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# Orthorhombic sphere packings. V. Trivariant lattice complexes of space groups belonging to crystal class 222

**Heidrun Sowa**

GZG Abt. Kristallographie, Georg-August-Universität Göttingen, Goldschmidtstr. 1, D-37077 Göttingen, Germany. Correspondence e-mail: heidrun.sowa@geo.uni-goettingen.de

This paper completes the derivation of all types of homogeneous sphere packing with orthorhombic symmetry. The nine orthorhombic trivariant lattice complexes belonging to the space groups of crystal class 222 were examined in regard to the existence of homogeneous sphere packings and of interpenetrating sets of layers of spheres. Altogether, sphere packings of 84 different types have been found; the maximal inherent symmetry is orthorhombic for only 36 of these types. In addition, interpenetrating sets of $6^3$ nets occur once. All lattice complexes with orthorhombic characteristic space group give rise to 260 different types of sphere packing in total. The maximal inherent symmetry is orthorhombic for 160 of these types. Sphere packings of 13 types can also be generated with cubic, those of seven types with hexagonal and those of 80 types with tetragonal symmetry. In addition, ten types of interpenetrating sphere packing and two types of sets of interpenetrating sphere layers are obtained. Most of the sphere packings can be subdivided into layer-like subunits perpendicular to one of the orthorhombic main axes.



## 1. Introduction

In this last part of a series of publications on homogeneous sphere packings with orthorhombic symmetry, all types of sphere packing and of interpenetrating sphere layers are tabulated that can be generated in the nine trivariant orthorhombic lattice complexes belonging to space groups of crystal class 222. The four previous papers present the sphere-packing types that refer to orthorhombic lattice complexes with less than three degrees of freedom (*cf.* Fischer *et al.*, 2006; Sowa *et al.*, 2007) and to the trivariant lattice complexes of space groups belonging to crystal class *mmm* (Sowa & Fischer, 2010; Sowa, 2012). Therefore, all sphere-packing types occurring with orthorhombic symmetry are completely derived now.

Information about the procedure of derivation of the sphere packings and all of the necessary definitions have been given in the preceding papers (Sowa *et al.*, 2003; Fischer *et al.*, 2006). Again, the investigated range of the lattice parameters was restricted if the affine normalizer of the space group under consideration interchanges two or three lattice directions (Fischer *et al.*, 2006).

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

## 2. Results

Table 1 gives information on all sphere-packing types that can be realised in the nine examined trivariant orthorhombic lattice complexes. For each lattice complex, the characteristic Wyckoff position and the investigated range of coordinate and lattice parameters are given.

In the second block of information, capital letters indicate the coordinate triplets of the centres of spheres that may be in contact with the reference sphere at $x$, $y$, $z$. The same letter may symbolize two or four neighbouring spheres if they are equidistant for symmetry reasons.

The third block specifies the types of sphere packing or interpenetrating sphere layer that can be generated in the lattice complex under consideration. In the first column, a symbol *n.j* denotes an $n$-dimensional parameter range, $j$ being a serial number. A prefix $n$ indicates a type of interpenetrating nets of spheres (*cf.* *I*222). In the second column, a symbol $k/m/fn$ (Fischer, 1971) characterizes the sphere-packing type: $k$ means the number of contacts per sphere, $m$ is the length of the shortest ring of spheres with mutual contact within the sphere packing, $f$ indicates the highest crystal family for a sphere packing of that type (*o*: orthorhombic, *t*: tetragonal, *h*: hexagonal, *c*: cubic), and $n$ is an arbitrary number. The sets of interpenetrating sphere layers occurring in space group *I*222 are symbolized by $t[6^3]^2$. This means that two sets of $6^3$ nets

**Table 1**
The sphere packings corresponding to the nine orthorhombic trivariant lattice complexes belonging to space groups of crystal class 222.

| | | | | | | |
|---|---|---|---|---|---|---|
| ***P*222 4u *x*, *y*, *z*** | | | $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b \le c}$ | | | |
| *A* | $-x, -y, z$ | *E* | $-x, y, -z + 1$ | *J* | $-x + 1, y, -z + 1$ | |
| *B* | $-x, y, -z$ | *F* | $x, -y, -z$ | *K* | $x, -y, -z + 1$ | |
| *C* | $x + 1, y, z$ | *G* | $-x + 1, -y, z$ | *L* | $x, -y + 1, -z$ | |
| | $x - 1, y, z$ | *H* | $-x + 1, y, -z$ | *M* | $x, -y + 1, -z + 1$ | |
| *D* | $-x, -y + 1, z$ | *I* | $-x + 1, -y + 1, z$ | | | |
| 0.1 | 12/3/*c*1 | *ABDEFGHIJKLM* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | 0.74048 |
| 0.2 | 10/3/*t*1 | *ABCDEGHIJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, 1$ | | | 0.69813 |
| 1.1 | 8/4/*c*1 | *ABDEGHIJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, 1$ | | | 0.68017 |
| 1.2 | 6/4/*c*1 | *ABCDE* | $0, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, 1$ | | | 0.52360 |
| ***P*222$_1$ 4*e* *x*, *y*, *z*** | | | $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b}$ | | | |
| *A* | $x, -y, -z$ | *D* | $x, y + 1, z$ | *H* | $-x + 1, y, -z + \frac{1}{2}$ | |
| *B* | $-x, y, -z + \frac{1}{2}$ | | $x, y - 1, z$ | *I* | $-x + 1, y, -z - \frac{1}{2}$ | |
| *C* | $x + 1, y, z$ | *E* | $-x, y, -z - \frac{1}{2}$ | *J* | $x, y, z + 1$ | |
| | $x - 1, y, z$ | *F* | $x, -y + 1, -z$ | | $x, y, z - 1$ | |
| | | *G* | $x, -y, -z + 1$ | | | |
| 0.1 | 8/3/*t*1 | *ABCDFH* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2(3)^{1/2}$ | | | 0.60460 |
| 0.2 | 8/3/*h*4 | *ABCEFHI* | $\frac{1}{4}, \frac{1}{4}, 0; \frac{1}{2}, \frac{1}{2}(3)^{1/2}$ | | | 0.60460 |
| 0.3 | 8/3/*h*4 | *ABEFHIJ* | $\frac{1}{4}, \frac{1}{4}, 0; \frac{1}{2}(3)^{1/2}, \frac{1}{2}$ | | | 0.60460 |
| 1.1 | 7/3/*o*1 | *ABCDF* | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}; 1, 2 + 3^{1/2}$ | | | 0.56119 |
| 1.1′ | 7/3/*o*1 | *ABCDH* | $\frac{1}{4}, 0, 1 - \frac{1}{2}(3)^{1/2}; 1, 2 + 3^{1/2}$ | | | 0.56119 |
| 1.2 | 6/3/*o*1 | *ABCFH* | $\frac{1}{4}, \frac{1}{4}, \frac{11}{8} - \frac{1}{8}(105)^{1/2}; \frac{1}{4}(21)^{1/2} - \frac{1}{4}(5)^{1/2}, \frac{1}{4}(7)^{1/2} + \frac{1}{4}(15)^{1/2}$ | | | 0.44226 |
| 1.3 | 6/4/*t*2 | *ABFHJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, \frac{2}{15}(15)^{1/2}$ | | | 0.55851 |
| 1.4 | 6/4/*c*1 | *ABCEF* | $0, \frac{1}{4}, 0; \frac{1}{2}, 1$ | | | 0.52360 |
| 1.5 | 6/4/*c*1 | *ABEFHI* | $\frac{1}{4}, \frac{1}{4}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | | | 0.52360 |
| 2.1 | 6/4/*c*1 | *ABCD* | $0, 0, \frac{1}{8}; 1, 4$ | | | 0.52360 |
| 2.2 | 5/4/*h*5 | *ABCF* | $0, \frac{1}{4}, \frac{1}{12}; \frac{1}{3}(3)^{1/2}, 3^{1/2}$ | | | 0.40307 |
| 2.3 | 4/6/*c*1 | *ABFH* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2^{1/2}$ | | | 0.34009 |
| ***P*2$_1$2$_1$2 4*c* *x*, *y*, *z*** | | | $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b}$ | | | |
| *A* | $-x, -y, z$ | *D* | $x + \frac{1}{2}, -y + \frac{1}{2}, -z$ | *H* | $-x + \frac{1}{2}, y + \frac{1}{2}, -z$ | |
| *B* | $x + 1, y, z$ | | $x - \frac{1}{2}, -y + \frac{1}{2}, -z$ | | $-x + \frac{1}{2}, y - \frac{1}{2}, -z$ | |
| | $x - 1, y, z$ | *E* | $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ | *I* | $-x + \frac{1}{2}, y + \frac{1}{2}, -z + 1$ | |
| *C* | $x, y, z + 1$ | | $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ | | $-x + \frac{1}{2}, y - \frac{1}{2}, -z + 1$ | |
| | $x, y, z - 1$ | *F* | $-x, -y + 1, z$ | *J* | $-x + 1, -y + 1, z$ | |
| | | *G* | $-x + 1, -y, z$ | | | |
| 0.1 | 12/3/*h*1 | *ACDEGHI* | $\frac{1}{4}, \frac{1}{6}, \frac{1}{4}; \frac{2}{3}(2)^{1/2}, \frac{1}{3}(3)^{1/2}$ | | | 0.74048 |
| 0.2 | 12/3/*c*1 | *ADEFGHIJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | 0.74048 |
| 0.3 | 10/3/*o*2 | *ABCDEG* | $\frac{1}{4}, \frac{3}{4} - \frac{1}{4}(6)^{1/2}, \frac{1}{4}; 3^{1/2} - 2^{1/2}, 3^{1/2} - 2^{1/2}$ | | | 0.66568 |
| 0.4 | 10/3/*t*1 | *ABDEFGJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, 1$ | | | 0.69813 |
| 1.1 | 11/3/*t*1 | *ACDEHI* | $\frac{1}{2}(2)^{1/2} - \frac{1}{2}, \frac{1}{2}(2)^{1/2} - \frac{1}{2}, \frac{1}{4}; 1, 2 - 2^{1/2}$ | | | 0.71868 |
| 1.2 | 10/3/*o*1 | *ADEGHI* | $\frac{1}{4}, \frac{1}{5}, \frac{1}{4}; \frac{2}{5}(6)^{1/2}, \frac{1}{5}(15)^{1/2}$ | | | 0.69813 |
| 1.3 | 9/3/*t*2 | *ABCDE* | $0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}; 1 - \frac{1}{2}(2)^{1/2}, 1 - \frac{1}{2}(2)^{1/2}$ | | | 0.61343 |
| 1.4 | 8/3/*o*1 | *ACDEG* | $\frac{1}{4}, \frac{1}{7}, \frac{1}{4}; \frac{2}{7}(3)^{1/2}, \frac{1}{7}(7)^{1/2}$ | | | 0.60460 |
| 1.5 | 8/3/*h*3 | *ABDEG* | $\frac{1}{4}, \frac{1}{6}, \frac{1}{4}; \frac{2}{9}(3)^{1/2}, \frac{1}{3}(3)^{1/2}$ | | | 0.53472 |
| 1.6 | 8/3/*h*4 | *ABDEF* | $0, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}(3)^{1/2}$ | | | 0.60460 |
| 1.7 | 8/3/*h*4 | *ACDEF* | $0, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}(3)^{1/2}, \frac{1}{2}$ | | | 0.60460 |
| 1.7′ | | *ACGHI* | | | | |
| 1.8 | 8/3/*h*4 | *ABCDG* | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{6}(3)^{1/2}, \frac{1}{6}(3)^{1/2}$ | | | 0.60460 |
| 1.9 | 8/3/*h*4 | *ACDGH* | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}(3)^{1/2}, \frac{1}{2}$ | | | 0.60460 |
| 1.10 | 8/4/*c*1 | *ADEFGJ* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, 1$ | | | 0.68017 |
| 2.1 | 10/3/*t*1 | *CDEHI* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, \frac{1}{3}(3)^{1/2}$ | | | 0.69813 |
| 2.2 | 9/3/*t*1 | *ADEHI* | $0.22150, 0.22150, \frac{1}{4}; 1, 0.74632$ | | | 0.69006 |
| 2.3 | 7/3/*o*1 | *ABCD* | $0, 1 - \frac{1}{2}(3)^{1/2}, 0; 2 - 3^{1/2}, 2 - 3^{1/2}$ | | | 0.56119 |
| 2.4 | 7/3/*o*5 | *ABDE* | $0, \frac{3}{2} - \frac{1}{2}(7)^{1/2}, \frac{1}{4}; 3 - 7^{1/2}, [2(7)^{1/2} - 5]^{1/2}$ | | | 0.48680 |
| 2.5 | 7/3/*o*5 | *ACDE* | $0, \frac{3}{2} - \frac{1}{2}(7)^{1/2}, \frac{1}{4}; [2(7)^{1/2} - 5]^{1/2}, 3 - 7^{1/2}$ | | | 0.48680 |
| 2.5′ | | *ACHI* | | | | |
| 2.6 | 7/3/*t*5 | *ACDH* | $\frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{4}(3)^{1/2} - \frac{1}{4}, 0; 1, \frac{1}{2}(6)^{1/2} - \frac{1}{2}(2)^{1/2}$ | | | 0.56119 |
| 2.7 | 6/4/*h*2 | *ADEG* | $\frac{1}{4}, \frac{1}{6}, \frac{1}{4}; \frac{1}{3}(2)^{1/2}, \frac{1}{3}(3)^{1/2}$ | | | 0.52360 |
| 2.8 | 6/4/*c*1 | *ADEF* | $0, \frac{1}{4}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | | | 0.52360 |
| 2.8′ | | *AGHI* | | | | |
| 2.9 | 6/4/*c*1 | *ACDF* | $0, \frac{1}{4}, 0; 1, \frac{1}{2}$ | | | 0.52360 |

**Table 1 (continued)**

| | | | | | | |
|---|---|---|---|---|---|---|
| 2.9′ | | *ACGH* | $\frac{1}{4}$, 0, 0; 1, $\frac{1}{2}$ | | | |
| 2.10 | 6/4/*c*1 | *ACDG* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{4}(2)^{1/2}$ | | | 0.52360 |
| 3.1 | 8/4/*c*1 | *DEHI* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; 1, $\frac{1}{2}(2)^{1/2}$ | | | 0.68017 |
| 3.2 | 6/4/*c*1 | *CDH* | $\frac{1}{4}$, $\frac{1}{4}$, 0; 1, $\frac{1}{2}$ | | | 0.52360 |
| 3.3 | 5/4/*t*6 | *ADE* | 0, $\frac{3}{16}$, $\frac{1}{4}$; $\frac{1}{2}$, $\frac{1}{2}$ | | | 0.44179 |
| 3.3′ | | *AHI* | | | | |
| 3.4 | 5/4/*h*5 | *ACD* | 0, $\frac{1}{6}$, 0; $\frac{1}{3}(3)^{1/2}$, $\frac{1}{3}$ | | | 0.40307 |
| 3.4′ | | *ACH* | | | | |
| ***P*2$_1$2$_1$2$_1$ 4*a* *x*, *y*, *z*** | | | $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b \le c}$ | | | |
| *A* | $-x+\frac{1}{2}, -y, z+\frac{1}{2}$ | *D* | $x+\frac{1}{2}, -y+\frac{1}{2}, -z$ | *G* | $-x, y+\frac{1}{2}, -z-\frac{1}{2}$ | |
| | $-x+\frac{1}{2}, -y, z-\frac{1}{2}$ | | $x-\frac{1}{2}, -y+\frac{1}{2}, -z$ | | $-x, y-\frac{1}{2}, -z-\frac{1}{2}$ | |
| *B* | $-x-\frac{1}{2}, -y, z+\frac{1}{2}$ | *E* | $x+\frac{1}{2}, -y-\frac{1}{2}, -z$ | *H* | $x, y+1, z$ | |
| | $-x-\frac{1}{2}, -y, z-\frac{1}{2}$ | | $x-\frac{1}{2}, -y-\frac{1}{2}, -z$ | | $x, y-1, z$ | |
| *C* | $x+1, y, z$ | *F* | $-x, y+\frac{1}{2}, -z+\frac{1}{2}$ | *I* | $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$ | |
| | $x-1, y, z$ | | $-x, y-\frac{1}{2}, -z+\frac{1}{2}$ | | $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$ | |
| 0.1 | 12/3/*h*1 | *ABCDEF* | 0, 0, $\frac{1}{12}$; $\frac{1}{4}(6)^{1/2}$, $\frac{3}{4}(2)^{1/2}$ | | | 0.74048 |
| 0.2 | 12/3/*c*1 | *ABDEFG* | 0, 0, 0; 1, 1 | | | 0.74048 |
| 0.3 | 12/3/*c*1 | *CDEFHI* | $\frac{1}{4}$, 0, $\frac{1}{8}$; 1, $2(2)^{1/2}$ | | | 0.74048 |
| 0.4 | 12/3/*c*1 | *ACDEFI* | $\frac{1}{4}$, 0, $\frac{1}{8}$; $\frac{1}{2}(2)^{1/2}$, $2^{1/2}$ | | | 0.74048 |
| 1.1 | 10/3/*o*1 | *ABDEF* | 0, 0, $\frac{1}{20}$; $\frac{1}{4}(10)^{1/2}$, $\frac{5}{12}(6)^{1/2}$ | | | 0.69813 |
| 1.2 | 10/3/*o*2 | *CDEFH* | 0, 0, $\frac{1}{4}(6)^{1/2} - \frac{1}{2}$; 1, $2^{1/2} + 3^{1/2}$ | | | 0.66568 |
| 1.3 | 10/3/*o*2 | *CDFHI* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{3}{4} - \frac{1}{4}(6)^{1/2}$; 1, $2^{1/2} + 3^{1/2}$ | | | 0.66568 |
| 1.4 | 10/3/*o*5 | *ACDEF* | $\frac{1}{8}$, 0, $\frac{1}{10}$; $\frac{1}{6}(15)^{1/2}$, $\frac{5}{4}$ | | | 0.69813 |
| 1.5 | 10/3/*o*6 | *ACDFI* | $\frac{1}{4}$, $\frac{1}{2} - \frac{1}{6}(6)^{1/2}$, $\frac{1}{8}(6)^{1/2} - \frac{1}{8}$; $\frac{1}{3}[18-6(6)^{1/2}]^{1/2}$, $\frac{2}{3}(3)^{1/2}$ | | | 0.66568 |
| 1.5′ | | *ABCDF* | | | | |
| 1.6 | 10/3/*t*1 | *ABCDE* | 0, 0, 0; $\frac{1}{3}(3)^{1/2}$, 1 | | | 0.69813 |
| 1.7 | 10/3/*t*1 | *ADEFI* | $\frac{1}{4}$, 0, $\frac{1}{8}$; 1, $\frac{2}{3}(6)^{1/2}$ | | | 0.69813 |
| 1.8 | 10/3/*t*1 | *CDEFI* | $\frac{1}{4}$, 0, $\frac{1}{8}$; $\frac{1}{3}(6)^{1/2}$, 2 | | | 0.69813 |
| 2.1 | 8/3/*o*1 | *CDEF* | 0, 0, $\frac{3}{28}$; $\frac{1}{6}(21)^{1/2}$, $\frac{7}{6}(3)^{1/2}$ | | | 0.60460 |
| 2.2 | 8/3/*o*5 | *ADFI* | $\frac{1}{4}$, $\frac{1}{8}$, $\frac{5}{28}$; $\frac{1}{7}(42)^{1/2}$, $\frac{1}{2}(7)^{1/2}$ | | | 0.60460 |
| 2.2′ | | *ABDF*, *ADEF* | | | | |
| 2.3 | 8/3/*t*1 | *CDFH* | 0, $\frac{1}{4}$, $\frac{1}{8}$; 1, $2(3)^{1/2}$ | | | 0.60460 |
| 2.4 | 8/3/*t*2 | *ACDF* | $\frac{1}{8}$, $\frac{1}{12}$, $\frac{1}{6}$; $\frac{2}{9}(6)^{1/2}$, 1 | | | 0.62056 |
| 2.5 | 8/3/*h*3 | *CDFI* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{6}$; $\frac{2}{3}$, $3^{1/2}$ | | | 0.53742 |
| 2.5′ | | *ABCD* | | | | |
| 2.6 | 8/3/*h*4 | *ACDE* | $\frac{1}{4}$, 0, 0; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(3)^{1/2}$ | | | 0.60460 |
| 2.7 | 8/3/*h*4 | *ACFI* | $\frac{1}{4}$, 0, $\frac{1}{4}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(3)^{1/2}$ | | | 0.60460 |
| 2.7′ | | *ABCF* | | | | |
| 2.8 | 8/4/*c*1 | *ABDE* | 0, 0, 0; $\frac{1}{2}(2)^{1/2}$, 1 | | | 0.68017 |
| 2.9 | 8/4/*c*1 | *DEFI* | $\frac{1}{4}$, 0, $\frac{1}{8}$; 1, 2 | | | 0.68017 |
| 3.1 | 6/3/*o*1 | *CDF* | 0, $\frac{1}{4}$, $\frac{1}{8}(105)^{1/2} - \frac{9}{8}$; $\frac{1}{4}(21)^{1/2} - \frac{1}{4}(5)^{1/2}$, $\frac{1}{4}(7)^{1/2} + \frac{1}{4}(15)^{1/2}$ | | | 0.44226 |
| 3.1′ | | *ACD* | | | | |
| 3.2 | 6/3/*c*1 | *ADF* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}$; 1, 1 | | | 0.48096 |
| 3.3 | 6/4/*t*2 | *ACF* | $\frac{1}{8}$, 0, $\frac{1}{4}$; $\frac{2}{15}(15)^{1/2}$, 1 | | | 0.55851 |
| 3.4 | 6/4/*h*2 | *DFI* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{6}$; $\frac{1}{4}(6)^{1/2}$, $3^{1/2}$ | | | 0.52360 |
| 3.4′ | | *ABD*, *DEF* | | | | |
| 3.5 | 6/4/*c*1 | *ADE* | $\frac{1}{4}$, 0, 0; 1, $2^{1/2}$ | | | 0.52360 |
| 3.5′ | | *AFI* | $\frac{1}{4}$, 0, $\frac{1}{4}$; 1, $2^{1/2}$ | | | |
| 3.5′ | | *ABF* | | | | |
| 4.1 | 4/6/*c*1 | *DF* | 0, $\frac{1}{4}$, $\frac{1}{8}$; 1, $2^{1/2}$ | | | 0.34009 |
| 4.1′ | | *AD*, *AF* | | | | |
| ***C*222$_1$ 8*c* *x*, *y*, *z*** | | | $\mathbf{0 \leqq x \leqq \frac{1}{4}, 0 \leqq y \leqq \frac{1}{4}, 0 \leqq z \leqq \frac{1}{4}; a \leqq b}$ | | | |
| *A* | $x, -y, -z$ | *F* | $x+\frac{1}{2}, y+\frac{1}{2}, z$ | *I* | $x, -y, -z+1$ | |
| *B* | $-x, y, -z+\frac{1}{2}$ | | $x-\frac{1}{2}, y+\frac{1}{2}, z$ | *J* | $-x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$ | |
| *C* | $x+1, y, z$ | | $x+\frac{1}{2}, y-\frac{1}{2}, z$ | | $-x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$ | |
| | $x-1, y, z$ | | $x-\frac{1}{2}, y-\frac{1}{2}, z$ | *K* | $-x+1, y, -z+\frac{1}{2}$ | |
| *D* | $-x, y, -z-\frac{1}{2}$ | *G* | $x, -y+1, -z$ | *L* | $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$ | |
| *E* | $x+\frac{1}{2}, -y+\frac{1}{2}, -z$ | *H* | $x, y, z+1$ | | $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$ | |
| | $x-\frac{1}{2}, -y+\frac{1}{2}, -z$ | | $x, y, z-1$ | *M* | $-x+1, y, -z-\frac{1}{2}$ | |
| 0.1 | 12/3/*c*1 | *ABEFGKL* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, 2 | | | 0.74048 |
| 0.2 | 11/3/*o*2 | *ABCEFK* | $\frac{1}{4}$, $\frac{1}{6}$, $\frac{3}{2}(2)^{1/2} - 2$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(2)^{1/2} + 1$ | | | 0.71868 |

**Table 1 (continued)**

| | | | | |
|---|---|---|---|---|
| 0.3 | 10/3/*t*1 | *ABEGJKL* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, \frac{2}{3}(3)^{1/2}$ | 0.69813 |
| 0.4 | 9/3/*o*1 | *ABCDEKM* | $\frac{1}{4}, 1 - \frac{1}{2}(3)^{1/2}, 0; 2 - 3^{1/2}, 2(3)^{1/2} - 3$ | 0.64801 |
| 0.5 | 9/3/*o*1 | *ABDHJKM* | $\frac{1}{4}, 1 - \frac{1}{2}(3)^{1/2}, 0; 2(3)^{1/2} - 3, 2 - 3^{1/2}$ | 0.64801 |
| 0.6 | 9/3/*t*2 | *ABDEJKM* | $\frac{1}{4}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0; 2^{1/2} - 1, 2^{1/2} - 1$ | 0.61343 |
| 0.7 | 8/3/*h*4 | *ABDEGJ* | $\frac{1}{8}, \frac{1}{4}, 0; 1, \frac{1}{2}(3)^{1/2}$ | 0.60460 |
| 0.7′ | | *ABIJKL* | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{2}(3)^{1/2}$ | |
| 0.8 | 8/3/*h*4 | *ABHIJK* | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{1}{6}(3)^{1/2}$ | 0.60460 |
| 1.1 | 10/3/*t*1 | *BCEFK* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, 2$ | 0.69813 |
| 1.2 | 10/3/*h*2 | *ABCEF* | $0, \frac{1}{6}, \frac{1}{4}(6)^{1/2} - \frac{1}{2}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2} + \frac{1}{3}(2)^{1/2}$ | 0.66568 |
| 1.3 | 9/3/*o*1 | *ABCFK* | $\frac{1}{4}, 0, 1 - \frac{1}{2}(3)^{1/2}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2} + 1$ | 0.64801 |
| 1.4 | 9/3/*o*5 | *ABEFK* | $\frac{1}{4}$, 0.19373, 0.12338; 0.74152, 1.97434 | 0.69006 |
| 1.5 | 9/3/*t*2 | *ABEFG* | $0, \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, 0; 1, 2^{1/2} + 1$ | 0.61343 |
| 1.5′ | | *ABFKL* | $\frac{1}{4}, 0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}; 1, 2^{1/2} + 1$ | |
| 1.6 | 8/4/*c*1 | *ABEGKL* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2^{1/2}$ | 0.68017 |
| 1.7 | 7/3/*o*1 | *ABCDE* | $0, 1 - \frac{1}{2}(3)^{1/2}, 0; 2 - 3^{1/2}, 4 - 2(3)^{1/2}$ | 0.56119 |
| 1.8 | 7/3/*o*2 | *ABDHJ* | $\frac{15}{64} - \frac{1}{64}(33)^{1/2}, \frac{7}{8} - \frac{1}{8}(33)^{1/2}, 0; \frac{3}{2}(3)^{1/2} - \frac{1}{2}(11)^{1/2}, \frac{7}{4} - \frac{1}{4}(33)^{1/2}$ | 0.43908 |
| 1.8′ | | *ABHIJ* | | |
| 1.9 | 7/3/*o*3 | *ABDEJ* | $\frac{4}{9} - \frac{1}{9}(7)^{1/2}, \frac{3}{2} - \frac{1}{2}(7)^{1/2}, 0; 7^{1/2} - 2, \frac{2}{3}[26(7)^{1/2} - 68]^{1/2}$ | 0.48680 |
| 1.10 | 7/3/*o*9 | *ABEJK* | $0, \frac{1}{6}, \frac{3}{4} - \frac{1}{4}(7)^{1/2}; \frac{1}{3}(3)^{1/2}, \frac{1}{9}[15 + 6(7)^{1/2}]^{1/2}$ | 0.50736 |
| 1.11 | 7/3/*o*10 | *ABCEK* | $\frac{1}{4}, \frac{1}{12}(7)^{1/2} - \frac{1}{12}, \frac{3}{4} - \frac{1}{4}(7)^{1/2}; \frac{1}{3}[6(7)^{1/2} - 15]^{1/2}, \frac{1}{3}[2(7)^{1/2} + 1]^{1/2}$ | 0.48680 |
| 1.12 | 7/3/*o*11 | *ABHJK* | $\frac{1}{4}$, 0.13061, 0.15994; 0.54240, 0.27571 | 0.58705 |
| 1.13 | 7/3/*o*12 | *ABEGJ* | $\frac{1}{32}(105)^{1/2} - \frac{5}{32}, \frac{1}{4}$, 0.04707; 1, 0.95602 | 0.57451 |
| 1.13′ | | *ABJKL* | $\frac{1}{4}, \frac{1}{32}(105)^{1/2} - \frac{5}{32}$, 0.20293; 1, 0.95602 | |
| 1.14 | 7/4/*o*1 | *ABDEKM* | $\frac{1}{4}, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{3}[12 - 3(13)^{1/2})]^{1/2}, \frac{1}{6}(13)^{1/2} - \frac{1}{6}$ | 0.60210 |
| 1.15 | 7/4/*o*1 | *ABDJKM* | $\frac{1}{4}, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{6}(13)^{1/2} - \frac{1}{6}, \frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$ | 0.60210 |
| 1.16 | 6/4/*c*1 | *ABDEG* | $0, \frac{1}{4}, 0; 1, 1$ | 0.52360 |
| 1.16′ | | *ABIKL* | $\frac{1}{4}, 0, \frac{1}{4}; 1, 1$ | |
| 1.17 | 6/4/*c*1 | *ABIJK* | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}$ | 0.52360 |
| 2.1 | 9/3/*o*1 | *BCEF* | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2} + 1$ | 0.64801 |
| 2.2 | 8/3/*o*2 | *ABEF* | $0, \frac{7}{32}, \frac{3}{28}; \frac{1}{2}(3)^{1/2}, \frac{7}{8}(7)^{1/2}$ | 0.60460 |
| 2.3 | 8/3/*h*4 | *ABCF* | $0, 0, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, \frac{4}{3}(3)^{1/2}$ | 0.60460 |
| 2.4 | 8/4/*c*1 | *BEFK* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, 2$ | 0.68017 |
| 2.5 | 7/4/*o*1 | *ABFK* | $\frac{1}{4}, 0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}; \frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}, \frac{1}{2}(13)^{1/2} + \frac{1}{2}$ | 0.60210 |
| 2.6 | 6/3/*o*2 | *ABCE* | $0, \frac{19}{64} - \frac{1}{64}(105)^{1/2}, \frac{1}{16}(105)^{1/2} - \frac{9}{16}; \frac{1}{4}(15)^{1/2} - \frac{1}{4}(7)^{1/2}, \frac{3}{16}(15)^{1/2} + \frac{1}{16}(7)^{1/2}$ | 0.44226 |
| 2.7 | 6/3/*o*30 | *ABEJ* | 0.18416, 0.18042, 0.04256; 0.66583, 0.65183 | 0.46960 |
| 2.8 | 6/3/*t*1 | *ABHJ* | 0.15314, 0.15314, $\frac{1}{8}$; 1, 0.31633 | 0.41915 |
| 2.9 | 6/4/*c*1 | *AEGJ* | $\frac{1}{4}, \frac{1}{4}, 0; 1, 1$ | 0.52360 |
| 2.9′ | | *BJKL* | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | |
| 2.10 | 5/4/*o*1 | *ABDJ* | $\frac{1}{7}, \frac{1}{6}, 0; \frac{1}{3}(7)^{1/2}, \frac{2}{21}(21)^{1/2}$ | 0.40307 |
| 2.10′ | | *ABIJ* | | 0.52360 |
| 2.11 | 5/4/*o*7 | *ABEK* | $\frac{1}{4}, \frac{3}{20}, \frac{3}{32}; \frac{1}{5}(5)^{1/2}, \frac{4}{5}$ | 0.44179 |
| 2.12 | 5/4/*o*8 | *ABJK* | $\frac{1}{4}$, 0.14839, 0.14839; 0.63751, 0.53756 | 0.46761 |
| 2.13 | 5/4/*t*6 | *ABEG* | $0, \frac{1}{4}, \frac{1}{16}; 1, 2^{1/2}$ | 0.44179 |
| 2.13′ | | *ABKL* | $\frac{1}{4}, 0, \frac{3}{16}; 1, 2^{1/2}$ | |
| 2.14 | 5/4/*h*5 | *ABDE* | $0, \frac{1}{6}, 0; \frac{1}{3}(3)^{1/2}, \frac{2}{3}$ | 0.40307 |
| 3.1 | 7/4/*o*1 | *BEF* | $0, \frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}; \frac{1}{2}[10 - 2(13)^{1/2}], \frac{1}{2}(13)^{1/2} + \frac{1}{2}$ | 0.60210 |
| 3.2 | 6/4/*c*1 | *ABF* | $0, 0, \frac{1}{8}; 1, 2(2)^{1/2}$ | 0.52360 |
| 3.3 | 5/4/*t*6 | *AEJ* | $\frac{1}{4}, \frac{3}{16}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.44179 |
| 3.4 | 4/6/*t*1 | *ABJ* | 0.16487, 0.16487, $\frac{1}{8}$; 1, 0.52024 | 0.35858 |
| 3.5 | 4/6/*h*2 | *ABE* | $0, \frac{1}{6}, \frac{1}{16}, \frac{1}{3}(3)^{1/2}, \frac{2}{3}(2)^{1/2}$ | 0.34009 |

***C*222 8*l* *x*, *y*, *z*** $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b}$

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

| | | | | |
|---|---|---|---|---|
| 0.1 | 9/3/*o*1 | *ABCDEKMN* | $\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{4}; 2 - 3^{1/2}, 2(3)^{1/2} - 3$ | 0.64801 |
| 0.2 | 9/3/*o*1 | *ACEHIJMN* | $\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{4}; 2(3)^{1/2} - 3, 2 - 3^{1/2}$ | 0.64801 |
| 0.3 | 9/3/*t*2 | *ABCEHIKMN* | $\frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}; 2^{1/2} - 1, 2^{1/2} - 1$ | 0.61343 |
| 0.4 | 7/3/*o*1 | *ABCDEF* | $0, 1 - \frac{1}{2}(3)^{1/2}, \frac{1}{4}; 2 - 3^{1/2}, 4 - 2(3)^{1/2}$ | 0.56119 |

**Table 1 (continued)**

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.5 | 6/4/*c*1 | *ABCEFG* | 0, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1 | | | 0.52360 |
| 0.5′ | | *BEHIKL* | $\frac{1}{4}$, 0, $\frac{1}{4}$; 1, 1 | | | |
| 1.1 | 7/4/*o*1 | *ABCEKMN* | $\frac{1}{4}$, $\frac{1}{24}(13)^{1/2} - \frac{1}{24}$, $\frac{1}{4}$, $\frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$, $\frac{1}{6}(13)^{1/2} - \frac{1}{6}$ | | | 0.60210 |
| 1.2 | 7/4/*o*1 | *ACEHIMN* | $\frac{1}{4}$, $\frac{1}{24}(13)^{1/2} - \frac{1}{24}$, $\frac{1}{4}$, $\frac{1}{6}(13)^{1/2} - \frac{1}{6}$, $\frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$ | | | 0.60210 |
| 1.3 | 7/3/*t*4 | *ACEHIJ* | $\frac{3}{4} - \frac{1}{4}(6)^{1/2}$, $\frac{3}{4} - \frac{1}{4}(6)^{1/2}$, $\frac{1}{4}$; 1, $3^{1/2} - 2^{1/2}$ | | | 0.42315 |
| 1.4 | 6/3/*t*5 | *ABCEHI* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{4}$; 1, $\frac{1}{2}$ | | | 0.37024 |
| 1.5 | 6/4/*o*2 | *ABCDE* | 0.06652, 0.12896, $\frac{1}{4}$; 0.26023, 0.51584 | | | 0.54992 |
| 1.6 | 6/4/*c*1 | *AEHJM* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{4}$ | | | 0.52360 |
| 1.7 | 5/4/*t*6 | *BEHIK* | $\frac{1}{4}$, $\frac{1}{16}$, $\frac{1}{4}$, $\frac{1}{2}(2)^{1/2}$, $\frac{1}{2}(2)^{1/2}$ | | | 0.44179 |
| 1.8 | 5/4/*h*5 | *ABCEF* | 0, $\frac{1}{6}$, $\frac{1}{4}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}$ | | | 0.40307 |
| 2.1 | 5/4/*t*4 | *AEHJ* | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0; 1, $1 - \frac{1}{2}(2)^{1/2}$ | | | 0.35934 |
| 2.2 | 5/4/*t*5 | *ACEHI* | [0.15, 0.11602, $\frac{1}{4}$; 0.77348, 0.40933] | | | >0.37024 |
| 2.3 | 4/4/*o*2 | *ABCE* | 0.08793, 0.14827, $\frac{1}{4}$; 0.79229, $\frac{1}{8}(33)^{1/2} - \frac{1}{8}$ | | | 0.31354 |
| 2.3′ | | *BEHI* | | | | |
| ***F*222 16*k* *x*, *y*, *z*** | | | **$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$, $a \le b \le c$** | | | |
| *A* | $-x, y, -z$ | *E* | $x + 1, y, z$ | *H* | $x, -y + \frac{1}{2}, -z + \frac{1}{2}$ | |
| *B* | $-x, -y, z$ | | $x - 1, y, z$ | *I* | $-x, -y + 1, z$ | |
| *C* | $-x + \frac{1}{2}, y, -z + \frac{1}{2}$ | *F* | $-x + \frac{1}{2}, -y + \frac{1}{2}, z$ | *J* | $x, -y, -z$ | |
| *D* | $-x - \frac{1}{2}, y, -z + \frac{1}{2}$ | *G* | $-x - \frac{1}{2}, -y + \frac{1}{2}, z$ | | | |
| 0.1 | 8/3/*t*5 | *ABCDEFG* | 0, $1 - \frac{1}{2}(3)^{1/2}$, $1 - \frac{1}{2}(3)^{1/2}$; $2 - 3^{1/2}$, 1 | | | 0.60148 |
| 0.2 | 7/3/*t*7 | *ABCDFGH* | 0, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $2^{1/2} - 1$, 1 | | | 0.50819 |
| 0.3 | 6/3/*c*2 | *ABCFHJ* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}$; 1, 1 | | | 0.37024 |
| 0.4 | 6/4/*c*1 | *ABFGHI* | 0, $\frac{1}{4}$, $\frac{1}{8}$; 1, 2 | | | 0.52360 |
| 1.1 | 6/4/*t*3 | *ABCEF* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}$; $\frac{1}{15}(15)^{1/2}$, 1 | | | 0.55851 |
| 1.2 | 6/4/*t*7 | *ABCDFG* | [0, 0.14, 0.14; 0.34641, 1] | | | >0.50819 |
| 1.3 | 5/3/*t*9 | *ABCFH* | 0.10727, 0.13626, 0.13626; 0.79693, 1 | | | 0.35003 |
| 1.4 | 5/4/*o*9 | *ABFGH* | 0, 0.17812, 0.13055; 0.65186, 1.36432 | | | 0.42583 |
| 2.1 | 4/4/*t*1 | *ABCF* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}$; $\frac{1}{2}(2)^{1/2}$, 1 | | | 0.34009 |
| 2.2 | 4/4/*t*2 | *ABFH* | 0.08990, 0.16010, $\frac{1}{8}$; 1, 1.28078 | | | 0.32392 |
| ***I*222 8*k* *x*, *y*, *z*** | | | **$0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$; $a \le b \le c$** | | | |
| *A* | $-x, y, -z$ | *E* | $-x, -y + 1, z$ | *J* | $-x + 1, -y, z$ | |
| *B* | $-x, -y, z$ | *F* | $-x, y, -z + 1$ | *K* | $x, -y, -z + 1$ | |
| *C* | $x + 1, y, z$ | *G* | $x, -y, -z$ | *L* | $-x + 1, y, -z$ | |
| | $x - 1, y, z$ | *H* | $-x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ | *M* | $-x + 1, -y + 1, z$ | |
| *D* | $x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$ | | $-x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ | *N* | $x, -y + 1, -z$ | |
| | $x - \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$ | *I* | $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$<br>$-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ | | | |
| 0.1 | 12/3/*c*1 | *ABDEGIJLMN* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, 2 | | | 0.74048 |
| 0.2 | 10/3/*t*1 | *ABCDEJLM* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; $\frac{1}{3}(3)^{1/2}$, 2 | | | 0.69813 |
| 0.3 | 10/3/*t*1 | *ADGHILN* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, $\frac{2}{3}(3)^{1/2}$ | | | 0.69813 |
| 0.4 | 9/3/*c*2 | *ABDGHI* | $\frac{3}{16}$, $\frac{3}{16}$, $\frac{3}{16}$; 1, 1 | | | 0.62478 |
| 1.1 | 8/3/*t*4 | *ABCDJL* | $\frac{1}{4}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $\frac{2}{3}(3)^{1/2} - \frac{1}{3}(6)^{1/2}$, 1 | | | 0.47912 |
| 1.2 | 8/3/*t*8 | *ADGHI* | 0.19823, 0.19823, 0.17410; 1, 1.02678 | | | 0.62073 |
| 1.3 | 8/4/*c*1 | *ADGILN* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; 1, $2^{1/2}$, | | | 0.68017 |
| 1.4 | 8/4/*c*1 | *ABDEJLM* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; $\frac{1}{2}(2)^{1/2}$, 2 | | | 0.68017 |
| 1.5 | 7/3/*o*1 | *ABCDE* | 0, $\frac{1}{4}$, $1 - \frac{1}{2}(3)^{1/2}$; $\frac{1}{2}$, $1 + \frac{1}{2}(3)^{1/2}$ | | | 0.56119 |
| 1.6 | 7/3/*o*13 | *BDGIJ* | $\frac{1}{4}$, 0.14855, 0.16950; 0.91396, 1.34798 | | | 0.55058 |
| 1.6′ | | *ADGHL* | | | | |
| 1.7 | 7/3/*t*6 | *ABDGJL* | $\frac{1}{4}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $2 - 2^{1/2}$, 1 | | | 0.50819 |
| 1.8 | 7/3/*t*15 | *ABDGI* | 0.19894, 0.19894, 0.15666; 1, 1.26991 | | | 0.58768 |
| 1.9 | 6/4/*c*1 | *AGHLN* | $\frac{1}{4}$, $\frac{1}{4}$, 0; 1, 1 | | | 0.52360 |
| 1.9′ | | *ABDEF* | 0, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1 | | | |
| 1.9′ | | *BGIJK* | $\frac{1}{4}$, 0, $\frac{1}{4}$; 1, 1 | | | |
| 2.1 | 7/3/*t*8 | *DGHI* | $\frac{1}{4}$, $\frac{1}{4}(3)^{1/2} - \frac{1}{4}$, $\frac{1}{4}(3)^{1/2} - \frac{1}{4}$; $[4(3)^{1/2} - 6]^{1/2}$, 1 | | | 0.60304 |
| 2.2 | 6/3/*o*31 | *BDGI* | 0.24970, 0.14877, 0.16949; 0.91435, 1.34704 | | | 0.55058 |
| 2.2′ | | *ADGH* | | | | |
| 2.3 | 6/3/*t*7 | *ABCD* | 0, $\frac{2}{5} - \frac{1}{10}(6)^{1/2}$, $\frac{2}{5} - \frac{1}{10}(6)^{1/2}$; $\frac{4}{5} - \frac{1}{5}(6)^{1/2}$, 1 | | | 0.40281 |
| 2.4 | 6/4/*t*6 | *ABDJL* | 0, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$; $2^{1/2} - 1$, 1 | | | 0.46680 |
| 2.5 | 6/4/*t*8 | *ADGI* | [0.21, 0.21, 0.15277; 1, 1.2] | | | >0.58768 |
| 2.6 | 5/3/*t*6 | *ABDG* | $\frac{3}{40}(10)^{1/2}$, $\frac{3}{20}$, $\frac{3}{20}$, $\frac{1}{5}(10)^{1/2}$, 1 | | | 0.50579 |
| 2.7 | 5/4/*o*10 | *BDGJ* | $\frac{1}{4}$, 0.14555, 0.15165; 0.62514, 1.03056 | | | 0.50664 |

**Table 1 (continued)**

| | | | | | | |
|---|---|---|---|---|---|---|
| 2.7′ | | *ADGL* | | | | |
| 2.8 | 5/4/*h*5 | *ABDE* | 0, $\frac{1}{4}$, $\frac{1}{6}$; $\frac{1}{2}(3)^{1/2}$, $\frac{3}{2}$ | | | 0.40307 |
| 2.8′ | | *AGHL*, *BGIJ* | | | | |
| 3.1 | 6/4/*c*1 | *DHI* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1 | | | 0.52360 |
| 3.2 | 5/4/*o*11 | *DGI* | $\frac{1}{4}$, 0.14882, 0.16949; 0.91443, 1.34684 | | | 0.55058 |
| 3.2′ | | *DGH* | | | | |
| 3.3 | 4/4/*o*22 | *BDG* | [0.24, 0.14902, 0.15401; 0.63106, 1.00696] | | | >0.50579 |
| 3.3′ | | *ADG* | | | | |
| 3.4 | 4/4/*t*5 | *ABD* | 0, $\frac{5}{8} - \frac{1}{8}(13)^{1/2}$, $\frac{5}{8} - \frac{1}{8}(13)^{1/2}$; $\frac{1}{2}[2(13)^{1/2} - 6]^{1/2}$, 1 | | | 0.32252 |
| 3.4′ | | *AGH*, *BGI* | | | | |
| *n*4.1 | *t*[$6^3$]$^2$ | *DG* | [0.21, 0.18, 0.16681; 0.96, 1.02] | | | >0.50579 |
| ***I*2$_1$2$_1$2$_1$ 8*d* *x*, *y*, *z*** | | | $\mathbf{0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b \le c}$ | | | |
| *A* | $x, -y, -z + \frac{1}{2}$ | *E* | $x + 1, y, z$ | *H* | $-x + \frac{1}{2}, y, -z + 1$ | |
| *B* | $x, -y, -z - \frac{1}{2}$ | | $x - 1, y, z$ | *I* | $-x - \frac{1}{2}, y, -z + 1$ | |
| *C* | $-x + \frac{1}{2}, y, -z$ | *F* | $-x, -y + \frac{1}{2}, z$ | *J* | $-x + 1, -y + \frac{1}{2}, z$ | |
| *D* | $-x - \frac{1}{2}, y, -z$ | *G* | $-x, -y - \frac{1}{2}, z$ | *K* | $-x + 1, -y - \frac{1}{2}, z$ | |
| 0.1 | 8/3/*h*4 | *ACEFGJK* | $\frac{1}{4}$, 0, $\frac{1}{8}$; $\frac{1}{3}(3)^{1/2}$, $\frac{4}{3}(3)^{1/2}$ | | | 0.60460 |
| 0.2 | 7/3/*o*1 | *ACDEFG* | 0, 0, $\frac{1}{2}(3)^{1/2} - \frac{3}{4}$; $\frac{1}{2}$, $\frac{1}{2}(3)^{1/2} + 1$ | | | 0.56119 |
| 0.3 | 6/4/*c*1 | *ABCDFG* | 0, 0, 0; 1, 1 | | | 0.52360 |
| 1.1 | 6/3/*o*3 | *ACEFJ* | $\frac{1}{4}$, 0.11409, 0.14822; 0.31387, 1.05877 | | | 0.38975 |
| 1.1′ | | *ACDEF* | | | | |
| 1.2 | 6/4/*o*1 | *ACEFG* | 0.08637, 0, 0.12146; 0.50763, 1.97462 | | | 0.54644 |
| 1.3 | 6/4/*c*1 | *ACFGJK* | $\frac{1}{4}$, 0, $\frac{1}{8}$; 1, $2(2)^{1/2}$ | | | 0.52360 |
| 1.4 | 5/4/*h*5 | *ACDFG* | 0, 0, $\frac{1}{12}$; $\frac{1}{2}(3)^{1/2}$, $\frac{3}{2}$ | | | 0.40307 |
| 2.1 | 5/4/*t*1 | *ACEF* | $\frac{1}{8}$, 0.10552, 0.14448; 0.29844, 1 | | | 0.37309 |
| 2.2 | 4/4/*o*1 | *ACFJ* | $\frac{1}{4}$, 0.14767, $\frac{11}{16} - \frac{1}{16}(73)^{1/2}$; 0.63979, 1.23702 | | | 0.28988 |
| 2.2′ | | *ACDF*, *ACFG* | | | | |
| 3.1 | 3/10/*c*1 | *ACF* | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}$; 1, 1 | | | 0.18512 |

(Shubnikov, 1916) are intertwined and the highest inherent symmetry of this type is tetragonal. The string of capital letters in the third column describes the centres of those spheres that are in contact with the reference sphere. However, depending on the choice of the asymmetric unit, the parameter region of a sphere-packing type may disintegrate into two or more disconnected parts. Then, each part corresponds to another string of capital letters and a symmetry operation either of the Euclidean or of the affine normalizer of the space group under consideration transforms both sets of symmetry operations into each other. In such a case the symbol in the first column is modified by a prime.

The last two columns refer to the sphere packing with minimal density belonging to the corresponding type: the fourth column gives the values of the coordinate parameters $x$, $y$, $z$ and of the axial ratios $a/b$ and $c/b$, the fifth column the value $\rho_m$ of the minimal density. If a sphere-packing type does not include an arrangement with minimal density, parameters for any other packing of that type are given in square brackets.

In total, the nine orthorhombic trivariant lattice complexes belonging to space groups of crystal class 222 give rise to sphere packings of 84 different types with contact numbers three to 12. Interpenetrating sphere packings do not occur in the lattice complexes under consideration but two sets of interpenetrating $6^3$ nets $t[6^3]^2$ may be obtained in the general position of *I*222. For 48 of the 84 types, the maximal inherent symmetry is higher than orthorhombic. This means that these types include at least one sphere packing with cubic (eight types), hexagonal (seven types) or tetragonal (33 types) symmetry as is indicated by the letters *c*, *h* or *t* in the sphere-packing symbol. For 36 types, the maximal inherent symmetry is orthorhombic. Thirty three of these occur also in lattice complexes with less than three degrees of freedom (*cf.* Fischer *et al.*, 2006; Sowa *et al.*, 2007). The sphere packings of the other three types, namely 4/4/*o*22, 6/3/*o*30 and 6/3/*o*31, can be exclusively generated with site symmetry 1. Type 6/3/*o*30 (Fig. 1) has been first derived by Blatov (2007) using net–subnet relations and is symbolized by **vbo** in the Reticular Chemistry

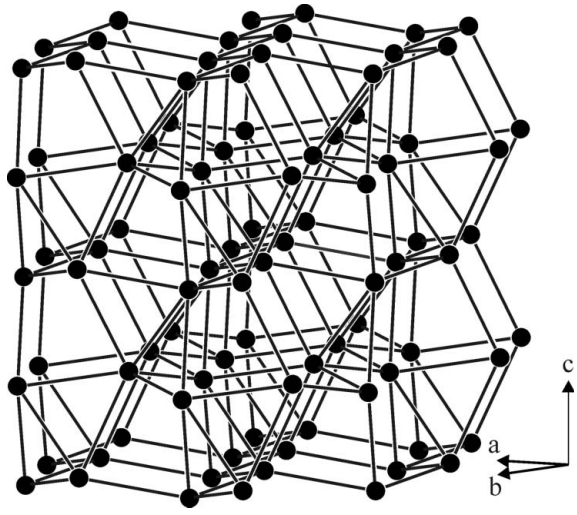


**Figure 1**
Sphere packing with minimal density of type 6/3/*o*30 (RCSR symbol **vbo**) ($C222_1$ 8*c*).

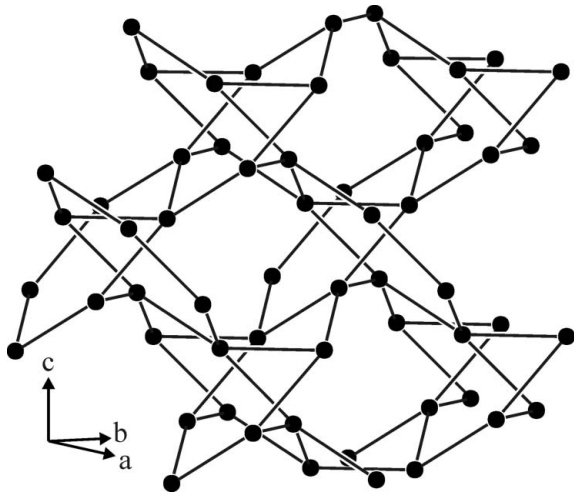


**Figure 2**
Sphere packing of type 4/4/*o*22 (*I*222 8*k*).

Structure Resource (RCSR) database (O'Keeffe *et al.*, 2008). A corresponding sphere packing shows symmetry $C222_1$ 8*c* and contains corrugated $6^3$ nets perpendicular to **a** and **c** and corrugated $3^2434$ nets perpendicular to **b**. Sphere packings of types 4/4/*o*22 (Fig. 2) and 6/3/*o*31 (Fig. 3) are not included in the RCSR database yet, but were derived by Blatov (2007) and can be found in the Topos TTD database (Blatov, 2006) as xfv-4-I222 and wfs-6-I222, respectively. They can be generated in the general position of *I*222. The parameter region of 4/4/*o*22 has three degrees of freedom and does not comprise an arrangement with minimal density.

The systems of interpenetrating sphere nets $t[6^3]^2$ have a four-dimensional parameter region in *I*222 8*k*. If each sphere of such a $6^3$ net has an additional contact to a certain sphere from a net of the other system, a sphere packing of type 4/4/*o*22 results. Two further contacts give rise to sphere packings of type 6/3/*o*31 with a two-dimensional parameter region. It can be described by stacking corrugated $6^3$ nets perpendicular to **a** or corrugated $3^2434$ nets perpendicular to **c**. The minimal density of this type is very close to that of type 7/3/*o*13 with an adjacent one-dimensional parameter region.

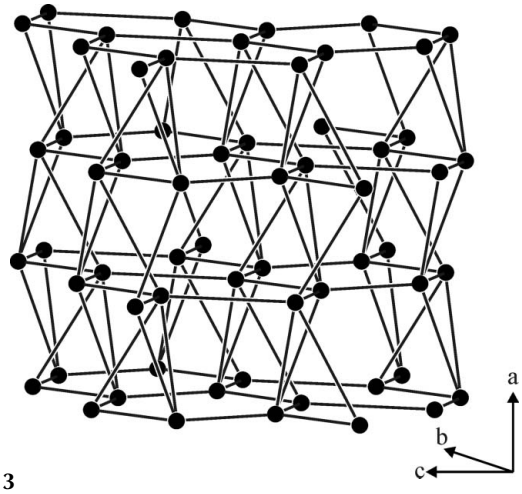


**Figure 3**
Sphere packing with minimal density of type 6/3/*o*31 (*I*222 8*k*).

## 3. Examples of crystal structures

Examples of atomic arrangements that correspond to sphere packings in one of the trivariant orthorhombic lattice complexes described above can be found, for instance, in the following crystal structures.

(i) One modification of tridymite $SiO_2$ crystallizes in space group $C222_1$ (Kihara *et al.*, 1986). The arrangement of the Si atoms located at the general position corresponds to a nearly ideal sphere packing of type 4/6/*h*2 (**lon**).

(ii) An almost undistorted sphere packing of the cubic type 4/6/*c*1 (**dia**) is formed by the Be atoms in $Be(OH)_2$ that crystallizes in space group $P2_12_12_1$ (Stahl *et al.*, 1998).

(iii) Selenic acid $H_2SeO_4$ crystallizes in space group $P2_12_12_1$ (Erfany-Far *et al.*, 1987). The Se atoms form a slightly distorted sphere packing of type 6/3/o1 (**sxd**).

(iv) The arrangement of the Te atoms at the general position of *C*222 in $Cs_2Ag_2ZrTe_4$ (Pell & Ibers, 1995) corresponds to a slightly distorted sphere packing of the tetragonal type 9/3/*t*2 (**nce**). The Ag atoms occupy one half and the Zr atoms one quarter of the tetrahedral voids. The Cs atoms are located in the cube-shaped voids.

## 4. Orthorhombic sphere packings

All lattice complexes with orthorhombic characteristic space group give rise to a total of 260 different types of sphere packing. One hundred and sixty of these show orthorhombic inherent symmetry, 13 types can also be generated with cubic, seven with hexagonal and 80 with tetragonal symmetry. In addition, ten types of interpenetrating sphere packing and two types of interpenetrating sphere layer are obtained. Looking at the underlying nets of the sphere packings (*cf. e.g.* Delgado-Friedrichs *et al.*, 2005; O'Keeffe, 2012), the sphere-packing graphs, it becomes apparent that five of the orthorhombic types are topologically identical with certain tetragonal sphere-packing types (Sowa, 2012). However, the orthorhombic variants can not be deformed into the analogous tetragonal ones without forming additional contacts, and the minimal densities for tetragonal and orthorhombic types may differ. These types may be identified in Tables 2 and 3 by special sphere-packing symbols like, for instance, 6/3/*o*25/*t*44. This symbol means that the orthorhombic type 6/3/*o*25 and the tetragonal type 6/3/*t*44 can be described with isomorphic sphere-packing graphs. Moreira de Oliveira & Eon (2013) applied graph-theoretical methods and found out that the periodic nets associated with the sphere-packing types 4/4*o*18, 4/4/*o*19 and 5/3/*o*6 display so-called collisions and, therefore, cannot be studied using *Systre* (Delgado-Friedrichs & O'Keeffe, 2003). By investigating the corresponding labelled quotient graphs, the authors discovered that all three types of sphere packing are associated with noncrystallographic nets. Their quotient graphs are related to that of **ths** and they could be presented as different kinds of double **ths**.

The complete list of orthorhombic sphere-packing types is given in Table 2. In the first column, the sphere-packing type is identified by its symbol *k*/*m*/*on*. The second column indicates

**Table 2**
Minimal densities and sample parameters of all orthorhombic sphere-packing types.

| Type | Symmetry | $df_{min}$ | $df_{max}$ | $x, y, z; a, b, c$ | $\rho_{min}$ | RCSR |
|---|---|---|---|---|---|---|
| **3/10/*o*1** | *Pnna* 8*e* | 3 | | 0.10000, 0.09375, 0.12500; 2.98142, 2.38514, 2.66667 | 0.22089 | **utp** |
| **3/10/*o*2** | *Fddd* 32*h* | 3 | | 0.04096, 0.18419, 0.41878; 1.73184, 5.24059, 6.09375 | 0.30295 | **utq** |
| **4/4/*o*1** | *Imma* 8*h* | 2 | 3 | 0.00000, 0.09650, 0.14767; 1.68470, 3.25733, 2.63321 | 0.28988 | **sra** |
| **4/4/*o*2** | *Cccm* 8*l* | 2 | 3 | 0.08793, 0.14827, 0.00000; 2.41817, 3.05213, 1.81013 | 0.31354 | **irl** |
| **4/4/*o*3** | *Cmcm* 16*h* | 2 | | 0.15350, 0.14522, 0.07383; 3.25733, 3.12602, 2.83822 | 0.28988 | **pcl** |
| **4/4/*o*4** | *Cmce* 16*g* | 2 | | 0.17431, 0.13380, 0.08715; 2.86852, 3.27410, 2.76575 | 0.32252 | **cag** |
| **4/4/*o*5** | *Cccm* 16*m* | 2 | | 0.10390, 0.14077, 0.13565; 2.58880, 2.99406, 3.68595 | 0.29323 | **umc** |
| **4/4/*o*6** | *Ibam* 16*k* | 2 | | 0.18272, 0.13108, 0.14571; 1.91107, 2.73009, 3.43143 | >0.42099 | |
| **4/4/*o*7** | *Ccce* 16*i* | 2 | | 0.07388, 0.16794, 0.13351; 2.53070, 2.76131, 3.47327 | 0.34516 | **uou** |
| **4/4/*o*8** | *Ccce* 16*i* | 2 | | 0.14640, 0.11354, 0.15000; 2.34399, 3.20289, 2.42439 | >0.45095 | |
| **4/4/*o*9** | *Ccce* 16*i* | 2 | | 0.20219, 0.11629, 0.13000; 2.10662, 3.66272, 2.01450 | >0.45095 | |
| **4/4/*o*10** | *Fddd* 32*h* | 2 | | 0.00000, 0.19275, 0.07898; 1.60400, 5.21707, 6.33043 | 0.31629 | **umv** |
| **4/4/*o*11** | *Fddd* 32*h* | 2 | | 0.00000, 0.19914, 0.17403; 1.75648, 4.70099, 5.78040 | 0.35104 | **uod** |
| **4/4/*o*12** | *Fddd* 32*h* | 2 | | 0.10754, 0.13788, 0.05694; 2.58781, 3.01269, 7.29463 | 0.29462 | **vbb** |
| **4/4/*o*13** | *Fddd* 32*h* | 2 | | 0.08578, 0.13388, 0.31804; 1.69975, 3.57241, 6.09724 | 0.45255 | **vba** |
| **4/4/*o*14** | *Fddd* 32*h* | 2 | | 0.05190, 0.14969, 0.42799; 1.90310, 3.27435, 6.80693 | 0.39501 | **uke** |
| **4/4/*o*15** | *Fddd* 32*h* | 2 | | 0.03399, 0.13423, 0.30017; 1.97833, 3.69121, 5.17404 | 0.44346 | **ukj** |
| **4/4/*o*16** | *Fddd* 32*h* | 2 | | 0.03813, 0.16523, 0.31862; 2.03428, 2.98954, 6.28123 | 0.43862 | **ukm** |
| **4/4/*o*17** | *Fddd* 32*h* | 3 | | 0.02000, 0.22715, 0.34339; 2.63750, 2.69045, 5.31318 | >0.44179 | |
| **4/4/*o*18** | *Fddd* 32*h* | 3 | | 0.07500, 0.15000, 0.39086; 2.47594, 3.09492, 4.25352 | >0.44889 | |
| **4/4/*o*19/*t*39** | *Fddd* 32*h* | 3 | | 0.10000, 0.13900, 0.35901; 2.36664, 3.19816, 3.23014 | >0.65226 | |
| **4/4/*o*20** | *Fddd* 32*h* | 3 | | 0.05000, 0.21000, 0.40957; 2.43627, 2.80449, 5.36252 | >0.45606 | |
| **4/4/*o*21** | *Fddd* 32*h* | 3 | | 0.10000, 0.13640, 0.36087; 2.20567, 3.31496, 3.38126 | >0.65192 | |
| **4/4/*o*22** | *I*222 8*k* | 3 | | 0.24000, 0.13351, 0.20000; 1.63773, 2.31477, 1.96527 | >0.50579 | |
| **4/6/*o*1** | *Fddd* 16*e* | 2 | 3 | 0.17995, 0.00000, 0.00000; 4.65290, 1.51661, 3.08490 | 0.38484 | **neb** |
| **4/6/*o*2** | *Pccn* 8*e* | 3 | | 0.12500, 0.07005, 0.15268; 1.51661, 2.57113, 2.79133 | 0.38484 | **mmt** |
| **4/6/*o*3** | *Pbcn* 8*d* | 3 | | 0.14849, 0.15056, 0.00847; 2.35130, 2.37565, 1.48178 | 0.50607 | **sow** |
| **5/3/*o*1** | *Pnna* 8*e* | 2 | | 0.08682, 0.13978, 0.09705; 1.75045, 2.93581, 2.49215 | 0.32707 | |
| **5/3/*o*2** | *Ccce* 16*i* | 1 | | 0.15612, 0.10965, 0.13897; 2.26468, 3.22438, 2.54413 | 0.45095 | **vbe** |
| **5/3/*o*3** | *Fddd* 32*h* | 1 | | 0.05798, 0.14503, 0.31166; 1.84127, 3.36809, 5.73423 | 0.47116 | **vdb** |
| **5/3/*o*4** | *Fddd* 32*h* | 2 | | 0.05802, 0.21593, 0.34241; 2.55843, 2.74478, 5.31529 | 0.44889 | **vbi** |
| **5/3/*o*5** | *Fddd* 32*h* | 2 | | 0.04768, 0.22355, 0.40921; 2.44394, 2.80685, 5.35571 | 0.45606 | **vbn** |
| **5/3/*o*6/*t*24** | *Fddd* 32*h* | 2 | | 0.09700, 0.14000, 0.35391; 2.31081, 3.21412, 3.40253 | >0.65226 | |
| **5/3/*o*7** | *Fddd* 32*h* | 2 | | 0.09332, 0.14000, 0.35138; 2.24762, 3.24197, 3.50132 | >0.65192 | |
| **5/4/*o*1** | *Cmcm* 8*g* | 2 | 3 | 0.16667, 0.14286, 0.25000; 3.00000, 2.64575, 1.30931 | 0.40307 | **noy** |
| **5/4/*o*2** | *Pnna* 8*e* | 2 | | 0.12230, 0.08452, 0.12500; 3.40308, 2.92564, 1.00000 | 0.42072 | **soe** |
| **5/4/*o*3** | *Pnna* 8*e* | 2 | | 0.10290, 0.07674, 0.10737; 3.35885, 1.00000, 3.28830 | 0.37925 | **sof** |
| **5/4/*o*4** | *Fddd* 16*e* | 1 | 2 | 0.15625, 0.00000, 0.00000; 3.20000, 1.60000, 3.57771 | 0.45734 | **fob** |
| **5/4/*o*5** | *Fddd* 16*e* | 1 | 2 | 0.08452, 0.00000, 0.00000; 5.91548, 1.00000, 3.36615 | 0.42072 | **zga** |
| **5/4/*o*6** | *Fdd*2 16*b* | 2 | | 0.17857, 0.05208, 0.00000; 2.44404, 4.68432, 1.60000 | 0.45734 | **vbf** |
| **5/4/*o*7** | *Cmce* 8*f* | 2 | 3 | 0.00000, 0.15000, 0.09375; 1.33333, 2.98142, 2.38514 | 0.44179 | **noz** |
| **5/4/*o*8** | *Cmce* 8*f* | 2 | 3 | 0.00000, 0.14839, 0.14839; 1.89198, 2.96776, 1.59536 | 0.46761 | **nov** |
| **5/4/*o*9** | *Fmmm* 16*m* | 1 | 2 | 0.00000, 0.17812, 0.13055; 1.82988, 2.80717, 3.82988 | 0.42583 | **skb** |
| **5/4/*o*10** | *Ibam* 8*j* | 2 | 3 | 0.14555, 0.15165, 0.00000; 2.34124, 2.41280, 1.46360 | 0.50664 | **skc** |
| **5/4/*o*11** | *Ibam* 8*j* | 2 | 3 | 0.14882, 0.16949, 0.00000; 1.83485, 2.47124, 1.67785 | 0.55058 | |
| **5/4/*o*12** | *Cmce* 16*g* | 2 | | 0.13204, 0.15467, 0.11297; 3.78666, 3.00264, 1.63982 | 0.44933 | **vbk** |
| **5/4/*o*13** | *Ibam* 16*k* | 2 | | 0.20000, 0.14382, 0.13744; 1.67173, 2.58496, 3.63795 | >0.50126 | |
| **5/4/*o*14** | *Ccce* 16*i* | 2 | | 0.08586, 0.13284, 0.15511; 1.61816, 3.61571, 3.09664 | 0.46239 | **vbj** |
| **5/4/*o*15** | *Ccce* 16*i* | 2 | | 0.15884, 0.12245, 0.18000; 2.39897, 3.52514, 1.79854 | >0.52446 | |
| **5/4/*o*16** | *Ccce* 16*i* | 2 | | 0.23454, 0.10864, 0.13000; 1.53823, 3.53302, 2.66297 | >0.51712 | |
| **5/4/*o*17** | *Fddd* 32*h* | 1 | | 0.00000, 0.16104, 0.06645; 1.66715, 3.10482, 7.52410 | 0.43021 | **vcd** |
| **5/4/*o*18** | *Fddd* 32*h* | 1 | | 0.00000, 0.13203, 0.20818; 1.78711, 3.78711, 5.36808 | 0.46118 | **vcb** |
| **5/4/*o*19** | *Fddd* 32*h* | 1 | | 0.00000, 0.17224, 0.18605; 1.78455, 2.90298, 6.97673 | 0.46358 | **vce** |
| **5/4/*o*20** | *Fddd* 32*h* | 1 | | 0.12500, 0.12500, 0.32544; 1.59642, 3.66762, 6.07713 | 0.47089 | **vbd** |
| **5/4/*o*21** | *Fddd* 32*h* | 2 | | 0.02764, 0.17932, 0.42466; 1.00000, 6.33576, 6.62626 | 0.39910 | **sog** |
| **5/4/*o*22/*t*49** | *Fddd* 32*h* | 2 | | 0.05000, 0.19549, 0.37347; 2.57768, 3.05833, 3.81799 | >0.52360 | |
| **5/4/*o*23** | *Fddd* 32*h* | 2 | | 0.04334, 0.20921, 0.40949; 2.35211, 2.87076, 5.40808 | 0.45883 | **vbc** |
| **5/4/*o*24** | *Fddd* 32*h* | 2 | | 0.03774, 0.21837, 0.34070; 2.31548, 2.90298, 5.41898 | 0.45999 | **vbg** |
| **5/4/*o*25** | *Fddd* 32*h* | 2 | | 0.06250, 0.17500, 0.41250; 2.43432, 2.72166, 5.44331 | 0.46459 | **soh** |
| **5/4/*o*26** | *Fddd* 32*h* | 2 | | 0.07500, 0.18000, 0.37377; 2.58279, 3.05416, 3.65176 | >0.54864 | |
| **5/4/*o*27** | *Fddd* 32*h* | 2 | | 0.10000, 0.13640, 0.35791; 2.20007, 3.30654, 3.48086 | >0.65192 | |
| **5/4/*o*28** | *Fddd* 32*h* | 2 | | 0.09300, 0.14103, 0.35586; 2.26227, 3.25929, 3.32447 | >0.65226 | |
| **5/4/*o*29/*t*48** | *Fddd* 32*h* | 2 | | 0.09500, 0.14000, 0.35142; 2.28357, 3.21776, 3.48201 | >0.65226 | |
| **5/4/*o*30** | *Fddd* 32*h* | 3 | | 0.10000, 0.13607, 0.36340; 2.28724, 3.26749, 3.26875 | >0.68017 | |
| **5/4/*o*31** | *Ibca* 16*f* | 2 | | 0.11286, 0.08406, 0.12417; 1.77137, 2.76176, 3.51944 | 0.48658 | **soi** |

**Table 2 (continued)**

| Type | Symmetry | $df_{min}$ | $df_{max}$ | $x, y, z; a, b, c$ | $\rho_{min}$ | RCSR |
|---|---|---|---|---|---|---|
| **6/3/o1** | *Imma* 4*e* | 1 | 3 | 0.00000, 0.25000, 0.09413; 1.00000, 1.70466, 2.77806 | 0.44226 | **sxd** |
| **6/3/o2** | *Cmcm* 8*f* | 1 | 2 | 0.00000, 0.13677, 0.07793; 1.00000, 3.25937, 2.90587 | 0.44226 | **osa** |
| **6/3/o3** | *Imma* 8*h* | 1 | 2 | 0.00000, 0.10178, 0.11409; 1.00000, 3.37328, 3.18604 | 0.38975 | **skd** |
| **6/3/o4** | *Fddd* 16*e* | 1 | 2 | 0.17084, 0.00000, 0.00000; 5.47036, 1.00000, 3.31284 | 0.46228 | **wky** |
| **6/3/o5** | *Pnma* 8*d* | 2 | | 0.18162, 0.07793, 0.16397; 1.91203, 2.90587, 1.70466 | 0.44226 | **osc** |
| **6/3/o6** | *Cmcm* 16*h* | 2 | | 0.17207, 0.15726, 0.11323; 2.90587, 1.78309, 3.65587 | 0.44226 | **vbx** |
| **6/3/o7** | *Cmce* 16*g* | 1 | | 0.13800, 0.16261, 0.07936; 3.62323, 2.95911, 1.71177 | 0.45648 | **vbw** |
| **6/3/o8** | *Cmce* 16*g* | 1 | | 0.18276, 0.14457, 0.11889; 2.73587, 1.85970, 3.54595 | 0.46435 | **vbr** |
| **6/3/o9** | *Ibam* 16*k* | 1 | | 0.15357, 0.16467, 0.13643; 1.80440, 2.52740, 3.66477 | 0.50126 | **vca** |
| **6/3/o10** | *Pccn* 8*e* | 2 | | 0.12500, 0.07916, 0.13417; 1.00000, 2.83372, 3.19765 | 0.46228 | **vbt** |
| **6/3/o11** | *Pccn* 8*e* | 2 | | 0.18320, 0.07858, 0.16744; 1.66938, 2.84326, 1.94962 | 0.45266 | **vbu** |
| **6/3/o12** | *Pbcn* 8*d* | 2 | | 0.14999, 0.14584, 0.01179; 2.41215, 2.36356, 1.44880 | 0.50712 | **vcz** |
| **6/3/o13** | *Pbcn* 8*d* | 2 | | 0.12500, 0.20000, 0.09375; 1.63299, 1.82574, 2.92119 | 0.48096 | **vbn** |
| **6/3/o14** | *Pbcn* 8*d* | 2 | | 0.14872, 0.16950, 0.00023; 1.83478, 2.47189, 1.67748 | 0.55058 | **soj** |
| **6/3/o15** | *Ccce* 16*i* | 1 | | 0.17511, 0.11878, 0.14373; 2.41022, 3.55338, 1.86514 | 0.52446 | **vbs** |
| **6/3/o16** | *Ccce* 16*i* | 1 | | 0.16144, 0.11603, 0.15849; 1.75988, 3.54610, 2.59593 | 0.51712 | **vbq** |
| **6/3/o17** | *Ccce* 16*i* | 1 | | 0.07047, 0.13708, 0.15954; 1.66885, 3.54507, 3.04613 | 0.46487 | **vbv** |
| **6/3/o18** | *Fddd* 32*h* | 1 | | 0.00000, 0.18106, 0.07510; 1.00000, 6.28122, 6.65779 | 0.40066 | **sok** |
| **6/3/o19** | *Fddd* 32*h* | 1 | | 0.09504, 0.13909, 0.35207; 2.23251, 3.25498, 3.53683 | 0.65192 | |
| **6/3/o20** | *Fddd* 32*h* | 1 | | 0.05882, 0.17340, 0.41256; 2.36823, 2.76936, 5.49155 | 0.46521 | **vbl** |
| **6/3/o21** | *Fddd* 32*h* | 1 | | 0.05770, 0.22221, 0.37693; 2.56191, 3.07132, 3.88125 | 0.54864 | **vda** |
| **6/3/o22** | *Fddd* 32*h* | 1 | | 0.09240, 0.14004, 0.35292; 2.26268, 3.24320, 3.40536 | >0.65226 | |
| **6/3/o23** | *Fddd* 32*h* | 1 | | 0.09316, 0.14128, 0.35354; 2.25417, 3.25195, 3.41455 | >0.65226 | |
| **6/3/o24** | *Fddd* 32*h* | 1 | | 0.05418, 0.18305, 0.33359; 2.35476, 2.64994, 5.59258 | 0.48012 | **vcf** |
| **6/3/o25/t44** | *Fddd* 32*h* | 1 | | 0.10882, 0.13562, 0.35893; 2.50430, 3.09103, 3.24558 | >0.65226 | **wia** |
| **6/3/o26** | *Fddd* 32*h* | 2 | | 0.10000, 0.13510, 0.36346; 2.21066, 3.31948, 3.32280 | >0.68623 | |
| **6/3/o27** | *Fddd* 32*h* | 2 | | 0.10095, 0.13871, 0.36021; 2.38242, 3.19080, 3.19399 | >0.69006 | |
| **6/3/o28** | *Fddd* 32*h* | 2 | | 0.09763, 0.13871, 0.36021; 2.38242, 3.19080, 3.19399 | >0.69006 | |
| **6/3/o29** | *Ibca* 16*f* | 1 | | 0.09554, 0.07936, 0.12007; 1.79922, 2.75147, 3.46185 | 0.48883 | **vbp** |
| **6/3/o30** | $C222_1$ 8*c* | 2 | | 0.18416, 0.18042, 0.04256; 1.82382, 2.73919, 1.78550 | 0.46960 | **vbo** |
| **6/3/o31** | *I*222 8*k* | 2 | | 0.24970, 0.14877, 0.16949; 1.67766, 1.83481, 2.47156 | 0.55058 | |
| | | | | | | |
| **6/4/o1** | *Imma* 8*h* | 1 | 2 | 0.00000, 0.12146, 0.16363; 1.96993, 3.88987, 1.00000 | 0.54664 | **ske** |
| **6/4/o2** | *Cccm* 8*l* | 1 | 2 | 0.06652, 0.12896, 0.00000; 1.00000, 3.84270, 1.98222 | 0.54992 | **vby** |
| **6/4/o3** | *Cccm* 16*m* | 1 | | 0.08644, 0.12759, 0.12595; 1.00000, 3.85985, 3.96989 | 0.54673 | **vbm** |
| **6/4/o4** | *Pbcn* 8*d* | 2 | | 0.16363, 0.15451, 0.06910; 2.42825, 1.81554, 1.67788 | 0.56628 | **sol** |
| **6/4/o5** | *Fddd* 32*h* | 1 | | 0.09573, 0.12696, 0.06197; 1.00000, 3.86542, 7.91869 | 0.54739 | **som** |
| **6/4/o6** | *Fddd* 32*h* | 1 | | 0.03713, 0.13107, 0.43581; 1.00000, 3.80418, 7.76830 | 0.56697 | |
| **6/4/o7** | *Fddd* 32*h* | 1 | | 0.00000, 0.14000, 0.19325; 1.23718, 3.57143, 6.92250 | >0.53190 | |
| **6/4/o8** | *Fddd* 32*h* | 1 | | 0.09156, 0.12724, 0.31410; 1.00000, 3.86311, 7.39854 | 0.58623 | **son** |
| **6/4/o9** | *Fddd* 32*h* | 1 | | 0.04324, 0.21869, 0.37504; 2.36852, 3.22337, 3.91644 | 0.56036 | **vcc** |
| **6/4/o10** | *Fddd* 32*h* | 2 | | 0.10100, 0.13500, 0.36337; 2.20082, 3.32571, 3.32951 | >0.68710 | |
| **6/4/o11** | *Fddd* 32*h* | 2 | | 0.10512, 0.13423, 0.34622; 2.29964, 3.26074, 3.26400 | >0.68017 | |
| | | | | | | |
| **7/3/o1** | *Cmmm* 4*g* | 0 | 2 | 0.13397, 0.00000, 0.00000; 3.73205, 1.00000, 1.00000 | 0.56119 | **svk** |
| **7/3/o2** | *Cmcm* 8*g* | 1 | 2 | 0.15693, 0.14462, 0.25000; 3.18614, 2.99422, 1.00000 | 0.43908 | **skf** |
| **7/3/o3** | *Cmcm* 8*g* | 1 | 2 | 0.17712, 0.15047, 0.25000; 2.82288, 1.82288, 1.67219 | 0.48680 | **osf** |
| **7/3/o4** | *Pnna* 8*e* | 1 | | 0.12151, 0.11945, 0.08235; 1.97269, 3.60821, 1.00000 | 0.58849 | **vcr** |
| **7/3/o5** | *Immm* 4*e* | 1 | 2 | 0.17712, 0.00000, 0.00000; 2.82288, 1.00000, 1.52410 | 0.48680 | **ose** |
| **7/3/o6** | *Fddd* 16*e* | 0 | 1 | 0.13397, 0.00000, 0.00000; 3.73205, 1.00000, 3.86370 | 0.58099 | **swl** |
| **7/3/o7** | *Fdd*2 16*b* | 1 | | 0.14226, 0.06002, 0.00000; 2.69074, 5.35894, 1.00000 | 0.58099 | **vck** |
| **7/3/o8** | *Fdd*2 16*b* | 1 | | 0.16667, 0.04428, 0.00000; 2.85052, 3.51975, 1.64575 | 0.50736 | **vcl** |
| **7/3/o9** | *Cmce* 8*f* | 1 | 2 | 0.00000, 0.16667, 0.08856; 1.64575, 2.85052, 1.75988 | 0.50736 | **vco** |
| **7/3/o10** | *Cmce* 8*f* | 1 | 2 | 0.00000, 0.13715, 0.08856; 1.00000, 3.20804, 2.68223 | 0.48680 | **ska** |
| **7/3/o11** | *Cmce* 8*f* | 1 | 2 | 0.00000, 0.13061, 0.15994; 1.96729, 3.62697, 1.00000 | 0.58705 | **vcn** |
| **7/3/o12** | *Cmce* 8*f* | 1 | 2 | 0.00000, 0.16397, 0.20293; 1.96837, 1.96837, 1.88180 | 0.57451 | **vcm** |
| **7/3/o13** | *Ibam* 8*j* | 1 | 2 | 0.14855, 0.16950, 0.00000; 1.83465, 2.47307, 1.67679 | 0.55058 | **vcg** |
| **7/3/o14** | *Cmce* 16*g* | 1 | | 0.12715, 0.13210, 0.12100; 3.93229, 3.67261, 1.00000 | 0.58009 | **vci** |
| **7/3/o15** | *Cmce* 16*g* | 1 | | 0.12642, 0.17164, 0.19469; 3.95515, 1.95515, 1.90380 | 0.56906 | **vcq** |
| **7/3/o16** | *Pbca* 8*c* | 2 | | 0.16160, 0.11690, 0.16397; 1.94180, 2.69768, 1.39185 | 0.57451 | **vcj** |
| **7/3/o17** | *Ccce* 16*i* | 1 | | 0.19179, 0.12200, 0.17441; 1.91113, 3.80847, 1.94986 | 0.59030 | **vcp** |
| **7/3/o18** | *Ccce* 16*i* | 1 | | 0.08460, 0.12771, 0.13307; 1.00000, 3.85856, 3.70322 | 0.58629 | **vch** |
| **7/3/o19** | *Fddd* 32*h* | 0 | | 0.00000, 0.13397, 0.06358; 1.00000, 3.73205, 7.86370 | 0.57092 | **soo** |
| **7/3/o20** | *Fddd* 32*h* | 0 | | 0.00000, 0.14645, 0.19581; 1.41421, 3.41421, 6.52395 | 0.53190 | **soq** |
| **7/3/o21** | *Fddd* 32*h* | 0 | | 0.09274, 0.14061, 0.35001; 2.24825, 3.23201, 3.53517 | 0.65226 | **sor** |
| **7/3/o22** | *Fddd* 32*h* | 0 | | 0.12500, 0.12500, 0.43402; 1.00000, 3.87298, 7.33708 | 0.58963 | |
| **7/3/o23** | *Fddd* 32*h* | 1 | | 0.09000, 0.14033, 0.35818; 2.30006, 3.24326, 3.24830 | >0.69103 | |
| **7/3/o24** | *Fddd* 32*h* | 1 | | 0.10400, 0.13323, 0.36529; 2.17542, 3.34663, 3.34947 | 0.68710 | |
| **7/3/o25** | *Fddd* 32*h* | 1 | | 0.09289, 0.14084, 0.35733; 2.26702, 3.26297, 3.26950 | >0.69256 | |
| **7/3/o26** | *Fddd* 32*h* | 1 | | 0.10010, 0.13786, 0.35944; 2.38428, 3.18702, 3.19496 | 0.69015 | |

**Table 2 (continued)**

| Type | Symmetry | $df_{min}$ | $df_{max}$ | $x, y, z; a, b, c$ | $\rho_{min}$ | RCSR |
|---|---|---|---|---|---|---|
| **7/4/*o*1** | *Fmmm* 8*g* | 1 | 3 | 0.14144, 0.00000, 0.00000; 3.53518, 1.28188, 1.53518 | 0.60210 | **sev** |
| **8/3/*o*1** | *Cmcm* 4*c* | 1 | 2 | 0.00000, 0.14286, 0.25000; 1.00000, 2.64575, 1.30931 | 0.60460 | **ecu** |
| **8/3/*o*2** | *Cmcm* 8*f* | 1 | 2 | 0.00000, 0.21875, 0.10714; 1.30931, 1.51186, 3.50000 | 0.60460 | **osb** |
| **8/3/*o*3** | *Fddd* 16*e* | 1 | 2 | 0.19110, 0.00000, 0.00000; 6.55041, 1.27227, 1.54316 | 0.65142 | **eev** |
| **8/3/*o*4** | *Pnma* 8*d* | 1 | | 0.14063, 0.10714, 0.17857; 1.97949, 3.50000, 1.00000 | 0.60460 | **osd** |
| **8/3/*o*5** | *Pnma* 4*c* | 2 | | 0.17857, 0.25000, 0.12500; 1.87083, 1.30931, 1.41421 | 0.60460 | **vcs** |
| **8/3/*o*6** | *Pccn* 8*e* | 1 | | 0.19940, 0.10654, 0.13649; 1.00000, 3.46750, 1.98973 | 0.60712 | **sos** |
| **8/3/*o*7** | *Pbcn* 8*d* | 1 | | 0.16378, 0.15199, 0.07041; 2.44384, 1.81374, 1.66855 | 0.56637 | **vcv** |
| **8/3/*o*8** | *Pbcn* 8*d* | 1 | | 0.17344, 0.18988, 0.04847; 1.91286, 1.91228, 1.85616 | 0.61693 | **vct** |
| **8/3/*o*9** | *Pbcn* 8*d* | 1 | | 0.12500, 0.15000, 0.11111; 1.00000, 1.93649, 3.48569 | 0.62056 | **vcu** |
| **8/3/*o*10** | *Fddd* 32*h* | 0 | | 0.00000, 0.13397, 0.19091; 1.00000, 3.73205, 7.32780 | 0.61267 | **sot** |
| **8/3/*o*11** | *Fddd* 32*h* | 0 | | 0.09209, 0.13954, 0.35639; 2.27573, 3.25335, 3.26770 | 0.69256 | **sou** |
| **9/3/*o*1** | *Fmmm* 8*g* | 0 | 2 | 0.13397, 0.00000, 0.00000; 3.73205, 1.00000, 1.73205 | 0.64801 | **nci** |
| **9/3/*o*2** | *Fddd* 16*e* | 0 | 1 | 0.06699, 0.00000, 0.00000; 7.46410, 1.00000, 1.73205 | 0.64801 | **ncm** |
| **9/3/*o*3** | *Fdd*2 16*b* | 0 | | 0.13668, 0.05792, 0.00000; 3.27209, 3.86091, 1.00000 | 0.66314 | **skg** |
| **9/3/*o*4** | *Fdd*2 16*b* | 1 | | 0.21713, 0.05810, 0.00000; 1.51749, 6.47273, 1.30278 | 0.65469 | **skh** |
| **9/3/*o*5** | *Cmce* 8*f* | 1 | | 0.00000, 0.19373, 0.12338; 1.19126, 1.60651, 3.17181 | 0.69006 | **vcx** |
| **9/3/*o*6** | *Pbca* 8*c* | 1 | | 0.18166, 0.11583, 0.16458; 1.91267, 1.93045, 1.71075 | 0.66314 | **vcy** |
| **9/3/*o*7** | *Pbca* 8*c* | 1 | | 0.14144, 0.11620, 0.17431; 1.97695, 3.23637, 1.00000 | 0.65469 | **vcw** |
| **10/3/*o*1** | *Cmcm* 4*c* | 1 | | 0.00000, 0.20000, 0.25000; 1.22474, 1.58114, 1.54919 | 0.69813 | **cco** |
| **10/3/*o*2** | *Cmcm* 4*c* | 0 | 1 | 0.00000, 0.13763, 0.25000; 1.00000, 3.14626, 1.00000 | 0.66568 | **chb** |
| **10/3/*o*3** | *Fddd* 8*a* | 0 | | 0.00000, 0.00000, 0.00000; 1.00000, 1.73205, 3.46410 | 0.69813 | **gpu** |
| **10/3/*o*4** | *Fddd* 16*e* | 0 | 1 | 0.18750, 0.00000, 0.00000; 6.92820, 1.00000, 1.73205 | 0.69813 | **tcf** |
| **10/3/*o*5** | *Pnma* 4*c* | 1 | | 0.15000, 0.25000, 0.12500; 1.93649, 1.54919, 1.00000 | 0.69813 | **tcg** |
| **10/3/*o*6** | *Pnma* 4*c* | 1 | | 0.18119, 0.25000, 0.15825; 1.90604, 1.00000, 1.65068 | 0.66568 | **feb** |
| **11/3/*o*1** | *Fdd*2 16*b* | 0 | | 0.16667, 0.06066, 0.00000; 1.73205, 6.73009, 1.00000 | 0.71868 | **ele** |
| **11/3/*o*2** | *Cmce* 8*f* | 0 | | 0.00000, 0.16667, 0.12132; 1.00000, 1.73205, 3.36504 | 0.71868 | **elb** |

**Table 3**
Layer descriptions for the 160 orthorhombic types of sphere packing.

RCSR names for the layers used in this work are hxl ($3^6$), sql ($4^4$) hcb ($6^3$), cem ($3^34^2$), tts ($3^2434$), fes ($48^2$).

| Type | Layer parallel to (100) | | | Layer parallel to (010) | | | Layer parallel to (001) | | |
|---|---|---|---|---|---|---|---|---|---|
| **3/10/*o*1** | – | | | – | | | – | | |
| **3/10/*o*2** | – | | | – | | | – | | |
| **4/4/*o*1** | $48^2$ | 1,0 1 | – – | $6^3$ | 1,0 2 | – + | – | | |
| **4/4/*o*2** | – | | | $6^3$ | 1,0 2 | – + | $4_c(8+2)^2$ | 1,0 1 | – – |
| **4/4/*o*3** | $6^3$ | 1,0 2 | – + | $48^2$ | 1,0 2 | – + | $48^2$ | 1,0 2 | – + |
| **4/4/*o*4** | $6^3$ | 1,0 2 | – + | $48^2$ | 1,0 2 | – + | $48^2$ | 1,0 2 | – + |
| | | | | $6^3$ | 1,0 2 | – + | | | |
| **4/4/*o*5** | – | | | $48^2$ | 1,0 2 | – + | $4_c(8+2)^2$ | 1,0 2 | – + |
| **4/4/*o*6** | – | | | $6^3$ | 1,0 2 | – + | $4_c(8+2)^2$ | 1,0 2 | – + |
| **4/4/*o*7** | $48^2$ | 1,0 2 | – + | $6^3$ | 1,0 2 | – + | $6^3$ | 1,0 2 | – + |
| **4/4/*o*8** | – | | | $4_c(8+2)^2$ | 1,0 2 | – + | $6^3$ | 1,0 2 | – + |
| | | | | | | | $4_c(8+2)^2$ | 1,0 2 | – + |
| **4/4/*o*9** | $6^3$ | 1,0 2 | – + | $4_c(8+2)^2$ | 1,0 2 | – + | $48^2$ | 1,0 2 | – + |
| **4/4/*o*10** | – | | | – | | | $6^3$ | 1,0 4 | + + |
| **4/4/*o*11** | – | | | – | | | $6^3$ | 1,0 4 | – + |
| **4/4/*o*12** | – | | | – | | | $4_c(8+2)^2$ | 1,0 4 | – + |
| **4/4/*o*13** | – | | | – | | | $6^3$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 1,0 4 | – + |
| **4/4/*o*14** | – | | | – | | | $6^3$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 1,0 4 | – + |
| **4/4/*o*15** | – | | | – | | | $48^2$ | 1,0 4 | – + |
| **4/4/*o*16** | – | | | – | | | $6^3$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 1,0 4 | – + |
| **4/4/*o*17** | – | | | – | | | – | | |
| **4/4/*o*18** | – | | | – | | | – | | |
| **4/4/*o*19/*t*39** | – | | | – | | | – | | |
| **4/4/*o*20** | – | | | – | | | – | | |
| **4/4/*o*21** | – | | | – | | | – | | |
| **4/4/*o*22** | – | | | – | | | $6^3$ | 1,0 2 | – + |

**Table 3 (continued)**

| Type | Layer parallel to (100) | | | Layer parallel to (010) | | | Layer parallel to (001) | | |
|---|---|---|---|---|---|---|---|---|---|
| **4/6/*o*1** | – | | | – | | | $6^3$ | 1,0 2 | – – |
| **4/6/*o*2** | – | | | $6^3$ | 1,0 2 | – + | $6^3$ | 1,0 2 | – + |
| **4/6/*o*3** | – | | | $6^3$ | 1,0 2 | – + | – | | |
| **5/3/*o*1** | – | | | $6^3$ | 2,0 2 | – + | – | | |
| **5/3/*o*2** | $6^3$ | 2,0 2 | – + | $4_t8^2$ | 1,0 2 | – + | $6^3$ | 2,0 2 | – + |
| | | | | | | | $4_t8^2$ | 1,0 2 | – + |
| **5/3/*o*3** | – | | | – | | | $6^3$ | 2,0 4 | – + |
| | | | | | | | $4_t8^2$ | 1,0 4 | – + |
| **5/3/*o*4** | – | | | – | | | – | | |
| **5/3/*o*5** | – | | | – | | | – | | |
| **5/3/*o*6/*t*24** | – | | | – | | | – | | |
| **5/3/*o*7** | – | | | – | | | – | | |
| **5/4/*o*1** | $4^4$ | 1,0 2 | – + | $6^3$ | 2,0 2 | – + | $48^2$ | 2,0 1 | – – |
| **5/4/*o*2** | $4^4$ | 1,0 2 | – + | $4^4$ | 1,0 2 | – + | – | | |
| | $4^4$ | 1,0 2 | – + | | | | | | |
| **5/4/*o*3** | $4^4$ | 1,0 2 | – + | – | | | $4^4$ | 1,0 2 | – + |
| **5/4/*o*4** | – | | | – | | | $6^3$ | 1,1 4 | + + |
| **5/4/*o*5** | $4^4$ | 1,0 4 | – + | – | | | $4^4$ | 1,0 2 | – – |
| **5/4/*o*6** | – | | | $6^3$ | 2,0 4 | – + | – | | |
| **5/4/*o*7** | $6^3$ | 2,0 1 | – – | $4^4$ | 1,0 2 | – + | $6^3$ | 2,0 2 | – + |
| | | | | $6^3$ | 2,0 2 | – + | | | |
| **5/4/*o*8** | $6^3$ | 1,1 2 | + + | $4^4$ | 1,0 2 | – + | – | | |
| | | | | $6^3$ | 2,0 2 | – + | | | |
| **5/4/*o*9** | $48^2$ | 1,1 2 | + + | $4^4$ | 1,0 2 | – + | $6^3$ | 1,1 4 | + + |
| **5/4/*o*10** | – | | | $4^4$ | 1,0 2 | – + | $4_c(8+2)^2$ | 2,0 1 | – – |
| **5/4/*o*11** | – | | | $4^4$ | 1,0 2 | – + | $6^3$ | 1,1 2 | + + |
| **5/4/*o*12** | $6^3$ | 1,1 4 | + + | $4^4$ | 1,0 2 | – + | – | | |
| | | | | $48^2$ | 2,0 2 | – + | | | |
| **5/4/*o*13** | – | | | $4^4$ | 1,0 2 | – + | $6^3$ | 1,1 4 | + + |
| **5/4/*o*14** | – | | | $6^3$ | 1,1 4 | + + | $4^4$ | 1,0 2 | – + |
| | | | | | | | $4_c(8+2)^2$ | 2,0 2 | – + |
| **5/4/*o*15** | $4^4$ | 1,0 2 | – + | $6^3$ | 1,1 4 | + + | – | | |
| **5/4/*o*16** | – | | | $6^3$ | 1,1 4 | + + | $4^4$ | 1,0 2 | – + |
| **5/4/*o*17** | – | | | – | | | $6^3$ | 1,1 8 | + + |
| **5/4/*o*18** | – | | | $6^3$ | 1,1 4 | – + | $4^4$ | 1,0 4 | – + |
| **5/4/*o*19** | – | | | – | | | $6^3$ | 1,1 8 | + + |
| **5/4/*o*20** | – | | | $6^3$ | 1,1 4 | + + | $4^4$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 2,0 4 | – + |
| **5/4/*o*21** | – | | | $4^4$ | 1,0 4 | – + | $4^4$ | 1,0 4 | – + |
| **5/4/*o*22/*t*49** | – | | | – | | | – | | |
| **5/4/*o*23** | – | | | – | | | $4^4$ | 1,0 4 | – + |
| **5/4/*o*24** | – | | | – | | | $4^4$ | 1,0 4 | + + |
| **5/4/*o*25** | – | | | – | | | $4^4$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 2,0 4 | – + |
| **5/4/*o*26** | – | | | $48^2$ | 1,1 4 | – + | – | | |
| **5/4/*o*27** | – | | | – | | | $4^4$ | 1,0 4 | – + |
| **5/4/*o*28** | – | | | – | | | – | | |
| **5/4/*o*29/*t*48** | – | | | – | | | $48^2$ | 2,0 4 | – + |
| **5/4/*o*30** | – | | | – | | | – | | |
| **5/4/*o*31** | – | | | $4^4$ | 1,0 2 | – + | $6^3$ | 1,1 4 | + + |
| **6/3/*o*1** | $6^3$ | 2,1 1 | – – | $3^34^2$ | 1,0 1 | – – | $4^4$ | 2,0 2 | – + |
| **6/3/*o*2** | $6^3$ | 2,1 2 | – – | $3^34^2$ | 1,0 2 | – + | $3^34^2$ | 1,0 2 | – + |
| | | | | $4^4$ | 2,0 2 | – + | | | |
| **6/3/*o*3** | $48^2$ | 2,1 1 | – – | $3^34^2$ | 1,0 2 | – + | $4^4$ | 2,0 2 | – + |
| **6/3/*o*4** | $4^4$ | 2,0 4 | – + | – | | | $3^34^2$ | 1,0 2 | – – |
| **6/3/*o*5** | $6^3$ | 2,1 2 | – + | $3^2434$ | 1,0 2 | – + | – | | |
| **6/3/*o*6** | $3^34^2$ | 1,0 2 | – + | $48^2$ | 2,1 2 | – + | $6^3$ | 2,1 4 | + + |
| **6/3/*o*7** | $6^3$ | 2,1 4 | + + | $3^34^2$ | 1,0 2 | – + | $48^2$ | 2,1 2 | – + |
| | | | | $48^2$ | 3,0 2 | – + | | | |
| **6/3/*o*8** | $3^34^2$ | 1,0 2 | – + | $6^3$ | 2,1 2 | – + | $6^3$ | 2,1 4 | + + |
| | | | | $48^2$ | 3,0 2 | – + | | | |
| **6/3/*o*9** | – | | | $3^34^2$ | 1,0 2 | – + | $6^3$ | 2,1 4 | + + |
| **6/3/*o*10** | – | | | $3^34^2$ | 1,0 2 | – + | $3^34^2$ | 1,0 2 | – + |
| | | | | | | | $4^4$ | 2,0 2 | – + |
| **6/3/*o*11** | – | | | $3^2434$ | 1,0 2 | – + | $6^3$ | 2,1 2 | – + |
| **6/3/*o*12** | $4^4$ | 2,1 2 | – + | $6^3$ | 3,0 2 | – + | – | | |
| **6/3/*o*13** | – | | | $6^3$ | 2,1 2 | – + | $3^2434$ | 1,0 2 | – + |
| | | | | | | | $6^3$ | 3,0 2 | – + |

**Table 3 (continued)**

| Type | Layer parallel to (100) | | | Layer parallel to (010) | | | Layer parallel to (001) | | |
|---|---|---|---|---|---|---|---|---|---|
| **6/3/*o*14** | – | | | $3^2434$ | 1,0 2 | – + | $6^3$ | 2,1 2 | – + |
| **6/3/*o*15** | $3^34^2$ | 1,0 2 | – + | $6^3$ | 2,1 4 | + + | $48^2$ | 2,1 2 | – + |
| **6/3/*o*16** | – | | | $6^3$ | 2,1 4 | + + | $3^34^2$ | 1,0 2 | – + |
| | | | | | | | $4_c(8+2)^2$ | 3,0 2 | – + |
| **6/3/*o*17** | $48^2$ | 2,1 2 | – + | $6^3$ | 2,1 4 | + + | $3^34^2$ | 1,0 2 | – + |
| | | | | | | | $4_c(8+2)^2$ | 3,0 2 | – + |
| **6/3/*o*18** | – | | | $4^4$ | 2,0 4 | – + | $3^34^2$ | 1,0 4 | + + |
| **6/3/*o*19** | – | | | – | | | $3^34^2$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 3,0 2 | – + |
| **6/3/*o*20** | – | | | – | | | $3^34^2$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 3,0 4 | – + |
| **6/3/*o*21** | – | | | $48^2$ | 2,1 4 | – + | – | | |
| **6/3/*o*22** | – | | | – | | | $48^2$ | 3,0 4 | – + |
| **6/3/*o*23** | – | | | – | | | $4^4$ | 2,0 4 | – + |
| **6/3/*o*24** | – | | | – | | | $3^34^2$ | 1,0 4 | – + |
| | | | | | | | $4_c(8+2)^2$ | 3,0 4 | – + |
| **6/3/*o*25/*t*44** | – | | | – | | | $4^4$ | 2,0 4 | – + |
| | | | | | | | $4_t8^2$ | 2,0 4 | – + |
| **6/3/*o*26** | – | | | – | | | – | | |
| **6/3/*o*27** | – | | | – | | | – | | |
| **6/3/*o*28** | – | | | – | | | – | | |
| **6/3/*o*29** | $6^3$ | 2,1 2 | – + | $3^34^2$ | 1,0 2 | – + | $6^3$ | 2,1 4 | + + |
| **6/3/*o*30** | $6^3$ | 2,1 2 | – + | $3^2434$ | 1,0 2 | – + | $6^3$ | 2,1 2 | – + |
| **6/3/*o*31** | $6^3$ | 2,1 2 | – + | – | | | $3^2434$ | 1,0 2 | – + |
| **6/4/*o*1** | $4^4$ | 1,1 2 | + + | $4^4$ | 1,1 4 | – + | – | | |
| **6/4/*o*2** | – | | | $4^4$ | 1,1 4 | + + | $4^4$ | 1,1 2 | + + |
| **6/4/*o*3** | – | | | $4^4$ | 1,1 4 | + + | $4^4$ | 1,1 4 | + + |
| **6/4/*o*4** | $4^4$ | 2,0 2 | – + | $6^3$ | 2,1 2 | – + | $6^3$ | 2,1 2 | – + |
| | | | | | | | $6^3$ | 2,1 2 | – + |
| **6/4/*o*5** | – | | | $4^4$ | 1,1 4 | + + | $4^4$ | 1,1 8 | + + |
| **6/4/*o*6** | – | | | $4^4$ | 1,1 4 | – + | $4^4$ | 1,1 8 | + + |
| **6/4/*o*7** | – | | | $6^3$ | 2,1 4 | – + | $6^3$ | 2,1 8 | + + |
| **6/4/*o*8** | – | | | $4^4$ | 1,1 4 | – + | $4^4$ | 1,1 8 | + + |
| **6/4/*o*9** | – | | | $48^2$ | 2,1 4 | – + | $4^4$ | 1,1 4 | + + |
| **6/4/*o*10** | – | | | $4^4$ | 1,1 4 | – + | – | | |
| **6/4/*o*11** | – | | | – | | | – | | |
| **7/3/*o*1** | $4^4$ | 2,1 4 | + + | $4^4$ | 2,1 1 | – – | $3^34^2$ | 1,1 1 | + + |
| **7/3/*o*2** | $3^6$ | 1,0 2 | – + | $3^34^2$ | 2,0 2 | – + | $48^2$ | 3,1 1 | – – |
| **7/3/*o*3** | $3^6$ | 1,0 2 | – + | $6^3$ | 3,1 1 | – + | $6^3$ | 2,2 2 | + + |
| **7/3/*o*4** | $4^4$ | 2,1 2 | – + | $4^4$ | 2,1 4 | + + | – | | |
| | $4^4$ | 2,1 2 | – + | | | | | | |
| **7/3/*o*5** | $3^6$ | 1,0 2 | – + | $6^3$ | 3,1 1 | – – | $3^34^2$ | 2,0 1 | – – |
| **7/3/*o*6** | $4^4$ | 2,1 4 | – + | – | | | $3^34^2$ | 1,1 4 | + + |
| **7/3/*o*7** | – | | | $4^4$ | 3,0 4 | – + | – | | |
| | | | | $3^34^2$ | 2,0 4 | – + | | | |
| **7/3/*o*8** | – | | | $6^3$ | 3,1 4 | – + | – | | |
| **7/3/*o*9** | $6^3$ | 2,2 2 | + + | $3^6$ | 1,0 2 | – + | $6^3$ | 3,1 2 | – + |
| | | | | $6^3$ | 4,0 2 | – + | | | |
| **7/3/*o*10** | $6^3$ | 3,1 1 | – – | $3^6$ | 1,0 2 | – + | $3^34^2$ | 2,0 2 | – + |
| | | | | $3^34^2$ | 2,0 2 | – + | | | |
| **7/3/*o*11** | $3^34^2$ | 1,1 2 | + + | $4^4$ | 2,1 4 | + + | – | | |
| **7/3/*o*12** | $3^2434$ | 1,1 2 | + + | $4^4$ | 2,1 2 | – + | $4^4$ | 2,1 2 | – + |
| | | | | $6^3$ | 3,1 2 | – + | | | |
| **7/3/*o*13** | – | | | $3^6$ | 1,0 2 | – + | $6^3$ | 2,2 2 | + + |
| **7/3/*o*14** | $3^34^2$ | 1,1 4 | + + | $4^4$ | 2,1 4 | + + | – | | |
| **7/3/*o*15** | $3^2434$ | 1,1 4 | + + | $4^4$ | 2,1 2 | – + | $4^4$ | 2,1 2 | – + |
| | | | | $48^2$ | 3,1 2 | – + | | | |
| **7/3/*o*16** | $4^4$ | 2,1 2 | – + | $4^4$ | 3,0 2 | – + | – | | |
| | $6^3$ | 3,1 2 | – + | $3^2434$ | 2,0 2 | – + | | | |
| **7/3/*o*17** | $4^4$ | 2,1 2 | – + | $3^2434$ | 1,1 4 | + + | $4^4$ | 2,1 2 | – + |
| **7/3/*o*18** | – | | | $3^34^2$ | 1,1 4 | + + | $4^4$ | 2,1 4 | + + |
| **7/3/*o*19** | – | | | $4^4$ | 2,1 4 | – + | $3^34^2$ | 1,1 8 | + + |
| **7/3/*o*20** | – | | | $6^3$ | 3,1 4 | – + | $6^3$ | 3,1 8 | + + |
| **7/3/*o*21** | – | | | – | | | $3^34^2$ | 2,0 4 | – + |
| | | | | | | | $4_t8^2$ | 3,0 4 | – + |
| **7/3/*o*22** | – | | | $3^34^2$ | 1,1 4 | + + | $4^4$ | 2,1 8 | + + |
| **7/3/*o*23** | – | | | – | | | – | | |
| **7/3/*o*24** | – | | | $4^4$ | 2,1 4 | – + | – | | |
| **7/3/*o*25** | – | | | $4^4$ | 2,1 4 | – + | – | | |

**Table 3 (continued)**

| Type | Layer parallel to (100) | | | Layer parallel to (010) | | | Layer parallel to (001) | | |
|---|---|---|---|---|---|---|---|---|---|
| **7/3/*o*26** | – | | | – | | | $48^2$ | 3,1 4 | – + |
| **7/4/*o*1** | $4^4$ | 2,1 4 | + + | $4^4$ | 3,0 1 | – – | $6^3$ | 2,2 2 | + + |
| **8/3/*o*1** | $4^4$ | 3,1 1 | – – | $3^6$ | 2,0 2 | – + | $3^34^2$ | 3,0 1 | – – |
| | | | | $4^4$ | 4,0 2 | – + | | | |
| **8/3/*o*2** | $3^34^2$ | 3,0 1 | – – | $6^3$ | 3,2 2 | – + | $4^4$ | 3,1 4 | + + |
| **8/3/*o*3** | $4^4$ | 2,2 8 | + + | – | | | $6^3$ | 3,2 2 | – – |
| **8/3/*o*4** | $4^4$ | 3,1 2 | – + | $4^4$ | 3,1 4 | + + | – | | |
| | $3^34^2$ | 2,1 2 | – + | | | | | | |
| **8/3/*o*5** | $4^4$ | 3,1 2 | – + | $3^2434$ | 3,0 1 | – – | – | | |
| **8/3/*o*6** | – | | | $4^4$ | 3,1 4 | + + | $3^34^2$ | 2,1 2 | – + |
| | | | | | | | $4^4$ | 3,1 2 | – + |
| **8/3/*o*7** | $3^6$ | 2,0 2 | – + | $6^3$ | 4,1 2 | – + | $6^3$ | 3,2 2 | – + |
| | | | | | | | $6^3$ | 3,2 2 | – + |
| **8/3/*o*8** | $4^4$ | 3,1 2 | – + | $3^2434$ | 2,1 2 | – + | $3^2434$ | 2,1 2 | – + |
| | | | | | | | $6^3$ | 4,1 2 | – + |
| **8/3/*o*9** | – | | | $3^34^2$ | 2,1 2 | – + | $4^4$ | 3,1 4 | + + |
| | | | | $4^4$ | 3,1 2 | – + | | | |
| **8/3/*o*10** | – | | | $3^34^2$ | 2,1 4 | – + | $3^34^2$ | 2,1 8 | + + |
| **8/3/*o*11** | – | | | $4^4$ | 2,2 4 | – + | $48^2$ | 4,1 4 | – + |
| **9/3/*o*1** | $3^6$ | 2,1 4 | + + | $4^4$ | 3,2 1 | – – | $3^34^2$ | 2,2 2 | + + |
| **9/3/*o*2** | $3^6$ | 2,1 8 | + + | – | | | $4^4$ | 3,2 2 | – – |
| **9/3/*o*3** | $4^4$ | 3,2 4 | – + | $4^4$ | 4,1 4 | – + | – | | |
| | | | | $3^34^2$ | 3,1 4 | – + | | | |
| **9/3/*o*4** | – | | | $4^4$ | 3,2 8 | + + | – | | |
| **9/3/*o*5** | $3^34^2$ | 4,0 1 | – – | $4^4$ | 3,2 2 | – + | $4^4$ | 3,2 4 | + + |
| | | | | $6^3$ | 4,2 2 | – + | | | |
| **9/3/*o*6** | $3^6$ | 2,1 2 | – + | $3^2434$ | 3,1 2 | – + | $4^4$ | 3,2 2 | – + |
| | $6^3$ | 5,1 2 | – + | $4^4$ | 4,1 2 | – + | $6^3$ | 4,2 2 | – + |
| **9/3/*o*7** | $3^6$ | 2,1 2 | – + | $4^4$ | 3,2 4 | + + | – | | |
| | $3^34^2$ | 3,1 2 | – + | | | | | | |
| **10/3/*o*1** | $3^6$ | 4,0 1 | – – | $4^4$ | 4,2 2 | – + | $4^4$ | 3,3 2 | + + |
| **10/3/*o*2** | $3^6$ | 3,1 1 | – – | $4^4$ | 4,2 4 | + + | $3^34^2$ | 4,1 1 | – – |
| **10/3/*o*3** | – | | | $4^4$ | 4,2 2 | – – | $3^6$ | 2,2 4 | + + |
| **10/3/*o*4** | $3^6$ | 2,2 8 | + + | – | | | $3^34^2$ | 3,2 2 | – – |
| **10/3/*o*5** | $3^6$ | 3,1 2 | – + | $4^4$ | 3,3 2 | + + | – | | |
| | $4^4$ | 5,1 2 | – + | | | | | | |
| **10/3/*o*6** | $3^6$ | 3,1 2 | – + | $3^2434$ | 4,1 1 | – – | $4^4$ | 4,2 2 | – + |
| **11/3/*o*1** | – | | | $3^6$ | 3,2 8 | + + | – | | |
| **11/3/*o*2** | $3^34^2$ | 5,1 1 | – – | $3^6$ | 3,2 2 | – + | $3^6$ | 3,2 4 | + + |
| | | | | $3^34^2$ | 4,2 2 | – + | | | |

that lattice complex where packings of this type occur with highest symmetry. Columns three and four show the minimal and maximal degrees of freedom *df* of the corresponding parameter regions. The next columns tabulate the coordinates and the lattice parameters for a sphere packing with minimal density, which is given in column six. If no such configuration exists, the parameter values of an arbitrarily chosen sphere packing of the type under consideration are shown. All lattice parameters refer to shortest distances $d = 1$ between neighbouring spheres. The last column lists the three-letter symbols from the RCSR database for the corresponding sphere-packing types.

One hundred and forty one out of the 160 orthorhombic sphere-packing types can be subdivided into layer-like subunits perpendicular to at least one of the orthorhombic main axes. Most of these flat or corrugated sphere layers correspond to vertex transitive nets (Shubnikov, 1916) and can be characterized, therefore, by their symbols $3^6$, $4^4$, $6^3$, $3^34^2$, $3^2434$ and $48^2$. The symbols for some special corrugated layers can be derived from those of plane nets. Figs. 4(*a*) and 4(*b*) show examples for corresponding nets of types $4_c(8+2)^2$ and $4_t8^2$ (*cf. e.g.* Fischer, 2005). In Table 3 the sphere-packing type is identified in column 1. The following three columns refer to different descriptions of the sphere packings with layers perpendicular to **a**, **b** and **c**. Each layer description consists of a layer symbol, three numbers and two signs. The first two numbers indicate how many contacts each sphere has to spheres of the neighbouring layers below and above. The third number is the number of layers per translation period. The first sign indicates whether the layer may be flat (+) or not (−) and the last sign is + if there is only one possibility to split the sphere packing into the corresponding layers, otherwise it is −.

Not only atomic arrangements in inorganic compounds may be described by means of sphere packings. Many complicated crystal structures, for instance, metal–organic framework materials (MOFs) can be characterized by three-periodic nets.

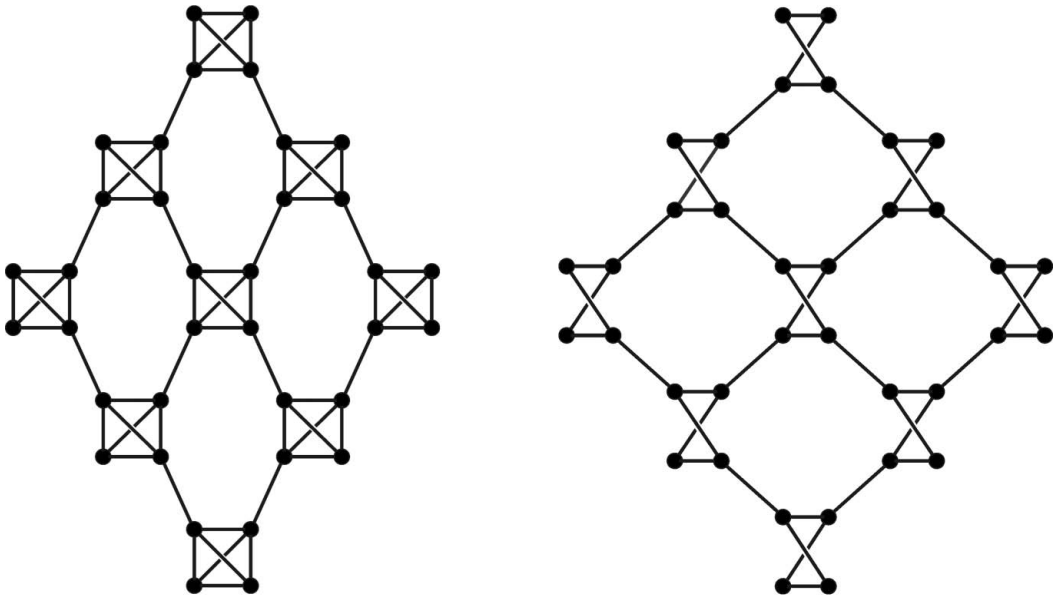


**Figure 4**
Sphere layers corresponding to non-planar graphs: (*a*) $4_t8^2$ layer, (*b*) $4_c(8+2)^2$ layer. $4_t8^2$ corresponds to KII or HIIIa and $4_c(8+2)^2$ to KIb or HIIa according to the nomenclature by Koch & Fischer (1978).

Corresponding investigations can be carried out using the *TOPOS* program package (Blatov, 2006). Analysing the Cambridge Structural Database (CSD), Alexandrov *et al.* (2011) found 5645 compounds containing metal atoms as well as organic molecules with underlying three-periodic single nets and 975 of such compounds which can be described by using interpenetrating nets. Also, the frameworks of hydrogen bonds in MOFs (*e.g.* Baburin, 2008) or organic materials (Baburin & Blatov, 2007) may be represented by three-periodic nets.

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## References

Alexandrov, E. V., Blatov, V. A., Kochetkov, A. V. & Proserpio, D. M. (2011). *CrystEngComm*, **13**, 3947.
Baburin, I. A. (2008). *Z. Kristallogr.* **233**, 371–381.
Baburin, I. A. & Blatov, V. A. (2007). *Acta Cryst.* B**63**, 791–802.
Blatov, V. A. (2006). *IUCr CompComm Newsletter*, **7**, 4–38; http://www.topos.ssu.samara.ru.
Blatov, V. A. (2007). *Acta Cryst.* A**63**, 329–343.
Delgado-Friedrichs, O., Foster, M. D., O'Keeffe, M., Proserpio, D. M., Treacy, M. M. & Yaghi, O. M. (2005). *J. Solid State Chem.* **178**, 2533–2554.
Delgado-Friedrichs, O. & O'Keeffe, M. (2003). *Acta Cryst.* A**59**, 351–360.
Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *Z. Kristallogr.* Suppl. Issue **1**.
Erfany-Far, H., Fuess, H. & Gregson, D. (1987). *Acta Cryst.* C**43**, 395–397.
Fischer, W. (1971). *Z. Kristallogr.* **133**, 18–42.
Fischer, W. (2005). *Acta Cryst.* A**61**, 435–444.
Fischer, W., Sowa, H. & Koch, E. (2006). *Acta Cryst.* A**62**, 413–418.
Kihara, K., Matsumoto, T. & Imamura, M. (1986). *Z. Kristallogr.* **177**, 39–52.
Koch, E. & Fischer, W. (1978). *Z. Kristallogr.* **148**, 107–152.
Moreira de Oliveira, M. Jr & Eon, J.-G. (2013). *Acta Cryst.* A**69**, 276–288.
O'Keeffe, M. (2012). *Struct. Chem.* **23**, 1079–1087.
O'Keeffe, M., Peskov, M. A., Ramsden, S. J. & Yaghi, O. M. (2008). *Acc. Chem. Res.* **41**, 1782–1789.
Pell, M. A. & Ibers, J. A. (1995). *J. Am. Chem. Soc.* **117**, 6284–6286.
Shubnikov, A. V. (1916). *Izv. Akad. Nauk. SSSR Ser. 6*, **10**, 755–799.
Sowa, H. (2012). *Acta Cryst.* A**68**, 763–777.
Sowa, H. & Fischer, W. (2010). *Acta Cryst.* A**66**, 292–300.
Sowa, H., Koch, E. & Fischer, W. (2003). *Acta Cryst.* A**59**, 317–326.
Sowa, H., Koch, E. & Fischer, W. (2007). *Acta Cryst.* A**63**, 354–364.
Stahl, R., Jung, C., Lutz, H. D., Kockelmann, W. & Jacobs, H. (1998). *Z. Anorg. Allg. Chem.* **624**, 1130–1136.