Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 14 February 2005
Accepted 7 March 2005

Hexagonal and trigonal sphere packings. III. Trivariant lattice complexes of hexagonal space groups

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All types of homogeneous sphere packing and interpenetrating sphere packings and layers were derived that correspond to point configurations of the 15 trivariant hexagonal lattice complexes. The respective sphere packings are assigned to 147 types. In total, sphere packings of 170 types can be realized with hexagonal symmetry. 103 types of sphere packing refer exclusively to trivariant hexagonal lattice complexes. For 23 of these types, the corresponding sphere packings can be generated only in hexagonal lattice complexes with less than three degrees of freedom or with trigonal or lower symmetry. In addition, seven types of interpenetrating sphere packings and two types of interpenetrating sphere layers were found. Interpenetrating 4.8^2 nets of spheres with 120° angles between the nets were assumed to be not possible, so far. The sphere packings belonging to 85 of the 170 hexagonal types can be split up into parallel layers of spheres with mutual contact and can be characterized by symbols derived from those for the Shubnikov nets. The sphere packings of 135 hexagonal types may be subdivided into rod-like subsets of spheres with mutual contact. Such rods may be described by rolling up a plane net. Only 23 types of sphere packing cannot be symbolized on the basis of layers or rods of spheres with mutual contact. Examples are given for crystal structures that can be described by means of sphere packings.

1. Introduction

In two previous papers (Sowa *et al.*, 2003; Sowa & Koch, 2004*a*), all types of sphere packing and interpenetrating sphere packings and layers have been presented that correspond to point configurations of the trigonal and hexagonal lattice complexes with less than three degrees of freedom.[1] All necessary definitions and information on the derivation of such sphere configurations may be taken from the preceding papers.

During the examination of the general position of $P6_222$ (Koch & Sowa, 2004), it became apparent that a purely graph-theoretical definition of sphere-packing types is inadequate and that the procedure for the assignment of sphere packings to types has to be modified. Sphere packings generated by identical symmetry operations may occur within two disjoint and non-congruent parameter regions with different minimal densities of the packings belonging to each region. Both variants, however, are characterized by isomorphic graphs. In the meantime, an analogous case with cubic symmetry has been described (Fischer, 2004).

[1] M. O'Keeffe kindly apprised us that the sphere packings in $R3c$ 18(*b*) assigned to type 8/3/*h*12 have cubic inherent symmetry and belong to type 8/3/*c*1.

The present paper gives characteristic data for the sphere packings and interpenetrating sphere packings and layers referring to the 15 trivariant lattice complexes of the hexagonal crystal system. Only some of the sphere packings with symmetry $P6_122$ 12*c* and $P6_222$ 12*k* have been known before (Sowa & Koch, 2002; Koch & Sowa, 2004).

2. Results

Significant data on all types of sphere packing, of interpenetrating sphere packings and of interpenetrating sphere layers corresponding to the 15 trivariant hexagonal lattice complexes are summarized in Table 1.

(1) Each lattice complex is identified by its characteristic Wyckoff position. In addition, the range of the coordinate parameters is given that has to be examined, *i.e.* one asymmetric unit of the Euclidean normalizer of the space group under consideration (*cf. e.g.* Koch *et al.*, 2002).

(2) In a second block, all possible neighbouring points of an original point at x, y, z are listed. For symmetry reasons, sets with two or more equidistant neighbouring points may be formed, irrespective of the choice of the free coordinate or

Table 1
Sphere packings, interpenetrating sphere packings and interpenetrating sphere layers corresponding to the 15 trivariant hexagonal lattice complexes.

P*$\bar{6}$ 6*l			**$0 < x \leq \frac{1}{3}; 0 \leq y \leq \frac{1}{2}x; 0 \leq z < \frac{1}{4}$**							
A	$x, y, -z$		*C*	$-y, x-y, z$	*D*	$-y+1, x-y, z$	*E*	$-y, x-y-1, z$		
B	$x, y, -z+1$			$-x+y, -x, z$		$-x+y+1, 1-x, z$		$-x+y+1, -x, z$		
0.1	8/3/*h*4	*ABCDE*	$\frac{1}{3}, 0, \frac{1}{4}; \frac{2}{3}\sqrt{3}$				0.60460			
1.1	6/3/*h*13	*ABCD*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{4}; 1$				0.45345	$1 \leq c < \frac{2}{3}\sqrt{3}$		
P*6/*m* 12*l			**$0, 2x-1 \leq y \leq \frac{1}{2}x; 0 < z \leq \frac{1}{4}$**							
A	$x, y, -z$		*C*	$x-y, x, z$	*D*	$-x+1, y, z$	*E*	$-y+1, x-y, z$		
B	$x, y, -z+1$			$y, -x+y, z$				$-x+y+1, -x+1, z$		
0.1	7/3/*h*13	*ABCDE*	$\frac{3}{7}, \frac{1}{7}, \frac{1}{4}; \frac{2}{7}\sqrt{7}$				0.51823			
1.1	5/3/*h*5	*ABDE*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, \frac{1}{4}; 4-2\sqrt{3}$				0.26045	$4-2\sqrt{3} \leq c < \frac{2}{7}\sqrt{7}$		
1.2	5/4/*h*5	*ABCD*	$\frac{1}{3}, 0, \frac{1}{4}; \frac{2}{3}$				0.40307	$\frac{2}{3} \leq c < \frac{2}{7}\sqrt{7}$		
1.3	6/3/*h*20	*ABDE*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{4}; \sqrt{3}-1$				0.48601	$\sqrt{3}-1 \leq c < \frac{2}{7}\sqrt{7}$		
P*6_3/*m* 12*i			**$0, 2x-1 \leq y \leq \frac{1}{2}x; 0 \leq z < \frac{1}{4}$**							
A	$y, -x+y, -z$		*B*	$x, y, -z+\frac{1}{2}$	*E*	$-y+1, x-y, z$	*F*	$-y, x-y, z$	*G*	$-y, x-y-1, z$
	$x-y, x, -z$		*C*	$x, y, -z-\frac{1}{2}$		$-x+y+1, -x+1, z$		$-x+y, -x, z$		$-x+y+1, -x, z$
			D	$-x+1, -y, -z$						
0.1	7/3/*h*13	*ABCDE*	$\frac{3}{7}, \frac{1}{7}, 0; \frac{2}{7}\sqrt{7}$				0.51823			
0.2	10/3/*h*2	*ABDEFG*	$\frac{1}{3}, 0, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$				0.66568			
1.1	5/3/*h*5	*BCDE*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, 0; 4-2\sqrt{3}$				0.26045	$4-2\sqrt{3} \leq c < \frac{2}{7}\sqrt{7}$		
1.2	5/4/*h*5	*ABCD*	$\frac{1}{3}, 0, 0; \frac{2}{3}$				0.40307	$\frac{2}{3} \leq c < \frac{2}{7}\sqrt{7}$		
1.3	6/3/*h*20	*ABCE*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, 0; \sqrt{3}-1$				0.48601	$\sqrt{3}-1 \leq c < \frac{2}{7}\sqrt{7}$		
1.4	6/3/*h*31	*ABDE*	0.41442, 0.12565, 0.07291; 1.14034				0.41914	$\frac{2}{7}\sqrt{7} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.5	7/3/*h*20	*ABEF*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; 1+\frac{1}{3}\sqrt{6}$				0.49926	$1+\frac{1}{3}\sqrt{6} \leq c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.6	6/3/*h*13	*BDEG*	$\frac{1}{2}, 0, \frac{1}{8}; 2$				0.45345	$2 \leq c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.1	4/3/*h*4	*BDE*	0.57018, 0.14036, 0.08796; 0.89321				0.19701	$4-2\sqrt{3} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.2	4/6/*h*2	*ABD*	$\frac{1}{3}, 0, \frac{1}{16}; \frac{2}{3}\sqrt{2}$				0.34009	$\frac{2}{3} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.3	5/3/*h*9	*ABE*	0.40475, 0.20238, 0.07778; 1.14060				0.38572	$\sqrt{3}-1 < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
P*622 12*n			**$0, 2x-1 \leq y \leq \frac{1}{2}x; 0 \leq z \leq \frac{1}{4}$**							
A	$x-y, -y, -z$		*D*	$x, x-y, -z+1$	*G*	$x, y, z+1$	*H*	$x-y, x, z$	*I*	$-y+1, x-y, z$
B	$x-y, -y, -z+1$		*E*	$-x+y+1, y, -z$		$x, y, z-1$		$y, -x+y, z$		$-x+y+1, -x+1, z$
C	$x, x-y, -z$		*F*	$-x+y+1, y, -z+1$					*J*	$-x+1, -y, z$
0.1	8/3/*h*15	*ABCDEFG*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{4}; \frac{1}{3}\sqrt{3}-\frac{1}{3}$				0.43201			
0.2	7/3/*h*14	*ABCDEFJ*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{4}; 1-\frac{1}{3}\sqrt{3}$				0.45821			
0.3	7/3/*h*15	*CDEFIJ*	$\frac{1}{3}\sqrt{6}-\frac{1}{3}, \frac{1}{3}\sqrt{6}-\frac{2}{3}, \frac{1}{4}; 2\sqrt{2}-\frac{4}{3}\sqrt{3}$				0.44882			
0.4	7/3/*h*16	*ABCDHJ*	$0.40013, 0.10722, \frac{1}{4}; 0.61389$				0.54567			
0.5	7/3/*h*17	*CDHIJ*	$\frac{3}{7}, \frac{1}{7}, \frac{1}{4}; \frac{2}{7}\sqrt{6}$				0.55975			
1.1	5/4/*h*17	*ACEG*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, 0; \frac{1}{2}-\frac{1}{6}\sqrt{3}$				0.32400	$\frac{1}{2}-\frac{1}{6}\sqrt{3} \leq c < \frac{1}{3}\sqrt{3}-\frac{1}{3}$		
1.2	6/4/*h*10	*ABCDEF*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{4}; \frac{1}{2}\sqrt{2}-\frac{1}{6}\sqrt{6}$				0.42089	$\frac{1}{3}\sqrt{3}-\frac{1}{3} < c < 1-\frac{1}{3}\sqrt{3}$		
1.3	5/4/*h*18	*ABCDJ*	$\{0.43301, 0.11603, \frac{1}{4}; \frac{1}{2}\}$				>0.45821	$1-\frac{1}{3}\sqrt{3} < c < 0.61389$		
1.4	5/4/*h*19	*CDEFJ*	$0.47385, 0.14051, \frac{1}{4}; 0.48675$				0.44621	$1-\frac{1}{3}\sqrt{3} < c < 2\sqrt{2}-\frac{4}{3}\sqrt{3}$		
1.5	5/3/*h*7	*CDIJ*	$\{0.47414, 0.14888, \frac{1}{4}; 0.55\}$				>0.44882	$2\sqrt{2}-\frac{4}{3}\sqrt{3} < c < \frac{2}{7}\sqrt{6}$		
1.6	5/3/*h*5	*EFIJ*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, \frac{1}{4}; 4-2\sqrt{3}$				0.26045	$2\sqrt{2}-\frac{4}{3}\sqrt{3} < c \leq 4-2\sqrt{3}$		
1.7	5/4/*h*5	*ABHJ*	$\frac{1}{3}, 0, \frac{1}{4}; \frac{2}{3}$				0.40307	$0.61389 < c \leq \frac{2}{3}$		
1.8	5/4/*h*20	*CDHJ*	$0.40396, 0.11227, \frac{1}{4}; 0.62688$				0.54522	$0.61389 < c < \frac{2}{7}\sqrt{6}$		
1.9	6/3/*h*20	*CDHI*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{4}; \sqrt{3}-1$				0.48601	$\frac{2}{7}\sqrt{6} < c \leq \sqrt{3}-1$		
*n*2.1	$h[6^3]^3$	*CDJ*	$\{0.45, 0.1275, \frac{1}{4}; \frac{1}{2}\}$				>0.44621	$1-\frac{1}{3}\sqrt{3} < c < \frac{2}{7}\sqrt{6}$		
P*$6_1$22 12*c			**$0, 2x-1 \leq y \leq \frac{1}{2}x; 0 \leq z < \frac{1}{2}$**							
A	$x, x-y, -z+\frac{1}{6}$		*G*	$x-y, -y, -z+1$	*M*	$-y+1, -x+1, -z+\frac{5}{6}$	*Q*	$-x+1, -x+y, -z+\frac{2}{3}$	*U*	$x+1, y, z$
B	$x-y, -y, -z$		*H*	$-y, -x, -z+\frac{5}{6}$	*N*	$-y+1, -x+1, -z-\frac{1}{6}$		$-x+1, -x+y+1, -z+\frac{2}{3}$		$x, y+1, z$
C	$-x+y+1, y, -z+\frac{1}{2}$		*I*	$x, x-y, -z+\frac{7}{6}$	*O*	$x-y, x, z+\frac{1}{6}$	*R*	$x-y, -y+1, -z$		$x+1, y+1, z$
D	$x, y, z+1$		*J*	$x-y, -y+1, -z+1$		$y, -x+y, z-\frac{1}{6}$		$x-y+1, -y+1, -z$		$x-1, y, z$
	$x, y, z-1$			$x-y+1, -y+1, -z+1$	*P*	$y, x-1, -z+\frac{1}{3}$	*S*	$x, x-y-1, -z+\frac{1}{6}$		$x, y-1, z$
E	$y, x, -z+\frac{1}{3}$		*K*	$-x+y+1, y, -z-\frac{1}{2}$		$y+1, x, -z+\frac{1}{3}$	*T*	$-x+2, -x+y+1, -z+\frac{2}{3}$		$x-1, y-1, z$
F	$-x, -x+y, -z+\frac{2}{3}$		*L*	$-x+y, y, -z+\frac{1}{2}$						
0.1	6/3/*h*32	*ABCDK*	$\frac{38}{103}+\frac{1}{103}\sqrt{105}, \frac{54}{103}-\frac{4}{103}\sqrt{105}, 0; \frac{54}{103}\sqrt{3}-\frac{12}{103}\sqrt{35}$				0.34737			
0.2	6/3/*h*33	*ABCDG*	$\frac{26}{97}+\frac{12}{97}\sqrt{2}, \frac{45}{97}-\frac{24}{97}\sqrt{2}, \frac{1}{4}; \frac{90}{97}-\frac{48}{97}\sqrt{2}$				0.37721			
0.3	6/3/*h*34	*ACDGI*	$\frac{1}{12911}(4250+2796\sqrt{2}-261\sqrt{105}+\frac{56}{3}\sqrt{210})$, $\frac{4}{12911}(376+138\sqrt{2}-96\sqrt{105}+\frac{169}{3}\sqrt{210}), \frac{1}{3}$; $\frac{12}{12911}(69\sqrt{3}+94\sqrt{6}+\frac{169}{2}\sqrt{35}-72\sqrt{70})$				0.38323			
0.4	5/4/*h*13	*ABCKN*	$\frac{2}{5}\sqrt{6}-\frac{2}{5}, \frac{4}{5}\sqrt{6}-\frac{9}{5}, 0; \frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3}$				0.27718			
0.5	6/3/*h*35	*ABCGO*	$\frac{27}{56}-\frac{1}{56}\sqrt{57}, \frac{25}{56}-\frac{3}{56}\sqrt{57}, \frac{1}{4}; \frac{3}{14}(11\sqrt{57}-73)^{1/2}$				0.44753			

Table 1 (continued)

0.6	6/3/*h*36	*ACGIO*	$\frac{27}{48}-\frac{1}{48}\sqrt{57}, \frac{7}{48}\sqrt{57}-\frac{15}{16}, \frac{1}{3}; \frac{3}{4}(9\sqrt{57}-67)^{1/2}$	0.51750	
0.7	6/4/*h*5	*ACIMO*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{3}; \frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$	0.54676	
0.8	6/3/*h*37	*CGIMO*	0.42523, 0.18415, 0.36939; 0.92606	0.50257	
0.9	6/3/*h*38	*CGHMO*	0.43726, 0.06274, 0.37215; 2.03611	0.53605	
0.10	7/3/*h*6	*CHMOQ*	$\frac{3}{5}-\frac{1}{15}\sqrt{6}, \frac{1}{15}\sqrt{6}-\frac{1}{10}, \frac{1}{6}+\frac{1}{12}\sqrt{6}; \frac{3}{5}+\frac{3}{5}\sqrt{6}$	0.53633	
0.11	6/4/*h*3	*CGHMQ*	$\frac{1}{2}, 0, \frac{3}{8}; \frac{3}{2}\sqrt{2}$	0.51013	
(0.11)		*ABCPS*	$\frac{1}{2}, 0, \frac{1}{8};$		
0.12	7/3/*h*8	*CFHOQ*	$\frac{1}{3}, 0, \frac{1}{3}; 2\sqrt{2}$	0.49365	
0.12′		*ACEOP*	$\frac{1}{3}, 0, \frac{1}{6};$		
0.13	7/3/*h*7	*FHMOQ*	$\frac{1}{3}, \frac{1}{6}, \frac{7}{12}-\frac{1}{12}\sqrt{7}; (5+2\sqrt{7})^{1/2}$	0.50736	
0.13′		*CFLOQ*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{12}+\frac{1}{12}\sqrt{7};$		
0.14	11/3/*h*1	*FHMQU*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{2}\sqrt{2}-\frac{1}{3}; 3\sqrt{3}+2\sqrt{6}$	0.71868	
0.14′		*CFLQU*	$\frac{1}{3}, \frac{1}{6}, 1-\frac{1}{2}\sqrt{2};$		
1.1	5/4/*h*27	*ABCD*	0.45926, 0.12213, 0.08941; 0.21501	0.33539	$0.21501 \le c < \frac{90}{97}-\frac{48}{97}\sqrt{2}$
1.2	5/4/*h*28	*CDGI*	0.46572, 0.12606, 0.47752; 0.21856	0.34656	$0.21856 \le c < \frac{12}{12911}(69\sqrt{3}+94\sqrt{6}+\frac{169}{2}\sqrt{35}-72\sqrt{70})$
1.3	4/4/*h*30	*ABCK*	0.51719, 0.14160, 0; 0.44117	0.24263	$\frac{54}{103}\sqrt{3}-\frac{12}{103}\sqrt{35} < c < \frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3}$
1.4	5/4/*h*29	*ACDG*	0.44496, 0.11729, 0.27438; 0.22765	0.37599	$0.22765 \le c < \frac{12}{12911}(69\sqrt{3}+94\sqrt{6}+\frac{169}{2}\sqrt{35}-72\sqrt{70})$
1.5	4/4/*h*31	*ABCG*	$0.42193, 0.09963, \frac{1}{4}; 0.37757$	0.32152	$\frac{90}{97}-\frac{48}{97}\sqrt{2} < c < \frac{3}{14}(11\sqrt{57}-73)^{1/2}$
1.6	4/6/*h*13	*ACGI*	$0.44058, 0.13031, \frac{1}{3}; 0.36551$	0.33492	$\frac{12}{12911}(69\sqrt{3}+94\sqrt{6}+\frac{169}{2}\sqrt{35}-72\sqrt{70}) < c < \frac{3}{4}(9\sqrt{57}-67)^{1/2}$
1.7	4/4/*h*32	*CGIM*	0.55516, 0.16255, 0.45700; 0.68319	0.25267	$\frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3} < c \le 0.92647$
1.8	5/3/*h*12	*ABCO*	0.33342, 0.00317, 0.17036; 1.11651	0.35785	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c < 2.03611$
1.8′		*CGHO*			
1.9	5/4/*h*15	*BCGO*	$\frac{16}{23}-\frac{6}{23}\sqrt{2}, 0, \frac{1}{4}; \frac{24}{23}\sqrt{2}-\frac{18}{23}$	0.43565	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c \le \frac{24}{23}\sqrt{2}-\frac{18}{23}$
1.10	5/4/*h*30	*ACGO*	0.36114, 0.07289, 0.27451; 0.72959	0.43527	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c \le 0.75533$
1.11	5/4/*h*31	*ACIO*	$\{0.40813, 0.17122, \frac{1}{3}; 0.74\}$	>0.51750	$\frac{3}{4}(9\sqrt{57}-67)^{1/2} < c < \frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$
1.12	5/3/*h*13	*CGIO*	0.41968, 0.17899, 0.36256; 0.87924	0.50123	$\frac{3}{4}(9\sqrt{57}-67)^{1/2} < c < 0.92606$
1.13	5/4/*h*32	*CIMO*	{0.42326, 0.19897, 0.35253; 0.85}	>0.50257	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 0.92606$
1.14	5/4/*h*33	*CGMO*	0.42850, 0.15033, 0.37010; 1.36494	0.45259	$0.92606 < c < 2.03611$
1.15	5/3/*h*14	*ACEO*	0.36626, 0.13279, 0.20657; 1.67944	0.33402	$0.92606 < c < 2\sqrt{2}$
1.15′		*GIMO*			
1.16	5/4/*h*34	*CHMO*	{0.43703, 0.06297, 0.37158; 2.05}	>0.53605	$2.03611 < c < \frac{3}{5}+\frac{3}{5}\sqrt{6}$
1.17	4/6/*h*14	*CGHM*	{0.44251, 0.05749, 0.37264; 2.05}	>0.51013	$2.03611 < c < \frac{3}{2}\sqrt{2}$
1.18	5/3/*h*15	*CELO*	0.29917, 0.09833, 0.23748; 2.57658	0.36081	$2.03611 < c < (5+2\sqrt{7})^{1/2}$
1.18′		*GHMO*			
(1.18′)		*CFLO*			
1.19	6/3/*h*3	*CMOQ*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{3}; 3\sqrt{3}-3$	0.45821	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c \le 3\sqrt{3}-3$
1.20	6/3/*h*7	*CHOQ*	0.37085, 0.03323, 0.34261; 2.51648	0.47900	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < 2\sqrt{2}$
1.21	6/3/*h*4	*HMOQ*	0.38027, 0.11973, 0.36661; 2.77353	0.48934	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < (5+2\sqrt{7})^{1/2}$
1.22	5/4/*h*6	*CHMQ*	{0.45918, 0.04082, 0.37330; 2.1}	>0.51013	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < \frac{3}{2}\sqrt{2}$
1.23	5/4/*h*5	*ACEP*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{6}; 2\sqrt{3}$	0.40307	$2\sqrt{2} < c \le 2\sqrt{3}$
(1.23)		*ABNR*	$\frac{2}{3}, \frac{1}{3}, 0;$		
(1.23)		*CMQT*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3};$		
1.24	6/3/*h*5	*CFOQ*	$\frac{1}{3}, 0.06833, 0.32081; 2.97518$	0.48107	$2\sqrt{2} < c < (5+2\sqrt{7})^{1/2}$
1.25	6/3/*h*6	*FHOQ*	$\frac{1}{3}, 0.06833, 0.34585; 2.97518$	0.48107	$2\sqrt{2} < c < (5+2\sqrt{7})^{1/2}$
1.26	5/4/*h*35	*FHMQ*	$\frac{1}{3}, \frac{1}{6}, 0.36927; 4.67170$	0.46271	$(5+2\sqrt{7})^{1/2} < c < 3\sqrt{3}+2\sqrt{6}$
1.26′		*CFLQ*	$\frac{1}{3}, \frac{1}{6}, 0.29739;$		
1.27	9/3/*h*3	*GHMU*	$\frac{1}{2}, 0, \frac{1}{6}+\frac{1}{6}\sqrt{3}; 6+3\sqrt{3}$	0.64801	$3\sqrt{3}+2\sqrt{6} < c \le 6+3\sqrt{3}$
(1.27)		*ABSU*	$\frac{1}{2}, 0, \frac{1}{3}-\frac{1}{6}\sqrt{3};$		
(1.27)		*CELU, CFLU*			
1.28	10/3/*h*2	*CEPU*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{12}\sqrt{6}; 6+2\sqrt{6}$	0.66568	$3\sqrt{3}+2\sqrt{6} < c \le 6+2\sqrt{6}$
(1.28)		*CQTU*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}-\frac{1}{12}\sqrt{6};$		
(1.28)		*FHQU*			
1.28′		*AEPU*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3}-\frac{1}{12}\sqrt{6};$		
(1.28′)		*ABRU*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{12}\sqrt{6}-\frac{1}{6};$		
(1.28′)		*MQTU*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{6}+\frac{1}{12}\sqrt{6};$		
(1.28′)		*GJMU*	$\frac{2}{3}, \frac{1}{3}, \frac{2}{3}-\frac{1}{12}\sqrt{6};$		
(1.28′)		*CFQU*			
1.29	10/3/*h*3	*HMQU*	$\frac{1}{2}, 0, \frac{3}{8}; 6\sqrt{3}$	0.69813	$3\sqrt{3}+2\sqrt{6} < c \le 6\sqrt{3}$
(1.29)		*APSU*	$\frac{1}{2}, 0, \frac{1}{8};$		
2.1	3/8/*h*4	*ABC*	0.48832, 0.11851, 0.10345; 0.71442	0.16434	$0.21501 < c < \frac{3}{2}\sqrt{2}$
(2.1)		*CGM*			
2.1′		*CGH*			
2.2	3/10/*h*2	*CGI*	0.50282, 0.14350, 0.45567; 0.51486	0.22740	$0.21856 < c < 0.92647$
2.3	3/10/*h*3	*ACG*	0.42689, 0.11006, 0.27909; 0.39107	0.31596	$0.22765 < c < 0.75533$
2.4	3/8/*h*2	*ABN*	$\frac{1}{8}\sqrt{33}-\frac{1}{8}, \frac{1}{4}\sqrt{33}-\frac{5}{4}, 0; \frac{9}{4}\sqrt{3}-\frac{3}{4}\sqrt{11}$	0.17248	$\frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3} < c < 2\sqrt{3}$
(2.4)		*ACE*			

Table 1 (continued)

2.4′		*GIM*			
2.5	4/4/*h*33	*BCO*	0.33172, 0, 0.17067; 1.11360	0.35782	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c < 2.03611$
2.5′		*CGO*	0.33172, 0, 0.32933;		
2.6	4/4/*h*34	*ACO*	0.34926, 0.07370, 0.20305; 1.43592	0.32018	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c < 2\sqrt{2}$
2.6′		*CHO*			
(2.6′)		*IMO*			
2.7	4/4/*h*35	*CIO*	{0.40749, 0.16922, 0.334; 0.74}	>0.50123	$\frac{3}{4}(9\sqrt{57}-67)^{1/2} < c < 0.92606$
2.8	4/4/*h*2	*CMO*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{3}; \frac{3}{2}\sqrt{6}-\frac{3}{2}\sqrt{2}$	0.42089	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 3\sqrt{3}-3$
2.9	4/4/*h*36	*CEO*	0.34922, 0.12575, 0.22199; 1.89787	0.32641	$0.92606 < c < (5+2\sqrt{7})^{1/2}$
2.9′		*GMO*			
(2.9′)		*CFO*			
2.10	4/4/*h*1	*CLO*	$\frac{1}{4}, 0, \frac{1}{4}; \frac{3}{2}\sqrt{3}$	0.34907	$2.03611 < c < (5+2\sqrt{7})^{1/2}$
(2.10)		*HMO*			
2.11	3/10/*h*1	*GHM*	$\frac{1}{2}, 0, \frac{7}{16}; 3\sqrt{2}$	0.25507	$2.03611 < c < 6+3\sqrt{3}$
(2.11)		*ABS*	$\frac{1}{2}, 0, \frac{1}{16};$		
(2.11)		*CEL*, *CFL*			
2.12	5/3/*h*3	*COQ*	0.39470, 0.16940, 0.32635; 2.45054	0.44912	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < (5+2\sqrt{7})^{1/2}$
2.12′		*MOQ*			
2.13	4/4/*h*4	*CMQ*	$\frac{1}{8}+\frac{1}{24}\sqrt{105}, \frac{1}{16}+\frac{1}{48}\sqrt{105}, \frac{1}{3}; \frac{3}{8}\sqrt{3}+\frac{3}{8}\sqrt{35}$	0.33170	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < 2\sqrt{3}$
(2.13)		*ACP*, *CHQ*			
2.14	5/4/*h*7	*HOQ*	0.36278, 0.06658, 0.34988; 2.70053	0.47377	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < (5+2\sqrt{7})^{1/2}$
2.15	4/6/*h*1	*HMQ*	$\frac{1}{2}, 0, \frac{3}{8}; 3\sqrt{2}$	0.39270	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < 6\sqrt{3}$
(2.15)		*APS*	$\frac{1}{2}, 0, \frac{1}{8};$		
2.16	5/4/*h*11	*FOQ*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{3}; 3$	0.46542	$2\sqrt{2} < c < (5+2\sqrt{7})^{1/2}$
2.17	4/6/*h*2	*AEP*	$\frac{2}{3}, \frac{1}{3}, \frac{7}{48}; 2\sqrt{6}$	0.34009	$2\sqrt{2} < c < 6+2\sqrt{6}$
(2.17)		*ABR*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{48};$		
(2.17)		*MQT*	$\frac{2}{3}, \frac{1}{3}, \frac{17}{48};$		
(2.17)		*GMJ*	$\frac{2}{3}, \frac{1}{3}, \frac{23}{48};$		
(2.17)		*CFQ*			
2.17′		*CEP*	$\frac{2}{3}, \frac{1}{3}, \frac{3}{16};$		
(2.17′)		*CQT*	$\frac{2}{3}, \frac{1}{3}, \frac{5}{16};$		
(2.17′)		*FHQ*			
2.18	8/3/*h*4	*FHU*	$0, 0, \frac{3}{8}; 12$	0.60460	$3\sqrt{3}+2\sqrt{6} < c \leq 12$
(2.18)		*ABU*	$0, 0, \frac{1}{24};$		
(2.18)		*AEU*	$0, 0, \frac{1}{8};$		
(2.18)		*ELU*	$0, 0, \frac{5}{24};$		
(2.18)		*FLU*	$0, 0, \frac{7}{24};$		
(2.18)		*GHU*	$0, 0, \frac{11}{24};$		
(2.18)		*CEU*, *CFU*, *GMU*			
2.19	9/3/*h*3	*CPU*	$\frac{1}{2}, 0, \frac{1}{6}\sqrt{3}-\frac{1}{12}; 6+3\sqrt{3}$	0.64801	$3\sqrt{3}+2\sqrt{6} < c \leq 6+3\sqrt{3}$
(2.19)		*CQU*	$\frac{1}{2}, 0, \frac{7}{12}-\frac{1}{6}\sqrt{3};$		
(2.19)		*MQU*, *HQU*, *APU*			
*i*2.1	$h[3/10/h1]^2$	*CHM*	{0.44829, 0.05171, 0.3725; 2.08}	>0.51013	$2.03611 < c < \frac{3}{2}\sqrt{2}$
3.1	3/12/*h*1	*CO*	$\frac{17}{24}-\frac{1}{24}\sqrt{97}, 0, \frac{1}{4}; \frac{1}{4}(102-6\sqrt{97})^{1/2}$	0.29229	$\frac{3}{14}(11\sqrt{57}-73)^{1/2} < c < (5+2\sqrt{7})^{1/2}$
(3.1)		*MO*			
3.2	3/10/*h*1	*CQ*	$\frac{1}{2}, 0, \frac{5}{16}; 3\sqrt{2}$	0.25507	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < 6+2\sqrt{6}$
(3.2)		*CP*	$\frac{1}{2}, 0, \frac{3}{16};$		
(3.2)		*MQ*, *HQ*, *AP*			
3.3	4/4/*h*3	*OQ*	$\frac{5}{8}-\frac{1}{24}\sqrt{33}, \frac{5}{16}-\frac{1}{48}\sqrt{33}, \frac{1}{3}; \frac{3}{8}+\frac{3}{8}\sqrt{33}$	0.44621	$\frac{3}{5}+\frac{3}{5}\sqrt{6} < c < (5+2\sqrt{7})^{1/2}$
$P6_222$ 12*k*			**$0, 2x-1 \leq y \leq \frac{1}{2}x; 0 \leq z < \frac{1}{2}$**		
A	$x-y, -y, -z$		*D* $-x+y+1, y, -z$	*H* $x-y, -y, -z+1$	*L* $-x+1, -y+1, z$
B	$x, x-y, -z+\frac{1}{3}$		*E* $-x+1, -y, z$	*I* $x, x-y, -z+\frac{4}{3}$	*M* $-y, -x, -z+\frac{2}{3}$
C	$x, y, z+1$		*F* $-x, -y, z$	*J* $-y+1, -x+1, -z+\frac{2}{3}$	*N* $-x+2, -y+1, z$
	$x, y, z-1$		*G* $-x+y+1, y, -z+1$	*K* $y, x, -z+\frac{2}{3}$	
0.1	6/3/*h*30	*BCGHI*	$\frac{1}{20514}(6582+560\sqrt{3}+1089\sqrt{35}-459\sqrt{105}),$ $\frac{1}{20514}(1995+3115\sqrt{3}+288\sqrt{35}-630\sqrt{105}), \frac{5}{12};$ $\frac{3}{3419}(-630+96\sqrt{3}+89\sqrt{35}+19\sqrt{105})$	0.37038	
0.2	7/3/*h*21	*ABCDGH*	$\frac{1}{3862}(1202-144\sqrt{3}+195\sqrt{35}-33\sqrt{105}),$ $\frac{3}{3862}(387+291\sqrt{3}-32\sqrt{35}-54\sqrt{105}), \frac{1}{4};$ $\frac{3}{1931}(387+291\sqrt{3}-32\sqrt{35}-54\sqrt{105})$	0.38553	
0.3	6/3/*h*29	*ABDEGH*	$\frac{1}{26}(94+48\sqrt{3}-21\sqrt{17}-11\sqrt{51}),$ $\frac{3}{78}(-225-129\sqrt{3}+54\sqrt{17}+32\sqrt{51}), \frac{1}{4};$ $\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51})$	0.34157	
0.4	5/4/*h*13	*BDEGJ*	$\frac{2}{5}\sqrt{6}-\frac{2}{5}, \frac{4}{5}\sqrt{6}-\frac{9}{5}, \frac{1}{4}; \frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3}$	0.27718	
0.5	5/4/*h*15	*ABEHM*	$\frac{16}{23}-\frac{6}{23}\sqrt{2}, 0, \frac{1}{4}; \frac{24}{23}\sqrt{2}-\frac{18}{23}$	0.43565	

Table 1 (continued)

0.6	6/4/*h*5	*BGHIJK*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{5}{12}; \frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$	0.54676	
0.7	5/3/*h*10	*BEGHJ*	0.44027, 0.16318, 0.35849; 0.99868	0.46396	
0.8	5/4/*h*24	*BEHJK*	0.40819, 0.15737, 0.35189; 1.15110	0.52432	
0.9	5/4/*h*23	*BEHKM*	$\frac{1}{2}+\frac{1}{3}\sqrt{3}-3^{1/4}(\frac{1}{4}\sqrt{2}+\frac{1}{12}\sqrt{6}), \frac{1}{6}\sqrt{3}-3^{1/4}(\frac{1}{4}\sqrt{2}-\frac{1}{12}\sqrt{6}), \frac{1}{3};$ $3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3}$	0.49270	
0.10	6/3/*h*3	*EGHJKL*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{5}{12}; 3\sqrt{3}-3$	0.45821	
0.11	5/3/*h*16	*BEFKM*	$\frac{1}{6}\sqrt{3}, \frac{1}{3}\sqrt{3}-\frac{1}{2}, \frac{1}{6}+\frac{1}{18}\sqrt{3}; \frac{3}{2}\sqrt{3}$	0.38733	
0.12	5/3/*h*2	*EFHKM*	$\frac{1}{6}\sqrt{3}, \frac{1}{3}\sqrt{3}-\frac{1}{2}, \frac{1}{2}-\frac{1}{18}\sqrt{3}; \frac{3}{2}\sqrt{3}$	0.38733	
0.13	5/3/*h*11	*ABDEL*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{6}\sqrt{2}-\frac{1}{6}; \frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6})$	0.37959	
(0.13)		*BEJKL*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{2};$		
0.14	5/4/*h*11	*EFHKL*	$\frac{1}{3}, \frac{1}{6}, \frac{5}{12}; 3$	0.46542	
0.15	5/4/*h*22	*ABEFL*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{3}\sqrt{3}-\frac{1}{2}; \frac{3}{2}+\sqrt{3}$	0.43201	
(0.15)		*BEFKL*	$\frac{1}{3}, \frac{1}{6}, \frac{5}{6}-\frac{1}{3}\sqrt{3};$		
0.16	5/4/*h*5	*BDELN*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{12}; 2\sqrt{3}$	0.40307	
(0.16)		*BEJLN*	$\frac{2}{3}, \frac{1}{3}, \frac{1}{4};$		
(0.16)		*EGJLN*	$\frac{2}{3}, \frac{1}{3}, \frac{5}{12};$		
1.1	5/4/*h*25	*ABCD*	0.45518, 0.12245, 0.07079; 0.21425	0.33304	$0.21425 \le c < \frac{3}{1931}(387+291\sqrt{3}-32\sqrt{35}-54\sqrt{105})$
1.1′		*CGHI*			
1.2	5/4/*h*16	*BCGH*	0.45469, 0.12378, 0.35630; 0.22385	0.36354	$0.22385 \le c < \frac{3}{1931}(387+291\sqrt{3}-32\sqrt{35}-54\sqrt{105})$
1.3	4/4/*h*25	*BGHI*	0.44811, 0.14176, $\frac{5}{12}$; 0.38651	0.30704	$\frac{3}{3419}(-630+96\sqrt{3}+89\sqrt{35}+19\sqrt{105}) < c < \frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2}$
1.4	5/4/*h*26	*ABDGH*	0.46116, 0.10610, $\frac{1}{4}$; 0.35625	0.34142	$\frac{3}{1931}(387+291\sqrt{3}-32\sqrt{35}-54\sqrt{105}) < c$ $< \frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51})$
1.5	4/4/*h*17	*BDEG*	0.53657, 0.14477, $\frac{1}{4}$; 0.50150	0.25657	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < \frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3}$
1.6	4/4/*h*23	*ABEH*	0.42259, 0.08038, $\frac{1}{4}$; 0.47041	0.31490	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < \frac{24}{23}\sqrt{2}-\frac{18}{23}$
1.7*a*	4/3/*h*9*a*	*ABDE*	0.45817, 0.11429, 0.09211; 1.07459	0.14815	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c$ $< \frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6})$
1.7*b*	4/3/*h*9*b*	*EGHJ*	0.43522, 0.17698, 0.39788; 1.50095	0.39382	$0.99868 < c < 3\sqrt{3}-3$
1.8	4/4/*h*16	*BEGJ*	0.55518, 0.16296, 0.29327; 0.68268	0.25155	$\frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3} < c < 0.99868$
1.9	4/4/*h*22	*BEHM*	0.33228, 0.02560, 0.29669; 0.88789	0.39328	$\frac{24}{23}\sqrt{2}-\frac{18}{23} < c < 3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3}$
1.10	4/4/*h*28	*BGHJ*	0.43941, 0.16555, 0.36026; 0.99085	0.46383	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 0.99868$
1.11	4/4/*h*24	*BHJK*	0.41580, 0.18577, 0.37326; 0.97670	0.49708	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 1.15110$
1.12	4/4/*h*2	*GHJK*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{5}{12}; \frac{3}{2}\sqrt{6}-\frac{3}{2}\sqrt{2}$	0.42089	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 3\sqrt{3}-3$
1.13	4/4/*h*27	*BEHJ*	{0.42537, 0.16069, 0.35516; 1.07}	>0.46396	$0.99868 < c < 1.15110$
1.14	4/4/*h*37	*BEHK*	0.35098, 0.10020, 0.33524; 1.20854	0.49211	$1.15110 < c < 3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3}$
1.15	4/4/*h*29	*BEJK*	0.41446, 0.18078, 0.27671; 2.12657	0.35647	$1.15110 < c < \frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6})$
1.16	4/4/*h*26	*EHJK*	0.41422, 0.17988, 0.40033; 1.76305	0.42629	$1.15110 < c < 3\sqrt{3}-3$
1.17	4/4/*h*38	*BEKM*	0.31767, 0.08512, 0.27401; 2.09506	0.36722	$3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3} < c < \frac{3}{2}\sqrt{3}$
1.18	4/4/*h*21	*EHKM*	0.31767, 0.08512, 0.39266; 2.09506	0.36722	$3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3} < c < \frac{3}{2}\sqrt{3}$
1.19	4/4/*h*3	*EHKL*	$\frac{5}{8}-\frac{1}{24}\sqrt{33}, \frac{5}{16}-\frac{1}{48}\sqrt{33}, \frac{5}{12}; \frac{3}{8}+\frac{3}{8}\sqrt{33}$	0.44621	$3\sqrt{3}-3 < c < 3$
1.20	4/4/*h*4	*EGJL*	$\frac{1}{8}+\frac{1}{24}\sqrt{105}, \frac{1}{16}+\frac{1}{48}\sqrt{105}, \frac{5}{12}; \frac{3}{8}\sqrt{3}+\frac{3}{8}\sqrt{35}$	0.33170	$3\sqrt{3}-3 < c < 2\sqrt{3}$
1.21	4/4/*h*1	*BEFM*	$\frac{1}{4}, 0, \frac{1}{4}; \frac{3}{2}\sqrt{3}$	0.34907	$c = \frac{3}{2}\sqrt{3}$
1.22	4/4/*h*39	*BEFK*	0.29053, 0.08105, 0.26254; 2.62436	0.38723	$\frac{3}{2}\sqrt{3} < c < \frac{3}{2}+\sqrt{3}$
1.23	4/4/*h*20	*ABEF*	0.26269, 0.02538, 0.08726; 2.86499	0.32022	$\frac{3}{2}\sqrt{3} < c < \frac{3}{2}+\sqrt{3}$
1.23′		*EFHM*			
1.24	4/4/*h*40	*EFHK*	$\{\frac{7}{24}, \frac{1}{12}$, 0.40476; 2.625}	>0.38733	$\frac{3}{2}\sqrt{3} < c < 3$
1.25	4/4/*h*18	*BDEL*	0.53061, 0.26531, 0.07959; 2.88698	0.31945	$\frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6}) < c < 2\sqrt{3}$
(1.25)		*BEJL*	0.53061, 0.26531, 0.25375;		
1.26	4/4/*h*19	*BEKL*	{0.39798, 0.19899, 0.26136; 2.8}	>0.37959	$\frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6}) < c < \frac{3}{2}+\sqrt{3}$
(1.26)		*ABEL*			
*i*1.1	$h[4/3/h9a]^2$	*BEGH*	0.45817, 0.11429, 0.31578; 0.53729	0.29631	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < 0.99868$
2.1*a*	3/4/*h*1*a*	*ABD*	0.45337, 0.12740, 0.07476; 0.90013	0.13918	$0.21425 < c < \frac{3}{2}(-1-\sqrt{2}+\sqrt{3}+\sqrt{6})$
2.1*a*′		*GHI*			
(2.1*a*)		*BJK*			
2.1*b*	3/4/*h*1*b*	*GHJ*	{0.43223, 0.18515, 0.38400; 1}	>0.39382	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 3\sqrt{3}-3$
2.2*a*	3/4/*h*2*a*	*ABE*	0.43559, 0.09867, 0.09899; 1.14900	0.14544	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < \frac{3}{2}+\sqrt{3}$
2.2*a*′		*EHM*			
2.2*b*	3/4/*h*2*b*	*EHJ*	{0.43126, 0.16211, 0.36; 1.07}	>0.39382	$0.99868 < c < 3\sqrt{3}-3$
2.3	3/4/*h*3	*BDE*	0.53120, 0.14951, 0.10710; 1.20898	0.12240	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < 2\sqrt{3}$
2.3′		*EGJ*			
2.4	3/8/*h*2	*BEJ*	$\frac{1}{8}\sqrt{33}-\frac{1}{8}, \frac{1}{4}\sqrt{33}-\frac{5}{4}, \frac{1}{4}; \frac{9}{4}\sqrt{3}-\frac{3}{4}\sqrt{11}$	0.17248	$\frac{24}{5}\sqrt{2}-\frac{18}{5}\sqrt{3} < c < 2\sqrt{3}$
2.5	3/12/*h*1	*BEM*	$\frac{17}{24}-\frac{1}{24}\sqrt{97}, 0, \frac{1}{4}; \frac{1}{4}(102-6\sqrt{97})^{1/2}$	0.29229	$\frac{24}{23}\sqrt{2}-\frac{18}{23} < c < \frac{3}{2}\sqrt{3}$
2.6	3/8/*h*5	*BHJ*	{0.42483, 0.19254, 0.38409; 0.9}	>0.46383	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 1.15110$
2.7	3/8/*h*6	*BEK*	0.37633, 0.14769, 0.27430; 2.15379	0.35115	$1.15110 < c < \frac{3}{2}+\sqrt{3}$
*i*2.1	$h[3/4/h1a]^2$	*BGH*	0.45337, 0.12740, 0.35048; 0.45007	0.27835	$0.22385 < c < 0.99868$
*i*2.2	$h[3/4/h2a]^2$	*BEH*	0.43559, 0.09867, 0.30202; 0.57450	0.29088	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c$ $< 3^{1/4}(\frac{3}{4}\sqrt{2}+\frac{3}{4}\sqrt{6})-\frac{3}{2}\sqrt{3}$
*i*2.3	$h[3/4/h3]^2$	*BEG*	0.53120, 0.14951, 0.28580; 0.60449	0.24480	$\frac{3}{13}(-129-75\sqrt{3}+32\sqrt{17}+18\sqrt{51}) < c < 0.99868$

Table 1 (continued)

*i*2.4	$h[3/4/h1a]^3$	*HJK*	0.41923, 0.19857, 0.40810; 1.55908	0.41753	$\frac{3}{4}\sqrt{6}-\frac{3}{4}\sqrt{2} < c < 3\sqrt{3}-3$		
*i*2.5	$h[3/4/h3]^3$	*EHK*	0.31929, 0.08711, 0.39290; 2.09402	0.36720	$1.15110 < c < 3$		
P*6₃22 12*i			**$0, 2x-1 \le y \le \frac{1}{2}x; 0 \le z \le \frac{1}{4}$**				
A	$x-y, -y, -z$		*E* $-x+y+1, y, -z-\frac{1}{2}$; *G* $-y, x-y, z$	*I*	$x-y, -y, -z+1$	*L*	$y, x, -z$
B	$x, x-y, -z+\frac{1}{2}$		*F* $x, y, z+1$; $-x+y, -x, z$	*J*	$-y, -x, -z+\frac{1}{2}$		
C	$x, x-y, -z-\frac{1}{2}$		$x, y, z-1$; *H* $-y+1, x-y, z$	*K*	$-y, x-y-1, z$		
D	$-x+y+1, y, -z+\frac{1}{2}$		$-x+y+1, -x+1, z$		$-x+y+1, -x, z$		
0.1	6/3/*h*28	*ABDFI*	$\frac{4}{9}, \frac{1}{9}, \frac{1}{4}; \frac{2}{9}$	0.35828			
0.2	7/3/*h*18	*ABCDEF*	$\frac{7}{15}, \frac{2}{15}, 0; \frac{2}{15}\sqrt{3}$	0.38694			
0.3	7/3/*h*19	*ABCDEH*	$\frac{1}{2}, \frac{1}{6}, 0; \frac{1}{3}\sqrt{2}$	0.37024			
0.4	5/4/*h*5	*ABDIJ*	$\frac{1}{3}, 0, \frac{1}{4}; \frac{2}{3}$	0.40307			
0.5	6/3/*h*20	*ABCHL*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, 0; \sqrt{3}-1$	0.48601			
0.6	7/3/*h*20	*ABGHL*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; 1+\frac{1}{3}\sqrt{6}$	0.49926			
0.7	10/3/*h*2	*ABDGHJK*	$\frac{1}{3}, 0, \frac{3}{4}-\frac{1}{4}\sqrt{6}; \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$	0.66568			
1.1	5/4/*h*36	*ABDF*	0.45274, 0.11941, 0.15653; 0.21777	0.34405	$0.21777 \le c < \frac{2}{15}\sqrt{3}$		
1.2	4/4/*h*5	*ABDI*	$\frac{5}{12}, \frac{1}{12}, \frac{1}{4}; \frac{1}{6}\sqrt{6}$	0.27768	$\frac{2}{9} < c < \frac{2}{3}$		
1.3	5/4/*h*21	*ABCDE*	0.48100, 0.14767, 0; 0.35182	0.34503	$\frac{2}{15}\sqrt{3} < c < \frac{1}{3}\sqrt{2}$		
1.4	5/3/*h*5	*ADEH*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, 0; 4-2\sqrt{3}$	0.26045	$\frac{1}{3}\sqrt{2} < c \le 4-2\sqrt{3}$		
1.5	5/3/*h*8	*ABCH*	0.48786, 0.17112, 0; 0.51627	0.36587	$\frac{1}{3}\sqrt{2} < c < \sqrt{3}-1$		
1.6	5/3/*h*17	*ABDH*	0.48468, 0.15135, 0.10120; 0.86476	0.26274	$\frac{1}{3}\sqrt{2} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.7	4/6/*h*2	*ABDJ*	$\frac{1}{3}, 0, \frac{3}{16}; \frac{2}{3}\sqrt{2}$	0.34009	$\frac{2}{3} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.8	5/3/*h*9	*ABHL*	0.40475, 0.20238, 0.07778; 1.14060	0.38572	$\sqrt{3}-1 < c < 1+\frac{1}{3}\sqrt{6}$		
1.9	6/3/*h*39	*ABGH*	$\frac{1}{3}$, 0.13512, 0.11788; 1.88844	0.48887	$1+\frac{1}{3}\sqrt{6} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.10	6/3/*h*13	*ADHK*	$\frac{1}{2}, 0, \frac{1}{8}; 2$	0.45345	$2 \le c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.1	3/6/*h*3	*ABD*	$\frac{1}{6}\sqrt{7}, \frac{1}{6}\sqrt{7}-\frac{1}{3}$, 0.14714; 0.60475	0.20537	$0.21777 < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.2	4/3/*h*4	*ADH*	0.57018, 0.14036, 0.08796; 0.89321	0.19701	$\frac{1}{3}\sqrt{2} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
2.3	4/3/*h*10	*ABH*	{0.47152, 0.14355, 0.11109; 1}	>0.26274	$\frac{1}{3}\sqrt{2} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
P*$\bar{6}$*m*2 12*o			**$0 < x \le \frac{1}{3}; 0 \le y < \frac{1}{2}x; 0 < z \le \frac{1}{4}$**				
A	$x, y, -z$		*B* $x, y, -z+1$; *C* $x, x-y, z$	*D*	$-x+y+1, y, z$	*E*	$-y, -x, z$
0.1	5/4/*h*5	*ABCDE*	$\frac{1}{3}, 0, \frac{1}{4}; \frac{2}{3}$	0.40307			
P*$\bar{6}$*c*2 12*l			**$0 < x \le \frac{1}{3}; 0 \le y \le \frac{1}{2}x; 0 \le z < \frac{1}{4}$**				
A	$x, y, -z+\frac{1}{2}$		*C* $x, x-y, -z$; *F* $-y, x-y, z$	*G*	$-y+1, x-y, z$	*H*	$-y, x-y-1, z$
B	$x, y, -z-\frac{1}{2}$		*D* $-x+y+1, y, -z$; $-x+y, -x, z$		$-x+y+1, -x+1, z$		$-x+y+1, -x, z$
			E $-y, -x, -z$				
0.1	5/4/*h*5	*ABCDE*	$\frac{1}{3}, 0, 0; \frac{2}{3}$	0.40307			
0.2	10/3/*h*2	*ACDEFGH*	$\frac{1}{3}, 0, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$	0.66568			
1.1	4/6/*h*2	*ACDE*	$\frac{1}{3}, 0, \frac{1}{16}; \frac{2}{3}\sqrt{2}$	0.34009	$\frac{2}{3} < c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
1.2	6/3/*h*13	*ACFG*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{8}; 2$	0.45345	$2 \le c < \frac{2}{3}\sqrt{2}+\frac{2}{3}\sqrt{3}$		
P*$\bar{6}$2*m* 12*l			**$0 < y; 2x-1 \le y \le \frac{1}{2}x; 0 < z \le \frac{1}{4}$**				
A	$x, y, -z$		*B* $x, y, -z+1$; *C* $x-y, -y, z$	*D*	y, x, z	*E*	$-y+1, x-y, z$ $-x+y+1, -x+1, z$
0.1	6/3/*h*20	*ABCDE*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{4}; \sqrt{3}-1$	0.48601			
1.1	5/3/*h*5	*ABCE*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, \frac{1}{4}; 4-2\sqrt{3}$	0.26045	$4-2\sqrt{3} \le c < \sqrt{3}-1$		
P*$\bar{6}$2*c* 12*i			**$0, 2x-1 \le y \le \frac{1}{2}x; 0 \le z < \frac{1}{4}$**				
A	$x, y, -z+\frac{1}{2}$		*C* $x-y, -y, -z$; *E* $-y, x-y, z$	*F*	$-y+1, x-y, z$	*G*	$-y, x-y-1, z$
B	$x, y, -z-\frac{1}{2}$		*D* $y, x, -z$; $-x+y, -x, z$		$-x+y+1, -x+1, z$		$-x+y+1, -x, z$
0.1	6/3/*h*20	*ABCDF*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, 0; \sqrt{3}-1$	0.48601			
0.2	7/3/*h*20	*ACDEF*	$\frac{1}{3}, \frac{1}{6}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; 1+\frac{1}{3}\sqrt{6}$	0.49926			
0.3	8/3/*h*4	*ACEFG*	$\frac{1}{3}, 0, \frac{1}{8}; \frac{4}{3}\sqrt{3}$	0.60460			
1.1	5/3/*h*5	*ABCF*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, 0; 4-2\sqrt{3}$	0.26045	$4-2\sqrt{3} \le c < \sqrt{3}-1$		
1.2	5/3/*h*9	*ACDF*	0.40475, 0.20238, 0.07778; 1.14060	0.38572	$\sqrt{3}-1 < c < 1+\frac{1}{3}\sqrt{6}$		
1.3	6/3/*h*40	*ACEF*	$\frac{1}{3}$, 0.12724, 0.11839; 1.91724	0.48632	$1+\frac{1}{3}\sqrt{6} < c < \frac{4}{3}\sqrt{3}$		
1.4	6/3/*h*13	*ACFG*	$\frac{1}{2}, 0, \frac{1}{8}; 2$	0.45345	$2 \le c < \frac{4}{3}\sqrt{3}$		
2.1	4/3/*h*4	*ACF*	0.57018, 0.14036, 0.08796; 0.89321	0.19701	$4-2\sqrt{3} < c < \frac{4}{3}\sqrt{3}$		
P*6/*mmm* 24*r			**$0, 2x-1 < y < \frac{1}{2}x; 0 < z \le \frac{1}{4}$**				
A	$x, y, -z$		*B* $x, y, -z+1$; *C* $x-y, -y, z$	*D*	$x, x-y, z$	*E*	$-x+y+1, y, z$
0.1	5/4/*h*17	*ABCDE*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{4}; 1-\frac{1}{3}\sqrt{3}$	0.32400			

Table 1 (continued)

P6/mcc* 24*m			**$0, 2x-1 \le y \le \frac{1}{2}x; 0 < z \le \frac{1}{4}$**		
A	$x, y, -z$		*C* $x-y, -y, -z+\frac{1}{2}$	*F* $x-y, x, z$	*G* $-y+1, x-y, z$; *H* $-x+1, -y, z$
B	$x, y, -z+1$		*D* $x, x-y, -z+\frac{1}{2}$	$y, -x+y, z$	$-x+y+1, -x+1, z$
			E $-x+y+1, y, -z+\frac{1}{2}$		
0.1	5/4/*h*17	*ABCDE*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{4}; 1-\frac{1}{3}\sqrt{3}$	0.32400	
0.2	5/3/*h*18	*ACDEH*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{1}{2}-\frac{1}{4}\sqrt{2}; 1+\sqrt{2}-\frac{1}{3}\sqrt{3}-\frac{1}{3}\sqrt{6}$	0.37959	
0.3	6/3/*h*41	*ADEGH*	$\frac{1}{3}\sqrt{6}-\frac{1}{3}, \frac{1}{3}\sqrt{6}-\frac{2}{3}, \frac{3}{4}-\frac{1}{4}\sqrt{6}; \frac{2}{3}\sqrt{3}$	0.40348	
0.4	6/3/*h*42	*ACDFH*	$\frac{1}{9}(3+2\sqrt{3})[1-(3\sqrt{3}-5)^{1/2}], \frac{1}{9}\sqrt{3}[1-(3\sqrt{3}-5)^{1/2}],$ $\frac{1}{4}(2+\sqrt{3})[1-(\sqrt{3}-1)^{1/2}];$ $\frac{1}{3}(\sqrt{2}+\sqrt{6})[1+(\sqrt{3}-1)^{1/2}][1-(3\sqrt{3}-5)^{1/2}]$	0.50321	
0.5	7/3/*h*22	*ADFGH*	$\frac{3}{7}, \frac{1}{7}, \frac{7}{4}-\frac{1}{4}\sqrt{42}; \frac{2}{7}\sqrt{6}+\frac{2}{7}\sqrt{7}$	0.53819	
1.1	4/4/*h*41	*ACDE*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, \frac{3}{16}; \sqrt{2}-\frac{1}{3}\sqrt{6}$	0.27338	$1-\frac{1}{3}\sqrt{3} < c < 1+\sqrt{2}-\frac{1}{3}\sqrt{3}-\frac{1}{3}\sqrt{6}$
1.2	5/3/*h*5	*AEGH*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, \frac{1}{8}; 8-4\sqrt{3}$	0.26045	$8-4\sqrt{3} \le c < \frac{2}{3}\sqrt{3}$
1.3	4/4/*h*42	*ADEH*	{0.47227, 0.13894, 0.14062; 1.1}	>0.37959	$1+\sqrt{2}-\frac{1}{3}\sqrt{3}-\frac{1}{3}\sqrt{6} < c < \frac{2}{3}\sqrt{3}$
1.4	4/4/*h*43	*ACDH*	{0.43150, 0.11562, 0.14016; 1.15}	>0.37959	$1+\sqrt{2}-\frac{1}{3}\sqrt{3}-\frac{1}{3}\sqrt{6} < c$ $< \frac{1}{3}(\sqrt{2}+\sqrt{6})[1+(\sqrt{3}-1)^{1/2}][1-(3\sqrt{3}-5)^{1/2}]$
1.5	5/3/*h*19	*ADGH*	{0.45647, 0.14678, 0.13285; 1.3}	>0.40348	$\frac{2}{3}\sqrt{3} < c < \frac{2}{7}\sqrt{6}+\frac{2}{7}\sqrt{7}$
1.6	5/4/*h*5	*ACFH*	$\frac{1}{3}, 0, \frac{1}{8}; \frac{4}{3}$	0.40307	$\frac{1}{3}(\sqrt{2}+\sqrt{6})[1+(\sqrt{3}-1)^{1/2}][1-(3\sqrt{3}-5)^{1/2}] < c \le \frac{4}{3}$
1.7	5/4/*h*37	*ADFH*	{0.41535, 0.12681, 0.13167; 1.4}	>0.50321	$\frac{1}{3}(\sqrt{2}+\sqrt{6})[1+(\sqrt{3}-1)^{1/2}][1-(3\sqrt{3}-5)^{1/2}] < c < \frac{2}{7}\sqrt{6}+\frac{2}{7}\sqrt{7}$
1.8	6/3/*h*20	*ADFG*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{8}; 2\sqrt{3}-2$	0.48601	$\frac{2}{7}\sqrt{6}+\frac{2}{7}\sqrt{7} < c \le 2\sqrt{3}-2$
*n*2.1	$h[48^2]^3$	*ADH*	{0.43397, 0.12641, 0.1355; $\frac{5}{4}$}	>0.37959	$1+\sqrt{2}-\frac{1}{3}\sqrt{3}-\frac{1}{3}\sqrt{6} < c < \frac{2}{7}\sqrt{6}+\frac{2}{7}\sqrt{7}$
$P6_3/mcm$* 24*l			**$0 < y; 2x-1 \le y \le \frac{1}{2}x; 0 \le z < \frac{1}{4}$**		
A	$x, y, -z+\frac{1}{2}$		*C* $x-y, -y, z$	*E* $x, x-y, -z$	*G* $-y+1, x-y, z$
B	$x, y, -z-\frac{1}{2}$		*D* y, x, z	*F* $-x+y+1, y, -z$	$-x+y+1, -x+1, z$
0.1	5/4/*h*17	*ABCEF*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, 0; 1-\frac{1}{3}\sqrt{3}$	0.32400	
0.2	6/3/*h*43	*ACEFG*	$\frac{1}{2}, \frac{1}{6}, \frac{1}{4}\sqrt{6}-\frac{1}{2}; \frac{1}{3}\sqrt{2}+\frac{1}{3}\sqrt{3}$	0.33284	
0.3	6/3/*h*20	*ACDEG*	$1-\frac{1}{3}\sqrt{3}, \frac{1}{2}-\frac{1}{6}\sqrt{3}, \frac{1}{8}; 2\sqrt{3}-2$	0.48601	
1.1	4/4/*h*44	*ACEF*	0.46429, 0.13096, 0.07778; 0.65853	0.25715	$1-\frac{1}{3}\sqrt{3} < c < \frac{1}{3}\sqrt{2}+\frac{1}{3}\sqrt{3}$
1.2	5/3/*h*5	*ACFG*	$\frac{1}{3}\sqrt{3}, \frac{2}{3}\sqrt{3}-1, \frac{1}{8}; 8-4\sqrt{3}$	0.26045	$\frac{1}{3}\sqrt{2}+\frac{1}{3}\sqrt{3} < c \le 8-4\sqrt{3}$
1.3	5/3/*h*20	*ACEG*	{0.46055, 0.18432, 0.12230; $\frac{5}{4}$}	>0.33284	$\frac{1}{3}\sqrt{2}+\frac{1}{3}\sqrt{3} < c < 2\sqrt{3}-2$
$P6_3/mmc$* 24*l			**$0, 2x-1 \le y < \frac{1}{2}x; 0 \le z < \frac{1}{4}$**		
A	$x, y, -z+\frac{1}{2}$		*B* $x, y, -z-\frac{1}{2}$	*C* $x-y, -y, -z$	*D* $x, x-y, z$; *E* $-x+y+1, y, z$; *F* $-y, -x, z$
0.1	5/4/*h*17	*ABCDE*	$\frac{1}{6}\sqrt{3}+\frac{1}{6}, \frac{1}{6}\sqrt{3}-\frac{1}{6}, 0; 1-\frac{1}{3}\sqrt{3}$	0.32400	
0.2	5/4/*h*5	*ACDEF*	$\frac{1}{3}, 0, \frac{1}{8}; \frac{4}{3}$	0.40307	
1.1	4/4/*h*45	*ACDE*	0.43760, 0.10427, 0.09522; 0.73995	0.23570	$1-\frac{1}{3}\sqrt{3} < c < \frac{4}{3}$

metrical parameters. Each such (set of) neighbouring point(s) is designated by a capital letter.

(3) The third block of information describes each corresponding type of sphere packing or of interpenetrating sphere packings or layers together with its parameter region: a symbol *n.j* in the first column indicates an *n*-dimensional parameter range. *j* is a serial number. In the case of interpenetrating sphere packings or layers, this symbol is preceded by the lower-case letter *i* or *n*, respectively.

The type of sphere configuration is identified in the second column. A sphere-packing type is designated by a symbol *k*/*m*/*hn*, 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, *h* indicates that the hexagonal crystal family is the highest family for a sphere packing of that type and *n* is an arbitrary number. Symbols of sphere packings generated by identical symmetry operations but occurring within two disjoint non-congruent parameter regions are supplemented by *a* or *b* (*cf.* Koch & Sowa, 2004).

Types of interpenetrating sphere packings are characterized by symbols $h[k/m/hn]^l$. Here, *k*/*m*/*hn* describes the type of the sphere packings that interpenetrate each other, *l* is the number of interpenetrating sphere packings and the first *h* indicates the highest possible crystal family for the type of interpenetrating sphere packing.

Interpenetrating sphere layers are identified by similar symbols: the usual symbols of the Shubnikov nets (Shubnikov, 1916), however, replace the symbols of the sphere-packing types, and *l* is the number of sets of parallel sphere layers, *i.e.* 3 in the hexagonal system.

A string of capital letters in the third column identifies all neighbouring points that give rise to sphere contacts.

The next two columns refer to those (interpenetrating) sphere packings or layers of the type under consideration that show minimal density: the 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. For each sphere-packing type occurring in the hexagonal crystal system, the sphere packing with minimal density is one with highest inherent symmetry, *i.e.* it corresponds to a point configuration belonging to a limiting complex, if possible. Parameter values given in braces indicate that the parameter region of the

Table 2
Layer and rod description for the 170 types of sphere packings that can be generated with hexagonal symmetry.

Type	Symmetry	Layer description			Rod description		
3/4/h1a	$P6_222$ 12k	–			–		
3/4/h1b	$P6_222$ 12k	–			–		
3/4/h2a	$P6_222$ 12k	–			–		
3/4/h2b	$P6_222$ 12k	–			–		
3/4/h3	$P6_222$ 12k	–			–		
3/6/h3	$P6_322$ 12i	–			–		
3/8/h2	$P6_222$ 6i	–			–		
3/8/h4	$P6_122$ 12c	–			–		
3/8/h5	$P6_222$ 12k	–			–		
3/8/h6	$P6_222$ 12k	–			–		
3/10/h1	$P6_222$ 6f	–			–		
3/10/h2	$P6_122$ 12c	–			–		
3/10/h3	$P6_122$ 12c	–			–		
3/12/h1	$P6_222$ 6g	–			–		
4/3/h3	$P6_3/mmc$ 6h	3.12^2	1,0 1	−−	$6^3(6,3)$	1,0	h
4/3/h4	$P6_3/mmc$ 12k	3.12^2	1,0 2	−+	$48^2(0,3)$	1,0	h
4/3/h9a	$P6_222$ 12k	–			–		
4/3/h9b	$P6_222$ 12k	–			–		
4/3/h10	$P6_322$ 12i	3.12^2	1,0 2	−+	–		
4/4/h1	$P6_222$ 6g	$4_c(8+2)^2$	1,0 $\frac{3}{2}$	−−	$4^4(0,2)$	1,0	h
4/4/h2	$P6_222$ 6i	–			–		
4/4/h3	$P6_222$ 6i	$4_c(8+2)^2$	1,0 $\frac{3}{2}$	−−	–		
4/4/h4	$P6_222$ 6i	$4_c(8+2)^2$	1,0 $\frac{3}{2}$	−−	–		
4/4/h5	$P6_3/mmc$ 12j	4.6.12	1,0 1	−−	$6^3(6,3)$	1,0	h
4/4/h16	$P6_222$ 12k	–			$4^4(0,2)$	1,0	t
4/4/h17	$P6_222$ 12k	–			$6^3(3,2)$	1,0	t
4/4/h18	$P6_222$ 12k	$4_c(8+2)^2$	1,0 3	−+	–		
4/4/h19	$P6_222$ 12k	$4_c(8+2)^2$	1,0 3	−+	–		
4/4/h20	$P6_222$ 12k	$4_c(8+2)^2$	1,0 3	−+	$4^4(0,2)$	1,0	h
4/4/h21	$P6_222$ 12k	48^2	1,0 3	−+	$6^3(0,2)$	1,0	h
4/4/h22	$P6_222$ 12k	–			$6^3(4,2)$	1,0	h
4/4/h23	$P6_222$ 12k	–			$6^3(6,4)$	1,0	h
4/4/h24	$P6_222$ 12k	–			$6^3(4,2)$	1,0	h
4/4/h25	$P6_222$ 12k	–			$6^3(6,4)$	1,0	h
					$6^3(3,2)$	1,0	t
4/4/h26	$P6_222$ 12k	48^2	1,0 3	−+	–		
4/4/h27	$P6_222$ 12k	–			–		
4/4/h28	$P6_222$ 12k	–			$4^4(0,2)$	1,0	t
4/4/h29	$P6_222$ 12k	48^2	1,0 3	++	–		
4/4/h30	$P6_122$ 12c	–			$6^3(3,2)$	1,0	t
4/4/h31	$P6_122$ 12c	–			$6^3(6,5)$	1,0	h
4/4/h32	$P6_122$ 12c	–			$4^4(0,2)$	1,0	t
4/4/h33	$P6_122$ 12c	–			$4^4(0,2)$	1,0	h
4/4/h34	$P6_122$ 12c	–			$4^4(0,2)$	1,0	h
4/4/h35	$P6_122$ 12c	–			$4^4(0,2)$	1,0	h
4/4/h36	$P6_122$ 12c	–			$4^4(0,2)$	1,0	h
4/4/h37	$P6_222$ 12k	–			$6^3(4,2)$	1,0	h
4/4/h38	$P6_222$ 12k	48^2	1,0 3	−+	$6^3(0,2)$	1,0	h
4/4/h39	$P6_222$ 12k	$4_c(8+2)^2$	1,0 3	−+	$4^4(0,2)$	1,0	h
		$4_c(8+2)^2$	1,0 3	−+			
4/4/h40	$P6_222$ 12k	$4_c(8+2)^2$	1,0 3	−+	$4^4(0,2)$	1,0	h
4/4/h41	$P6/mcc$ 24m	4.6.12	1,0 2	−+	$6^3(0,6)$	1,0	h
					$6^3(0,3)$	1,0	t
4/4/h42	$P6/mcc$ 24m	$4_c6(12+6)$	1,0 2	−+	$6^3(0,3)$	1,0	t
4/4/h43	$P6/mcc$ 24m	$4_c(6+3)12$	1,0 2	−+	$6^3(0,6)$	1,0	h
4/4/h44	$P6_3/mcm$ 24l	4.6.12	1,0 2	−+	$48^2(0,3)$	1,0	h
					$6^3(0,3)$	1,0	t
4/4/h45	$P6_3/mmc$ 24l	4.6.12	1,0 2	−+	$48^2(0,3)$	1,0	h
4/5/h3	$P6_122$ 6b	–			–		
4/5/h4	$P6_122$ 6b	–			$6^3(6,5)$	1,0	h
4/6/h1	$P6_222$ 3c	–			–		
4/6/h2	$P6_3/mmc$ 4f	6^3	1,0 2	−+	$6^3(0,3)$	1,0	h
4/6/h3	$P6_122$ 6a	–			$6^3(3,2)$	1,0	t
4/6/h13	$P6_122$ 12c	–			$6^3(6,5)$	1,0	h
					$6^3(3,2)$	1,0	t
4/6/h14	$P6_122$ 12c	–			$6^3(3,2)$	1,0	t
5/3/h2	$P6_222$ 12k	4_t8^2	1,0 3	−+	$3^34^2(0,2)$	1,0	h
5/3/h3	$P6_122$ 12c	–			–		
5/3/h5	$P6/mmm$ 6l	3.12^2	1,1 1	++	$4^4(0,12)$	1,0	h
					$4^4(0,3)$	1,0	t
5/3/h6	$P6_2$ 6c	–			–		
5/3/h7	$P6/mcc$ 12l	3.12^2	1,1 2	++	$4^4(0,3)$	1,0	t
5/3/h8	$P6_3/mcm$ 12j	3.12^2	1,1 2	++	$6^3(6,3)$	1,1	h
					$4^4(0,3)$	1,0	t
5/3/h9	$P6_3/mmc$ 12k	3464	1,0 2	−+	$6^3(0,3)$	1,1	h
5/3/h10	$P6_222$ 12k	–			$4^4(0,2)$	2,0	t
5/3/h11	$P6_222$ 12k	4_t8^2	1,0 3	−+	–		
5/3/h12	$P6_122$ 12c	–			$3^6(1,2)$	1,0	h
5/3/h13	$P6_122$ 12c	–			$3^6(1,2)$	1,0	h
5/3/h14	$P6_122$ 12c	–			$3^6(1,2)$	1,0	h
5/3/h15	$P6_122$ 12c	–			$3^6(1,2)$	1,0	h
5/3/h16	$P6_222$ 12k	4_t8^2	1,0 3	−+	$3^34^2(0,2)$	1,0	h
		$4_c(8+2)^2$	2,0 3	−+			
5/3/h17	$P6_322$ 12i	3.12^2	2,0 2	−+	–		
5/3/h18	$P6/mcc$ 24m	$4_t6.12$	1,0 2	−+	$6^3(0,6)$	2,0	h
					$6^3(0,3)$	2,0	t
5/3/h19	$P6/mcc$ 24m	3.12^2	1,1 4	++	$4^4(0,3)$	1,0	t
5/3/h20	$P6_3/mcm$ 24l	3.12^2	1,1 4	++	$48^2(0,3)$	1,1	h
					$4^4(0,3)$	1,0	t
5/4/h5	$P6/mmm$ 2c	6^3	1,1 1	++	$4^4(0,6)$	q	h
5/4/h6	$P6_122$ 12c	–			$4^4(0,2)$	1,1	t
5/4/h7	$P6_122$ 12c	–			$4^4(0,2)$	1,1	h
5/4/h11	$P6_222$ 6i	6^3	1,1 3	++	$4^4(0,2)$	1,1	h
5/4/h13	$P6_222$ 6i	–			$4^4(2,12)$	1,0	h
					$4^4(1,3)$	1,0	t
5/4/h15	$P6_222$ 6g	–			$4^4(2,6)$	1,0	h
					$4^4(1,6)$	1,0	t
5/4/h16	$P6_222$ 12k	–			$4^4(4,12)$	1,0	h
					$4^4(2,6)$	1,0	t
5/4/h17	$P6/mmm$ 12p	4.6.12	1,1 1	++	$4^4(0,12)$	1,0	h
					$4^4(0,6)$	1,0	t
5/4/h18	$P6/mcc$ 12l	$4_c(6+3)12$	2,0 1	−−	$4^4(6,6)$	1,0	h
5/4/h19	$P6/mcc$ 12l	$4_t6(12+6)$	2,0 1	−−	$4^4(3,3)$	1,0	t
5/4/h20	$P6/mcc$ 12l	6^3	1,1 2	+−	$4^4(0,6)$	1,0	h
5/4/h21	$P6_3/mcm$ 12j	4.6.12	2,0 1	−−	$6^3(6,3)$	2,0	h
					$4^4(3,3)$	1,0	t
5/4/h22	$P6_222$ 12k	6^3	1,1 6	++	$4^4(0,2)$	1,1	h
5/4/h23	$P6_222$ 12k	48^2	1,1 3	++	$4^4(0,4)$	1,0	h
5/4/h24	$P6_222$ 12k	48^2	1,1 3	−+	$6^3(4,2)$	1,1	h
5/4/h25	$P6_222$ 12k	–			$4^4(2,12)$	1,0	h
					$4^4(1,6)$	1,0	t
5/4/h26	$P6_222$ 12k	–			$6^3(6,4)$	2,0	h
					$6^3(3,2)$	2,0	t
5/4/h27	$P6_122$ 12c	–			$4^4(1,12)$	1,0	h
					$4^4(1,6)$	1,0	t
5/4/h28	$P6_122$ 12c	–			$4^4(1,12)$	1,0	h
					$4^4(2,6)$	1,0	t
5/4/h29	$P6_122$ 12c	–			$4^4(5,12)$	1,0	h
					$4^4(1,6)$	1,0	t
5/4/h30	$P6_122$ 12c	–			$4^4(2,5)$	1,0	h
5/4/h31	$P6_122$ 12c	–			$4^4(2,6)$	1,0	h
					$6^3(3,2)$	1,1	t
5/4/h32	$P6_122$ 12c	–			$4^4(0,2)$	1,1	h
					$4^4(0,2)$	1,1	t
5/4/h33	$P6_122$ 12c	–			$4^4(0,2)$	1,1	h
5/4/h34	$P6_122$ 12c	–			$4^4(0,2)$	1,1	h
5/4/h35	$P6_122$ 12c	6^3	2,0 6	−+	–		
5/4/h36	$P6_322$ 12i	–			$4^4(3,12)$	1,0	h
					$4^4(0,6)$	1,0	t
5/4/h37	$P6/mcc$ 24m	6^3	1,1 4	++	$4^4(0,6)$	1,0	h
6/3/h3	$P6_222$ 6i	4_t8^2	2,0 $\frac{3}{2}$	−−	–		
6/3/h4	$P6_122$ 12c	–			$4^4(0,2)$	2,1	h
6/3/h5	$P6_122$ 12c	6^3	2,1 6	−+	$4^4(0,2)$	2,1	h
6/3/h6	$P6_122$ 12c	6^3	2,1 6	−+	$3^6(1,2)$	1,1	h
6/3/h7	$P6_122$ 12c	–			$4^4(0,2)$	2,1	h
6/3/h10	$P6_122$ 6b	–			$4^4(0,2)$	r	h
6/3/h12	$P6_122$ 6b	–			$3^34^2(6,5)$	t	h
					$4^4(1,3)$	2,0	t

Table 2 (continued)

Type	Symmetry	Layer description			Rod description		
6/3/h13	*P6/mmm 3f*	3636	1,1 1	++	4^4(0,6)	*c*	*h*
					4^4(0,3)	*c*	*t*
6/3/h17	$P6_122$ 6*a*	–			4^4(1,6)	2,0	*h*
					3^34^2(3,2)	1,0	*t*
6/3/h20	*P6/mmm 6l*	3464	1,1 1	++	4^4(0,6)	1,1	*h*
					4^4(0,3)	1,1	*t*
6/3/h21	$P6_3/mmc$ 6*h*	3.12^2	2,1 1	−−	3^34^2(6,3)	*t*	*h*
					4^4(0,3)	2,0	*t*
6/3/h22	$P6_3/mmc$ 6*h*	3464	2,0 1	−−	4^4(3,3)	1,1	*h*
6/3/h26	$P6_1$ 6*a*	–			–		
6/3/h27	$P\bar{6}2c$ 6*h*	3636	1,1 2	++	4^4(0,3)	1,1	*h*
6/3/h28	$P6_3/mmc$ 12*j*	4.6.12	2,1 1	−−	3^34^2(6,3)	1,0	*h*
					4^4(0,6)	2,0	*t*
6/3/h29	$P6_222$ 12*k*	–			6^3(6,4)	3,0	*h*
					6^3(3,2)	3,0	*t*
6/3/h30	$P6_222$ 12*k*	–			3^34^2(6,4)	1,0	*h*
					3^34^2(3,2)	1,0	*t*
6/3/h31	$P6_3/m$ 12*i*	3^46	1,0 2	−+	6^3(0,3)	2,1	*h*
6/3/h32	$P6_122$ 12*c*	–			4^4(1,12)	2,0	*h*
					3^34^2(3,2)	1,0	*t*
6/3/h33	$P6_122$ 12*c*	–			3^34^2(6,5)	1,0	*h*
					4^4(1,6)	2,0	*t*
6/3/h34	$P6_122$ 12*c*	–			3^34^2(6,5)	1,0	*h*
					3^34^2(3,2)	1,0	*t*
6/3/h35	$P6_122$ 12*c*	–			3^34^2(1,6)	1,0	*h*
6/3/h36	$P6_122$ 12*c*	–			3^34^2(1,6)	1,0	*h*
					6^3(3,2)	2,1	*t*
6/3/h37	$P6_122$ 12*c*	–			3^6(1,2)	1,1	*h*
					4^4(0,2)	2,1	*t*
6/3/h38	$P6_122$ 12*c*	–			3^6(1,2)	1,1	*h*
6/3/h39	$P6_322$ 12*i*	3636	1,1 4	++	4^4(0,3)	1,1	*h*
6/3/h40	$P\bar{6}2c$ 12*i*	3636	1,1 4	++	4^4(0,3)	1,1	*h*
6/3/h41	*P6/mcc 24m*	3.12^2	2,1 4	++	3^34^2(0,3)	1,0	*t*
6/3/h42	*P6/mcc 24m*	6^3	2,1 4	++	3^34^2(0,6)	1,0	*h*
6/3/h43	$P6_3/mcm$ 24*l*	3.12^2	2,1 4	++	48^2(0,3)	2,1	*h*
					3^34^2(0,3)	1,0	*t*
6/4/h2	$P6_3/mmc$ 2*c*	6^3	3,0 1	−−	4^4(3,3)	*c*	*h*
6/4/h3	$P6_222$ 3*c*	–			4^4(2,6)	*c*	*h*
					4^4(1,3)	*c*	*t*
6/4/h5	$P6_222$ 6*i*	–			4^4(2,6)	1,1	*h*
					4^4(1,3)	1,1	*t*
6/4/h6	$P6_122$ 6*b*	–			4^4(1,6)	1,1	*h*
					4^4(1,3)	1,1	*t*
6/4/h10	*P6/mcc 12l*	4.6.12	3,0 1	−−	4^4(6,6)	2,0	*h*
					4^4(3,3)	2,0	*t*
7/3/h6	$P6_122$ 12*c*	–			4^4(0,2)	2,2	*h*
7/3/h7	$P6_122$ 12*c*	6^3	3,1 6	−+	3^6(1,2)	2,1	*h*
7/3/h8	$P6_122$ 12*c*	6^3	2,2 6	++	3^6(1,2)	2,1	*h*
7/3/h12	$P6_2$ 6*c*	–			4^4(2,6)	2,1	*h*
					4^4(1,3)	2,1	*t*
7/3/h13	*P6/m 6j*	3^46	1,1 2	++	4^4(0,6)	2,1	*h*
					4^4(0,3)	2,1	*t*
7/3/h14	*P6/mcc 12l*	4,6.12	3,0 1	−−	4^4(6,6)	3,0	*h*
					4^4(3,3)	3,0	*t*
7/3/h15	*P6/mcc 12l*	3.12^2	2,2 2	++	3^6(0,3)	1,0	*t*
7/3/h16	*P6/mcc 12l*	6^3	2,2 2	++	3^6(0,6)	1,0	*t*
7/3/h17	*P6/mcc 12l*	3^46	1,1 2	++	4^4(0,6)	2,1	*h*
					4^4(0,3)	2,1	*t*
7/3/h18	$P6_3/mcm$ 12*j*	4.6.12	3,1 1	−−	3^34^2(6,3)	2,0	*h*
					3^6(3,6)	1,0	*t*
7/3/h19	$P6_3/mcm$ 12*j*	3.12^2	2,2 2	++	6^3(6,3)	3,1	*h*
					3^6(0,3)	1,0	*t*
7/3/h20	$P6_3/mmc$ 12*k*	3636	2,1 4	++	3^34^2(0,3)	1,1	*h*
7/3/h21	$P6_222$ 12*k*	–			3^34^2(6,4)	2,0	*h*
					3^34^2(3,2)	2,0	*t*
7/3/h22	*P6/mcc 24m*	3^46	1,1 4	++	4^4(0,6)	2,1	*h*
					4^4(0,3)	2,1	*t*
8/3/h3	$P6_3/mmc$ 2*c*	6^3	4,1 1	−−	3^6(3,6)	*t*	*h*
8/3/h4	*P6/mmm 1a*	3^6	1,1 1	++	4^4(0,3)	*q*	*t*
8/3/h6	$P6_122$ 6*b*	–			3^34^2(1,6)	*c*	*h*
8/3/h10	$P6_3/mmc$ 6*h*	3636	2,2 2	++	3^6(0,3)	1,1	*h*
8/3/h11	$P6_3/mmc$ 6*h*	3464	3,1 1	−−	3^6(3,6)	1,1	*h*
					4^4(0,3)	2,2	*t*
8/3/h13	$P6_1$ 6*a*	–			4^4(0,2)	3,1	*h*
					4^4(1,3)	3,1	*t*
8/3/h14	$P6_3/m$ 6*h*	3^46	3,0 1	−−	4^4(3,3)	3,1	*h*
8/3/h15	*P6/mcc 12l*	4.6.12	4,1 1	−−	3^6(6,12)	2,0	*h*
					3^6(3,6)	2,0	*t*
9/3/h3	$P6_222$ 6*f*	3^6	2,1 6	−−	4^4(0,2)	*d*	*h*
10/3/h2	$P6_3/mmc$ 4*f*	3^6	3,1 4	++	3^34^2(0,3)	*c*	*h*
10/3/h3	$P6_222$ 3*c*	3^6	2,2 3	++	4^4(0,2)	*r*	*h*
10/3/h5	$P6_3/m$ 6*h*	3^46	4,1 1	−−	3^6(3,6)	2,1	*h*
11/3/h1	$P6_122$ 12*c*	3^6	3,2 12	++	–		
12/3/h1	$P6_3/mmc$ 2*c*	3^6	3,3 2	++	3^6(0,3)	*c*	*h*

corresponding type does not include an arrangement with minimal density. Then the given parameters refer to an arbitrarily chosen sphere packing of that type.

For each type of sphere configuration with free parameters, the corresponding range of the axial ratio *c*/*a* is shown in the sixth column.

If the asymmetric unit of the Euclidean normalizer of a space group is not totally bounded by mirror planes, a complicated situation may occur for the parameter regions of some types of sphere configuration: the connected parameter region – represented by a string of capital letters – is not completely located within the chosen asymmetric unit but it belongs to two or more different asymmetric units. In such a case, the parameter region corresponding to a certain type disintegrates into two or more disconnected parts, each of them belonging to the asymmetric unit under consideration but referring to another string of capital letters. The corresponding symmetry operations can be transformed into another by a symmetry operation of the space group itself or by a symmetry operation of the Euclidean normalizer. A modification of the symbol in the first column of Table 1 by parentheses or by a prime, respectively, indicates such a disconnected parameter range. Fischer (1991) has discussed in detail a corresponding tetragonal example.

3. Discussion

15 lattice complexes with three degrees of freedom belong to the hexagonal crystal system. Their point configurations give rise to sphere packings of altogether 147 types. 103 of these types refer exclusively to trivariant hexagonal lattice complexes, *i.e.* none of their sphere packings can be generated with site symmetry other than 1. The other 44 sphere-packing types were already known from the investigation of lattice complexes with less than three degrees of freedom (Sowa *et al.*, 2003; Sowa & Koch, 2004*a*). In total, sphere packings of 170 types can be realized with hexagonal symmetry. For 23 of these types, however, the corresponding sphere packings can be generated only in hexagonal lattice complexes with less than three degrees of freedom or with trigonal or lower

symmetry. The hexagonal closest packings of spheres belongs to these types.

In principle, all types of homogeneous sphere packings with three contacts per sphere have already been derived by Koch & Fischer (1995) using a combinatorial method. The present investigation, however, shows that three types of such sphere packings had been overlooked, namely 3/10/*h*2 and 3/10/*h*3 with symmetry $P6_122$ and 3/8/*h*6 with symmetry $P6_222$.

Sphere packings with 11 contacts per sphere are comparatively rare. Until now, only six types of such sphere packing have been described (*cf.* Koch & Fischer, 1999). One of these, namely 11/3/*h*1, refers to lattice complex $P6_122$ 12*c*. The respective sphere packings are composed of triangular nets of spheres with three and two contacts per sphere to the nets above and below. The translation period in the *c* direction corresponds to 12 triangular nets.

Systematic removal of one of the contacts between spheres from neighbouring nets results in sphere packings with contact number 10. The corresponding types – 10/3/*h*3 and 10/3/*h*2 – refer to one-dimensional parameter regions in $P6_122$ 12*c*. Sphere packings of both types can also be generated with higher symmetry (*cf.* Sowa *et al.*, 2003). The maximal generating symmetry for 10/3/*h*3 is $P6_222$ 3*c*. Here, the number of triangular nets per translation period is only 3. Sphere packings of type 10/3/*h*2 occur with highest symmetry in $P6_3/mmc$ 4*f* and the corresponding number of triangular nets per translation period is 4.

Type10/3/*h*2 exhibits a noteworthy property: lattice complex $P6_122$ 12*c* contains $P6_3/mmc$ 4*f* as a limiting complex at $\frac{2}{3}\frac{1}{3}z$ (*cf.* Engel *et al.*, 1984). Accordingly, the minimal density for sphere packings of type 10/3/*h*2 in $P6_122$ 12*c* refers to the parameters $\frac{2}{3}, \frac{1}{3}, z$ with $z = \frac{1}{12}\sqrt{6}$ and $c/a = 6 + 2\sqrt{6}$. The Euclidean normalizer $N_E(P6_122) = P6_222$ $(\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$ (*cf.* Koch *et al.*, 2002) contains, however, at $\frac{2}{3}\frac{1}{3}z$ only a threefold screw axis. As a consequence, the two halves of the one-dimensional parameter region of type 10/3/*h*2 cannot be mapped onto each other by a symmetry operation of $N_E(P6_122)$. Therefore, the sphere packings at both sides of $\frac{2}{3}, \frac{1}{3}, \frac{1}{12}\sqrt{6}$ are not congruent, although their *z* and *c*/*a* values and their densities agree pairwise. Moreover, the sequence of distances from a central atom to all the other atoms in the various coordination shells is also the same. Sphere packings of such a pair, however, are not homometric because the calculated reflection intensities for the two corresponding hypothetical crystal structures do not agree. An analogous case has not been described before.

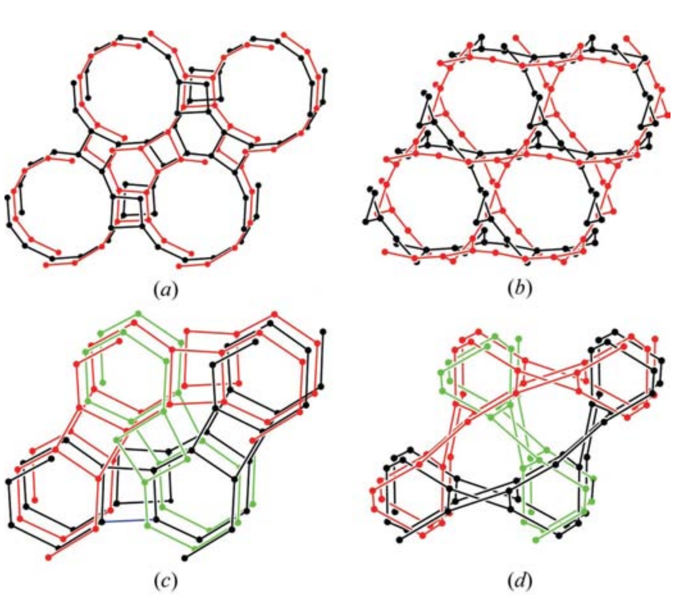

Figure 1
Interpenetrating sphere packings: (*a*) type $h[3/4/h1a]^2$, (*b*) type $h[3/4/h3]^2$, (*c*) type $h[3/4/h1a]^3$, (*d*) type $h[3/4/h3]^3$.

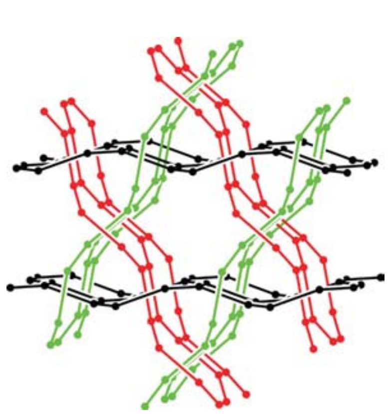

Figure 2
Interpenetrating sphere layers of type $h[48^2]^3$.

Seven types of interpenetrating sphere packings occur with hexagonal symmetry. Two congruent sphere packings interpenetrate one another in five cases, three congruent sphere packings in two cases. Interpenetration of three sphere packings with hexagonal symmetry was unknown before. $P6_222$ 12*k* gives rise to six types of interpenetrating sphere packings, $P6_122$ 12*c* to one type. It is worth noting that the interpenetrating sphere packings with symmetry $P6_222$ 12*k* are built up from individual packings of those types whose remarkable properties were discussed in detail in a previous paper (Koch & Sowa, 2004): two or three individual packings of type 3/4/*h*1*a* or type 3/4/*h*3 may be fitted into each other thus forming interpenetrating sphere packings of type $h[3/4/h1a]^2$ or $h[3/4/h3]^2$ and of type $h[3/4/h1a]^3$ or $h[3/4/h3]^3$, respectively (*cf.* Fig. 1). Only two packings of type 3/4/*h*2*a* and 4/3/*h*9*a* may be combined to interpenetrating sphere packings of type $h[3/4/h2a]^2$ and $h[4/3/h9a]^2$. Sphere packings of the denser variants 3/4/*h*1*b*, 3/4/*h*2*b* and 4/3/*h*9*b* cannot be fitted into each other.

Three sets of interpenetrating 6^3 layers of spheres $h[6^3]^3$ are found in *P*622 12*n*. They have already been described before in *P*6/*mcc* 12*l* with site symmetry *m*..[2] (Sowa & Koch, 2004*a*). Three sets of parallel 48^2 layers interpenetrate each other in *P*6/*mcc* 24*m* (*cf.* Fig. 2) forming configurations of type $h[48^2]^3$. Just as the interpenetrating honeycomb layers, the 48^2 layers have necessarily to be corrugated to prevent contacts between spheres from different layers.

[2] Inadvertently, incorrect parameters for $h[6^3]^3$ in *P*6/*mcc* 12*l* were given by Sowa & Koch (2004*a*). Correct values are for instance $x = 0.45145$, $y = 0.135$, $c/a = 0.55$.

Table 2 gives a survey of all the 170 types of hexagonal sphere packings. The first two columns show the symbols of the sphere-packing type and of that lattice complex where packings of the type under consideration can be generated with highest site symmetry.

Most of the hexagonal sphere packings may be subdivided either into connected layer-like or rod-like subunits or into both of these. These subunits may be used to construct some kind of 'descriptive symbols' that reflect certain properties of the sphere packings but are not sufficient to discriminate all types. Columns 3 and 4 give information on such layer-like and rod-like subunits, respectively, and on their mutual arrangement.

(i) The sphere packings of 85 hexagonal types may be split up into connected layer-like arrangements of spheres perpendicular to **c**. Most of these – either flat or corrugated – sphere layers correspond directly to one of the vertex-transitive plane nets (Shubnikov, 1916) and are characterized by the corresponding well known symbols 3^6, 6^3, 3.12^2, 3^46, 48^2, 3636, 3464 and 4.6.12. All further sphere layers are necessarily corrugated and do not correspond to planar graphs. They may be described, however, by symbols derived either from 48^2, namely 4_t8^2 and $4_c(8+2)^2$, or from 4.6.12, namely $4_t6.12$, $4_c(6+3)12$ and $4_c6(12+6)$. The corresponding sphere layers are illustrated in Fig. 3. Each layer symbol is followed by three numbers and two signs (+ or −). The first two numbers indicate the number of contacts of a certain sphere to spheres from the layers above and below. The third number is the number of sphere layers per translation period. A similar symbolism has already been introduced to describe sphere packings with high contact numbers derived from plane triangular or square nets (Koch & Fischer, 1999). The first sign shows whether or not a sphere packing of the regarded type can be composed of plane sphere layers. The second sign is + if there is only one possibility to split the sphere packing into the corresponding corrugated layers, otherwise it is −.

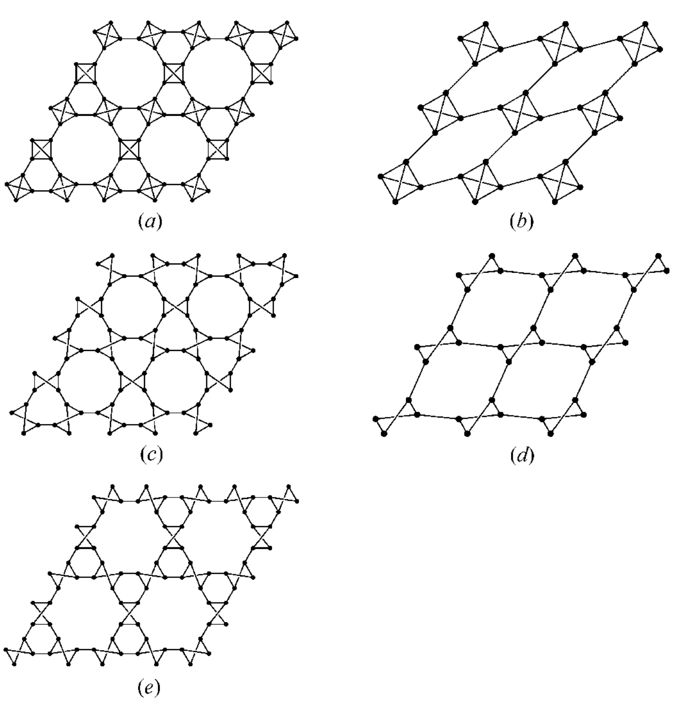

Figure 3
Sphere layers corresponding to non-planar graphs: (*a*) $4_t6.12$ layer, (*b*) $4_c(6+3)12$ layer, (*c*) $4_c6(12+6)$ layer, (*d*) 4_t8^2 layer, (*e*) $4_t(8+2)^2$ layer.

(ii) The sphere packings of 135 hexagonal types may be subdivided into connected rod-like arrangements of spheres parallel to **c**. Such a rod can be regarded as part of a plane net that is rolled up, *i.e.* certain spheres out of the infinite net are identified. (Chains of spheres are disregarded.) For a given plane net different possibilities exist for employing this procedure. In order to identify uniquely a type of rod-like arrangement of spheres, it is sufficient to supplement the symbol of the Shubnikov net with the vector between the centres of two arbitrary spheres of the plane net that coincide when the rolling operation is performed. Such symbols have already been used and are explained in detail in a paper on the sphere packings for crystallographic point groups, rod groups and layer groups (Koch & Fischer, 1978). Furthermore, all types of rod-like sphere packings have been illustrated by figures in that paper. Each sphere is in contact with other spheres from one or from two neighbouring rods. The corresponding numbers follow the symbols for the rod-like arrangements. In a few cases, a sphere packing may be split up into congruent rods of spheres but neighbouring rods have part of their spheres in common. Then, the arrangement of these common spheres is described by a lower-case letter: *r* means one or two rows of spheres without mutual contact, *d* a row of dumb-bells of spheres, *c* a chain of spheres, *t* a triangular ribbon of spheres and *q* a quadrangular ribbon of spheres. The last item describes the position of the rod axes with respect to a hexagonal unit cell: *h* means rods around $00z$ (hexagonal axes), whereas *t* designates rods around $\frac{2}{3}\frac{1}{3}z$ and $\frac{1}{3}\frac{2}{3}z$ (trigonal axes).

Only the sphere packings of 23 hexagonal types cannot be subdivided either into connected layer-like or into connected rod-like subunits. This is necessarily the case for all sphere packings with three contacts per sphere (14 hexagonal types).

4. Structural examples

Sphere packings are a useful tool especially for the description of simple crystal structures. In this connection, the atoms forming a sphere packing have not necessarily to be linked by bonds or shortest distances but it is sufficient that the symmetrically equivalent neighbours are nearly equidistant.

(i) The high-temperature modification of $FePO_4$ crystallizes in space group $P6_422$. It corresponds to the structure of β-quartz with doubled lattice parameter *c*. Accordingly, the O atoms form a slightly distorted sphere packing of type 6/3/*h*3. Their coordinate parameters $x = 0.579$, $y = 0.776$ and $z = 0.592$ (*cf.* Haines *et al.*, 2003) are rather close to the ideal sphere-packing parameters $x = \frac{1}{3}\sqrt{3} \approx 0.5774$, $y = \frac{1}{2} + \frac{1}{6}\sqrt{3} \approx 0.7887$ and $z = \frac{7}{12} \approx 0.5833$. The observed axial ratio $c/a = 2.2031$ is in good agreement with the theoretical value $c/a = 3\sqrt{-3} \approx 2.1962$. Like the Si atoms in quartz, the Fe and the P atoms together are arranged in a sphere packing of type 4/6/*h*1.

(ii) $CoNb_3S_6$ (*cf.* Parkin *et al.*, 1983) and a large number of other sulfides with the same structure type crystallize in space group $P6_322$. The S atoms are arranged in a nearly ideal sphere packing of type 10/3/*h*2. Such a packing consists of parallel 3^6 nets with three and one contacts per sphere to the neighbouring nets below and above. The S-atom coordinates (0.3322, 0.0009, 0.3694) correspond well with the theoretical values $(\frac{1}{3}, 0, \frac{1}{4}\surd 6 - \frac{1}{4} = 0.3624)$, whereas the observed axial ratio $c/a = 2.067$ is somewhat smaller than the theoretical value $c/a = \frac{2}{3}\surd 2 + \frac{2}{3}\surd 3 = 2.0975$. In alternating layers, two kinds of voids are formed, namely nearly ideal octahedra and slightly flattened trigonal prisms. Co atoms occupy one third of the former voids, Nb atoms one half of the latter.

(iii) The low-temperature phase of FeS, troilite, with symmetry $P\bar{6}2c$ is usually described as related to the nickel arsenide type (*cf.* Keller-Besrest & Collin, 1990). The three symmetrically inequivalent kinds of S atoms together form a slightly distorted hexagonal closest sphere packing with a standard deviation $s = 3.6\%$ calculated for the 12 shortest S—S distances of the three kinds of S atoms (*cf.* Sowa & Koch, 2004*b*). The axial ratio $c/a = \frac{4}{3}\surd 2 = 1.8856$ for an undistorted hexagonal closest packing in $P\bar{6}2c$ is somewhat smaller than the observed value $c/a = 1.9708$. The Fe atoms occupy all octahedral voids in the S-atom configuration but they are not located at the centres of these voids. As a consequence, the Fe atoms are not arranged in a primitive hexagonal lattice – as in the nickel arsenide type – but they correspond to a sphere packing of type 4/3/*h*4 [the respective net is called 'augmented **acs**' by Delgado Friedrichs *et al.* (2003)]. A sphere packing of the same type 4/3/*h*4, but with the distinctly smaller axial ratio $c/a = 1.023$, is formed by the Au atoms in $K_4Au_6S_5$ (*cf.* Klepp & Bronger, 1988).

(iv) $Nd_3UO_6Cl_3$ (*cf.* Henche *et al.*, 1993) crystallizes in space group $P6_3/m$. The O-atom arrangement at Wyckoff position 12*i* corresponds to a sphere packing of type 5/3/*h*5. It consists of almost flat 3.12^2 nets stacked directly upon each other. The Cl atoms form columns of octahedra in the large channels around 00*z*. The U atoms occupy half of the trigonal prismatic voids within the O-atom arrangement, whereas six O and two Cl atoms coordinate each Nd atom.

(v) Microporous silica, SSZ-24, with symmetry *P*6/*mcc* and composition $SiO_{2.267}$ (*cf.* Bialek *et al.*, 1991) is the silica analogue of $AlPO_4$-5 (zeolite framework type AFI). The Si atoms form in good approximation a sphere packing of type 4/4/*h*41. This type occurs in *P*6/*mcc* within the one-dimensional parameter range $0.4226 < c/a < 1.0204$. The parameter values of the Si-atom arrangement ($x = 0.4568$, $y = 0.3358$, $z = 0.1898$; $c/a = 0.6092$) correspond well with the parameters referring to the minimal density for sphere packings of this type ($x = \frac{1}{6} + \frac{1}{6}\surd 3 = 0.4553$, $y = \frac{1}{3}$, $z = \frac{3}{16}$; $c/a = \surd 2 - \frac{1}{3}\surd 6 = 0.5977$). $AlPO_4$-5 crystallizes in the subgroup *P*6*cc* of *P*6/*mcc* (*cf.* Klap *et al.*, 2000). Here, the Al and the P atoms together form an analogous heterogeneous sphere packing.

(vi) The zeolite GME is named after the mineral gmelinite, $Na_{8.08}Si_{16.26}Al_{7.69}O_{48}(H_2O)_{14.4}$. It crystallizes with space group $P6_3/mmc$. The Si and the Al atoms are statistically distributed. Their arrangement corresponds well with a sphere packing of type 4/4/*h*45 that occurs within a one-dimensional parameter range in the general position of $P6_3/mmc$. Again, the structural parameters [$x = 0.4421$, $y = 0.1058$, $z = 0.0942$, $c/a = 0.7319$, *cf.* Sacerdoti *et al.* (1995)] are very close to the parameters of the sphere packing with minimal density ($x = 0.4376$, $y = 0.1043$, $z = 0.0952$, $c/a = 0.7400$).

We would like to thank Professor Werner Fischer for many helpful discussions and the Deutsche Forschungsgemeinschaft for the support of this work under KO 1139/1-1.

References

Bialek, R., Meier, W. M., Davis, M. & Annen, M. J. (1991). *Zeolites*, **11**, 438–442.

Delgado Friedrichs, O., O'Keeffe, M. & Yaghi, O. M. (2003). *Acta Cryst.* A**59**, 515–525.

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

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

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

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

Haines, J., Cambon, O. & Hull, S. (2003). *Z. Kristallogr.* **218**, 193–200.

Henche, G., Fiedler, K. & Gruehn, R. (1993). *Z. Anorg. Allg. Chem.* **619**, 77–87.

Keller-Besrest, F. & Collin, G. (1990). *J. Solid State Chem.* **84**, 194–210.

Klap, G. J., van Koningsveld, H., Graafsma, H. & Schreurs, A. M. M. (2000). *Microporous Mesoporous Mater.* **38**, 403–412.

Klepp, K. O. & Bronger, W. (1988). *J. Less Common Met.* **137**, 13–20.

Koch, E. & Fischer, W. (1978). *Z. Kristallogr.* **148**, 107–152.

Koch, E. & Fischer, W. (1995). *Z. Kristallogr.* **210**, 407–414.

Koch, E. & Fischer, W. (1999). *International Tables for Crystallography*, Vol. C, 2nd ed., edited by A. J. C. Wilson & E. Prince, Section 9.1. Dordrecht/Boston/London: Kluwer Academic Publishers.

Koch, E., Fischer, W. & Müller, U. (2002). *International Tables for Crystallography*, Vol. A, 5th ed., edited by Th. Hahn, Section 15.3.5. Dordrecht/Boston/London: Kluwer Academic Publishers.

Koch, E. & Sowa, H. (2004). *Acta Cryst.* A**60**, 239–245.

Parkin, S. S. P., Marseglia, E. A. & Brown, P. J. (1983). *J. Phys. C*, **16**, 2765–2778.

Sacerdoti, M., Passaglia, E. & Carnevali, R. (1995). *Zeolites*, **15**, 276–281.

Shubnikov, A. V. (1916). *Izv. Akad. Nauk SSSR Ser. 6*, **10,** 755–799.

Sowa, H. & Koch, E. (2002). *Acta Cryst.* A**58**, 327–333.

Sowa, H. & Koch, E. (2004*a*). *Acta Cryst.* A**60**, 158–166.

Sowa, H. & Koch, E. (2004*b*). *Eur. J. Mineral.* **16**, 255–260.

Sowa, H., Koch, E. & Fischer, W. (2003). *Acta Cryst.* A**59**, 317–326.