Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 31 May 2002
Accepted 17 July 2002

Homogeneous sphere packings with triclinic symmetry

W. Fischer and E. Koch*

Institut für Mineralogie, Petrologie und Kristallographie der Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany. Correspondence e-mail: kochelke@mailer.uni-marburg.de

All homogeneous sphere packings with triclinic symmetry have been derived by studying the characteristic Wyckoff positions $P\bar{1}$ 1*a* and $P\bar{1}$ 2*i* of the two triclinic lattice complexes. These sphere packings belong to 30 different types. Only one type exists that has exclusively triclinic sphere packings and no higher-symmetry ones. The inherent symmetry of part of the sphere packings is triclinic for 18 types. Sphere packings of all but six of the 30 types may be realized as stackings of parallel planar nets.

1. Introduction

Up to now, complete information on homogeneous sphere packings is available for the cubic (*cf.* Fischer, 1973, 1974) and the tetragonal crystal systems (*cf.* Fischer, 1991*a*,*b*, 1993). Beyond it, only sporadic information exists on sphere packings with hexagonal (Sowa & Koch, 2002), trigonal (Zobetz, 1983; Sowa & Koch, 1999) and orthorhombic symmetry (Sowa, 2000*a*,*b*, 2001; Sowa & Koch, 2001). Sphere packings with three contacts per sphere have completely been derived by Koch & Fischer (1995), some with 10 or more contacts are described in Chapter 9 of *International Tables for Crystallography* (1999), Vol. C.

A set of non-intersecting spheres with the symmetry of a crystallographic group is called a *sphere packing* if any two spheres are connected by a chain of spheres with mutual contact. In a *homogenous* sphere packing, all spheres are symmetrically equivalent. As the number of such sphere packings is infinite, a classification into types is useful: Two sphere packings are assigned to the same *sphere-packing type* if a biunique mapping exists that sends the spheres of one sphere packing onto the spheres of the other one under preservation of all contact relationships between the spheres (*cf. e.g.* Fischer, 1991*a*). Very often, sphere packings of the same type may be generated using different symmetry, *i.e.* within Wyckoff positions belonging either to the same space group or to space groups of the same type or even to space groups of different types. In all such cases, the corresponding Wyckoff positions are either assigned to the same lattice complex or they are related by some limiting-complex relationships (*cf. International Tables for Crystallography*, 2002, Vol. A, ch. 14). As a consequence and in analogy to point configurations, the inherent symmetry of a sphere packing may be higher than the space-group symmetry used for its derivation. Moreover, sphere packings of the same type may show different inherent symmetry. In such a case, they may be generated either with the same or with different space-group symmetry. Then there exists a uniquely defined lattice complex for each sphere-packing type, where all corresponding sphere packings show the analogous highest inherent symmetry.

Recently, Michael O'Keeffe (private communication) raised the question of whether there exists any sphere-packing type with the property that all its sphere packings show triclinic inherent symmetry. This gave the impulse to complement our existing material on triclinic sphere packings and to prepare it for publication.

As all Wyckoff positions of triclinic space groups belong to only two lattice complexes (*cf. International Tables for Crystallography*, 2002, Vol. A, ch. 14), it is sufficient for the derivation of all triclinic sphere packings to study the Wyckoff positions $P\bar{1}$ 1*a* and $P\bar{1}$ 2*i*.

2. Sphere packings corresponding to lattice complex $P\bar{1}$ 1*a*

All point configurations of $P\bar{1}$ 1*a* form point lattices and, accordingly, the corresponding sphere-packing types are well known. Table 1 contains information on the five types of sphere packings that can be derived from point lattices.

In the first column, the sphere-packing type is designated by a symbol *k*/*m*/*sn* as was first introduced by Fischer (1971): *k* means the number of contacts per sphere, *m* is the length of the shortest mesh within the sphere packing, *s* indicates the highest crystal family for a sphere packing of that type [*c*: cubic, *h*: hexagonal/trigonal, *t*: tetragonal, *o*: orthorhombic, *m*: monoclinic, *a*: anorthic (triclinic)], and *n* is an arbitrary number. 12/3/*c*1 is the type of the cubic closest packings; 8/4/*c*1 and 6/4/*c*1 are the types corresponding to the body-centred and the primitive cubic lattices, respectively. 10/3/*t*1 refers to body-centred tetragonal lattices with the special axial ratio $c/a = \frac{1}{3} \times 6^{1/2}$ giving rise to 10 contacts per sphere, and 8/3/*h*1 belongs to primitive hexagonal lattices with $c/a = 1$.

Table 1
Sphere packings generated in $P\bar{1}$ 1*a* ($a = b = c$).

Symbol	Net	Stacking	Symmetry operations	f	Minimal symmetry	ρ_{min}	cos α, cos β, cos γ	Maximal symmetry
12/3/*c*1	3^6	3, 3 3	*t*(100), *t*(010), *t*(001), *t*(101), *t*(011), *t*(111)	0	$Fm\bar{3}m$ 4*a*	0.74048	$-\frac{1}{2}, -\frac{1}{2}, 0$	$Fm\bar{3}m$ 4*a*
10/3/*t*1	3^6	2, 2 2	*t*(100), *t*(010), *t*(001), *t*(110), *t*(101)	1	*Immm* 2*a*	0.69813	$-\frac{1}{2}, -\frac{1}{2}, \frac{1}{4}$	*I*4/*mmm* 2*a*
8/4/*c*1	4^4	2, 2 2	*t*(100), *t*(010), *t*(001), *t*(111)	2	*Immm* 2*a*	0.68017	$-\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$	$Im\bar{3}m$ 2*a*
8/3/*h*4	3^6	1, 1 1	*t*(100), *t*(010), *t*(001), *t*(110)	2	$P\bar{1}$ 1*a*	0.60460	$0, 0, -\frac{1}{2}$	*P*6/*mmm* 1*a*
6/4/*c*1	4^4	1, 1 1	*t*(100), *t*(010), *t*(001)	3	$P\bar{1}$ 1*a*	0.52360	0, 0, 0	$Pm\bar{3}m$ 1*a*

Table 2
Sphere packings generated in $P\bar{1}$ 2*i*.

Symbol	Net	Stacking	Symmetry operations	f	Minimal symmetry	ρ_{min}	$x, y, z; a, b, c$; cos α, cos β, cos γ	Maximal symmetry
12/3/*c*1	3^6	3, 3 3	*ABCDEGHJK*	0	$Fm\bar{3}m$ 4*a*	0.74048	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1, 3^{1/2}; -\frac{1}{6} \times 3^{1/2}, \frac{1}{6} \times 3^{1/2}, -\frac{1}{2}$	$Fm\bar{3}m$ 4*a*
			ABDEFGHIJK	0	$Fm\bar{3}m$ 4*a*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1, 2^{1/2}; 0, 0, 0$	
12/3/*h*1	3^6	3, 3 2	*ABCDFGHJK*	0	$P6_3/mmc$ 2*c*	0.74048	$\frac{1}{6}, \frac{1}{3}, \frac{1}{4}; 1, 1, \frac{2}{3} \times 6^{1/2}; 0, 0, -\frac{1}{2}$	$P6_3/mmc$ 2*c*
11/3/*m*1	3^6	3, 2 12	*ABCDGHJK*	1	*C*2/*m* 4*i*	0.71868	$\frac{1}{2} \times 2^{1/2} - \frac{1}{2}, 1 - \frac{1}{2} \times 2^{1/2}, \frac{9}{2} - 3 \times 2^{1/2}; 1, 1, 1 + \frac{1}{2} \times 2^{1/2}; \frac{1}{4} \times 2^{1/2} - \frac{1}{2}, \frac{1}{2} - \frac{1}{4} \times 2^{1/2}, -\frac{1}{2}$	*C*2/*m* 4*i*
10/3/*h*4	3^6	3, 1 6	*ABCDHJK*	2	$P\bar{1}$ 2*i*	0.66568	$\frac{1}{2} - \frac{1}{6} \times 6^{1/2}, 1 - \frac{1}{3} \times 6^{1/2}, \frac{3}{2} - \frac{1}{2} \times 6^{1/2}; 1, 1, \frac{1}{3}(18 + 6 \times 6^{1/2})^{1/2}; \frac{1}{4}(6 - 2 \times 6^{1/2})^{1/2}, 0, -\frac{1}{2}$	$R\bar{3}m$ 6*c*
10/3/*t*1	3^6	2, 2 2	*ABCDEHI*	2	*C*2/*m* 4*i*	0.69813	$\frac{1}{4}, 0, \frac{1}{4}; 1, 1, 3^{1/2}; 0, 0, -\frac{1}{2}$	*I*4/*mmm* 2*a*
			ABDEGHJK	1	*C*2/*m* 4*i*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1, \frac{1}{2}(10)^{1/2}; 1 - \frac{1}{2}(10)^{1/2}, \frac{1}{2}(10)^{1/2} - 1, -\frac{1}{4}$	
			ADEFGHIJK	1	*Immm* 2*a*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, \frac{1}{2} \times 6^{1/2}, \frac{1}{2} \times 6^{1/2}; 0, 0, 0$	
10/3/*o*3	3^6	2, 2 4	*ABCDGHI*	2	$P\bar{1}$ 2*i*	0.69813	$\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; 1, 1, \frac{1}{2}(13)^{1/2}; \frac{1}{13}(13)^{1/2}, -\frac{1}{26}(13)^{1/2}, -\frac{1}{2}$	*Fddd* 8*a*
10/3/*o*1	4^4	3, 3 2	*ABDFGHJK*	1	*Cmcm* 4*c*	0.69813	$\frac{2}{10}, \frac{3}{10}, \frac{1}{4}; 1, 1, \frac{2}{5}(15)^{1/2}; 0, 0, -\frac{1}{4}$	*Cmcm* 4*c*
10/3/*o*2	4^4	4, 2 4	*ABDFHIJK*	1	*C*2/*m* 4*i*	0.66568	$\frac{3}{4} - \frac{1}{4} \times 6^{1/2}, \frac{1}{4}, \frac{3}{2} - \frac{1}{2} \times 6^{1/2}; 1, 1, \frac{1}{2}(6 + 2 \times 6^{1/2})^{1/2}; 0, -\frac{1}{6}(18 - 6 \times 6^{1/2})^{1/2}, 0$	*Cmcm* 4*c*
9/3/*t*2	4^4	4, 1 4	*ABDHIJK*	2	$P\bar{1}$ 2*i*	0.61343	$\frac{1}{2} - \frac{1}{4} \times 2^{1/2}, \frac{1}{2} - \frac{1}{4} \times 2^{1/2}, 1 - \frac{1}{2} \times 2^{1/2}; 1, 1, (2 + 2^{1/2})^{1/2}; -\frac{1}{4}(4 - 2 \times 2^{1/2})^{1/2}, -\frac{1}{4}(4 - 2 \times 2^{1/2})^{1/2}, 0$	*I*4/*mmm* 4*e*
9/3/*o*1	3^6	2, 1 4	*ABCDHI*	3	$P\bar{1}$ 2*i*	0.64801	$1 - \frac{1}{2} \times 3^{1/2}, 0, 2 - 3^{1/2}; 1, 1, \frac{1}{2} \times 6^{1/2} + \frac{1}{2} \times 2^{1/2}; \frac{1}{8} \times 6^{1/2} - \frac{1}{8} \times 2^{1/2}, \frac{1}{4} \times 2^{1/2} - \frac{1}{4} \times 6^{1/2}, -\frac{1}{2}$	*Fmmm* 8*i*
9/3/*m*1	4^4	3, 2 –	*ABDGHJK*	2	*C*2/*m* 4*i*	0.69006	0.22150, 0.27850, 0.25325; 1, 1, 1.59618; −0.09098, 0.09098, −0.29044	*C*2/*m* 4*i*
9/3/*a*1	4^4	3, 2 –	*ABDFHJK*	2	$P\bar{1}$ 2*i*	0.65469	0.11620, 0.26759, 0.26759; 1, 1, 1.67415; 0, −0.25345, −0.15139	$P\bar{1}$ 2*i*
8/4/*c*1	4^4	2, 2 2	*ABDGHK*	3	*C*2/*m* 4*i*	0.68017	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1, \frac{2}{3} \times 6^{1/2}; 0, 0, -\frac{1}{3}$	$Im\bar{3}m$ 2*a*
			DEFGHIJK	2	*Immm* 2*a*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{2}{3} \times 3^{1/2}, \frac{2}{3} \times 3^{1/2}, \frac{2}{3} \times 3^{1/2}; 0, 0, 0$	
8/3/*h*3			*ADEHIJK*	2	$P2_1/m$ 2*e*	0.53742	$\frac{1}{4}, \frac{1}{6}, \frac{1}{3}; 1, \frac{3}{2}, \frac{3}{2}; -\frac{1}{2}, 0, 0$	$P6_3/mmc$ 2*c*
8/3/*h*4	3^6	1, 1 1	*ABCDH*	4	$P\bar{1}$ 2*i*	0.60460	$0, 0, \frac{1}{4}; 1, 1, 2; 0, 0, -\frac{1}{2}$	*P*6/*mmm* 1*a*
			ABDEHI	3	$P\bar{1}$ 2*i*		$\frac{1}{4}, 0, \frac{1}{4}; 1, 1, 3^{1/2}; 0, 0, 0$	
			ADEGHJK	2	$P\bar{1}$ 2*i*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 2^{1/2}, 2^{1/2}; -\frac{1}{4}, \frac{1}{4} \times 2^{1/2}, -\frac{1}{4} \times 2^{1/2}$	
8/3/*t*1	4^4	2, 2 4	*ABDFHI*	3	$P\bar{1}$ 2*i*	0.60460	$\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; 1, 1, \frac{1}{2}(14)^{1/2}; \frac{1}{14}(14)^{1/2}, -\frac{1}{14}(14)^{1/2}, 0$	$I4_1/amd$ 4*a*
8/3/*o*1			*ADFHIJK*	2	$P2_1/m$ 2*e*	0.60460	$\frac{1}{7}, \frac{1}{4}, \frac{2}{7}; 1, \frac{2}{7}(21)^{1/2}, 2^{1/2}; 0, -\frac{1}{4} \times 2^{1/2}, 0$	*Cmcm* 4*c*
8/3/*m*1	4^4	3, 1 32	*ABDHJK*	3	$P\bar{1}$ 2*i*	0.60460	$\frac{1}{8}, \frac{9}{56}, \frac{2}{7}; 1, 1, \frac{1}{2}(14)^{1/2}; -\frac{1}{14}(14)^{1/2}, -\frac{5}{98}(14)^{1/2}, -\frac{1}{7}$	*C*2/*m* 4*i*
8/3/*m*2	4^4	2, 2 4	*ABDEHK*	3	$P\bar{1}$ 2*i*	0.65142	$\frac{1}{4}$, 0.13221, 0.26442; 1, 1, 1.71223; −0.29202, 0.05568, −0.19066	*C*2/*c* 4*e*
7/3/*o*1	4^4	2, 1 4	*ABDHI*	4	$P\bar{1}$ 2*i*	0.56119	$1- \frac{1}{2} \times 3^{1/2}, 0, 2 - 3^{1/2}; 1, 1, \frac{1}{2} \times 2^{1/2} + \frac{1}{2} \times 6^{1/2}; 0, \frac{1}{4} \times 2^{1/2} - \frac{1}{4} \times 6^{1/2}, 0$	*Cmmm* 4*g*
7/3/*o*5			*ADHIJK*	3	$P\bar{1}$ 2*i*	0.48680	$\frac{3}{2} - \frac{1}{2} \times 7^{1/2}, \frac{3}{2} - \frac{1}{2} \times 7^{1/2}, 3 - 7^{1/2}; 1, \frac{1}{2}(4 + 2 \times 7^{1/2})^{1/2}, \frac{1}{2}(6 + 2 \times 7^{1/2})^{1/2}; -\frac{1}{4}(2 \times 7^{1/2} - 2)^{1/2}, -\frac{1}{2}(3 - 7^{1/2})^{1/2}, 0$	*Immm* 4*e*
7/4/*o*1	4^4	2, 1 4	*ABDHK*	4	$P\bar{1}$ 2*i*	0.60210	$\frac{7}{24} - \frac{1}{24}(13)^{1/2}, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, \frac{7}{12} - \frac{1}{12}(13)^{1/2}; 1, 1, \frac{1}{6} \times 6^{1/2} + \frac{1}{6}(78)^{1/2}; \frac{1}{9} \times 6^{1/2} - \frac{1}{18}(78)^{1/2}, \frac{1}{9} \times 6^{1/2} - \frac{1}{18}(78)^{1/2}, \frac{2}{9} - \frac{1}{9} \times (13)^{1/2}$	*Fmmm* 8*i*
7/3/*m*1	$3^3 4^2$	1, 1 2	*ADFHJK*	3	$P\bar{1}$ 2*i*	0.57451	$\frac{11}{8} - \frac{1}{8}(105)^{1/2}, \frac{35}{16} - \frac{3}{16}(105)^{1/2}, \frac{35}{16} - \frac{3}{16}(105)^{1/2}; 1, \frac{1}{4}(14)^{1/2} + \frac{1}{12}(30)^{1/2}, \frac{1}{4}(14)^{1/2} + \frac{1}{12}(30)^{1/2}; 0, \frac{1}{24}(30)^{1/2} - \frac{1}{8}(14)^{1/2}, \frac{1}{24}(30)^{1/2} - \frac{1}{8}(14)^{1/2}$	*C*2/*m* 4*i*
6/4/*c*1	4^4	1, 1 1	*ABDH*	5	$P\bar{1}$ 2*i*	0.52360	$0, 0, \frac{1}{4}; 1, 1, 2; 0, 0, 0$	$Pm\bar{3}m$ 1*a*
			ADFHJ	4	$P\bar{1}$ 2*i*		$0, \frac{1}{4}, \frac{1}{4}; 1, 2^{1/2}, 2^{1/2}; 0, 0, 0$	
			DEGHJK	3	$P\bar{1}$ 2*i*		$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 2^{1/2}, 2^{1/2}, 2^{1/2}; -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$	
6/4/*h*2			*DEHIJK*	3	$P2_1/m$ 2*e*	0.52360	$\frac{1}{4}, \frac{1}{6}, \frac{1}{3}; \frac{2}{3} \times 3^{1/2}, 2^{1/2}, 2^{1/2}; -\frac{1}{2}, 0, 0$	$P6_3/mmc$ 2*c*
6/4/*t*2	4^4	1, 1 2	*ADGHJ*	4	$P\bar{1}$ 2*i*	0.55851	$\frac{1}{8}, \frac{1}{4}, \frac{1}{4}; 1, \frac{1}{4}(34)^{1/2}, \frac{1}{4}(34)^{1/2}; -\frac{2}{17}, \frac{1}{17}(34)^{1/2}, -\frac{1}{17}(34)^{1/2}$	$I4_1/amd$ 4*a*
6/3/*o*1			*ADHJK*	4	$P\bar{1}$ 2*i*	0.44226	$\frac{11}{8} - \frac{1}{8}(105)^{1/2}, \frac{11}{4} - \frac{1}{4}(105)^{1/2}, \frac{13}{8} - \frac{1}{8}(105)^{1/2}; 1, \frac{1}{4} \times 5^{1/2} + \frac{1}{4}(21)^{1/2}, \frac{1}{4} \times 5^{1/2} + \frac{1}{4}(21)^{1/2}; -\frac{1}{2}, 0, \frac{1}{8} \times 5^{1/2} - \frac{1}{8}(21)^{1/2}$	*Imma* 4*e*
5/4/*h*5	6^3	1, 1 1	*ADHJ*	5	$P\bar{1}$ 2*i*	0.40307	$0, \frac{1}{6}, \frac{1}{3}; 1, 3^{1/2}, 3^{1/2}; -\frac{1}{2}, 0, 0$	*P*6/*mmm* 2*c*
5/4/*t*6	6^3	1, 1 2	*DHIJK*	4	$P\bar{1}$ 2*i*	0.44179	$\frac{3}{16}, \frac{3}{16}, \frac{3}{8}; \frac{4}{3}, \frac{4}{3}, \frac{2}{3} \times 6^{1/2}; -\frac{1}{6} \times 6^{1/2}, -\frac{1}{6} \times 6^{1/2}, 0$	*I*4/*mmm* 4*e*
4/6/*c*1			*DFHI*	5	$P\bar{1}$ 2*i*	0.34009	$\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; \frac{2}{3} \times 6^{1/2}, \frac{2}{3} \times 6^{1/2}, \frac{2}{3} \times 6^{1/2}; \frac{1}{2}, -\frac{1}{2}, 0$	$Fd\bar{3}m$ 8*a*

Table 3
Symmetry operations giving rise to sphere contacts in $P\bar{1}$ 2*i*.

Symbol	Symmetry operations	Symbol	Symmetry operation	Symbol	Symmetry operation
A	$t(100)$, $t(\bar{1}00)$	*D*	$\bar{1}(000)$	*H*	$\bar{1}(00\frac{1}{2})$
B	$t(010)$, $t(0\bar{1}0)$	*E*	$\bar{1}(\frac{1}{2}00)$	*I*	$\bar{1}(\frac{1}{2}0\frac{1}{2})$
C	$t(110)$, $t(\bar{1}\bar{1}0)$	*F*	$\bar{1}(0\frac{1}{2}0)$	*J*	$\bar{1}(0\frac{1}{2}\frac{1}{2})$
		G	$\bar{1}(\frac{1}{2}\frac{1}{2}0)$	*K*	$\bar{1}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

The second column shows the simplest plane nets of spheres from which the sphere packings may be constructed, *i.e.* triangular nets 3^6 and quadrangular nets 4^4. Column 3 contains information on the stacking of these nets (*cf. International Tables for Crystallography*, 1999, Vol. C, ch. 9): the contact numbers to the nets above and below, and the number of layers per translation period in the direction perpendicular to the layers.

The next column shows the symmetry operations (translations) that give rise to sphere contacts. Without restriction of the generality, the unit cell may always be chosen such that the translations parallel to **a**, **b** and **c** correspond to sphere contacts. The number f of degrees of freedom for the sphere-packing type is given in the fifth column. The minimal symmetry of a sphere packing of that type when generated in $P\bar{1}$ 1*a* is displayed in column 6.

The last three columns only refer to special sphere packings of the regarded type, namely to those with minimal density $\rho_{\rm min}$. cos α, cos β and cos γ are the corresponding metrical parameters. The ninth column shows the maximal symmetry of a sphere packing of that type. In all cases, it is also the inherent symmetry of the sphere packings with minimal density.

Obviously, maximal and minimal symmetry have to agree for type 12/3/*c*1. For 10/3/*t*1 and 8/4/*c*1, the minimal symmetry is reduced to that of an orthorhombic body-centred lattice. Among all sphere packings of $P\bar{1}$ 1*a*, only part of those belonging to types 8/3/*h*4 and 6/4/*c*1 may show $P\bar{1}$ 1*a* as inherent symmetry.

3. Sphere packings corresponding to lattice complex $P\bar{1}$ 2*i*

As there exist only two points per unit cell for $P\bar{1}$ 2*i*, a procedure similar to that described by Sinogowitz (1943) has been used to derive sphere packings with that symmetry.

The spheres are arranged in layers parallel to the **ab** plane with two layers per unit cell. Without restriction of the generality, it may be assumed in the following: (i) that the length of the shortest distance between spheres is $d = 1$; (ii) that **a** is the shortest lattice vector; and (iii) that $1 \leq a \leq b \leq c$ and $90 \leq \gamma \leq 120°$ hold. Then, shortest distances between spheres from the same layer necessarily correspond to lattice translations and run parallel to [100], [010] or [110]. The following cases may be distinguished:

(1) $a = b = d = 1$, $\gamma = 120°$: the spheres are arranged in triangular nets 3^6. Sphere contacts refer to the translations $t(100)$, $t(\bar{1}00)$, $t(010)$, $t(0\bar{1}0)$, $t(110)$ and $t(\bar{1}\bar{1}0)$.

(2) $a = b = d = 1$, $90 \leq \gamma < 120°$: the spheres are arranged in quadrangular nets 4^4. Sphere contacts refer to the translations $t(100)$, $t(\bar{1}00)$, $t(010)$ and $t(0\bar{1}0)$.

(3) $a = d = 1$, $b > 1$, $90 \leq \gamma < 120°$: the spheres form rows parallel to **a**. Sphere contacts refer to the translations $t(100)$ and $t(\bar{1}00)$.

(4) $1 < a \leq b$, $90 \leq \gamma < 120°$: no contact exists between spheres within the same layer.

In order to form a sphere packing, in each of the four cases contacts between spheres of neighbouring layers are necessary in addition. As all spheres of a certain layer are translationally equivalent, each sphere has to be in contact with up to four spheres from the layer above and, independently, with up to four spheres from the layer below. All contacts between spheres from different layers necessarily correspond to inversions through some inversion centres $\bar{1}$.

The special situation where the two spheres within a unit cell belong to the same plane net need not be investigated separately. Such a situation occurs only if – for cases (3) and (4) – the z parameter is specialized to $z = 0$ or $\frac{1}{2}$. Because $1 < b \leq c$ must hold, contact to spheres from neighbouring layers cannot correspond to translations but only to inversions.

The cases (1) to (4) together with the various possibilities for contacts between spheres of different layers have systematically been studied. The result is gathered in Table 2. In analogy to Table 1, sphere-packing symbols, plane nets and stacking information are given in the first three columns. In the fourth column, a string of capital letters – explained in Table 3 – symbolizes the symmetry operations that give rise to sphere contacts. Columns 5, 6, 7 and 9 are analogous to the respective columns in Table 1. Column 8 shows those parameters that refer to a sphere packing of the regarded type with minimal density. These values have been calculated with the aid of the PC program *EUREKA: THE SOLVER* (1987), but most of them could be verified by solving the corresponding equations directly.

In contrast to $P\bar{1}$ 1*a*, sphere packings of one and the same type may be generated by different non-equivalent sets of

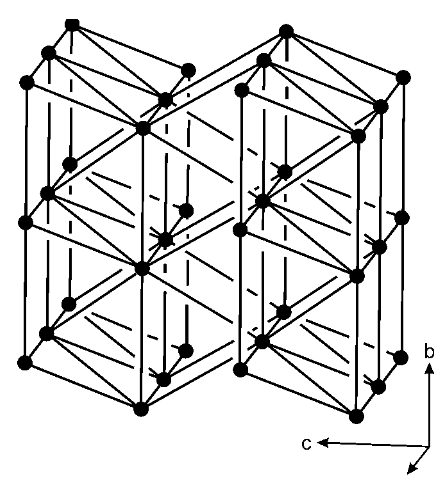

Figure 1
Sphere packing of type 9/3/*a*1 with minimal density.

Table 4
Sphere packings of so far unknown types generated with maximal symmetry.

Symbol	$\rho_{\min}$	$x, y, z; a, b, c; \cos\alpha, \cos\beta, \cos\gamma$	Symmetry
9/3/*m*1	0.69006	0.22150, 0, 0.24675; 1.60651, 1.19126, 1.59618; 0, −0.11327, 0	*C*2/*m* 4*i* *x*0*z*
8/3/*m*1	0.60460	$\frac{1}{8}, 0, \frac{3}{14}; \frac{4}{7} \times 7^{1/2}, \frac{2}{7}(21)^{1/2}, \frac{1}{2}(14)^{1/2}; 0, \frac{1}{4} \times 2^{1/2}, 0$	*C*2/*m* 4*i* *x*0*z*
8/3/*m*2	0.65142	$0, 0.13221, \frac{1}{4}; 1, 3.27521, 1; 0, -0.19066, 0$	*C*2/*c* 4*e* $0y\frac{1}{4}$
7/3/*m*1	0.57451	$\frac{35}{16} - \frac{3}{16}(105)^{1/2}, 0, \frac{11}{8} - \frac{1}{8}(105)^{1/2}; \frac{1}{2} \times 7^{1/2} + \frac{1}{6}(15)^{1/2}, \frac{1}{2} \times 7^{1/2} + \frac{1}{6}(15)^{1/2}, 1; 0, \frac{1}{12}(15)^{1/2} - \frac{1}{4} \times 7^{1/2}, 0$	*C*2/*m* 4*i* *x*0*z*
7/3/*o*5	0.48680	$\frac{3}{2} - \frac{1}{2} \times 7^{1/2}, 0, 0; \frac{3}{2} + \frac{1}{2} \times 7^{1/2}, \frac{1}{2}(4 + 2 \times 7^{1/2})^{1/2}, 1; 0, 0, 0$	*Immm* 4*e* *x*00

symmetry operations in $P\bar{1}\,2i$. Then, the corresponding numbers *f* of degrees of freedom may also differ.

4. Discussion

As lattice complex $P\bar{1}\,1a$ forms a limiting complex of $P\bar{1}\,2i$, all sphere packings of $P\bar{1}\,1a$ have also been found in $P\bar{1}\,2i$. In total, sphere packings of 30 different types may be generated with symmetry $P\bar{1}\,2i$.

Only one type exists where the maximal inherent symmetry of the corresponding sphere packings is triclinic, namely 9/3/*a*1 (*cf*. Fig. 1). In this case, the spheres form plane nets of rhombi 4^4 parallel to the **ab** plane that cannot be deformed to square nets. Each sphere is connected to three spheres from one neighbouring net and to two spheres from the other net.

Five types are found, the maximal inherent symmetry of which is monoclinic: 11/3/*m*1, 9/3/*m*1, 8/3/*m*1, 8/3/*m*2 and 7/3/*m*1. Except 11/3/*m*1 [*cf. International Tables for Crystallography* (1999), Vol. C, ch. 9], all these types have not been known before. 11/3/*m*1 refers to triangular nets parallel to **a** and **b** with three contacts per sphere to one neighbouring net and two contacts to the other net. Nets of rhombi parallel to **a** and **b** are formed within the sphere packings of types 9/3/*m*1, 8/3/*m*1 and 8/3/*m*2. Each sphere touches three spheres from one neighbouring net and two or one from the other net for 9/3/*m*1 and 8/3/*m*1, respectively. Two contacts per sphere to both neighbouring nets exist for 8/3/*m*2. In the case of type 7/3/*m*1, $3^3 4^2$ nets with ribbons of triangles and rhombi perpendicular to $[01\bar{1}]$ are formed. Here, each sphere is in contact with only one sphere from each neighbouring net. For the new types 9/3/*m*1, 8/3/*m*1, 8/3/*m*2 and 7/3/*m*1, sphere-packing parameters referring to the maximal symmetry (*C*2/*m* 4*i* or *C*2/*c* 2*e*) are tabulated in Table 4.

In addition to the one triclinic sphere-packing type, 18 further ones comprise sphere packings with inherent symmetry $P\bar{1}\,2i$. For the other 11 types, the minimal inherent symmetry is higher than triclinic. In five of these cases, namely for types 12/3/*c*1, 12/3/*h*1, 11/3/*m*1, 10/3/*o*1 and 9/3/*m*1, the minimal inherent symmetry coincides with the maximal symmetry.

Sphere packings of all but six of the 30 types may be realized as stackings of parallel planar nets. In the case of a sphere packing with maximal inherent symmetry, these nets are undistorted in many but not all cases. In addition to triangular nets 3^6 and quadrangular nets 4^4, honeycomb nets 6^3 and nets with ribbons of triangles and rhombi $3^3 4^2$ occur twice and once, respectively. It has to be noticed that the number of layers per translation period in the direction perpendicular to the layers (last entry in column 3) refers only to sphere packings with minimal density. For other packings of the same type, this number may be higher and even infinite. Type 8/3/*m*1 shows the remarkably high number of 32 layers per translation period perpendicular to the 4^4 nets in the case of a sphere packing with minimal density. For two types, namely 9/3/*m*1 and 9/3/*a*1, not even in this special case does there exist a translation vector running perpendicular to the nets of rhombi, *i.e.* perpendicular to the **ab** plane.

Most of the sphere-packing types referring to $P\bar{1}\,1a$ and $P\bar{1}\,2i$ have been known before. In addition to the one new triclinic and the four new monoclinic ones, mentioned above, only the orthorhombic type 7/3/*o*5 (*cf*. also Table 4) was unknown before. The reason for this situation is because all but one (9/3/*a*1) of the 30 sphere-packing types correspond to limiting complexes of the lattice complex $P\bar{1}\,2i$. All these limiting complexes are connected not only with specialized coordinates but also with specialized metrical parameters and, therefore, have not been tabulated as 'non-characteristic orbits' by Engel *et al.* (1984). 12 of these sphere-packing types are related to cubic, hexagonal or tetragonal invariant lattice complexes, namely 12/3/*c*1 to *cF*, 8/4/*c*1 to *cI*, 6/4/*c*1 to *cP*, 4/6/*c*1 to *cD*, 12/3/*h*1, 8/3/*h*1 and 6/4/*h*2 to *hE*, 8/3/*h*4 to *hP*, 5/4/*h*5 to *hG*, 10/3/*t*1 to *tI*, and 8/3/*t*1 and 6/4/*t*1 to t^vD.

We thank Michael O'Keeffe not only for the impulse to this paper but also for correcting an error with respect to the maximal symmetry of 8/3/*m*2.

References

Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *Z. Kristallogr.* Suppl. Issue 1.
EUREKA: THE SOLVER (1987). Borland International, Inc., Scotts Valley, USA.
Fischer, W. (1971). *Z. Kristallogr.* **133**, 18–42.
Fischer, W. (1973). *Z. Kristallogr.* **138**, 129–146.
Fischer, W. (1974). *Z. Kristallogr.* **140**, 50–74.
Fischer, W. (1991*a*). *Z. Kristallogr.* **194**, 67–85.
Fischer, W. (1991*b*). *Z. Kristallogr.* **194**, 87–110.
Fischer, W. (1993). *Z. Kristallogr.* **205**, 9–26.
International Tables for Crystallography (1999). Vol. C, 2nd ed., edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.
International Tables for Crystallography (2002). Vol. A, 5th ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.
Koch, E. & Fischer, W. (1995). *Z. Kristallogr.* **210**, 407–414.

Sinogowitz, U. (1943). *Z. Kristallogr.* **105**, 23–52.
Sowa, H. (2000*a*). *Acta Cryst.* A**56**, 288–299.
Sowa, H. (2000*b*). *Z. Kristallogr.* **215**, 335–342.
Sowa, H. (2001). *Acta Cryst.* A**57**, 176–182.
Sowa, H. & Koch, E. (1999). *Z. Kristallogr.* **215**, 316–323.
Sowa, H. & Koch, E. (2001). *Acta Cryst.* A**57**, 406–413.
Sowa, H. & Koch, E. (2002). *Acta Cryst.* A**58**, 327–333.
Zobetz, E. (1983). *Z. Kristallogr.* **163**, 167–180.