$	0.68017	
2.8	8/4/c1	EFI	$\frac{1}{8}, \frac{1}{4}, 2, 1$	0.68017	
2.9	6/3/o1	ADE	$0, \frac{11}{8}-\frac{1}{8}\sqrt{105}; \frac{1}{4}\sqrt{21}-\frac{1}{4}\sqrt{5}, \frac{1}{4}\sqrt{7}+\frac{1}{4}\sqrt{15}$	0.44226	
2.10	6/3/o1	AEH	$0, \frac{1}{8}\sqrt{105}-\frac{9}{8}, \frac{1}{4}\sqrt{5}+\frac{1}{4}\sqrt{21}, \frac{3}{4}\sqrt{3}+\frac{1}{4}\sqrt{35}$	0.44226	
2.11	6/4/t2	ACE	$0, \frac{1}{8}, 1, \frac{2}{15}\sqrt{15}$	0.55851	
2.12	6/4/h2	AEG	$\frac{1}{4}, \frac{1}{12}, \frac{1}{3}\sqrt{6}, \sqrt{3}$	0.52360	
2.13	6/4/c1	ABE	$0, 0; \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$	0.52360	
2.14	6/4/c1	AEI	$0, \frac{1}{4}, \sqrt{2}, 1$	0.52360	
3.1	6/4/h2	EF	$\frac{1}{6}, 0; \frac{3}{2}\sqrt{2}, \frac{1}{2}\sqrt{6}$	0.52360	
3.2	6/4/c1	AF	$\frac{1}{4}, \frac{1}{4}, \sqrt{2}, 1$	0.52360	
3.3	4/6/c1	AE	$0, \frac{1}{8}, 1, \sqrt{2}$	0.34009	

Table 1 (continued)

Cmcm 8f 0, y, z			$0 \leq y \leq \frac{1}{4}, 0 \leq z < \frac{1}{4}$			
A	0, y, $-z + \frac{1}{2}$		E	0, $-y + 1$, $-z$	G	1, y, z
B	0, y, $-z - \frac{1}{2}$		F	$\frac{1}{2}, y + \frac{1}{2}, z$		$-1, y, z$
C	0, $-y$, $-z$			$\frac{1}{2}, y - \frac{1}{2}, z$	H	0, $y + 1$, z
D	$\frac{1}{2}, -y + \frac{1}{2}, -z$			$-\frac{1}{2}, y + \frac{1}{2}, z$		0, $y - 1$, z
	$-\frac{1}{2}, -y + \frac{1}{2}, -z$			$-\frac{1}{2}, y - \frac{1}{2}, z$		
0.1	10/3/h2	ACDFG		$\frac{1}{6}, \frac{1}{4}\sqrt{6} - \frac{1}{2}, \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{2 + \frac{2}{3}}\sqrt{3}$		0.66568
0.2	9/3/o1	ACEFH		$\frac{1}{4}, \frac{1}{2}\sqrt{3} - \frac{3}{4}, \sqrt{3}, 2 + \sqrt{3}$		0.64801
0.3	9/3/t2	ACDEF		$\frac{1}{4}, \frac{1}{4}\sqrt{2} - \frac{1}{4}, 1, 1 + \sqrt{2}$		0.61343
0.4	7/3/o1	ABCDG		$1 - \frac{1}{2}\sqrt{3}, 0; 2 - \sqrt{3}, 4 - 2\sqrt{3}$		0.56119
0.5	6/4/c1	ABCDE		$\frac{1}{4}, 0; 1, 1$		0.52360
1.1	9/3/o1	ADFG		$\frac{1}{4}, \frac{1}{2}\sqrt{3} - \frac{3}{4}, \frac{1}{3}\sqrt{3}, 1 + \frac{2}{3}\sqrt{3}$		0.64801
1.2	8/3/o2	ACDF		$\frac{7}{32}, \frac{3}{28}, \frac{1}{2}\sqrt{3}, \frac{7}{8}\sqrt{7}$		0.60460
1.3	8/3/h4	ACFG		$0, \frac{1}{8}, \frac{1}{3}\sqrt{3}, \frac{4}{3}\sqrt{3}$		0.60460
1.4	8/3/h4	ACFH		$0, \frac{1}{8}, \sqrt{3}, 4$		0.60460
1.5	7/4/o1	ACEF		$\frac{1}{4}, \frac{1}{24}\sqrt{13} - \frac{1}{24}, \frac{1}{6}(30 + 6\sqrt{13})^{1/2}, (4 + \sqrt{13})^{1/2}$		0.60210
1.6	6/3/o2	ACDG		$\frac{19}{64} - \frac{1}{64}\sqrt{105}, \frac{1}{16}\sqrt{105} - \frac{9}{16}, \frac{1}{4}\sqrt{15} - \frac{1}{4}\sqrt{7}, \frac{3}{16}\sqrt{15} + \frac{1}{16}\sqrt{7}$		0.44226
1.7	5/4/h5	ABCD		$\frac{1}{6}, 0; \frac{1}{3}\sqrt{3}, \frac{2}{3}$		0.40307
1.8	5/4/t6	ACDE		$\frac{1}{4}, \frac{1}{16}, 1, \sqrt{2}$		0.44179
2.1	7/4/o1	ADF		$\frac{1}{4}, \frac{1}{24}\sqrt{13} - \frac{1}{24}, \frac{1}{2}(10 - 2\sqrt{13})^{1/2}, \frac{1}{2} + \frac{1}{2}\sqrt{13}$		0.60210
2.2	6/4/c1	ACF		$0, \frac{1}{8}, 1, 2\sqrt{2}$		0.52360
2.3	4/6/h2	ACD		$\frac{1}{6}, \frac{1}{16}, \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{2}$		0.34009
Cmcm 8g x, y, $\frac{1}{4}$			$0 < x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}$			
A	$-x, y, \frac{1}{4}$		E	$x, y + 1, \frac{1}{4}$	G	$-x + \frac{1}{2}, -y + \frac{1}{2}, \frac{3}{4}$
B	$x, -y, \frac{3}{4}$			$x, y - 1, \frac{1}{4}$		$-x + \frac{1}{2}, -y + \frac{1}{2}, -\frac{1}{4}$
	$x, -y, -\frac{1}{4}$		F	$x, y, \frac{3}{4}$	H	$x, -y + 1, \frac{3}{4}$
C	$-x + 1, y, \frac{1}{4}$			$x, y, -\frac{3}{4}$		$x, -y + 1, -\frac{1}{4}$
D	$-x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}$					
	$-x + \frac{1}{2}, y - \frac{1}{2}, \frac{1}{4}$					
0.1	9/3/o1	ABFGH		$1 - \frac{1}{2}\sqrt{3}, \frac{1}{4}, 1 + \frac{2}{3}\sqrt{3}, \frac{1}{3}\sqrt{3}$		0.64801
0.2	9/3/o1	ABDEH		$1 - \frac{1}{2}\sqrt{3}, \frac{1}{4}, 2 + \sqrt{3}, \sqrt{3}$		0.64801
0.3	9/3/t2	ABDGH		$\frac{1}{2} - \frac{1}{4}\sqrt{2}, \frac{1}{4}, 1 + \sqrt{2}, 1$		0.61343
0.4	8/3/h4	ABCFG		$\frac{1}{4}, \frac{1}{8}, \frac{1}{3}\sqrt{3}, \frac{1}{6}\sqrt{3}$		0.60460
0.5	8/3/h4	ABCDG		$\frac{1}{4}, \frac{1}{8}, 1, \frac{1}{2}\sqrt{3}$		0.60460
1.1	7/3/o1	ABDE		$1 - \frac{1}{2}\sqrt{3}, 0; 2 + \sqrt{3}, 2$		0.56119
1.2	7/3/o2	ABFG		$\frac{7}{8} - \frac{1}{8}\sqrt{33}, \frac{15}{64} - \frac{1}{64}\sqrt{33}; \frac{3}{8}\sqrt{3} + \frac{1}{8}\sqrt{11}, \frac{5}{16}\sqrt{3} - \frac{1}{16}\sqrt{11}$		0.43908
1.3	7/3/o3	ABDG		$\frac{3}{2} - \frac{1}{2}\sqrt{7}, \frac{4}{9} - \frac{1}{9}\sqrt{7}; \frac{2}{3} + \frac{1}{3}\sqrt{7}, \frac{2}{9}(14\sqrt{7} - 20)^{1/2}$		0.48680
1.4	7/4/o1	ABGH		$\frac{7}{24} - \frac{1}{24}\sqrt{13}, \frac{1}{4}, \frac{1}{2} + \frac{1}{2}\sqrt{13}, \frac{1}{3}(10 - 2\sqrt{13})^{1/2}$		0.60210
1.5	7/4/o1	ABDH		$\frac{7}{24} - \frac{1}{24}\sqrt{13}, \frac{1}{4}, (4 + \sqrt{13})^{1/2}, \frac{1}{6}(30 + 6\sqrt{13})^{1/2}$		0.60210
1.6	6/4/c1	ABCG		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\sqrt{2}, \frac{1}{2}$		0.52360
1.7	6/4/c1	ABCD		$\frac{1}{4}, 0; 1, 1$		0.52360
1.8	6/4/c1	ACDG		$\frac{1}{4}, \frac{1}{4}, 1, 1$		0.52360
2.1	5/4/o1	ABG		$\frac{1}{6}, \frac{1}{7}, \frac{3}{7}\sqrt{7}, \frac{2}{7}\sqrt{3}$		0.40307
2.2	5/4/t6	ADG		$\frac{1}{16}, \frac{1}{4}, \sqrt{2}, 1$		0.44179
2.3	5/4/h5	ABD		$\frac{1}{6}, 0; \sqrt{3}, \frac{2}{3}\sqrt{3}$		0.40307
Cmce 8f 0, y, z			$0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$			
A	0, $-y$, $-z$		F	0, y, $z - 1$	J	0, $y + \frac{1}{2}$, $-z + \frac{1}{2}$
B	$\frac{1}{2}, y$, $-z + \frac{1}{2}$			0, y, $z + 1$		0, $y - \frac{1}{2}$, $-z + \frac{1}{2}$
	$-\frac{1}{2}, y$, $-z + \frac{1}{2}$		G	1, y, z	K	0, $y + 1$, z
C	$\frac{1}{2}, y$, $-z - \frac{1}{2}$			$-1, y, z$		0, $y - 1$, z
	$-\frac{1}{2}, y$, $-z - \frac{1}{2}$		H	0, $-y + 1$, $-z$	L	0, $-y$, $-z + 1$
D	0, $-y + \frac{1}{2}$, $z + \frac{1}{2}$		I	$\frac{1}{2}, y + \frac{1}{2}, z$		
	0, $-y + \frac{1}{2}$, $z - \frac{1}{2}$			$\frac{1}{2}, y - \frac{1}{2}, z$		
E	$\frac{1}{2}, -y + \frac{1}{2}, -z$			$-\frac{1}{2}, y + \frac{1}{2}, z$		
	$-\frac{1}{2}, -y + \frac{1}{2}, -z$			$-\frac{1}{2}, y - \frac{1}{2}, z$		
0.1	12/3/c1	ABEHIJ		$\frac{1}{4}, \frac{1}{8}, 1, 2$		0.74048
0.2	11/3/o2	ABEGI		$\frac{1}{6}, \frac{3}{2}\sqrt{2} - 2; \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{2} + 1$		0.71868
0.3	10/3/t1	ABDEHJ		$\frac{1}{4}, \frac{1}{8}, 1, \frac{2}{3}\sqrt{3}$		0.69813
0.4	10/3/t1	AHIJK		$\frac{1}{4}, \frac{1}{8}, \sqrt{3}, 2\sqrt{3}$		0.69813
0.5	9/3/o1	ABCDF		$1 - \frac{1}{2}\sqrt{3}, 0; 2\sqrt{3} - 3, 2 - \sqrt{3}$		0.64801
0.6	9/3/o1	ABCEG		$1 - \frac{1}{2}\sqrt{3}, 0; 2 - \sqrt{3}, 2\sqrt{3} - 3$		0.64801
0.7	9/3/t2	ABCDE		$\frac{1}{2} - \frac{1}{4}\sqrt{2}, 0; \sqrt{2} - 1, \sqrt{2} - 1$		0.61343
0.8	8/3/h4	ABDFL		$\frac{1}{8}, \frac{1}{4}, \frac{1}{3}\sqrt{3}, \frac{1}{6}\sqrt{3}$		0.60460
0.9	8/3/h4	ABDJL		$\frac{1}{8}, \frac{1}{4}, 1, \frac{1}{2}\sqrt{3}$		0.60460

Table 1 (continued)

1.1	10/3/r1	BEGI	$\frac{1}{4}, \frac{1}{8}, \frac{1}{3}\sqrt{3}, 2$	0.69813
1.2	9/3/o5	ABEI	0.19373, 0.12338; 0.74152, 1.97434	0.69006
1.3	9/3/o1	ABGI	$0, 1-\frac{1}{2}\sqrt{3}; \frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}+1$	0.64801
1.4	9/3/o1	AIJK	$0, 1-\frac{1}{2}\sqrt{3}; \sqrt{3}, \sqrt{3}+2$	0.64801
1.5	9/3/t2	ABJI	$0, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1, 1+\sqrt{2}$	0.61343
1.6	8/4/c1	ABEHJ	$\frac{1}{4}, \frac{1}{8}, 1, \sqrt{2}$	0.68018
1.7	8/4/c1	AHIJ	$\frac{1}{4}, \frac{1}{8}, \sqrt{2}, 2, \sqrt{2}$	0.68018
1.8	7/4/o1	ABCD	$\frac{7}{24}-\frac{1}{24}\sqrt{13}, 0; \frac{1}{6}\sqrt{13}-\frac{1}{6}, \frac{1}{3}(12-3\sqrt{13})^{1/2}$	0.60210
1.9	7/4/o1	ABCE	$\frac{7}{24}-\frac{1}{24}\sqrt{13}, 0; \frac{1}{3}(12-3\sqrt{13})^{1/2}, \frac{1}{6}\sqrt{13}-\frac{1}{6}$	0.60210
1.10	7/3/o9	ABDE	$\frac{1}{6}, \frac{3}{4}-\frac{1}{4}\sqrt{7}; \frac{1}{3}\sqrt{3}, \frac{1}{9}(15+6\sqrt{7})^{1/2}$	0.50736
1.11	7/3/o10	ABEG	$\frac{1}{12}\sqrt{7}-\frac{1}{12}, \frac{3}{4}-\frac{1}{4}\sqrt{7}; \frac{1}{3}(6\sqrt{7}-15)^{1/2}, \frac{1}{3}(1+2\sqrt{7})^{1/2}$	0.48680
1.12	7/3/o11	ABDF	0.13061, 0.15994; 0.54240, 0.27571	0.58705
1.13	7/3/o12	ABDJ	0.16397, 0.20293; 1, 0.95602	0.57451
1.14	6/4/c1	ADEH	$\frac{1}{4}, 0; 1, 1$	0.52360
1.15	6/4/c1	ABDL	$\frac{1}{8}, \frac{1}{4}, \frac{1}{2}\sqrt{2}, \frac{1}{2}$	0.52360
1.16	6/4/c1	ABJL	$0, \frac{1}{4}, 1, 1$	0.52360
2.1	8/4/c1	BEI	$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\sqrt{2}, 2$	0.68018
2.2	7/4/o1	ABI	$0, \frac{7}{24}-\frac{1}{24}\sqrt{13}; \frac{1}{3}(10-2\sqrt{13})^{1/2}, \frac{1}{2}+\frac{1}{2}\sqrt{13}$	0.60210
2.3	7/4/o1	AIJ	$0, \frac{7}{24}-\frac{1}{24}\sqrt{13}; \frac{1}{6}(30+6\sqrt{13})^{1/2}, (4+\sqrt{13})^{1/2}$	0.60210
2.4	6/4/c1	BDJ	$\frac{1}{4}, \frac{1}{4}, 1, 1$	0.52360
2.5	5/4/o7	ABE	$\frac{3}{20}, \frac{3}{32}, \frac{1}{5}\sqrt{5}, \frac{4}{5}$	0.44179
2.6	5/4/o8	ABD	0.14839, 0.14839; 0.63751, 0.53756	0.46761
2.7	5/4/t6	ADE	$\frac{3}{16}, 0; \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$	0.44179
2.8	5/4/t6	ABJ	$0, \frac{3}{16}, 1, \sqrt{2}$	0.44179
Cmmm 8n 0, y, z			$0 < y \leq \frac{1}{4}, 0 < z \leq \frac{1}{4}$	
A	0, y, -z		$\frac{1}{2}, -y+\frac{1}{2}, z$	
B	0, -y, z		$-\frac{1}{2}, -y+\frac{1}{2}, z$	
C	1, y, z		0, -y+1, z	
	-1, y, z		0, y, -z+1	
0.1	7/3/o1	ABCDF	$1-\frac{1}{2}\sqrt{3}, \frac{1}{4}, 2-\sqrt{3}, 4-2\sqrt{3}$	0.56119
0.2	6/4/c1	ABDEF	$\frac{1}{4}, \frac{1}{4}, 1, 1$	0.52360
1.1	5/4/h5	ABDF	$\frac{1}{6}, \frac{1}{4}, \frac{1}{3}\sqrt{3}, \frac{2}{3}$	0.40307
Cmmm 8p x, y, 0			$0 < x \leq \frac{1}{4}, 0 < y \leq \frac{1}{4}, a \leq b$	
A	-x, y, 0		x, y, 1	D -x+1, y, 0
B	x, -y, 0		x, y, -1	E -x+\frac{1}{2}, -y+\frac{1}{2}, 0
0.1	6/4/c1	ABCDE	$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}, \frac{1}{4}$	0.52360
1.1	5/4/t4	ABCE	$\frac{1}{2}-\frac{1}{4}\sqrt{2}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1, 1-\frac{1}{2}\sqrt{2}$	0.35934
Cccm 8l x, y, 0			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, a \leq b$	
A	-x, -y, 0		-x, y, \frac{1}{2}	I x+1, y, 0
B	x, -y, \frac{1}{2}		-x, y, -\frac{1}{2}	J x-1, y, 0
	x, -y, -\frac{1}{2}		x, y, 1	K -x-\frac{1}{2}, -y+\frac{1}{2}, 0
C	-x+1, -y, 0		x, y, -1	
D	-x+\frac{1}{2}, -y+\frac{1}{2}, 0		-x+1, y, \frac{1}{2}	
E	-x+\frac{1}{2}, -y-\frac{1}{2}, 0		-x+1, y, -\frac{1}{2}	
0.1	9/3/o1	BDFGH	$\frac{1}{4}, \frac{1}{2}\sqrt{3}-\frac{3}{4}, 2\sqrt{3}-3, 2-\sqrt{3}$	0.64801
0.2	9/3/o1	ACDFHI	$\frac{1}{4}, \frac{1}{2}\sqrt{3}-\frac{3}{4}, 2-\sqrt{3}, 2\sqrt{3}-3$	0.64801
0.3	9/3/t2	ABCDFH	$\frac{1}{4}, \frac{1}{4}\sqrt{2}-\frac{1}{4}, \sqrt{2}-1, \sqrt{2}-1$	0.61343
0.4	7/3/o1	ADFI	$0, 1-\frac{1}{2}\sqrt{3}; 2-\sqrt{3}, 4-2\sqrt{3}$	0.56119
0.5	6/4/c1	ABCDE	$\frac{1}{4}, 0; 1, 1$	0.52360
0.5'		ADFJK	$0, \frac{1}{4}, 1, 1$	
1.1	7/4/o1	ACDFH	$\frac{1}{4}, \frac{1}{24}\sqrt{13}-\frac{1}{24}, \frac{1}{3}(12-3\sqrt{13})^{1/2}, \frac{1}{6}\sqrt{13}-\frac{1}{6}$	0.60210
1.2	7/4/o1	BDFH	$\frac{1}{4}, \frac{1}{24}\sqrt{13}-\frac{1}{24}, \frac{1}{6}\sqrt{13}-\frac{1}{6}, \frac{1}{3}(12-3\sqrt{13})^{1/2}$	0.60210
1.3	7/3/t4	BDFG	$\frac{3}{4}-\frac{1}{4}\sqrt{6}, \frac{3}{4}-\frac{1}{4}\sqrt{6}; 1, \sqrt{3}-\sqrt{2}$	0.42315
1.4	6/4/o2	ADFI	0.06652, 0.12896; 0.26023, 0.51584	0.54992
1.5	6/3/t5	ABDF	$\frac{1}{8}, \frac{1}{8}, 1, \frac{1}{2}$	0.37024
1.6	5/4/t6	ABCD	$\frac{1}{4}, \frac{1}{16}, \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$	0.44179
1.7	5/4/h5	ADFJ	$0, \frac{1}{6}, \frac{1}{3}\sqrt{3}, \frac{2}{3}$	0.40307
2.1	5/4/t5	BDF	{0.15, 0.11602; 0.77348, 0.40933}	>0.37024
2.2	4/4/o2	ADF	0.08793, 0.14827; 0.79229, 0.59307	0.31354
2.2'		ABD		

Table 1 (continued)

Cmme 8m 0, y, z			$0 \leq y < \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$			
A	0, -y, -z		E	$\frac{1}{2}, -y, z$	G	0, -y, -z+1
B	$\frac{1}{2}, y, -z$			$-\frac{1}{2}, -y, z$	H	$\frac{1}{2}, y, -z+1$
	$-\frac{1}{2}, y, -z$		F	1, y, z		$-\frac{1}{2}, y, -z+1$
C	0, $-y+\frac{1}{2}, z$			-1, y, z	I	0, $-y-\frac{1}{2}, z$
D	0, y, z+1					
	0, y, z-1					
0.1	9/3/o1	ABCDGH		$\frac{1}{2}\sqrt{3}-\frac{3}{4}, \frac{1}{4}, 2\sqrt{3}-3, 2-\sqrt{3}$		0.64801
0.2	9/3/o1	BCEFH		$\frac{1}{2}\sqrt{3}-\frac{3}{4}, \frac{1}{4}, 2-\sqrt{3}, 2\sqrt{3}-3$		0.64801
0.3	9/3/t2	ABCEGH		$\frac{1}{4}\sqrt{2}-\frac{1}{4}, \frac{1}{4}, \sqrt{2}-1, \sqrt{2}-1$		0.61343
0.4	6/4/c1	ACEGI		$0, \frac{1}{4}, 1, 1$		0.52360
1.1	7/4/o1	ABCGH		$\frac{1}{24}\sqrt{13}-\frac{1}{24}, \frac{1}{6}, \frac{1}{6}\sqrt{13}-\frac{1}{6}, \frac{1}{3}(12-3\sqrt{13})^{1/2}$		0.60210
1.2	7/4/o1	BCEH		$\frac{1}{24}\sqrt{13}-\frac{1}{24}, \frac{1}{6}, \frac{1}{3}(12-3\sqrt{13})^{1/2}, \frac{1}{6}\sqrt{13}-\frac{1}{6}$		0.60210
1.3	6/4/c1	ABCD		$\frac{1}{8}, 0, \frac{1}{2}, \frac{1}{4}$		0.52360
1.4	5/4/t6	ACEG		$\frac{1}{16}, \frac{1}{4}, \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$		0.44179
Fmmm 16m 0, y, z			$0 < y \leq \frac{1}{4}, 0 < z \leq \frac{1}{4}, b \leq c$			
A	0, y, -z		D	$\frac{1}{2}, -y+\frac{1}{2}, z$	F	$\frac{1}{2}, y, -z+\frac{1}{2}$
B	0, -y, z			$-\frac{1}{2}, -y+\frac{1}{2}, z$		$-\frac{1}{2}, y, -z+\frac{1}{2}$
C	1, y, z		E	0, $-y+1, z$	G	0, $-y+\frac{1}{2}, -z+\frac{1}{2}$
	-1, y, z					
0.1	8/3/t5	ABCDF		$1-\frac{1}{2}\sqrt{3}, 1-\frac{1}{2}\sqrt{3}; 2-\sqrt{3}, 1$		0.60148
0.2	7/3/t7	ABDFG		$\frac{1}{2}-\frac{1}{4}\sqrt{2}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; \sqrt{2}-1, 1$		0.50819
0.3	6/4/c1	ABDEG		$\frac{1}{4}, \frac{1}{8}, 1, 2$		0.52360
1.1	6/4/t7	ABDF		{0.145, 0.145; 0.4, 1}		>0.50819
1.2	5/4/o9	ABDG		0.17812, 0.13055; 0.65186, 1.36432		0.42583
Immm 8l 0, y, z			$0 < y \leq \frac{1}{4}, 0 < z \leq \frac{1}{4}, b \leq c$			
A	0, y, -z		C	1, y, z	E	$\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$
B	0, -y, z			-1, y, z		$-\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$
			D	0, $-y+1, z$	F	0, y, $-z+1$
0.1	7/3/o1	ABCDE		$\frac{1}{4}, 1-\frac{1}{2}\sqrt{3}; \frac{1}{2}, 1+\frac{1}{2}\sqrt{3}$		0.56119
0.2	6/4/c1	ABDEF		$\frac{1}{4}, \frac{1}{4}, 1, 1$		0.52360
1.1	6/3/t7	ABCE		$\frac{2}{5}-\frac{1}{10}\sqrt{6}, \frac{2}{5}-\frac{1}{10}\sqrt{6}; \frac{4}{5}-\frac{1}{5}\sqrt{6}, 1$		0.40281
1.2	5/4/h5	ABDE		$\frac{1}{4}, \frac{1}{6}, \frac{1}{2}\sqrt{3}, \frac{3}{2}$		0.40307
2.1	4/4/t5	ABE		0.17431, 0.17431; 0.55025, 1		0.32252
Ibam 8j x, y, 0			$0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, a \leq b$			
A	-x, -y, 0		E	-x, y, $\frac{1}{2}$	H	x, y, 1
B	x, -y, $\frac{1}{2}$			-x, y, $-\frac{1}{2}$		x, y, -1
	x, -y, $-\frac{1}{2}$		F	-x+1, y, $\frac{1}{2}$	I	$x+\frac{1}{2}, -y+\frac{1}{2}, 0$
C	-x+1, -y, 0			-x+1, y, $-\frac{1}{2}$		$x-\frac{1}{2}, -y+\frac{1}{2}, 0$
D	$-x+\frac{1}{2}, y+\frac{1}{2}, 0$		G	x+1, y, 0	J	$-x+\frac{1}{2}, -y+\frac{1}{2}, \frac{1}{2}$
	$-x+\frac{1}{2}, y-\frac{1}{2}, 0$			x-1, y, 0	K	$-x+\frac{1}{2}, -y+\frac{1}{2}, -\frac{1}{2}$
						-x, -y+1, 0
0.1	12/3/c1	ABCEFIJ		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}, \frac{1}{2}$		0.74048
0.2	10/3/t1	ABCDIJ		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\sqrt{3}, \frac{1}{2}\sqrt{3}$		0.69813
0.3	10/3/t1	ACEFGI		$\frac{1}{4}, \frac{1}{8}, \frac{1}{6}\sqrt{3}, \frac{1}{2}$		0.69813
0.4	10/3/t1	BEFHJ		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}, \frac{1}{6}\sqrt{3}$		0.69813
1.1	8/3/t4	BEHJ		$\frac{1}{2}-\frac{1}{4}\sqrt{2}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1, \frac{2}{3}\sqrt{3}-\frac{1}{3}\sqrt{6}$		0.47912
1.2	8/4/c1	ABCIJ		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2}$		0.68017
1.3	8/4/c1	ACEFI		$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}\sqrt{2}, \frac{1}{2}$		0.68017
1.4	8/4/c1	BEFJ		$\frac{1}{4}, \frac{1}{8}, \frac{1}{2}, \frac{1}{4}\sqrt{2}$		0.68017
1.5	7/3/o1	AEGI		0, $1-\frac{1}{2}\sqrt{3}; 2-\sqrt{3}, 4-2\sqrt{3}$		0.56119
1.6	7/3/o13	AEIJ		0.14855, 0.16950; 0.74185, 0.67802		0.55058
1.6'		ABDJ				
1.7	7/3/t6	ABEJ		$\frac{1}{2}-\frac{1}{4}\sqrt{2}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1, 2-\sqrt{2}$		0.50819
1.8	7/3/t8	ADIJ		$\frac{1}{4}\sqrt{3}-\frac{1}{4}, \frac{1}{4}\sqrt{3}-\frac{1}{4}, 1, (4\sqrt{3}-6)^{1/2}$		0.60304
1.9	6/4/c1	ABCD		$\frac{1}{4}, 0, 1, 1$		0.52360
1.9'		AEIK		0, $\frac{1}{4}, 1, 1$		
2.1	6/4/t6	BEJ		$\frac{1}{2}-\frac{1}{4}\sqrt{2}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1, \sqrt{2}-1$		0.46680
2.2	6/4/c1	DIJ		$\frac{1}{4}, \frac{1}{4}, 1, 1$		0.52360
2.3	5/4/o10	AEJ		0.14555, 0.15165; 0.97034, 0.60660		0.50664
2.3'		ABJ				
2.4	5/4/o11	AIJ		0.14882, 0.16949, 0.74248, 0.67895		0.55058
2.4'		ADJ				

Table 1 (continued)

2.5	5/4/h5	AEI	$0, \frac{1}{6}, \frac{1}{3}\sqrt{3}, \frac{2}{3}$	0.40307
2.5'		ABD		
n3.1	$t[6^3]^2$	AJ	$\frac{3}{20}, \frac{3}{20}, 1, \frac{1}{5}\sqrt{10}$	0.50579
Imma 8h 0, y, z				
A	0, -y, -z		$0 \leq y < \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$	
B	1, y, z		D	0, y, z+1
	-1, y, z		E	0, y, z-1
C	0, -y+ $\frac{1}{2}$, z			$\frac{1}{2}, y, -z+\frac{1}{2}$
0.1	8/3/h4	ABCEF		$-\frac{1}{2}, y, -z+\frac{1}{2}$
0.2	8/3/h4	ACDEF		0, -y, -z
0.3	7/3/o1	ABCEG		0, -y, -z+1
0.4	7/3/o1	ACDEH		0, -y, -z-1
0.5	6/4/c1	ACEGH		0, -y, -z+1
1.1	6/3/o3	ABCE		
1.2	6/4/o1	ACDE		
1.3	6/4/c1	ACEF		
1.4	5/4/h5	ACEG		
1.5	5/4/h5	ACEH		
2.1	4/4/o1	ACE		

their distances from the original point are necessarily equal 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-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* is 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 with contact to the original sphere. If the parameter region of the regarded type disintegrates into two or more disconnected parts, then each part refers to another string of capital letters. A modification of the symbols in the first column of Table 1 indicates such disconnected parameter regions: a transformation by a symmetry operation from the space group is symbolized by parentheses, a transformation by an operation from the Euclidean or affine normalizer 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 two coordinate parameters *x*, *y* or *z* and of *a/b* and *c/b*, the fifth column the value of ρ_{mv} , the minimal density. Some types of sphere packings do not include an arrangement with minimal density. In such a case, parameters for any other sphere packing of that type are tabulated in braces.

3. Discussion

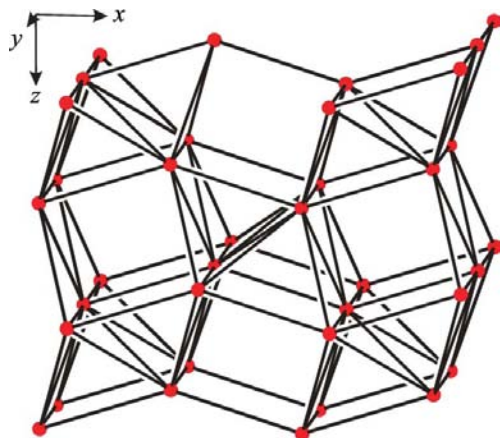
In total, the orthorhombic bivalent lattice complexes give rise to sphere packings of 90 different types. For only 47 of them,

the maximal inherent symmetry is orthorhombic. Owing to limiting-complex relationships,² all other types comprehend at least one sphere packing with tetragonal (31 types), hexagonal (7) or cubic (5) symmetry as indicated by the letter *t*, *h* or *c* in the symbol.

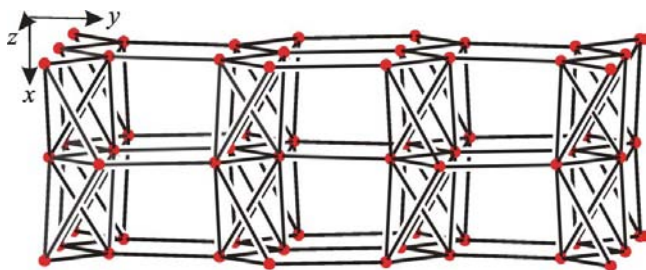
16 of the 47 orthorhombic types have already been listed in the first paper of this series (*cf.* Fischer *et al.*, 2006), whereas sphere packings of the other 31 types occur with highest symmetry in one of the orthorhombic bivalent lattice complexes. These are two types with contact number 4 (4/4/o1, 4/4/o2), seven types with contact number 5 (5/4/o1, 5/4/o6 to 5/4/o11), four types with contact number 6 (6/3/o2, 6/3/o3, 6/4/o1, 6/4/o2), nine types with contact number 7 (7/3/o2, 7/3/o3, 7/3/o7 to 7/3/o13), two types with contact number 8 (8/3/o2, 8/3/o5), three types with contact number 9 (9/3/o3 to 9/3/o5), two types with contact number 10 (10/3/o5, 10/3/o6) and two types with contact number 11 (11/3/o1, 11/3/o2). Type 8/3/o2 with symmetry *Cmcm 8f* has already been mentioned by Sowa (2001), types 5/4/o1, 7/3/o2, 7/3/o3 and 8/3/o2 with symmetry *Cmcm 8g* by Sowa & Koch (2001). Sphere packings of types 11/3/o1 and 11/3/o2 can be described as stacking of triangular nets of spheres (case 5 and case 3, respectively, in Table 9.1.1.2 of *International Tables for Crystallography*, 1999, Vol. C), those of type 10/3/o5 as stacking of square nets (case 14).

The **feb** net from the Reticular Chemistry Structure Resource (RCSR) data base (*cf.* <http://rcsr.anu.edu.au>) corresponds to the sphere-packing type 10/3/o6. The arrangement of the Fe atoms in FeB (Kapfenberger *et al.*, 2006) is closely related to such a sphere packing. Type 10/3/o6 is remarkable because its sphere packings cannot be subdivided into plane nets of spheres (*cf.* Fig. 1). Only three other such types with contact number 10 or higher are known so far,

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


Figure 1

Sphere packing of type $10/3/o6$ ($Pnma$ 4c): the triangular nets 3^6 perpendicular to **a**, the square nets 4^4 perpendicular to **c** and the $3^2 4^3$ nets perpendicular to **b** are necessarily corrugated.


Figure 2

Sphere packing of type $7/3/o9$ ($Cmce$ 8f) with flat honeycomb nets 6^3 perpendicular to **a**.

namely $11/3/t1$ (case 8), the famous rutile arrangement, $10/3/t2$ (case 19) and $10/3/h5$ (Sowa & Koch, 2004).

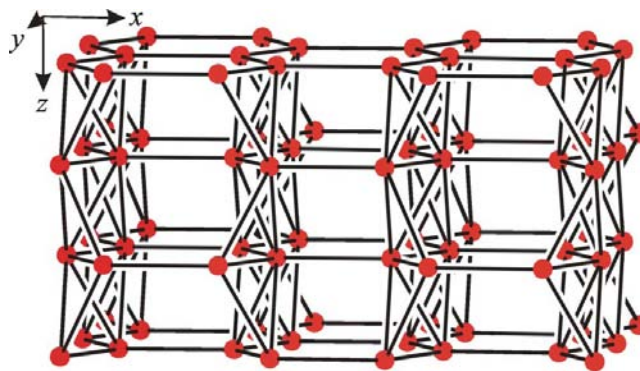
Orthorhombic lattice complexes with two degrees of freedom are incompatible with interpenetrating sphere packings, but $Ibam$ 8j enables two sets of interpenetrating 6^3 nets $t[6^3]^2$ (cf. Koch *et al.*, 2006).

4. Examples of crystal structures

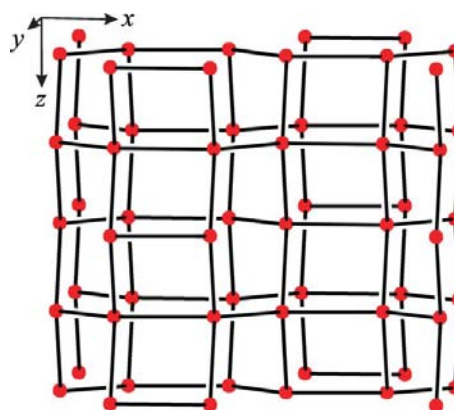
The following examples show four arbitrarily chosen examples of crystal structures with the property that some of the atoms are arranged similar to a sphere packing of one of the 31 orthorhombic types mentioned above.

(i) The O atoms in the crystal structure of $\text{KNa}_2(\text{AuO}_2)$ with symmetry $Pnmm$ (Wagner & Hoppe, 1986) form nearly a sphere packing of type $8/3/o1$ (cf. Fig. 3 of Fischer *et al.*, 2006). The Au atoms are roughly located at the middle of some of the O–O bonds, whereas the Na and the K atoms lie near the centres of some triangles or quadrangles of O atoms, respectively.

(ii) Under ambient conditions, Ga metal (cf. Sharma & Donohue, 1962) shows symmetry $Cmce$ and its atomic arrangement corresponds in good approximation to a sphere packing of type $7/3/o9$. Fig. 2 shows the minimal-density configuration of such a sphere packing.


Figure 3

Sphere packing of type $7/3/o3$ ($Cmcm$ 8g) with flat honeycomb nets 6^3 perpendicular to **c**.


Figure 4

Sphere packing of type $4/4/o1$ ($Imma$ 8j).

(iii) The Si atoms in the crystal structure of $\text{Si}_2\text{N}_2(\text{NH})$ (cf. Peters & Jacobs, 1989) occupy Wyckoff position $8b$ of space group $Cmcm$ 8g. The Si atoms form a slightly distorted sphere packing of type $7/3/o3$ (cf. Fig. 3).

(iv) BaZn_2 (Bruzzone *et al.*, 1985) with symmetry $Imma$ crystallizes together with a large number of other compounds in the SrAl_2 structure type. The arrangement of the Zn atoms corresponds to a sphere packing of type $4/4/o1$ (cf. Fig. 4) that has already been described as ‘ SrAl_2 net’ by O’Keeffe & Hyde (1996). The Ba atoms occupy large voids with 12 Zn neighbours.

This work was supported by the Deutsche Forschungsgemeinschaft under KO 1139/1-1,3.

References

- Bohm, J. & Dornberger-Schiff, K. (1967). *Acta Cryst.* **23**, 913–933.
 Bruzzone, G., Ferretti, M. & Merlo, F. (1985). *J. Less-Common Met.* **114**, 305–310.
 Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *Z. Kristallogr. Suppl.* Issue 1.
 Fischer, W. (1971). *Z. Kristallogr.* **133**, 18–42.
 Fischer, W., Sowa, H. & Koch, E. (2006). *Acta Cryst.* **A62**, 413–418.

- International Tables for Crystallography* (1999). Vol. C, 2nd ed., edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.
- Kapfenberger, Ch., Albert, B., Pöttgen, R. & Huppertz, H. (2006). *Z. Kristallogr.* **21**, 477–481.
- Koch, E. & Fischer, W. (1978). *Z. Kristallogr.* **148**, 107–152.
- Koch, E., Fischer, W. & Sowa, H. (2006). *Acta Cryst.* **A62**, 152–167.
- O’Keeffe, M. & Hyde, B. G. (1996). *Crystal Structures. I. Patterns and Symmetry*. Mineralogical Society of America.
- Peters, D. & Jacobs, H. (1989). *J. Less-Common Met.* **146**, 241–249.
- Sharma, B. D. & Donohue, J. (1962). *Z. Kristallogr.* **117**, 293–300.
- Sowa, H. (2001). *Acta Cryst.* **A57**, 176–182.
- Sowa, H. & Koch, E. (2001). *Acta Cryst.* **A57**, 406–413.
- Sowa, H. & Koch, E. (2004). *Acta Cryst.* **A60**, 158–166.
- Sowa, H. & Koch, E. (2005). *Acta Cryst.* **A61**, 331–342.
- Sowa, H. & Koch, E. (2006). *Acta Cryst.* **A62**, 379–399.
- Sowa, H., Koch, E. & Fischer, W. (2003). *Acta Cryst.* **A59**, 317–326.
- Wagner, G. & Hoppe, R. (1986). *Z. Anorg. Allg. Chem.* **537**, 115–122.