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Hexagonal and trigonal sphere packings. II. Bivariant lattice complexes

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All homogeneous sphere packings were derived which correspond to point configurations of the 26 bivariant lattice complexes belonging to the hexagonal crystal family. They may be assigned to 109 sphere-packing types. Among these, there is a type of sphere packing with contact number 10 that was not described before. For seven of the 109 types, the inherent symmetry of the sphere packings with minimal density is cubic. In addition, three types of interpenetrating sphere packings were found and one type of interpenetrating 6^3 sphere layers. Such an arrangement was unknown so far. Some frequently occurring structure types that can be related to sphere packings are described as examples.

1. Introduction

In a recent paper, all types of sphere packings and of interpenetrating sphere packings have been tabulated that correspond to point configurations of the invariant and univariant lattice complexes belonging to the hexagonal crystal family (Sowa *et al.*, 2003).[1] In the meantime, these investigations were extended to the 26 bivariant lattice complexes of the hexagonal crystal family. $R\bar{3}m$ 18*h* is the only one of these lattice complexes that has been investigated before (*cf.* Sowa & Koch, 1999).

All definitions and all information necessary for the derivation of sphere packings and interpenetrating sphere packings can be taken from the previous paper. In addition, all those sphere configurations were derived that disintegrate into layer-like partial configurations that interpenetrate each other. Such sphere configurations have been named *interpenetrating sphere layers* (Fischer & Koch, 1990).

2. Results

Relevant data on all types of sphere packings and of interpenetrating sphere packings and layers that correspond to the 26 bivariant lattice complexes of the hexagonal crystal family are summarized in Table 1:

(i) Each lattice complex is identified by its characteristic Wyckoff position, the respective site symmetry and a coordinate triplet of a reference point. The range of the coordinate parameters that was investigated complements this information. It is sufficient to consider one asymmetric unit of the Euclidean normalizer of the characteristic space group of the corresponding lattice complex (*cf. e.g.* Koch & Fischer, 2002).

(ii) All possible neighbouring points are listed in a second block of information. Two or more neighbouring points may be equidistant for symmetry reasons and form a set, irrespective of the choice of the free coordinate or metrical parameters. Each such (set of) neighbouring point(s) is designated by a capital letter.

(iii) The third block of information lists the corresponding types of sphere packings or of interpenetrating sphere packings or layers together with their parameter regions: a zero-, one- or two-dimensional parameter range for a sphere-packing type is designated in the first column by 0.*j*, 1.*j* or 2.*j*, respectively, with *j* being a serial number. In case of interpenetrating sphere packings or layers, these symbols are replaced by *i*1.*j*, *i*2.*j* or *n*2.*j*, respectively.

The type of sphere packing or of interpenetrating sphere packing or layer is identified in the second column. Each sphere-packing type is designated by a symbol *k*/*m*/*fn*, as was first introduced by Fischer (1971): *k* is the number of contacts per sphere, *m* is the length of the shortest mesh within the sphere packing, *f* indicates the highest crystal family for a sphere packing of that type (*c*: cubic, *h*: hexagonal) and *n* is an arbitrary number. Symbols for types of interpenetrating sphere packings have the form $f_1[k/m/fn]^l$. Here, *k*/*m*/*fn* describes the type of the sphere packings that interpenetrate each other, *l* is the number of interpenetrating sphere packings (two within the present paper) and f_1 indicates the highest crystal family for the type of interpenetrating sphere packing. *f* and f_1 may differ in principle. Interpenetrating sphere layers are identified by similar symbols: the symbol of the sphere-packing type, however, is replaced by one of the usual symbols for the Shubnikov nets (Shubnikov, 1916) and *l* means the number of sets of parallel sphere layers. A string of capital letters in the third column describes all neighbouring points

[1] The cited paper contains two errors: (i) interpenetrating sphere packings of type $h[4/3/h1]^2$ are found in lattice complex $R\bar{3}c$ 18*e*, not in $R\bar{3}m$ 18*e* (p. 321); (ii) the oxygen atoms of $Re_{1.16}O_3$ form a hexagonal closest packing of type 12/3/*h*1, not a cubic one (p. 325).

Table 1
The sphere packings, interpenetrating sphere packings and interpenetrating sphere layers corresponding to the 26 bivariant hexagonal lattice complexes.

***$P3_2$* 3*a* 1**		***x*, *y*, *z***	$\mathbf{0 \le x \le \frac{1}{3}; 0 \le y \le \frac{1}{2}x; z = 0}$			
A	$-x+y, -x, \frac{1}{3}+z$	$-y, x-y, -\frac{1}{3}+z$		*E*	$1+x, y, z$	$-1+x, y, z$
B	$x, y, 1+z$	$x, y, -1+z$			$x, 1+y, z$	$x, -1+y, z$
C	$1-x+y, 1-x, \frac{1}{3}+z$	$1-y, x-y, -\frac{1}{3}+z$			$1+x, 1+y, z$	$-1+x, -1+y, z$
D	$1-x+y, -x, \frac{1}{3}+z$	$-y, -1+x-y, -\frac{1}{3}+z$				
0.1	8/4/*c*1	*ABCD*	$\frac{1}{3}, 0; \frac{1}{4}\sqrt{6}$		0.68017	
0.2	12/3/*c*1	*ACDE*	$\frac{1}{3}, 0; \sqrt{6}$		0.74048	
1.1	6/4/*h*3	*ABC*	$\frac{1}{3}, \frac{1}{6}; \frac{3}{8}\sqrt{2}$		0.51013	$\frac{3}{8}\sqrt{2} \le c < \frac{1}{4}\sqrt{6}$
1.2	6/4/*c*1	*ACD*	$\frac{1}{3}, 0; \frac{1}{2}\sqrt{6}$		0.52360	$\frac{1}{4}\sqrt{6} < c < \sqrt{6}$
1.3	10/3/*h*3	*ACE*	$\frac{1}{3}, \frac{1}{6}; \frac{3}{2}\sqrt{3}$		0.69813	$\sqrt{6} < c \le \frac{3}{2}\sqrt{3}$
2.1	4/6/*h*1	*AC*	$\frac{1}{3}, \frac{1}{6}; \frac{3}{4}\sqrt{2}$		0.39270	$\frac{3}{8}\sqrt{2} < c \le \frac{3}{2}\sqrt{3}$
2.2	8/3/*h*4	*AE*	$0, 0; 3$		0.60460	$\sqrt{6} < c \le 3$
***R*3 9*b* 1**		***x*, *y*, *z***	$\mathbf{0 < x \le \frac{1}{3}; 0 \le y \le \frac{1}{2}x; z = 0}$			
A	$-x+y, -x, z$	$-y, x-y, z$		*D*	$1-x+y, 1-x, z$	$1-y, x-y, z$
B	$x, y, 1+z$	$x, y, -1+z$		*E*	$\frac{1}{3}-x+y, \frac{2}{3}-x, -\frac{1}{3}+z$	$\frac{2}{3}-y, \frac{1}{3}+x-y, \frac{1}{3}+z$
C	$\frac{2}{3}-x+y, \frac{1}{3}-x, \frac{1}{3}+z$	$\frac{1}{3}-y, -\frac{1}{3}+x-y, -\frac{1}{3}+z$		*F*	$1-x+y, -x, z$	$-y, -1+x-y, z$
0.1	8/3/*h*7	*ABCE*	$3-\frac{1}{3}\sqrt{69}, \frac{3}{2}-\frac{1}{6}\sqrt{69}; \frac{9}{2}-\frac{1}{2}\sqrt{69}$		0.65402	
0.2	8/3/*c*2	*ACDE*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{2}\sqrt{6}$		0.55536	
0.3	8/3/*h*4	*ACDF*	$\frac{1}{3}, 0; \sqrt{3}$		0.60460	
1.1	6/4/*h*7	*ABC*	$3-2\sqrt{2}, 0; 3\sqrt{3}-2\sqrt{6}$		0.48054	$3\sqrt{3}-2\sqrt{6} \le c < \frac{9}{2}-\frac{1}{2}\sqrt{69}$
1.2	6/4/*h*1	*BCE*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{8}\sqrt{6}$		0.51013	$\frac{1}{8}\sqrt{6} \le c < \frac{9}{2}-\frac{1}{2}\sqrt{69}$
1.3	6/3/*h*14	*ACE*	$\frac{4}{15}, \frac{2}{15}; \frac{1}{5}\sqrt{15}$		0.44959	$\frac{9}{2}-\frac{1}{2}\sqrt{69} < c < \frac{1}{2}\sqrt{6}$
1.4	6/3/*h*18	*ACD*	$\frac{1}{3}, \frac{4}{15}-\frac{1}{15}\sqrt{6}; \frac{1}{5}(15+15\sqrt{6})^{1/2}$		0.50729	$\frac{1}{2}\sqrt{6} < c < \sqrt{3}$
2.1	4/3/*h*1	*AC*	$\frac{1}{5}, 0; \frac{1}{5}\sqrt{15}$		0.29202	$3\sqrt{3}-2\sqrt{6} < c < \sqrt{3}$
2.2	4/6/*c*2	*CE*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{4}\sqrt{6}$		0.39270	$\frac{1}{8}\sqrt{6} < c < \frac{1}{2}\sqrt{6}$
***R*3*m* 18*c* 1**		***x*, *y*, *z***	$\mathbf{0 < x \le \frac{1}{3}; 0 \le y < \frac{1}{2}x; z = 0}$			
A	$x, x-y, z$			*D*	$-y, -x, z$	
B	$x, y, 1+z$	$x, y, -1+z$		*E*	$1-x+y, y, z$	
C	$\frac{2}{3}-x+y, \frac{1}{3}-x, \frac{1}{3}+z$	$\frac{1}{3}-y, -\frac{1}{3}+x-y, -\frac{1}{3}+z$				
0.1	6/4/*h*9	*ABCD*	$\frac{9}{19}-\frac{2}{19}\sqrt{6}, 0; \frac{9}{19}-\frac{2}{19}\sqrt{6}$		0.50701	
0.2	5/4/*h*5	*ACDE*	$\frac{1}{3}, 0; 1$		0.40307	
1.1	5/4/*h*14	*ABC*	$\frac{1}{3}, \frac{16}{15}-\frac{2}{5}\sqrt{6}; \frac{4}{5}\sqrt{6}-\frac{9}{5}$		0.27718	$\frac{4}{5}\sqrt{6}-\frac{9}{5} \le c < \frac{9}{19}-\frac{2}{19}\sqrt{6}$
1.2	4/4/*c*1	*ACD*	$\frac{1}{4}, 0; \frac{1}{4}\sqrt{6}$		0.27768	$\frac{9}{19}-\frac{2}{19}\sqrt{6} < c < 1$
2.1	3/8/*h*1	*AC*	$\frac{1}{3}, \frac{19}{24}-\frac{1}{8}\sqrt{33}; \frac{9}{8}-\frac{1}{8}\sqrt{33}$		0.17248	$\frac{4}{5}\sqrt{6}-\frac{9}{5} < c < 1$
***R*3*c* 18*b* 1**		***x*, *y*, *z***	$\mathbf{0 < x \le \frac{1}{3}; 0 \le y \le \frac{1}{2}x; z = 0}$			
A	$-x+y, -x, z$	$-y, x-y, z$		*F*	$\frac{1}{3}-x+y, -\frac{1}{3}+y, \frac{1}{6}+z$	$\frac{2}{3}-x+y, \frac{1}{3}+y, -\frac{1}{6}+z$
B	$x, x-y, \frac{1}{2}+z$	$x, x-y, -\frac{1}{2}+z$		*G*	$\frac{1}{3}-y, \frac{2}{3}-x, \frac{1}{6}+z$	$\frac{2}{3}-y, \frac{1}{3}-x, -\frac{1}{6}+z$
C	$-y, -x, \frac{1}{2}+z$	$-y, -x, -\frac{1}{2}+z$		*H*	$\frac{1}{3}+x, -\frac{1}{3}+x-y, \frac{1}{6}+z$	$-\frac{1}{3}+x, -\frac{2}{3}+x-y, -\frac{1}{6}+z$
D	$x, y, 1+z$	$x, y, -1+z$		*I*	$1-x+y, 1-x, z$	$1-y, x-y, z$
E	$\frac{2}{3}-x+y, \frac{1}{3}-x, \frac{1}{3}+z$	$\frac{1}{3}-y, -\frac{1}{3}+x-y, -\frac{1}{3}+z$		*J*	$1-x+y, -x, z$	$-y, -1+x-y, z$
0.1	8/3/*h*8	*BCDE*	$\frac{27}{49}-\frac{12}{49}\sqrt{2}, 0; \frac{18}{49}\sqrt{3}-\frac{8}{49}\sqrt{6}$		0.60791	
0.2	8/3/*h*9	*ABCE*	$\frac{9}{8}-\frac{1}{8}\sqrt{57}, 0; \frac{9}{4}\sqrt{2}-\frac{1}{4}\sqrt{114}$		0.65695	
0.3	8/3/*h*2	*BEFG*	$\frac{1}{3}, \frac{1}{14}\sqrt{57}-\frac{17}{42}; \frac{1}{7}(54\sqrt{57}-390)^{1/2}$		0.52528	
0.4	8/3/*h*12	*ABEF*	$\frac{5}{24}, \frac{1}{24}; \frac{1}{4}\sqrt{6}$		0.64284	
0.5	8/3/*h*7	*ABFG*	$3-\frac{1}{3}\sqrt{69}, \frac{3}{2}-\frac{1}{6}\sqrt{69}; 9-\sqrt{69}$		0.65402	
0.6	8/3/*h*3	*EFGH*	$\frac{1}{3}, 0; \frac{2}{3}\sqrt{3}$		0.53742	
0.7	12/3/*h*1	*AFGHIJ*	$\frac{1}{3}, 0; 2\sqrt{2}$		0.74048	
1.1	6/3/*h*15	*BDE*	$\frac{1}{3}, \frac{64}{141}-\frac{12}{47}\sqrt{2}; \frac{16}{47}\sqrt{6}-\frac{18}{47}\sqrt{3}$		0.31648	$\frac{16}{47}\sqrt{6}-\frac{18}{47}\sqrt{3} \le c < \frac{18}{49}\sqrt{3}-\frac{8}{49}\sqrt{6}$
1.2	6/4/*h*8	*BCE*	0.19854, 0; 0.32962		0.56721	$\frac{18}{49}\sqrt{3}-\frac{8}{49}\sqrt{6} < c < \frac{9}{4}\sqrt{2}-\frac{1}{4}\sqrt{114}$
1.3	6/3/*h*23	*ABE*	0.19810, 0.02599; 0.57605		0.63644	$\frac{9}{4}\sqrt{2}-\frac{1}{4}\sqrt{114} < c < \frac{1}{4}\sqrt{6}$
1.4	6/3/*h*24	*BEF*	0.31333, 0.12281; 0.59534		0.52006	$6\sqrt{3}-4\sqrt{6} \le c < \frac{1}{4}\sqrt{6}$
1.5	6/4/*h*1	*BFG*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{4}\sqrt{6}$		0.51013	$\frac{1}{7}(54\sqrt{57}-390)^{1/2} < c < 9-\sqrt{69}$
1.6	6/3/*h*16	*EFG*	$\frac{1}{3}$, 0.08820; 0.89096		0.45502	$\frac{1}{7}(54\sqrt{57}-390)^{1/2} < c < \frac{2}{3}\sqrt{3}$
1.7	6/3/*h*19	*AEF*	$\frac{3}{4}-\frac{1}{4}\sqrt{5}, 0; \frac{3}{2}\sqrt{3}-\frac{1}{2}\sqrt{15}$		0.59542	$\frac{1}{4}\sqrt{6} < c \le \frac{3}{2}\sqrt{3}-\frac{1}{2}\sqrt{15}$
1.8	6/3/*h*25	*ABF*	0.21983, 0.07254; 0.65523		0.63022	$\frac{1}{4}\sqrt{6} < c < 9-\sqrt{69}$
1.9	6/3/*h*14	*AFG*	$\frac{4}{15}, \frac{2}{15}; \frac{2}{5}\sqrt{15}$		0.44959	$9-\sqrt{69} < c < \sqrt{6}$
1.10	6/4/*h*2	*FGH*	$\frac{1}{3}, 0; \sqrt{2}$		0.52360	$\frac{2}{3}\sqrt{3} < c < 2\sqrt{2}$
1.11	8/3/*c*2	*AFGI*	$\frac{1}{3}, \frac{1}{6}; \sqrt{6}$		0.55536	$\sqrt{6} \le c < 2\sqrt{2}$

2.1	4/5/*h*1	*BE*	$\frac{1}{3}$, 0.09720; 0.25508		0.28622	$\frac{16}{47}\sqrt{6}-\frac{18}{47}\sqrt{3} < c < \frac{1}{4}\sqrt{6}$
2.2	4/5/*h*2	*EF*	0.26212, 0; 0.90800		0.41845	$6\sqrt{3}-4\sqrt{6} < c < \frac{2}{3}\sqrt{3}$
2.3	4/6/*h*7	*BF*	{0.235, 0.08896; 0.65116}		>0.51013	$6\sqrt{3}-4\sqrt{6} < c < 9-\sqrt{69}$
2.4	4/6/*c*2	*FG*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{2}\sqrt{6}$		0.39270	$\frac{1}{7}(54\sqrt{57}-390)^{1/2} < c < 2\sqrt{2}$
2.5	4/3/*h*2	*AF*	$\frac{5}{4}-\frac{1}{4}\sqrt{17}, 0; \frac{1}{2}(18\sqrt{17}-66)^{1/2}$		0.41571	$\frac{1}{4}\sqrt{6} < c < 2\sqrt{2}$
*i*2.1	$h[4/3/h1]^2$	*AE*	{0.18667, 0; 0.6}		>0.59542	$\frac{9}{4}\sqrt{2}-\frac{1}{4}\sqrt{114} < c < \frac{3}{2}\sqrt{3}-\frac{1}{2}\sqrt{15}$
P*$\bar{3}$1*m* 6*k* ..*m		***x*, 0, *z***	$\mathbf{0 < x \le \frac{1}{2}; 0 \le z \le \frac{1}{4}}$			
A	*x*, *x*, −*z*	0, −*x*, − *z*		*E*	*x*, *x*, 1−*z*	0, −*x*, 1− *z*
B	*x*, 0, 1+*z*	*x*, 0, −1+*z*		*F*	1−*x*, 0, 1−*z*	
C	1−*x*, 0, −*z*			*G*	1, *x*, *z*	1−*x*, 1−*x*, *z*
D	0, *x*, *z*	−*x*, −*x*, *z*			0, −1+*x*, *z*	1−*x*, −*x*, *z*
0.1	8/3/*h*3	*ABCEF*	$\frac{1}{3}, \frac{1}{4}; \frac{2}{9}\sqrt{3}$		0.53742	
0.2	12/3/*h*1	*ACDEFG*	$\frac{1}{3}, \frac{1}{4}; \frac{2}{3}\sqrt{2}$		0.74048	
1.1	5/4/*h*5	*ABC*	$\frac{1}{3}, 0; \frac{1}{3}$		0.40307	$\frac{1}{3} \le c < \frac{2}{9}\sqrt{3}$
1.2	6/4/*h*2	*ACEF*	$\frac{1}{3}, \frac{1}{4}; \frac{1}{3}\sqrt{2}$		0.52360	$\frac{2}{9}\sqrt{3} < c < \frac{2}{3}\sqrt{2}$
1.3	6/3/*h*13	*CFG*	$\frac{1}{2}, \frac{1}{4}; 1$		0.45345	$\frac{2}{3}\sqrt{2} < c \le 1$
***P*$\bar{3}$*m*1 6*i* .*m*.**		***x*, −*x*, *z***	$\mathbf{0 < x < \frac{1}{3}; \frac{1}{3} < x \le \frac{1}{2}; 0 \le z \le \frac{1}{4}}$			
A	2*x*, *x*, −*z*	−*x*, −2*x*, −*z*		*E*	1−2*x*, −*x*, *z*	*x*, −1+2*x*, *z*
B	−2*x*, −*x*, *z*	*x*, 2*x*, *z*		*F*	1−*x*, −1+*x*, −*z*	
C	2*x*, *x*, 1−*z*	−*x*, −2*x*, 1−*z*		*G*	1−*x*, −1+*x*, 1−*z*	
D	*x*, −*x*, 1+*z*	*x*, −*x*, −1+*z*		*H*	2−2*x*, −*x*, *z*	*x*, −2+2*x*, *z*
0.1	6/3/*h*21	*DEFG*	$\frac{3}{7}, \frac{1}{4}; \frac{2}{7}$		0.29613	
0.2	8/3/*h*11	*ACDE*	$\frac{1}{5}, \frac{1}{4}; \frac{2}{5}$		0.58042	
0.3	8/3/*h*10	*ABCE*	$\frac{1}{6}, \frac{1}{4}; \frac{1}{3}\sqrt{6}$		0.55536	
0.4	6/3/*h*13	*EFGH*	$\frac{1}{2}, \frac{1}{4}; 1$		0.45345	
1.1	5/3/*h*5	*DEF*	$1-\frac{1}{3}\sqrt{3}, 0; 2-\sqrt{3}$		0.26045	$2-\sqrt{3} \le c < \frac{2}{7}$
1.2	6/3/*h*20	*ADE*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}, 0; \frac{1}{2}\sqrt{3}-\frac{1}{2}$		0.48601	$\frac{1}{2}\sqrt{3}-\frac{1}{2} \le c < \frac{2}{5}$
1.3	4/3/*h*3	*EFG*	$\frac{7}{6}-\frac{1}{6}\sqrt{19}, \frac{1}{4}; \frac{1}{3}(6\sqrt{19}-24)^{1/2}$		0.24427	$\frac{2}{7} < c < 1$
1.4	6/3/*h*22	*ACE*	$\frac{13}{24}-\frac{1}{24}\sqrt{73}, \frac{1}{4}; \frac{1}{6}(39-3\sqrt{73})^{1/2}$		0.51755	$\frac{2}{5} < c < \frac{1}{3}\sqrt{6}$
R*$\bar{3}$*m* 18*h* .*m		***x*, −*x*, *z***	$\mathbf{0 < x \le \frac{1}{6}; 0 \le z < \frac{1}{2}}$			
A	−2*x*, −*x*, *z*	*x*, 2*x*, *z*		*E*	$\frac{1}{3}-x, -\frac{1}{3}+x, \frac{2}{3}-z$	
B	2*x*, *x*, −*z*	−*x*, −2*x*, −*z*		*F*	$\frac{1}{3}-x, -\frac{1}{3}+x, -\frac{1}{3}-z$	
C	2*x*, *x*, 1−*z*	−*x*, −2*x*, 1−*z*		*G*	$-\frac{1}{3}+2x, -\frac{2}{3}+x, \frac{1}{3}-z$	$\frac{2}{3}-x, \frac{1}{3}-2x, \frac{1}{3}-z$
D	*x*, −*x*, 1+*z*	*x*, −*x*, −1+*z*		*H*	1−2*x*, −*x*, *z*	*x*, −1+2*x*, *z*
0.1	6/3/*h*1	*BDEF*	$\frac{70}{339}-\frac{1}{113}\sqrt{105}, \frac{1}{12}; \frac{4}{113}\sqrt{105}-\frac{18}{113}$		0.45038	
0.2	7/3/*h*1	*BCDE*	$\frac{18}{73}-\frac{1}{73}\sqrt{105}, \frac{1}{4}; \frac{36}{73}-\frac{2}{73}\sqrt{105}$		0.49102	
0.3	7/3/*h*2	*ABCE*	$\frac{1}{11}, \frac{1}{4}; \frac{2}{11}\sqrt{6}$		0.49569	
0.4	6/4/*h*1	*BEFG*	$\frac{1}{6}, \frac{1}{12}; \frac{1}{4}\sqrt{6}$		0.51013	
0.5	7/3/*h*3	*ABEG*	0.12209, 0.15794; 0.94675		0.56478	
0.6	8/3/*c*2	*ABGH*	$\frac{1}{6}, \frac{1}{12}; \sqrt{6}$		0.55536	
0.7	7/3/*h*4	*AEGH*	$\frac{1}{6}, \frac{1}{6}\sqrt{6}-\frac{1}{6}; \frac{3}{2}+\frac{1}{2}\sqrt{6}$		0.49926	
(0.7)		*ACEH*	$\frac{1}{6}, \frac{5}{6}-\frac{1}{6}\sqrt{6}$			
1.1	5/4/*h*1	*CDE*	0.11180, 0.44375; 0.19488		0.41330	$0.19488 \le c < \frac{36}{73}-\frac{2}{73}\sqrt{105}$
1.1′		*BDF*				
1.2	5/4/*h*2	*BDE*	0.11388, 0.11679; 0.20286		0.44786	$0.20286 \le c < \frac{36}{73}-\frac{2}{73}\sqrt{105}$
1.3	4/6/*h*4	*BEF*	$0.12762, \frac{1}{12}; 0.37082$		0.35482	$\frac{4}{113}\sqrt{105}-\frac{18}{113} < c < \frac{1}{4}\sqrt{6}$
1.4	5/4/*h*3	*BCE*	$0.10084, \frac{1}{4}; 0.31100$		0.44750	$\frac{36}{73}-\frac{2}{73}\sqrt{105} < c < \frac{2}{11}\sqrt{6}$
1.5	5/3/*c*3	*ACE*	$\frac{1}{3}-\frac{1}{6}\sqrt{2}, \frac{1}{6}+\frac{1}{6}\sqrt{2}; \frac{1}{2}\sqrt{6}$		0.22327	$\frac{2}{11}\sqrt{6} < c < \frac{3}{2}+\frac{1}{2}\sqrt{6}$
1.6	5/4/*h*4	*BEG*	0.15403, 0.11849; 0.73426		0.47896	$\frac{1}{4}\sqrt{6} < c < 0.94675$
1.7	6/3/*h*2	*ABG*	0.13263, 0.10444; 1.55532		0.44076	$0.94675 < c < \sqrt{6}$
1.8	5/3/*h*1	*AEG*	0.13343, 0.22397; 1.75278		0.39824	$0.94675 < c < \frac{3}{2}+\frac{1}{2}\sqrt{6}$
*i*1.1	$c[5/3/c3]^2$	*ABE*	$\frac{1}{3}-\frac{1}{6}\sqrt{2}, \frac{2}{3}-\frac{1}{3}\sqrt{2}; \frac{1}{4}\sqrt{6}$		0.44653	$\frac{2}{11}\sqrt{6} < c < 0.94675$
2.1	3/6/*h*1	*CE*	0.11987, 0.43494; 0.83119		0.16799	$0.19488 < c < \frac{3}{2}+\frac{1}{2}\sqrt{6}$
(2.1)		*EG*				
2.1′		*BF*				
2.2	4/6/*c*2	*BG*	$\frac{1}{6}, \frac{1}{12}; \frac{1}{2}\sqrt{6}$		0.39270	$\frac{1}{4}\sqrt{6} < c < \sqrt{6}$
*i*2.1	$h[3/6/h1]^2$	*BE*	0.11987, 0.13013; 0.41559		0.33598	$0.20286 < c < 0.94675$
***P*6$_1$ 6*a* 1**		***x*, *y*, *z***	$\mathbf{0, 2x-1 \le y \le \frac{1}{2}x; z = 0}$			
A	$x-y, x, \frac{1}{6}+z$	$y, -x+y, -\frac{1}{6}+z$		*F*	$1+x-y, x, \frac{1}{6}+z$	$y, 1-x+y, -\frac{1}{6}+z$
B	*x*, *y*, 1+*z*	*x*, *y*, −1+*z*		*G*	1+*x*, *y*, *z*	−1+*x*, *y*, *z*
C	$1-x, -y, \frac{1}{2}+z$	$1-x, -y, -\frac{1}{2}+z$			*x*, 1+*y*, *z*	*x*, −1+*y*, *z*
D	$1-y, x-y, \frac{1}{3}+z$	$1-x+y, 1-x, -\frac{1}{3}+z$			1+*x*, 1+*y*, *z*	−1+*x*, −1+*y*, *z*
E	$x-y, -1+x, \frac{1}{6}+z$	$1+y, 1-x+y, -\frac{1}{6}+z$				

0.1	8/3/*h*13	*ABCD*	$\frac{6710}{10129}-\frac{584}{10129}\sqrt{15}, \frac{615}{10129}+\frac{188}{10129}\sqrt{15}; 6(\frac{137}{10129}-\frac{24}{10129}\sqrt{15})^{1/2}$		0.56792	
0.2	8/3/*h*6	*ACDE*	$\frac{15}{14}-\frac{1}{14}\sqrt{57}, \frac{8}{7}-\frac{1}{7}\sqrt{57}; \frac{3}{7}(18\sqrt{57}-130)^{1/2}$		0.52528	
0.3	8/3/*h*3	*ADEF*	$\frac{2}{3}, \frac{1}{3}; 2$		0.53742	
0.4	12/3/*h*1	*AEFG*	$\frac{2}{3}, \frac{1}{3}; 2\sqrt{6}$		0.74048	
1.1	6/3/*h*12	*BCD*	$\frac{10}{47}+\frac{24}{47}\sqrt{2}, \frac{12}{47}\sqrt{2}-\frac{27}{47}; \frac{48}{47}\sqrt{2}-\frac{54}{47}$		0.31648	$\frac{48}{47}\sqrt{2}-\frac{54}{47} \le c < 6(\frac{137}{10129}-\frac{24}{10129}\sqrt{15})^{1/2}$
1.2	6/3/*h*17	*ABC*	$\frac{70}{113}-\frac{3}{113}\sqrt{105}, 0; \frac{12}{113}\sqrt{35}-\frac{18}{113}\sqrt{3}$		0.45038	$\frac{12}{113}\sqrt{35}-\frac{18}{113}\sqrt{3} \le c < 6(\frac{137}{10129}-\frac{24}{10129}\sqrt{15})^{1/2}$
1.3	6/4/*h*6	*ABD*	$\frac{70}{73}-\frac{8}{219}\sqrt{210}, \frac{35}{73}-\frac{4}{219}\sqrt{210}; \frac{6}{73}\sqrt{105}-\frac{24}{73}\sqrt{2}$		0.51632	$\frac{6}{73}\sqrt{105}-\frac{24}{73}\sqrt{2} \le c < 6(\frac{137}{10129}-\frac{24}{10129}\sqrt{15})^{1/2}$
1.4	6/3/*h*26	*ACD*	0.46984, 0.10615; 0.73677		0.43125	$6(\frac{137}{10129}-\frac{24}{10129}\sqrt{15})^{1/2} < c < \frac{3}{7}(18\sqrt{57}-130)^{1/2}$
1.5	6/4/*h*3	*ACE*	$\frac{1}{2}, 0; \frac{3}{4}\sqrt{2}$		0.51013	$\frac{3}{7}(18\sqrt{57}-130)^{1/2} < c \le \frac{3}{4}\sqrt{2}$
1.6	6/3/*h*10	*ADE*	0.57846, 0.15693; 1.54319		0.45502	$\frac{3}{7}(18\sqrt{57}-130)^{1/2} < c < 2$
1.7	6/4/*h*2	*AEF*	$\frac{2}{3}, \frac{1}{3}; \sqrt{6}$		0.52360	$2 < c < 2\sqrt{6}$
1.8	10/3/*h*3	*AEG*	$\frac{1}{2}, 0; 3\sqrt{3}$		0.69813	$2\sqrt{6} < c \le 3\sqrt{3}$
2.1	4/5/*h*4	*CD*	0.56947, 0.13894; 0.44182		0.28622	$\frac{48}{47}\sqrt{2}-\frac{54}{47} < c < \frac{3}{7}(18\sqrt{57}-130)^{1/2}$
2.2	4/6/*h*3	*AC*	0.38285, 0; 0.64227		0.35482	$\frac{12}{113}\sqrt{35}-\frac{18}{113}\sqrt{3} < c < \frac{3}{4}\sqrt{2}$
2.3	4/5/*h*3	*AD*	0.47297, 0.23648; 1.00012		0.31367	$\frac{6}{73}\sqrt{105}-\frac{24}{73}\sqrt{2} < c < 2$
2.4	4/6/*h*1	*AE*	$\frac{1}{2}, 0; \frac{3}{2}\sqrt{2}$		0.39270	$\frac{3}{7}(18\sqrt{57}-130)^{1/2} < c < 3\sqrt{3}$
2.5	8/3/*h*4	*AG*	0, 0; 6		0.60460	$2\sqrt{6} < c \le 6$
***P*6$_2$ 6*c* 1**		***x*, *y*, *z***	**$0, 2x-1 \le y \le \frac{1}{2}x; z = 0$**			
A	$-x, -y, z$			*E*	$1-x, 1-y, z$	
B	$x-y, x, \frac{1}{3}+z$	$y, -x+y, -\frac{1}{3}+z$		*F*	$1-x+y, 1-x, \frac{1}{3}+z$	$1-y, x-y, -\frac{1}{3}+z$
C	$x, y, 1+z$	$x, y, -1+z$		*G*	$2-x, 1-y, z$	
D	$1-x, -y, z$					
0.1	7/3/*h*12	*BCDF*	$\frac{305}{403}-\frac{16}{403}\sqrt{69}, \frac{81}{806}+\frac{5}{806}\sqrt{69}; 3(\frac{32}{403}-\frac{3}{403}\sqrt{69})^{1/2}$		0.57359	
0.2	6/3/*h*3	*BDEF*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \frac{3}{2}\sqrt{3}-\frac{3}{2}$		0.45821	
0.3	5/4/*h*11	*ABDE*	$\frac{1}{3}, \frac{1}{6}; \frac{3}{2}$		0.46542	
0.4	5/4/*h*5	*DEFG*	$\frac{2}{3}, \frac{1}{3}; \sqrt{3}$		0.40307	
1.1	5/4/*h*13	*CDF*	$\frac{2}{5}\sqrt{6}-\frac{2}{5}, \frac{4}{5}\sqrt{6}-\frac{9}{5}; \frac{12}{5}\sqrt{2}-\frac{9}{5}\sqrt{3}$		0.27718	$\frac{12}{5}\sqrt{2}-\frac{9}{5}\sqrt{3} \le c < 3(\frac{32}{403}-\frac{3}{403}\sqrt{69})^{1/2}$
1.2	5/4/*h*15	*BCD*	$\frac{16}{23}-\frac{6}{23}\sqrt{2}, 0; \frac{12}{23}\sqrt{2}-\frac{9}{23}$		0.43565	$\frac{12}{23}\sqrt{2}-\frac{9}{23} \le c < 3(\frac{32}{403}-\frac{3}{403}\sqrt{69})^{1/2}$
1.3	6/4/*h*5	*BCF*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \frac{3}{8}\sqrt{6}-\frac{3}{8}\sqrt{2}$		0.54676	$\frac{3}{8}\sqrt{6}-\frac{3}{8}\sqrt{2} \le c < 3(\frac{32}{403}-\frac{3}{403}\sqrt{69})^{1/2}$
1.4	5/3/*h*6	*BDF*	0.42374, 0.18110; 0.81651		0.42661	$3(\frac{32}{403}-\frac{3}{403}\sqrt{69})^{1/2} < c < \frac{3}{2}\sqrt{3}-\frac{3}{2}$
1.5	4/4/*h*3	*BDE*	$\frac{5}{8}-\frac{1}{24}\sqrt{33}, \frac{5}{16}-\frac{1}{48}\sqrt{33}; \frac{3}{16},+\frac{3}{16}\sqrt{33}$		0.44621	$\frac{3}{2}\sqrt{3}-\frac{3}{2} < c < \frac{3}{2}$
1.6	4/4/*h*4	*DEF*	$\frac{1}{8}+\frac{1}{24}\sqrt{105}, \frac{1}{16}+\frac{1}{48}\sqrt{105}; \frac{3}{16}\sqrt{3}+\frac{3}{16}\sqrt{35}$		0.33170	$\frac{3}{2}\sqrt{3}-\frac{3}{2} < c < \sqrt{3}$
1.7	4/4/*h*1	*ABD*	$\frac{1}{4}, 0; \frac{3}{4}\sqrt{3}$		0.34907	$\frac{3}{4}\sqrt{3} \le c < \frac{3}{2}$
2.1	3/8/*h*2	*DF*	$\frac{1}{8}\sqrt{33}-\frac{1}{8}, \frac{1}{4}\sqrt{33}-\frac{5}{4}; \frac{9}{8}\sqrt{3}-\frac{3}{8}\sqrt{11}$		0.17248	$\frac{12}{5}\sqrt{2}-\frac{9}{5}\sqrt{3} < c < \sqrt{3}$
2.2	3/12/*h*1	*BD*	$\frac{17}{24}-\frac{1}{24}\sqrt{97}, 0; \frac{1}{8}(102-6\sqrt{97})^{1/2}$		0.29229	$\frac{12}{23}\sqrt{2}-\frac{9}{23} < c < \frac{3}{2}$
2.3	4/4/*h*2	*BF*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$		0.42089	$\frac{3}{8}\sqrt{6}-\frac{3}{8}\sqrt{2} < c < \frac{3}{2}\sqrt{3}-\frac{3}{2}$
***P*$\bar{6}$ 3*j m*..**		***x*, *y*, 0**	**$0 < x \le \frac{1}{3}; 0 \le y \le \frac{1}{2}x$**			
A	$-y, x-y, 0$	$-x+y, -x, 0$		*C*	$1-y, x-y, 0$	$1-x+y, 1-x, 0$
B	$x, y, 1$	$x, y, -1$		*D*	$-y, -1+x-y, 0$	$1-x+y, -x, 0$
0.1	8/3/*h*4	*ABCD*	$\frac{1}{3}, 0; \frac{1}{3}\sqrt{3}$		0.60460	
1.1	6/3/*h*13	*ABC*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{2}$		0.45345	$\frac{1}{2} \le c < \frac{1}{3}\sqrt{3}$
***P*6/*m* 6*j m*..**		***x*, *y*, 0**	**$0, 2x-1 \le y \le \frac{1}{2}x$**			
A	$x-y, x, 0$	$y, -x+y, 0$		*C*	$1-x, -y, 0$	
B	$x, y, 1$	$x, y, -1$		*D*	$1-y, x-y, 0$	$1-x+y, 1-x, 0$
0.1	7/3/*h*13	*ABCD*	$\frac{3}{7}, \frac{1}{7}; \frac{1}{7}\sqrt{7}$		0.51823	
1.1	5/3/*h*5	*BCD*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1; 2-\sqrt{3}$		0.26045	$2-\sqrt{3} \le c < \frac{1}{7}\sqrt{7}$
1.2	5/4/*h*5	*ABC*	$\frac{1}{3}, 0; \frac{1}{3}$		0.40307	$\frac{1}{3} \le c < \frac{1}{7}\sqrt{7}$
1.3	6/3/*h*20	*ABD*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \frac{1}{2}\sqrt{3}-\frac{1}{2}$		0.48601	$\frac{1}{2}\sqrt{3}-\frac{1}{2} \le c < \frac{1}{7}\sqrt{7}$
***P*6$_3$/*m* 6*h m*..**		***x*, *y*, $\frac{1}{4}$**	**$0, 2x-1 \le y \le \frac{1}{2}x$**			
A	$-y, x-y, \frac{1}{4}$	$-x+y, -x, \frac{1}{4}$		*D*	$1-x, -y, \frac{3}{4}$	$1-x, -y, -\frac{1}{4}$
B	$x-y, x, \frac{3}{4}$	$y, -x+y, \frac{3}{4}$		*E*	$1-y, x-y, \frac{1}{4}$	$1-x+y, 1-x, \frac{1}{4}$
	$x-y, x, -\frac{1}{4}$	$y, -x+y, -\frac{1}{4}$		*F*	$-y, -1+x-y, \frac{1}{4}$	$1-x+y, -x, \frac{1}{4}$
C	$x, y, \frac{5}{4}$	$x, y, -\frac{3}{4}$				
0.1	10/3/*h*5	*BCDE*	$\frac{46}{73}-\frac{20}{219}\sqrt{6}, \frac{14}{219}\sqrt{6}-\frac{3}{73}; 2(\frac{13}{73}-\frac{4}{73}\sqrt{6})^{1/2}$		0.63648	
0.2	12/3/*h*1	*ABDEF*	$\frac{1}{3}, 0; \frac{2}{3}\sqrt{2}$		0.74048	
1.1	6/3/*h*21	*CDE*	$\frac{4}{7}, \frac{1}{7}; \frac{2}{7}$		0.29613	$\frac{2}{7} \le c < 2(\frac{13}{73}-\frac{4}{73}\sqrt{6})^{1/2}$
1.2	8/3/*h*3	*BCD*	$\frac{1}{3}, 0; \frac{2}{9}\sqrt{3}$		0.53742	$\frac{2}{9}\sqrt{3} \le c < 2(\frac{13}{73}-\frac{4}{73}\sqrt{6})^{1/2}$
1.3	8/3/*h*11	*BCE*	$\frac{2}{5}, \frac{1}{5}; \frac{2}{5}$		0.58042	$\frac{2}{5} \le c < 2(\frac{13}{73}-\frac{4}{73}\sqrt{6})^{1/2}$
1.4	8/3/*h*14	*BDE*	0.38762, 0.09006; 0.57982		0.59135	$2(\frac{13}{73}-\frac{4}{73}\sqrt{6})^{1/2} < c < \frac{2}{3}\sqrt{2}$
1.5	8/3/*h*10	*ABE*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{3}\sqrt{6}$		0.55536	$\frac{1}{3}\sqrt{6} \le c < \frac{2}{3}\sqrt{2}$
1.6	6/3/*h*13	*DEF*	$\frac{1}{2}, 0; 1$		0.45345	$\frac{2}{3}\sqrt{2} < c \le 1$

2.1	4/3/*h*3	*DE*	$\frac{1}{6}\sqrt{19}-\frac{1}{6}, \frac{1}{3}\sqrt{19}-\frac{4}{3}; \frac{1}{3}(6\sqrt{19}-24)^{1/2}$		0.24427	$\frac{2}{7}<c<1$
2.2	6/4/*h*2	*BD*	$\frac{1}{3}, 0; \frac{1}{3}\sqrt{2}$		0.52360	$\frac{2}{9}\sqrt{3}<c<\frac{2}{3}\sqrt{2}$
2.3	6/3/*h*22	*BE*	$\frac{13}{12}-\frac{1}{12}\sqrt{73}, \frac{13}{24}-\frac{1}{24}\sqrt{73}; \frac{1}{6}(39-3\sqrt{73})^{1/2}$		0.51755	$\frac{2}{5}<c<\frac{2}{3}\sqrt{2}$
P*$\bar{6}$*m*2 6*l m..		***x, y*, 0**	**$0<x\le\frac{1}{3}; 0\le y<\frac{1}{2}x$**			
A	*x*, *x*−*y*, 0			*C*	−*y*, −*x*, 0	
B	*x*, *y*, 1	*x*, *y*, −1		*D*	1−*x*+*y*, *y*, 0	
0.1	5/4/*h*5	*ABCD*	$\frac{1}{3}, 0; \frac{1}{3}$		0.40307	
P*$\bar{6}$*m*2 6*n .m.		***x*, −*x*, *z***	**$0<x\le\frac{1}{6}; 0<z\le\frac{1}{4}$**			
A	*x*, −*x*, −*z*			*C*	*x*, −*x*, 1−*z*	
B	*x*, 2*x*, *z*	−2*x*, −*x*, *z*		*D*	*x*, −1+2*x*, *z*	1−2*x*, −*x*, *z*
0.1	6/3/*h*13	*ABCD*	$\frac{1}{6}, \frac{1}{4}; 1$		0.45345	
P*$\bar{6}$*c*2 6*k m..		***x, y*, $\frac{1}{4}$**	**$0<x\le\frac{1}{3}; 0\le y\le\frac{1}{2}x$**			
A	−*y*, *x*−*y*, $\frac{1}{4}$	−*x*+*y*, −*x*, $\frac{1}{4}$		*E*	−*y*, −*x*, $\frac{3}{4}$	−*y*, −*x*, $-\frac{1}{4}$
B	*x*, *x*−*y*, $\frac{3}{4}$	*x*, *x*−*y*, $-\frac{1}{4}$		*F*	1−*y*, *x*−*y*, $\frac{1}{4}$	1−*x*+*y*, 1−*x*, $\frac{1}{4}$
C	*x*, *y*, $\frac{5}{4}$	*x*, *y*, $-\frac{3}{4}$		*G*	−*y*, −1+*x*−*y*, $\frac{1}{4}$	1−*x*+*y*, −*x*, $\frac{1}{4}$
D	1−*x*+*y*, *y*, $\frac{3}{4}$	1−*x*+*y*, *y*, $-\frac{1}{4}$				
0.1	8/3/*h*3	*BCDE*	$\frac{1}{3}, 0; \frac{2}{9}\sqrt{3}$		0.53742	
0.2	12/3/*h*1	*ABDEFG*	$\frac{1}{3}, 0; \frac{2}{3}\sqrt{2}$		0.74048	
1.1	6/4/*h*2	*BDE*	$\frac{1}{3}, 0; \frac{1}{3}\sqrt{2}$		0.52360	$\frac{2}{9}\sqrt{3}<c<\frac{2}{3}\sqrt{2}$
1.2	6/3/*h*13	*ABF*	$\frac{1}{3}, \frac{1}{6}; 1$		0.45345	$\frac{2}{3}\sqrt{2}<c\le 1$
P*$\bar{6}$2*m* 6*i ..m		***x*, 0, *z***	**$0<x\le\frac{1}{2}; 0<z\le\frac{1}{4}$**			
A	*x*, 0, −*z*			*D*	0, −1+*x*, *z*	1−*x*, −*x*, *z*
B	0, *x*, *z*	−*x*, −*x*, *z*			1, *x*, *z*	1−*x*, 1−*x*, *z*
C	*x*, 0, 1−*z*					
0.1	8/3/*h*4	*ABCD*	$\frac{1}{3}, \frac{1}{4}; \frac{2}{3}\sqrt{3}$		0.60460	
1.1	6/3/*h*13	*ACD*	$\frac{1}{2}, \frac{1}{4}; 1$		0.45345	$1\le c<\frac{2}{3}\sqrt{3}$
P*$\bar{6}$2*m* 6*j m..		***x, y*, 0**	**$0<y; 2x-1\le y\le\frac{1}{2}x$**			
A	*x*−*y*, −*y*, 0			*C*	1−*y*, *x*−*y*, 0	1−*x*+*y*, 1−*x*, 0
B	*x*, *y*, 1	*x*, *y*, −1		*D*	*y*, *x*, 0	
0.1	6/3/*h*20	*ABCD*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \frac{1}{2}\sqrt{3}-\frac{1}{2}$		0.48601	
1.1	5/3/*h*5	*ABC*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1; 2-\sqrt{3}$		0.26045	$2-\sqrt{3}\le c<\frac{1}{2}\sqrt{3}-\frac{1}{2}$
P*$\bar{6}$2*c* 6*h m..		***x, y*, $\frac{1}{4}$**	**$0, 2x-1\le y\le\frac{1}{2}x$**			
A	−*y*, *x*−*y*, $\frac{1}{4}$	−*x*+*y*, −*x*, $\frac{1}{4}$		*D*	1−*y*, *x*−*y*, $\frac{1}{4}$	1−*x*+*y*, 1−*x*, $\frac{1}{4}$
B	*x*−*y*, −*y*, $\frac{3}{4}$	*x*−*y*, −*y*, $-\frac{1}{4}$		*E*	−*y*, −1+*x*−*y*, $\frac{1}{4}$	1−*x*+*y*, −*x*, $\frac{1}{4}$
C	*x*, *y*, $\frac{5}{4}$	*x*, *y*, $-\frac{3}{4}$		*F*	*y*, *x*, $\frac{3}{4}$	*y*, *x*, $-\frac{1}{4}$
0.1	8/3/*h*11	*BCDF*	$\frac{2}{5}, \frac{1}{5}; \frac{2}{5}$		0.58042	
0.2	8/3/*h*10	*ABDF*	$\frac{1}{3}, \frac{1}{6}; \frac{1}{3}\sqrt{6}$		0.55536	
0.3	8/3/*h*4	*ABDE*	$\frac{1}{3}, 0; \frac{2}{3}\sqrt{3}$		0.60460	
1.1	6/3/*h*21	*BCD*	$\frac{4}{7}, \frac{1}{7}; \frac{2}{7}$		0.29613	$\frac{2}{7}\le c<\frac{2}{5}$
1.2	6/3/*h*22	*BDF*	$\frac{13}{12}-\frac{1}{12}\sqrt{73}, \frac{13}{24}-\frac{1}{24}\sqrt{73}; \frac{1}{6}(39-3\sqrt{73})^{1/2}$		0.51755	$\frac{2}{5}<c<\frac{1}{3}\sqrt{6}$
1.3	6/3/*h*27	*ABD*	$\frac{1}{3}, \frac{4}{15}-\frac{1}{15}\sqrt{6}; \frac{2}{15}(15+15\sqrt{6})^{1/2}$		0.50729	$\frac{1}{3}\sqrt{6}<c<\frac{2}{3}\sqrt{3}$
1.4	6/3/*h*13	*BDE*	$\frac{1}{2}, 0; 1$		0.45345	$1\le c<\frac{2}{3}\sqrt{3}$
2.1	4/3/*h*3	*BD*	$\frac{1}{6}\sqrt{19}-\frac{1}{6}, \frac{1}{3}\sqrt{19}-\frac{4}{3}; \frac{1}{3}(6\sqrt{19}-24)^{1/2}$		0.24427	$\frac{2}{7}<c<\frac{2}{3}\sqrt{3}$
P*6/*mmm* 12*n ..m		***x*, 0, *z***	**$0<x<\frac{1}{2}; 0<z\le\frac{1}{4}$**			
A	*x*, 0, −*z*			*C*	*x*, 0, 1−*z*	
B	0, −*x*, *z*	*x*, *x*, *z*		*D*	1−*x*, 0, *z*	
0.1	5/4/*h*5	*ABCD*	$\frac{1}{3}, \frac{1}{4}; \frac{2}{3}$		0.40307	
P*6/*mmm* 12*o .m.		***x*, 2*x*, *z***	**$0<x<\frac{1}{3}; \frac{1}{3}<x<\frac{1}{2}; 0<z\le\frac{1}{4}$**			
A	*x*, 2*x*, −*z*			*D*	1−*x*, 2−2*x*, *z*	
B	−*x*, *x*, *z*	2*x*, *x*, *z*		*E*	*x*, 1−*x*, *z*	1−2*x*, 1−*x*, *z*
C	*x*, 2*x*, 1−*z*					
0.1	5/3/*h*5	*ACDE*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{4}; 4-2\sqrt{3}$		0.26045	
0.2	6/3/*h*20	*ABCE*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{4}; \sqrt{3}-1$		0.48601	
P*6/*mmm* 12*p m..		***x, y*, 0**	**$0, 2x-1<y<\frac{1}{2}x$**			
A	*x*−*y*, −*y*, 0			*C*	1−*x*+*y*, *y*, 0	
B	*x*, *y*, 1	*x*, *y*, −1		*D*	*x*, *x*−*y*, 0	
0.1	5/4/*h*17	*ABCD*	$\frac{1}{6}+\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{3}-\frac{1}{6}; \frac{1}{2}-\frac{1}{6}\sqrt{3}$		0.32400	

P6/mcc* 12*l* *m..	***x, y,* 0**	**$0, 2x-1 \le y \le \frac{1}{2}x$**				
A	$x-y, x, 0$	$y, -x+y, 0$		*E*	$1-y, x-y, 0$	$1-x+y, 1-x, 0$
B	$x-y, -y, \frac{1}{2}$	$x-y, -y, -\frac{1}{2}$		*F*	$x, y, 1$	$x, y, -1$
C	$1-x, -y, 0$			*G*	$1-x+y, y, \frac{1}{2}$	$1-x+y, y, -\frac{1}{2}$
D	$x, x-y, \frac{1}{2}$	$x, x-y, -\frac{1}{2}$				
0.1	8/3/*h*15	*BDFG*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}; \frac{1}{3}\sqrt{3}-\frac{1}{3}$		0.43201	
0.2	7/3/*h*14	*BCDG*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}; 1-\frac{1}{3}\sqrt{3}$		0.45821	
0.3	7/3/*h*15	*CDEG*	$\frac{1}{3}\sqrt{6}-\frac{1}{3}, \frac{1}{3}\sqrt{6}-\frac{2}{3}; 2\sqrt{2}-\frac{4}{3}\sqrt{3}$		0.44882	
0.4	7/3/*h*16	*ABCD*	0.40013, 0.10722; 0.61389		0.54567	
0.5	7/3/*h*17	*ACDE*	$\frac{3}{7}, \frac{1}{7}; \frac{2}{7}\sqrt{6}$		0.55975	
1.1	6/4/*h*10	*BDG*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}; \frac{1}{2}\sqrt{2}-\frac{1}{6}\sqrt{6}$		0.42089	$\frac{1}{3}\sqrt{3}-\frac{1}{3} < c < 1-\frac{1}{3}\sqrt{3}$
1.2	5/4/*h*18	*BCD*	{0.418, 0.11200; 0.55201}		>0.45821	$1-\frac{1}{3}\sqrt{3} < c < 0.61389$
1.3	5/4/*h*19	*CDG*	0.47385, 0.14051; 0.48675		0.44621	$1-\frac{1}{3}\sqrt{3} < c < 2\sqrt{2}-\frac{4}{3}\sqrt{3}$
1.4	5/3/*h*7	*CDE*	{0.47414, 0.14888; 0.55}		>0.44882	$2\sqrt{2}-\frac{4}{3}\sqrt{3} < c < \frac{2}{7}\sqrt{6}$
1.5	5/3/*h*5	*CEG*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1; 4-2\sqrt{3}$		0.26045	$2\sqrt{2}-\frac{4}{3}\sqrt{3} < c \le 4-2\sqrt{3}$
1.6	5/4/*h*5	*ABC*	$\frac{1}{3}, 0; \frac{2}{3}$		0.40307	$0.61389 < c \le \frac{2}{3}$
1.7	5/4/*h*20	*ACD*	0.40396, 0.11227; 0.62688		0.54522	$0.61389 < c < \frac{2}{7}\sqrt{6}$
1.8	6/3/*h*20	*ADE*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \sqrt{3}-1$		0.48601	$\frac{2}{7}\sqrt{6} < c \le \sqrt{3}-1$
*n*2.1	$h[6^3]^3$	*CD*	{0.5, 0.15; 0.44721}		>0.44621	$1-\frac{1}{3}\sqrt{3} < c < \frac{2}{7}\sqrt{6}$
$P6_3/mcm$ 12*j* *m..*	**$x, y, \frac{1}{4}$**	**$0 < y; 2x-1 \le y \le \frac{1}{2}x$**				
A	$x-y, -y, \frac{1}{4}$			*D*	$x, y, \frac{5}{4}$	$x, y, -\frac{3}{4}$
B	$x, x-y, \frac{3}{4}$	$x, x-y, -\frac{1}{4}$		*E*	$1-x+y, y, \frac{3}{4}$	$1-x+y, y, -\frac{1}{4}$
C	$1-y, x-y, \frac{1}{4}$	$1-x+y, 1-x, \frac{1}{4}$		*F*	$y, x, \frac{1}{4}$	
0.1	7/3/*h*18	*ABDE*	$\frac{7}{15}, \frac{2}{15}; \frac{2}{15}\sqrt{3}$		0.38694	
0.2	7/3/*h*19	*ABCE*	$\frac{1}{2}, \frac{1}{6}; \frac{1}{3}\sqrt{2}$		0.37024	
0.3	6/3/*h*20	*ABCF*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}; \sqrt{3}-1$		0.48601	
1.1	5/4/*h*21	*ABE*	0.48100, 0.14767; 0.35182		0.34503	$\frac{2}{15}\sqrt{3} < c < \frac{1}{3}\sqrt{2}$
1.2	5/3/*h*8	*ABC*	0.48786, 0.17112; 0.51627		0.36587	$\frac{1}{3}\sqrt{2} < c < \sqrt{3}-1$
1.3	5/3/*h*5	*ACE*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1; 4-2\sqrt{3}$		0.26045	$\frac{1}{3}\sqrt{2} < c \le 4-2\sqrt{3}$
$P6_3/mcm$ 12*k* *..m*	***x,* 0, *z***	**$0 < x \le \frac{1}{2}; 0 \le z < \frac{1}{4}$**				
A	$x, x, -z$	$0, -x, -z$		*E*	$1, x, z$	$1-x, 1-x, z$
B	$0, x, z$	$-x, -x, z$			$0, -1+x, z$	$1-x, -x, z$
C	$x, 0, \frac{1}{2}-z$			*F*	$x, 0, -\frac{1}{2}-z$	
D	$1-x, 0, -z$					
0.1	5/4/*h*5	*ACDF*	$\frac{1}{3}, 0; \frac{2}{3}$		0.40307	
0.2	10/3/*h*2	*ABCDE*	$\frac{1}{3}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		0.66568	
1.1	4/6/*h*2	*ACD*	$\frac{1}{3}, \frac{1}{16}; \frac{2}{3}\sqrt{2}$		0.34009	$\frac{2}{3} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$
1.2	6/3/*h*13	*CDE*	$\frac{1}{2}, \frac{1}{8}; 2$		0.45345	$2 \le c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$
$P6_3/mmc$ 12*j* *m..*	**$x, y, \frac{1}{4}$**	**$0 \le y; 2x-1 < y < \frac{1}{2}x$**				
A	$x, x-y, \frac{1}{4}$			*D*	$x, y, \frac{5}{4}$	$x, y, -\frac{3}{4}$
B	$x-y, -y, \frac{3}{4}$	$x-y, -y, -\frac{1}{4}$		*E*	$-y, -x, \frac{1}{4}$	
C	$1-x+y, y, \frac{1}{4}$					
0.1	6/3/*h*28	*ABCD*	$\frac{4}{9}, \frac{1}{9}; \frac{2}{9}$		0.35828	
0.2	5/4/*h*5	*ABCE*	$\frac{1}{3}, 0; \frac{2}{3}$		0.40307	
1.1	4/4/*h*5	*ABC*	$\frac{5}{12}, \frac{1}{12}; \frac{1}{6}\sqrt{6}$		0.27768	$\frac{2}{9} < c < \frac{2}{3}$
$P6_3/mmc$ 12*k* *.m.*	***x,* 2*x*, *z***	**$0 < x < \frac{1}{3}; \frac{1}{3} < x \le \frac{1}{2}; 0 \le z < \frac{1}{4}$**				
A	$-x, x, -z$	$2x, x, -z$		*E*	$x, 1-x, z$	$1-2x, 1-x, z$
B	$x, 2x, \frac{1}{2}-z$			*F*	$x, 2-x, z$	$2-2x, 2-x, z$
C	$1-x, 2-2x, -z$			*G*	$x, 2x, -\frac{1}{2}-z$	
D	$x, -x, z$	$-2x, -x, z$				
0.1	5/3/*h*5	*BCEG*	$1-\frac{1}{3}\sqrt{3}, 0; 4-2\sqrt{3}$		0.26045	
0.2	6/3/*h*20	*ABEG*	$\frac{1}{2}-\frac{1}{6}\sqrt{3}, 0; \sqrt{3}-1$		0.48601	
0.3	7/3/*h*20	*ABDE*	$\frac{1}{6}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \frac{1}{3}\sqrt{6}+1$		0.49926	
0.4	6/3/*h*13	*BCEF*	$\frac{1}{2}, \frac{1}{8}; 2$		0.45345	
1.1	4/3/*h*4	*BCE*	0.42982, 0.08796; 0.89321		0.19701	$4-2\sqrt{3} < c < 2$
1.2	5/3/*h*9	*ABE*	0.20238, 0.07778; 1.14060		0.38572	$\sqrt{3}-1 < c < \frac{1}{3}\sqrt{6}+1$

that give rise to sphere contacts. The next two columns relate to those special (interpenetrating) sphere packings of the regarded type that show minimal density: the corresponding coordinate parameters and the axial ratio *c*/*a* are given in the fourth column, the value ρ_m of the minimal density in the fifth column. Some types of sphere configuration do not include an arrangement with minimal density. In such a case, parameters for any other sphere configuration of that type are tabulated in braces (*cf. e.g.* 4/6/*h*7 in *R*3*c* 18*b*). For each type of sphere configuration with free parameters, the range of the axial ratio *c*/*a* is shown in the sixth column.

Concerning the parameter regions of some types of sphere configuration, a complicated situation may occur if the asymmetric unit of the Euclidean normalizer of a space group is not totally bounded by mirror planes. A connected parameter region represented by a string of capital letters does not necessarily belong completely to the asymmetric unit under consideration. In such a case, the parameter region of the relevant type disintegrates into two or more disconnected parts, each of them referring to another string of capital letters. Within the present material, such a situation is found only for lattice complex $R\bar{3}m$ 18*h*. 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 or from the Euclidean normalizer is symbolized by parentheses or by a prime, respectively. Fischer (1991) has discussed in detail a corresponding tetragonal example.

3. Discussion

The hexagonal bivariant lattice complexes lead to sphere packings of altogether 109 types. 62 of these types have already been described during the examination of the hexagonal lattice complexes with zero or one degree of freedom (Sowa *et al.*, 2003).

Owing to limiting-complex relationships, the sphere packings of a certain type with minimal density may show cubic inherent symmetry. This applies to the following types: 4/4/*c*1 occurs in lattice complex *R*3*m* 18*c* with limiting complex $Im\bar{3}m$ 12*d*; 4/6/*c*2 occurs in lattice complexes $R\bar{3}m$ 18*h*, *R*3*c* 18*b* and *R*3 9*b* with limiting complex $Im\bar{3}m$ 12*b*; 8/3/*c*2 occurs in lattice complexes $R\bar{3}m$ 18*h*, *R*3*c* 18*b* and *R*3 9*b* with limiting complex $Pm\bar{3}m$ 3*c*; 5/3/*c*3 occurs in lattice complex $R\bar{3}m$ 18*h* with limiting complex $Pm\bar{3}m$ 6*e*; types 6/4/*c*1, 8/4/*c*1 and 12/3/*c*1 occur in lattice complex $P3_2$ 3*a* with limiting complexes $Pm\bar{3}m$ 1*a*, $Im\bar{3}m$ 2*a* and $Fm\bar{3}m$ 4*a*, respectively.

Only three hexagonal and one cubic sphere-packing types that correspond to invariant or univariant hexagonal lattice complexes were not also found in bivariant ones.

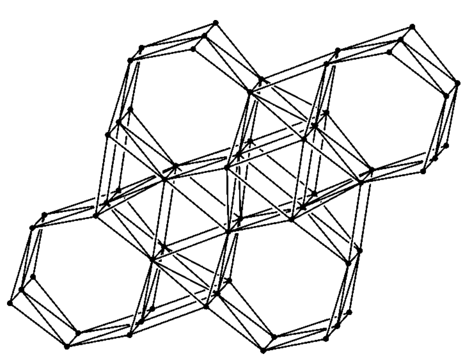

Figure 1
Sphere packing of type 10/3/*h*5.

Three types of interpenetrating sphere packing were derived. In all cases, two sphere packings interpenetrate one another. Types $h[3/6/h1]^2$ and $c[5/3/c3]^2$ occur in $R\bar{3}m$ 18*h*, but have not been found in a hexagonal lattice complex with less than two degrees of freedom. Though generated with symmetry $R\bar{3}m$, interpenetrating sphere packings of type $c[5/3/c3]^2$ can show cubic inherent symmetry since $Im\bar{3}m$ 12*e* forms a limiting complex of $R\bar{3}m$ 18*h*. $h[4/3/h1]^2$ occurs in *R*3*c* 18*b* and has already been described in $R\bar{3}c$ 18*e* (Sowa *et al.*, 2003).

Among the sphere packings of $P6_3/m$ 6*h*, there is one type with ten contacts per sphere that has never been described before, namely 10/3/*h*5 (*cf.* Fig. 1). Unlike most sphere packings with contact number 10 (*cf.* Koch & Fischer, 1999), it cannot be described by stacking of planar layers of spheres.

Another outstanding type of sphere configuration has symmetry *P*6/*mcc* 12*l*. Contrary to previous expectations (*cf.* Fischer & Koch, 1990), a type of interpenetrating sphere layer $h[6^3]^3$ with hexagonal symmetry was found. Three sets of parallel honeycomb nets 6^3 interpenetrate each other (*cf.* Fig. 2). The honeycomb layers have necessarily to be corrugated to avoid contacts between spheres from layers in different orientations.

4. Examples of crystal structures

Frequently, atomic arrangements within crystal structures may be interpreted as sphere packings, independently of whether or not the corresponding atoms are spheres in contact. For this approach, it is sufficient that the shortest distances between the atoms are (approximately) equal.

(I) Crystal structures are often related to cubic or hexagonal closest packings of spheres. Both occur in the hexagonal crystal family with different symmetries. Numerous such crystal structures are listed in a previous paper where the closest packings correspond to invariant or univariant lattice complexes (Sowa *et al.* 2003). Further examples of hexagonal

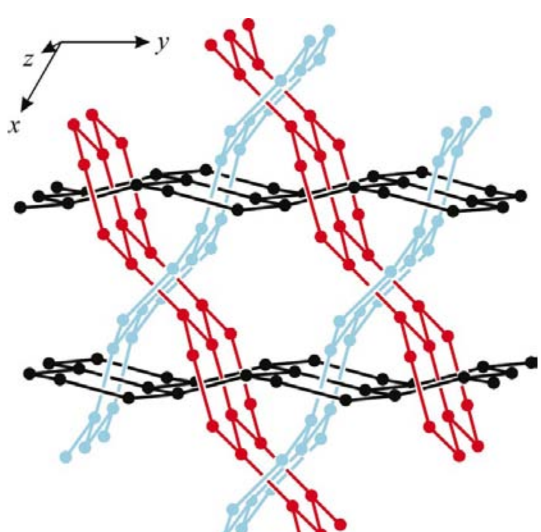

Figure 2
Interpenetrating honeycomb nets 6^3 of type $h[6^3]^3$

closest packings related to hexagonal bivariant lattice complexes are the following:

(i) Ag in Ag_6O_2 (Beesk *et al.*, 1981), O in $Li_2Pt(OH)_6$ (Trömel & Lupprich, 1975), O in UCr_2O_6 (Collomb *et al.*, 1976) and Cr in Cr_2N (Kim *et al.*, 1990): lattice complex $P\bar{3}1m$ 6*k*.

(ii) B in BI_3 (Albert & Schmitt, 2001): lattice complex $P6_3/m$ 6*h*.

(iii) Cl in $RuCl_3$ (Fletcher *et al.*, 1967), I in $LiScI_3$ (Lachgar *et al.*, 1991): lattice complex $P\bar{6}c2$ 6*k*.

(II) The oxygen arrangement in ReO_3 or in idealized perovskite refers to a sphere packing of type 8/3/*c*2. The small cations are located in octahedral voids whereas the larger cations centre the cuboctahedral voids that are empty in ReO_3-type structures. Sphere packings of type 8/3/*c*2 occur also in rhombohedral space groups. In lattice complex $R\bar{3}c$ 18*e* $x0\frac{1}{4}$, this sphere-packing type has one degree of freedom and the octahedra may be rotated around their threefold axes parallel to **c**. Such an octahedral rotation leads from the ReO_3 type to the VF_3 type (*c.f.* Hepworth *et al.*, 1957; Moreau *et al.*, 1970; Michel *et al.*, 1971; Megaw & Darlington, 1975; Sowa, 1997; Sowa *et al.*, 2003).

During the rotation of the octahedra, each cuboctahedral void splits up into two smaller ones that are symmetrically equivalent with respect to $R\bar{3}c$. Only one of these voids, however, can be occupied by the larger cation in perovskite-related structures. As a consequence, the deformation in such compounds happens in the subgroup $R3c$ of $R\bar{3}c$, where the two voids are no longer equivalent. Parameters $x = \frac{1}{3}$, $y = \frac{1}{6}$ and $c/a = \surd 6$ refer to the ideal cubic anion arrangement. Fig. 3 shows the rotation angle φ *versus* c/a for an ideal sphere packing of type 8/3/*c*2 (solid line). φ may be calculated as

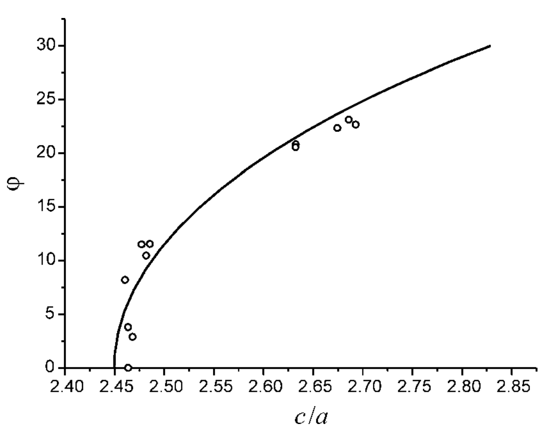

Figure 3
Rotation angle φ *versus* c/a for an ideal sphere packing of type 8/3/*c*2 (solid line) in lattice complex $R3c$ 18*b*. Open circles represent the anion arrangements in the following crystal structures. Rhombohedral perovskites: $Pb_{0.94}Sr_{0.06}Zr_{0.60}Ti_{0.40}O_3$ (Bedoya *et al.*, 2000); $PbZr_{0.9}Ti_{0.1}O_3$ (Ito *et al.*, 1983); $PbHf_{0.8}Ti_{0.2}O_3$ (Muller *et al.*, 2000); $Na_{0.5}Bi_{0.5}TiO_3$ (Jones & Thomas, 2002); $AgTaO_3$ (Wołcyrz & Łukaszewski, 1986); $BiFe_{0.780}Mn_{0.213}O_3$ (Sosnowska *et al.*, 2000); $LiNbO_3$ type: $MnTiO_3$ (Ko & Prewitt, 1988); $ReLiO_3$ (Cava *et al.*, 1982); $LiTaO_3$, $LiNbO_3$ (Hsu *et al.*, 1997); $FeTiO_3$ (Leinenweber *et al.*, 1995).

$$\tan\varphi = \frac{x - 2y}{2 - 3x}\sqrt{3}. \quad (1)$$

An octahedral rotation by $\varphi = 30°$ yields a hexagonally closest packed arrangement with parameters $x = \frac{1}{3}$, $y = 0$ and $c/a = 2\surd 2$. The open circles in Fig. 3 correspond to some related crystal structures. The structures are described as rhombohedrally distorted perovskite-type structures if the octahedra are rotated up to about 11°. Those with larger rotation angles (~20 to 24°) belong to the $LiNbO_3$ type (*cf. e.g.* Leinenweber *et al.*, 1995). In contrast to VF_3-type compounds, $LiNbO_3$-type compounds may not show a nearly ideal hexagonally closest-packed anion arrangement because the cations of the second type are too large to occupy octahedral voids in closest packings.

(III) 8/3/*h*10 is another sphere-packing type that can be related to many crystal structures. It occurs with no degree of freedom in $P\bar{3}m1$ 6*i* $x, -x, z$ at $x = \frac{1}{6}$, $z = \frac{1}{4}$, $c/a = \frac{1}{3}\surd 6$. K_2ReF_6 (Clark & Russell, 1978) represents a large number of other compounds, so-called 'hexagonal perovskites', with an anion arrangement corresponding to a sphere packing of type 8/3/*h*10. Similar to perovskite, the smaller cations are octahedrally coordinated and the larger cations occupy 12-coordinated voids. In contrast to perovskite, however, the octahedra share faces and form piles parallel to **c**. A similar anion packing occurs in the structures of $Tl_2Pt_4F_6$ (Bronger & Bonsmann, 1995) and $K_2Li_4UO_6$ (Wolf & Hoppe, 1987) where, in addition, further positions are occupied by cations.

(IV) $LaBr_3$ (Krämer *et al.*, 1989) crystallizes in space group $P6_3/m$. It belongs to the UCl_3 structure type that is adopted by trihalides of numerous 4*f* and 5*f* elements and also by trihydroxides of lanthanides. The anions occupy Wyckoff position 6*h* and correspond in good approximation to a sphere packing of type 8/3/*h*14 (*cf.* Fig. 4) that is described for the first time in the present paper. Type 8/3/*h*14 occurs with one degree of freedom in $P6_3/m$. The ends of its parameter range refer to type 10/3/*h*5 (*cf.* Fig. 1) at the lowest axial ratio and to type 12/3/*h*1 (hexagonal closest packing) at the highest axial ratio.

The coordination polyhedra of the cations in UCl_3-type structures are tricapped trigonal prisms with nine almost equal cation–anion distances and site symmetry $\bar{6}$. Ideal tricapped trigonal prisms are formed if equation (2) is fulfilled:

$$ya^2 = \tfrac{1}{4}c^2. \quad (2)$$

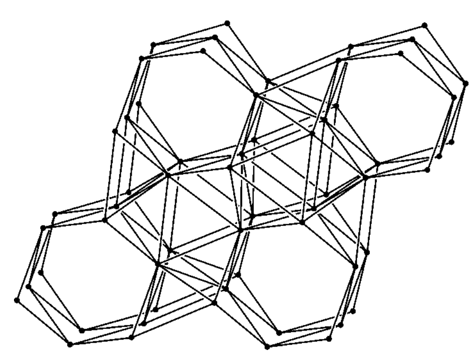

Figure 4
Sphere packing of type 8/3/*h*14.

The corresponding sphere-packing parameters $x = 0.38596$, $y = 0.08772$ and $c/a = 0.59235$ as well as the density $\rho = 0.59156$ differ only very slightly from those values given in Table 1 for the sphere packings with minimal density. At lower axial ratios, the nine-coordinated void splits up into a trigonal prism and three distorted tetrahedra, at higher axial ratios it disintegrates into two distorted trigonal antiprisms with a common large triangular face.

In addition, Na, K and Ag cations are located in the wide channels around the 6_3 axes in the crystal structures of addition/substitution derivatives of the UCl_3 type (Wickleder & Meyer, 1998). $[HOSO_3]^-$ tetrahedra replace the anions of the UCl_3 type in hydrogensulfates of rare-earth elements $M(HSO_4)_3$ (M = La, Ce–Nd) (Wickleder, 1998). The sulfur atoms fulfil the sphere-packing condition for type 8/3/*h*14 to good approximation.

Some further examples for crystal structures that can be described by means of sphere packings in $R\bar{3}m$ 18*h* have already been presented by Sowa & Koch (1999).

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