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# Interpenetration of homogeneous sphere packings and of two-periodic layers of spheres

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All systems of interpenetrating sphere packings that occur with highest symmetry in the cubic, hexagonal or tetragonal crystal family are tabulated. Homogeneous sphere packings belonging to 49 different types may be intertwined to systems of interpenetrating sphere packings belonging to 74 types. For all compatible lattice complexes, the coordinate and lattice parameters are given. The corresponding patterns of interpenetration are analysed. For the interpenetration of two, three, four, five and eight sphere packings, eleven, three, five, one and two different patterns, respectively, are distinguished. In addition, four types of interpenetrating layers of spheres were found. Each such sphere configuration splits into two or three subsets of parallel sphere layers with an angle of 90° or of 120°, respectively, between the directions of the normals of the layers. A single sphere layer corresponds either to a honeycomb net or to a net built up from quadrangles and octagons.

## 1. Introduction

Already in 1975, Wells realized that the crystal structures of certain inorganic compounds might be described by means of interpenetrating two- or three-periodic nets. Well known examples are the $H_2O$ modifications ice VII, VIII and X (*cf. e.g.* Pruznan *et al.*, 1993) and the mineral cuprite $Cu_2O$ (*cf. e.g.* Restori & Schwarzenbach, 1986), which each consist of two interpenetrating cristobalite-like networks. Even the crystal structures of certain organic substances may be looked at as interpenetrating three-periodic nets if one takes into account hydrogen bonds in addition to covalent bonds (*cf. e.g.* Ermer, 1988; Ermer & Eling, 1988; Ermer & Lindenberg, 1991).

In the last decade, the geometry and topology of infinite networks has attained much attention, especially in the field of crystal engineering of new porous solids like metal–organic framework materials that may lead to important applications like catalysis, gas separation or gas storage. One-, two- or three-periodic nets are used for the description and the classification of porous structures, since, on the basis of covalent and non-covalent bonds, the complicated structures can be attributed to nets, which may more easily be identified. In many metal–organic structures, two or more interpenetrating nets have been found. Batten & Robson (1998) and Carlucci *et al.* (2003) presented a large number of examples. The atomic arrangement of a number of inorganic compounds can also be described by means of interpenetrating nets (Baburin *et al.*, 2005). Many structural examples with this property are listed by Batten (2001).

Often the underlying nets are rather simple even in complicated crystal structures (*cf. e.g.* Delgado Friedrichs *et al.*, 2003; Blatov *et al.*, 2004). In many cases, they correspond to homogeneous sphere packings. Important nets that are found in structures based on interpenetrating networks are, for instance, the cubic and the tetragonal (10, 3) nets and the diamond net (Wells, 1975). These nets correspond to homogeneous sphere packings of type 3/10/*c*1 (Fischer, 1973, 2004), 3/10/*t*4 (Fischer, 1991*a*, 2005) and 4/6/*c*1 (Fischer, 1973, 2004), respectively.

Up to now, insufficient information on homogeneous interpenetrating sphere packings has been published. Tables of the types of interpenetrating sphere packings with cubic symmetry (Fischer & Koch, 1976) do not contain information on coordinates or lattice parameters. The tetragonal types were presented only on a congress poster (Fischer & Koch, 1990) and information on the hexagonal types is strewn across several papers dealing with homogeneous hexagonal sphere packings (Sowa *et al.*, 2003, Sowa & Koch, 2004, 2005, 2006).

In order to fill this gap, the present paper gives detailed information on all types of homogeneous interpenetrating sphere packings and of interpenetrating two-periodic sphere layers that occur with highest symmetry in the cubic, tetragonal or hexagonal crystal families.

## 2. Fundamentals

A *point configuration* is the set of all points that are generated from an original point by application of all symmetry operations of a given space group $G$, *i.e.* it is the orbit[1] of a given point under the action of a space group $G$.

[1] As 'orbit' is a very general mathematical term, comparable to the term 'group', it should be avoided without further specification.

Each point configuration can uniquely be assigned to a set of spheres, called *sphere configuration*, in the following way: (i) each point is the centre of a sphere; (ii) all spheres are equal in size; (iii) each sphere is in contact with at least one other sphere; (iv) no spheres overlap.

A sphere configuration with symmetry $G$ is called a (homogeneous) *sphere packing* if a chain of spheres with mutual contact connects any two of its spheres. Otherwise, the sphere configuration disintegrates into *partial configurations*. The symmetry group of each such partial configuration is a subgroup of $G$. It may be a point group, a rod group, a layer group or again a space group.

In the latter case, the sphere configuration consists of finitely many partial configurations that interpenetrate each other without mutual contact. Each such partial configuration, regarded by itself, forms a sphere packing with symmetry $H$, where $H$ is a subgroup of $G$ with index $i$, and $i$ is the number of sphere packings that interpenetrate each other. The entire arrangement, therefore, may be called a *system of interpenetrating sphere packings*.

In all other cases, the number of partial configurations is infinite. If a sphere configuration is built up from two-periodic configurations, then either all these layer-like partial configurations are oriented parallel to each other or two or three sets of parallel sphere layers exists. In contrast to the more general types of two-periodic net, parallel sphere layers can never be catenated or interwoven. Sphere layers running in different directions, however, necessarily must interpenetrate each other. A corresponding sphere configuration is called a *system of interpenetrating sphere layers*.

Let us regard a sphere configuration with space group $G$ and let $s$ be the order of the site-symmetry group of any of the spheres. Then, exactly $s$ symmetry operations[2] of $G$ map this sphere onto any other sphere of the sphere configuration. The set of all those symmetry operations of $G$ that map a certain original sphere onto its contacting neighbour spheres forms a set of generators of a subgroup of $G$, namely of the symmetry group $H$ of the respective partial configuration.

If $G$ and $H$ are identical, only one partial configuration exists and the sphere configuration is a sphere packing. If $H$ is a space group but $G$ and $H$ are different, then the sphere configuration splits up into $i$ interpenetrating sphere packings, where $i$ is the index of $H$ in $G$. Then, all symmetry operations of $H$ map, for example, a first individual sphere packing onto itself, whereas each left coset of $H$ in $G$ maps this sphere packing onto one of the other $i - 1$ ones.

Each sphere packing can uniquely be assigned to a graph, its *sphere-packing graph*, as follows: (i) each centre of a sphere is replaced by a vertex of the graph; (ii) two vertices of the graph are connected by an edge if and only if the corresponding spheres are in contact (*cf.* Fischer, 1971; *Mittelpunktsfigur*, Heesch & Laves, 1933).

Two sphere packings are assigned to the same *sphere-packing type* if the spheres of one sphere packing can be mapped onto the spheres of the other one and *vice versa* under preservation of all contact relationships between the spheres, *i.e.* if the corresponding sphere-packing graphs are isomorphic[3] (*cf. e.g.* Fischer, 1991*a*).

Each sphere-packing type is designated by a symbol $k/m/fn$, as was first introduced by Fischer (1971): $k$ means the number of contacts per sphere, $m$ is the length of the shortest ring within the sphere packing, $f$ indicates the highest crystal family for a sphere packing of that type ($c$: cubic, $h$: hexagonal, $t$: tetragonal, $o$: orthorhombic) and $n$ is an arbitrary number.

Closer inspection of interpenetrating sphere packings shows that the definition of types can be transferred from sphere packings to systems of interpenetrating sphere packings only if the details of the interpenetration are considered. Sphere packings of the same type can be intertwined in different ways: (i) various numbers of sphere packings of a given type may be combined; (ii) the rings in the sphere packings may be differently catenated or the screws in the individual packings may be differently arranged; (iii) the individual packings may be oriented differently with respect to each other. Such differences must be taken into account when defining types of interpenetrating sphere packings (*cf.* examples below).

Two systems of interpenetrating sphere packings belong to the same *type of interpenetrating sphere packings* if the individual sphere packings belong to the same sphere-packing type and if, in addition, the sphere packings are analogously intertwined in both systems (*cf.* also Fischer & Koch, 1976), *i.e.* if the numbers of individual packings are equal and the catenation of the rings, the arrangement of the screws and the mutual orientation of the individual packings are analogous in the two systems.

A type of interpenetrating sphere packings can be characterized by a symbol $g[k/m/fn]^i$, where $k/m/fn$ symbolizes the type of the partial configuration and $i$ is their number. The preceding letter indicates the highest possible symmetry for that type of interpenetrating sphere packing ($c$: cubic, $h$: hexagonal, $t$: tetragonal). If $i$ sphere packings of the same type can interpenetrate in different ways, Roman numbers as lower indices discriminate between these cases.

*Example:* Two sphere packings of type $3/3/c1$ can be combined to interpenetrating sphere packings belonging to three different types, namely to $c[3/3/c1]^2{}_{\mathrm{I}}$, $c[3/3/c1]^2{}_{\mathrm{II}}$ and $c[3/3/c1]^2{}_{\mathrm{III}}$ (*cf.* Fig. 1 and Table 1; Fischer, 1976; Fischer & Koch, 1976). The two sphere packings are directly congruent in the first two cases, whereas they are enantiomorphic in the third case. For each individual sphere packing, one 20-membered ring is emphasized in Fig. 1. The red and black rings in $c[3/3/c1]^2{}_{\mathrm{III}}$ are catenated in the same way as two circular links of a chain, *i.e.* the black ring winds itself once round the red one and *vice versa*. In the other cases, the catenation of the two rings is more complicated: the first ring winds itself twice round the second one in $c[3/3/c1]^2{}_{\mathrm{I}}$ and three times in $c[3/3/c1]^2{}_{\mathrm{II}}$.

[2] These $s$ symmetry operations form a left coset of the site-symmetry group under consideration.

[3] Only recently, the authors identified a few cases where this purely graph-theoretical definition does not sufficiently discriminate between sphere packings of different types (*cf.* Koch & Sowa, 2004; Fischer, 2004).

**Table 1**
Interpenetrating sphere packings occurring with highest symmetry in the cubic, hexagonal or tetragonal crystal family.

For all corresponding lattice complexes the parameters are tabulated. For orthorhombic space groups the lattice parameters are $a = b, c$.

| Sphere-packing type | Pattern of interpenetr. | | Interp. class | Group | Subgroup | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Symbol | Min. surf. | | $G$ | $H$ | $df$ | $\rho$ | $x, y, z$ | $a$ or $a = b, c$ | $d$ |
| $c[3/3/c1]^2_{\mathrm{I}}$ | *c-e* | $NO3^2$-$c4$ | Ia | $I4_132$ | $P4_332$ | 2 | 0.14411* | 0.01434, 0.11000, 0.61434 | 5.58699 | 1.19697 |
| | | | | | $P4_132$ | | | −0.01434, 0.11000, 0.11434 | | |
| $c[3/3/c1]^2_{\mathrm{II}}$ | *c-f* | – | IIa | $I4_132$ | $I2_13$ | 2 | 0.19282* | 0.01000, 0.01712, 0.15288 | 5.07029 | 1.25978 |
| $c[3/3/c1]^2_{\mathrm{III}}$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ – ..2 | $I4_132$ – ..2 | 0 | 0.11103 | 0.12500, 0.05801, 0.19199 | 6.09441 | 2.70138 |
| | | | IIa | $I\bar{4}3d$ | $I2_13$ | 2 | | 0.12500, 0.05801, 0.19199 | 6.09441 | |
| | | | IIa | $Ia\bar{3}$ | $I2_13$ | 2 | | 0.12500, 0.05801, 0.19199 | 6.09441 | |
| $h[3/4/c1]^2$ | *r-bc* | *rPD* | Ia | $R\bar{3}m$ | $R\bar{3}m$ (−**a**, −**b**, 2**c**) | 2 | 0.22327 | 0.28452, 0.06904, 0.36193 | 6.82843, 2.09077 | 1.39897 |
| $c[3/4/c5]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.24885* | 0.18099, 0.20915, −0.05000 | 5.86735 | 1.61710 |
| $c[3/4/c6]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.15115 | 0.16667, 0.16667, 0.00000 | 6.92820 | 2.51661 |
| $c[3/4/c7]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.12450 | 0.18750, 0.18750, 0.02589 | 7.39104 | 2.86042 |
| $h[3/4/h1a]^2$ | *h-q* | $NO3^2$-$h10$ | Ia | $P6_222$ | $P6_422$ (**a**, **b**, 2**c**) | 2 | 0.27835 | 0.45337, 0.12740, 0.35048 | 3.86895, 1.74129 | 1.34268 |
| $h[3/4/h2a]^2$ | *h-q* | $NO3^2$-$h10$ | Ia | $P6_222$ | $P6_422$ (**a**, **b**, 2**c**) | 2 | 0.29088 | 0.43559, 0.09867, 0.30202 | 3.51466, 2.01917 | 1.35954 |
| $h[3/4/h3]^2$ | *h-q* | $NO3^2$-$h10$ | Ia | $P6_222$ | $P6_422$ (**a**, **b**, 2**c**) | 2 | 0.24480 | 0.53120, 0.14951, 0.28580 | 3.66002, 2.21245 | 1.18738 |
| $t[3/4/t1]^2_{\mathrm{I}}$ | *t-b* | *tD* | Ia | $P4_2/nnm$ – ..$m$ | $I4_1/amd$ – .$m$. (**a**−**b**, **a**+**b**, 2**c**) | 2 | 0.23110 | 0.15350, 0.15350, 0.11075 | 2.79237, 2.32456 | 1.84222 |
| | | | IIa | $I4_1/acd$ | $I\bar{4}2d$ | 3 | | 0.15350, 0.00000, 0.05538 | 3.94901, 4.64911 | |
| | | | Ia | $P\bar{4}n2$ | $I\bar{4}2d$ (**a**−**b**, **a**+**b**, 2**c**) | 3 | | 0.15350, 0.15350, 0.11075 | 2.79237, 2.32456 | |
| | | | Ia | $P4_222$ | $I4_122$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | | 0.34650, 0.15350, 0.11075 | 2.79237, 2.32456 | |
| | | | IIa | $I4_1/acd$ | $I4_1/a$ | 3 | | 0.00000, 0.15350, 0.05538 | 3.94901, 4.64911 | |
| | | | Ia | $P4_2/n$ | $I4_1/a$ (**a**−**b**, **a**+**b**, 2**c**) | 3 | | 0.15350, 0.15350, 0.11075 | 2.79237, 2.32456 | |
| | | | IIa | $I4_1/acd$ | $Fddd$ (**a**−**b**, **a**+**b**, **c**) | 2 | | 0.15350, 0.00000, 0.30538 | 3.94901, 4.64911 | |
| | | | IIa | $I4_1/acd$ | $I4_122$ | 2 | | 0.00000, 0.15350, 0.30538 | 3.94901, 4.64911 | |
| | *o-b* | *oD* | Ia | $Pnnn$ | $Fddd$ (2**a**, 2**b**, 2**c**) | 3 | | 0.15350, 0.15350, 0.11075 | 2.79237, 2.32456 | |
| $t[3/4/t1]^2_{\mathrm{II}}$ | *t-b* | *tD* | IIa | $I4_1/acd$ | $Fddd$ (**a**−**b**, **a**+**b**, **c**) | 2 | 0.33199* | 0.12500, 0.05178, 0.87500 | 3.69552, 3.69552 | 1.16342 |
| $t[3/4/t2]^2_{\mathrm{I}}$ | *t-b* | *tD* | Ia | $P4_222$ | $I4_122$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | 0.22765 | 0.32625, 0.09162, 0.15574 | 2.54549, 2.83980 | 1.59671 |
| $t[3/4/t2]^2_{\mathrm{II}}$ | *t-a* | *tG* | IIa | $I4_1/acd$ | $I4_122$ | 2 | 0.22765 | 0.13269, 0.04106, 0.17213 | 3.59986, 5.67959 | 1.86066 |
| $t[3/4/t3]^2$ | *t-b* | *tD* | Ia | $P4_2/nnm$ | $I4_1/amd$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | 0.19875 | 0.27787, 0.10039, 0.11299 | 3.98413, 2.65552 | 1.86893 |
| $c[3/6/c3]^2$ | *c-b* | *D* | Ia | $Pn\bar{3}m$ – ..$m$ | $Fd\bar{3}m$ – ..$m$ (2**a**, 2**b**, 2**c**) | 1 | 0.32398* | 0.10445, 0.10445, 0.36000 | 3.38503 | 1.18252 |
| | | | IIa | $Fd\bar{3}c$ | $F4_132$ | 1 | | 0.05222, 0.05222, 0.18000 | 6.77006 | |
| | | | Ia | $P4_232$ | $F4_132$ (2**a**, 2**b**, 2**c**) | 1 | | 0.10445, 0.10445, 0.36000 | 3.38503 | |
| | | | IIa | $Fd\bar{3}c$ | $Fd\bar{3}$ | 2 | | 0.05222, 0.05222, 0.32000 | 6.77006 | |
| | | | Ia | $Pn\bar{3}$ | $Fd\bar{3}$ (2**a**, 2**b**, 2**c**) | 2 | | 0.10445, 0.10445, 0.36000 | 3.38503 | |
| $c[3/6/c5]^2$ | *c-c* | *P* | IIa | $Ia\bar{3}d$ | $Ia\bar{3}$ | 2 | 0.41603* | 0.15000, 0.00000, −0.01514 | 4.94367 | 1.29178 |
| $h[3/6/h1]^2$ | *r-bc* | *rPD* | Ia | $R\bar{3}m$ – .$m$ | $R\bar{3}m$ – .$m$ (−**a**, −**b**, 2**c**) | 2 | 0.33598 | 0.11987, −0.11987, 0.13013 | 4.27156, 1.77523 | 1.53610 |
| | | | IIa | $R\bar{3}c$ | $R32$ | 2 | | 0.23974, 0.11987, 0.31506 | 4.27156, 3.55047 | |
| | | | Ia | $R32$ | $R32$ (−**a**, −**b**, 2**c**) | 2 | | 0.23974, 0.11987, 0.36987 | 4.27156, 1.77523 | |
| | | | IIa | $R\bar{3}c$ | $R\bar{3}$ | 3 | | 0.23974, 0.11987, 0.06506 | 4.27156, 3.55047 | |
| | | | Ia | $R\bar{3}$ | $R\bar{3}$ (−**a**, −**b**, 2**c**) | 3 | | 0.23974, 0.11987, 0.36987 | 4.27156, 1.77523 | |
| $c[3/8/c2]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.52595* | 0.06419, 0.16146, −0.04000 | 4.57202 | 1.05076 |
| $t[3/8/t1]^2_{\mathrm{I}}$ | *t-b* | *tD* | IIa | $I4_1/amd$ | $I4_1md$ | 3 | 0.39969* | 0.20290, 0.12500, 0.19600 | 4.00000, 2.62000 | 1.01080 |
| | | | IIa | $I4_1/acd$ | $I4_1/a$ | 3 | 0.49111* | 0.18978, 0.11600, −0.05700 | 3.55992, 2.69211 | 1.02190 |
| $t[3/8/t1]^2_{\mathrm{II}}$ | *t-b* | *tD* | IIa | $I4_1/acd$ | $Fddd$ (**a**−**b**, **a**+**b**, **c**) | 2 | 0.53772* | 0.21786, 0.09000, −0.05900 | 2.12120, 6.92518 | 1.06933 |
| $t[3/8/t5]^2$ | *t-a* | *tG* | IIa | $I4_1/acd$ | $I4_122$ | 2 | 0.49503* | 0.17471, 0.12136, −0.06000 | 2.35046, 6.12648 | 1.02004 |
| $c[3/10/c1]^2_{\mathrm{I}}$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ – .32 | $I4_132$ – .32 | 0 | 0.37024 | $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | 2.82843 | 1.22474 |
| | | | IIa | $I\bar{4}3d$ – .3. | $I2_13$ – .3. | 1 | | $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | 2.82843 | |
| | | | IIa | $Ia\bar{3}$ – .3. | $I2_13$ – .3. | 1 | | $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | 2.82843 | |
| | *t-a* | *tG* | IIa | $I4_1/acd$ – ..2 | $I4_122$ – ..2 | 1 | | $\frac{3}{8}, \frac{3}{8}, \frac{1}{4}$ | 2.82843, 2.82843 | |
| | | | IIa | $I4_1cd$ | $I4_1$ | 2 | | $\frac{3}{8}, \frac{3}{8}, z$ | 2.82843, 2.82843 | |
| | | | IIa | $I4_1/a$ | $I4_1$ | 3 | | $\frac{3}{8}, \frac{3}{8}, \frac{1}{4}$ | 2.82843, 2.82843 | |
| | | | IIa | $I\bar{4}2d$ | $I2_12_12_1$ | 2 | | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}$ | 2.82843, 2.82843 | |
| | *o-a* | *oG* | IIa | $Ibca$ | $I2_12_12_1$ | 3 | | $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ | 2.82843, 2.82843 | |
| $t[3/10/c1]^2_{\mathrm{II}}$ | *t-b* | *tD* | Ia | $P4_322$ | $P4_32_12$ (**a**−**b**, **a**+**b**, **c**) | 3 | 0.44414* | 0.12500, 0.25500, 0.31250 | 1.93758, 2.51219 | 1.00717 |
| | | | IIa | $I4_122$ | $I4_1$ | 3 | 0.59386* | 0.20700, 0.02100, 0.16600 | 2.40312, 2.44279 | 1.01140 |
| $h[3/10/h1]^2$ | *h-n* | – | IIa | $P6_122$ | $P3_112$ | 2 | 0.52724* | 0.44829, 0.05171, 0.37250 | 1.87727, 3.90471 | 1.01969 |
| | | | Ia | $P3_221$ | $P3_121$ (**a**, **b**, 2**c**) | 3 | 0.57101* | 0.41000, 0.07341, 0.42000 | 1.79416, 1.97358 | 1.02564 |
| $t[3/10/t4]^2_{\mathrm{I}}$ | *t-b* | *tD* | Ia | $P4_22_12$ | $P4_32_12$ (**a**, **b**, 2**c**) | 3 | 0.51038* | 0.12500, 0.22297, 0.23000 | 1.98145, 2.09039 | 1.01297 |
| | | | | | $P4_12_12$ (**a**, **b**, 2**c**) | | | 0.22297, 0.12500, 0.23000 | | |
| $t[3/10/t4]^2_{\mathrm{II}}$ | *t-b* | *tD* | IIa | $I\bar{4}2d$ | $Fdd2$ (**a**−**b**, **a**+**b**, **c**) | 3 | 0.68110* | 0.21630, 0.02500, 0.15650 | 2.29636, 2.33252 | 1.01637 |
| $c[4/3/c1]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ – 2.22 | $I4_132$ – 2.22 | 0 | 0.36072 | $\frac{1}{8}, 0, \frac{1}{4}$ | 3.26599 | 1.52753 |
| | | | IIa | $I\bar{4}3d$ – 2.. | $I2_13$ – 2.. | 1 | | $\frac{1}{8}, 0, \frac{1}{4}$ | 3.26599 | |
| | | | IIa | $Ia\bar{3}$– 2.. | $I2_13$ – 2.. | 1 | | $\frac{1}{8}, 0, \frac{1}{4}$ | 3.26599 | |
| | | | IIa | $Pa\bar{3}$ | $P2_13$ | 2 | | $\frac{1}{8}, 0, \frac{1}{4}$ | 3.26599 | |
| $c[4/3/c4]^2$ | *c-a* | *G* | IIa | $Ia\bar{3}d$ – ..2 | $I4_132$ – ..2 | 0 | 0.41017 | 0.12500, 0.22855, 0.02145 | 3.94239 | 1.35401 |
| | | | IIa | $I\bar{4}3d$ | $I2_13$ | 1 | | 0.12500, 0.22855, 0.02145 | 3.94239 | |
| | | | IIa | $Ia\bar{3}$ | $I2_13$ | 1 | | 0.12500, 0.22855, 0.02145 | 3.94239 | |
| $c[4/3/c6]^2$ | *c-b* | *D* | Ia | $Pn\bar{3}m$ – .3$m$ | $Fd\bar{3}m$ – .3$m$ (2**a**, 2**b**, 2**c**) | 0 | 0.24708 | 0.13763, 0.13763, 0.13763 | 2.56891 | 1.90604 |
| | *t-b* | *tD* | Ia | $P4_2/nnm$ – ..$m$ | $I4_1/amd$ – .$m$. (**a**−**b**, **a**+**b**, 2**c**) | 1 | | 0.13763, 0.13763, 0.13763 | 2.56891, 2.56891 | |

**Table 1 (continued)**

| Sphere-packing type | Pattern of interpenetr. Symbol | Min. surf. | Interp. class | Group $G$ | Subgroup $H$ | $df$ | $\rho$ | $x, y, z$ | $a$ or $a = b, c$ | $d$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | IIa | $I4_1/acd$ | $I\bar{4}2d$ | 2 | | 0.13763, 0.00000, 0.06882 | 3.63299, 5.13783 | |
| | | | Ia | $P\bar{4}n2$ | $I\bar{4}2d$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | | 0.13763, 0.13763, 0.13763 | 2.56891, 2.56891 | |
| | | | Ia | $P4_222$ | $I4_122$ (**a**−**b**, **a**+**b**, 2**c**) | 1 | | 0.36237, 0.13763, 0.13763 | 2.56891, 2.56891 | |
| | | | IIa | $I4_1/acd$ | $I4_1/a$ | 2 | | 0.00000, 0.13763, 0.06882 | 3.63299, 5.13783 | |
| | | | Ia | $P4_2/n$ | $I4_1/a$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | | 0.13763, 0.13763, 0.13763 | 2.56891, 2.56891 | |
| | | | IIa | $I4_1/acd$ | $Fddd$ (**a**−**b**, **a**+**b**, **c**) | 1 | | 0.13763, 0.00000, 0.31882 | 3.63299, 5.13783 | |
| | | | IIa | $I4_1/acd$ | $I4_122$ | 1 | | 0.00000, 0.13763, 0.31882 | 3.63299, 5.13783 | |
| | $o$-$b$ | $oD$ | Ia | $Pnnn$ | $Fddd$ (2**a**, 2**b**, 2**c**) | 2 | | 0.13763, 0.13763, 0.13763 | 2.56891, 2.56891 | |
| $c[4/3/c11]^2$ | $c$-$c$ | $P$ | Ia | $I23$ | $P23$ | 1 | 0.50078 | 0.35061, 0.14939, 0.08277 | 2.92766 | 1.03772 |
| $c[4/3/c13]^2$ | $c$-$d$ | – | Ia | $Ia\bar{3}$ | $Pa\bar{3}$ | 2 | 0.59893* | 0.11768, 0.15587, −0.06400 | 3.47500 | 1.02152 |
| $c[4/3/c14]^2$ | $c$-$b$ | $D$ | IIa | $Fd\bar{3}c$ | $F4_132$ | 1 | 0.51930 | 0.14968, 0.08599, −0.00876 | 5.78489 | 1.04596 |
| $c[4/3/c15]^2_{\mathrm{I}}$ | $c$-$b$ | $D$ | Ia | $P4_232$ | $F4_132$ (2**a**, 2**b**, 2**c**) | 1 | 0.32686 | 0.30830, 0.12461, 0.08011 | 3.37505 | 1.54337 |
| $c[4/3/c15]^2_{\mathrm{II}}$ | $c$-$b$ | $D$ | IIa | $Fd\bar{3}c$ | $F4_132$ | 1 | 0.32686 | 0.15415, 0.06231, 0.04006 | 6.75011 | 1.47460 |
| $c[4/3/c20]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.60174* | 0.05500, 0.14971, −0.03706 | 4.37141 | 1.02443 |
| $c[4/3/c22]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.48730* | 0.14636, 0.03404, −0.02500 | 4.68984 | 1.02054 |
| $c[4/3/c23]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.41442* | 0.04640, 0.16028, 0.00000 | 4.95007 | 1.31489 |
| $c[4/3/c24]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.35316* | 0.10019, 0.13419, −0.01500 | 5.22114 | 1.44316 |
| $c[4/3/c25]^2$† | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.25124 | 0.13390, 0.10116, 0.00000 | 5.84872 | 1.68919 |
| $c[4/3/c26]^2$† | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 1 | 0.30002 | 0.16497, 0.04257, 0.03154 | 5.51284 | 1.62771 |
| $c[4/3/c27]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 0 | 0.15784 | 0.17678, 0.17678, 0.00000 | 6.82843 | 2.51564 |
| $h[4/3/h1]^2$ | $r$-$bc$ | $rPD$ | IIa | $R\bar{3}c$ – .2 | $R32$ – .2 | 1 | 0.61302* | 0.18667, 0.00000, 0.25000 | 3.09295, 1.85577 | 1.02291 |
| | | | IIa | $R3c$ | $R3$ | 2 | | 0.18667, 0.00000, $z$ | 3.09295, 1.85577 | |
| | | | IIa | $R\bar{3}$ | $R3$ | 3 | | 0.18667, 0.00000, 0.25000 | 3.09295, 1.85577 | |
| $h[4/3/h5]^2_{\mathrm{I}}$ | $r$-$bc$ | $rPD$ | Ia | $R32$ | $R32$ (−**a**, −**b**, 2**c**) | 2 | 0.42202 | 0.19127, 0.05734, 0.28951 | 3.39581, 2.23625 | 1.18905 |
| $h[4/3/h5]^2_{\mathrm{II}}$ | $r$-$bc$ | $rPD$ | IIa | $R\bar{3}c$ | $R32$ | 2 | 0.42202 | 0.19127, 0.05734, 0.35525 | 3.39581, 4.47250 | 1.36708 |
| $h[4/3/h9a]^2$ | $h$-$q$ | $NO3^2$-$h10$ | Ia | $P6_222$ | $P6_422$ (**a**, **b**, 2**c**) | 1 | 0.29631 | 0.45817, 0.11429, 0.31578 | 3.57190, 1.91916 | 1.40323 |
| $t[4/4/t1]^2$ | $t$-$b$ | $tD$ | IIa | $I4_1/amd$ – $.m.$ | $I4_1md$ – $.m.$ | 3 | 0.68999* | 0.00000, 0.22000, 0.34500 | 2.29840, 2.29840 | 1.00946 |
| | | | IIa | $I4_122$ | $I4_1$ | 3 | | 0.00000, 0.22000, 0.34500 | 2.29840, 2.29840 | |
| | | | IIa | $I4_1/a$ | $I4_1$ | 3 | | 0.00000, 0.22000, 0.34500 | 2.29840, 2.29840 | |
| | | | IIa | $I\bar{4}2d$ | $Fdd2$ (**a**−**b**, **a**+**b**, **c**) | 3 | | 0.00000, 0.22000, 0.34500 | 2.29840, 2.29840 | |
| | $o$-$b$ | $oD$ | IIa | $Fddd$ | $Fdd2$ | 4 | | 0.11000, 0.11000, 0.34500 | 3.25043, 2.29840 | |
| $t[4/4/t3]^2$ | $t$-$b$ | $tD$ | IIa | $I4_1/acd$ | $I4_1/a$ | 2 | 0.57796* | 0.16650, 0.11052, −0.04600 | 3.44817, 2.43823 | 1.01338 |
| $c[5/3/c3]^2$ | $c$-$c$ | $P$ | Ia | $Im\bar{3}m$ – $4m.m$ | $Pm\bar{3}m$ – $4m.m$ | 0 | 0.44653 | 0.29289, 0.00000, 0.00000 | 2.41421 | 1.39897 |
| | | | IIa | $Ia\bar{3}d$ | $Ia\bar{3}$ | 1 | | 0.14645, 0.00000, 0.00000 | 4.82843 | |
| | $r$-$bc$ | $rPD$ | Ia | $R\bar{3}m$ – $.m$ | $R\bar{3}m$ – $.m$ (−**a**, −**b**, 2**c**) | 1 | | 0.09763, 0.19526, 0.19526 | 3.41421; 2.09077 | |
| | | | IIa | $R\bar{3}c$ | $R32$ | 1 | | 0.19526, 0.09763, 0.34763 | 3.41421; 4.18154 | |
| | | | Ia | $R32$ | $R32$ (−**a**, −**b**, 2**c**) | 1 | | 0.19526, 0.09763, 0.30474 | 3.41421; 2.09077 | |
| | | | IIa | $R\bar{3}c$ | $R\bar{3}$ | 2 | | 0.19526, 0.09763, 0.09763 | 3.41421; 4.18154 | |
| | | | Ia | $R\bar{3}$ | $R\bar{3}$ (−**a**, −**b**, 2**c**) | 2 | | 0.19526, 0.09763, 0.30474 | 3.41421; 2.09077 | |
| $c[5/3/c10]^2$ | $c$-$b$ | $D$ | Ia | $Pn\bar{3}m$ – $..m$ | $Fd\bar{3}m$ – $..m$ (2**a**, 2**b**, 2**c**) | 0 | 0.34973 | 0.10714, 0.10714, 0.32143 | 3.29983 | 1.37437 |
| | | | IIa | $Fd\bar{3}c$ | $F4_132$ | 0 | | 0.05357, 0.05357, 0.16071 | 6.59966 | |
| | | | Ia | $P4_232$ | $F4_132$ (2**a**, 2**b**, 2**c**) | 0 | | 0.10714, 0.10714, 0.32143 | 3.29983 | |
| | | | IIa | $Fd\bar{3}c$ | $Fd\bar{3}$ | 1 | | 0.30357, 0.30357, 0.41071 | 6.59966 | |
| | | | Ia | $Pn\bar{3}$ | $Fd\bar{3}$ (2**a**, 2**b**, 2**c**) | 1 | | 0.10714, 0.10714, 0.32143 | 3.29983 | |
| $c[5/3/c19]^2$ | $c$-$b$ | $D$ | IIa | $Fd\bar{3}c$ | $F4_132$ | 1 | 0.50248 | 0.13390, 0.10116, 0.00000 | 5.84872 | 1.10750 |
| $c[5/3/c28]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 0 | 0.59847 | 0.05908, 0.15230, −0.03414 | 4.37935 | 1.06459 |
| $c[5/3/c29]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 0 | 0.35121 | 0.15441, 0.05741, 0.00000 | 5.23077 | 1.40363 |
| $c[5/3/c30]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 0 | 0.27768 | $\frac{1}{8}, \frac{1}{8}, 0$ | 5.65685 | 1.73205 |
| $c[5/3/c31]^2$ | $c$-$a$ | $G$ | IIa | $Ia\bar{3}d$ | $I4_132$ | 0 | 0.30293 | 0.03921, 0.16789, 0.03921 | 5.49509 | 1.66618 |
| $t[5/3/t1]^2$ | $t$-$b$ | $tD$ | IIa | $I4_1/amd$ – $.m.$ | $I4_1md$ – $.m.$ | 2 | 0.69156* | 0.00000, 0.21771, 0.34300 | 2.29666, 2.29666 | 1.00998 |
| | | | IIa | $I4_122$ | $I4_1$ | 2 | | 0.00000, 0.21771, 0.34300 | 2.29666, 2.29666 | |
| | | | IIa | $I4_1/a$ | $I4_1$ | 2 | | 0.00000, 0.21771, 0.34300 | 2.29666, 2.29666 | |
| | | | IIa | $I\bar{4}2d$ | $Fdd2$ (**a**−**b**, **a**+**b**, **c**) | 2 | | 0.00000, 0.21771, 0.34300 | 2.29666, 2.29666 | |
| | $o$-$b$ | $oD$ | IIa | $Fddd$ | $Fdd2$ | 3 | | 0.10885, 0.10885, 0.34300 | 3.24797, 2.29666 | |
| $t[5/3/t22]^2$ | $t$-$b$ | $tD$ | IIa | $I4_1/acd$ | $I4_1/a$ | 2 | 0.57600* | 0.17090, 0.10907, −0.04510 | 3.39633, 2 52178 | 1.01228 |
| $c[6/3/c25]^2$ | $c$-$b$ | $D$ | IIa | $Fd\bar{3}c$ | $F4_132$ | 0 | 0.52282 | 0.14017, 0.08663, 0.00000 | 5.77186 | 1.14412 |
| $h[3/4/h1a]^3$ | $h$-$o$ | | Ia | $P6_222$ | $P6_222$ (**a**−**b**, **a**+2**b**, **c**) | 2 | 0.41753 | 0.41923, 0.19857, 0.40810 | 2.23374, 3.48257 | 1.02801 |
| $h[3/4/h3]^3$ | $h$-$o$ | | Ia | $P6_222$ | $P6_222$ (**a**−**b**, **a**+2**b**, **c**) | 2 | 0.36720 | 0.31929, 0.08711, 0.39290 | 2.11312, 4.42491 | 1.00766 |
| $c[3/4/t1]^3$ | $c$-$l$ | | IIa | $I\bar{4}3d$ | $I\bar{4}2d$ (**a**, **b**, **c**; **b**, **c**, **a**; **c**, **a**, **b**) | 2 | 0.35311* | 0.00000, 0.10000, 0.31750 | 4.14424 | 1.25436 |
| $t[3/4/t1]^3$ | $t$-$m$ | | Ia | $I4_1/amd$ – $.m.$ | $I4_1/amd$ – $.m.$ (**a**, **b**, 3**c**) | 2 | 0.34665 | 0.00000, 0.15350, 0.33387 | 3.94901, 1.54970 | 1.18113 |
| | | | Ia | $I\bar{4}2d$ | $I\bar{4}2d$ (**a**, **b**, 3**c**) | 3 | | 0.00000, 0.15350, 0.33387 | 3.94901, 1.54970 | |
| | | | Ia | $I4_122$ | $I4_122$ (**a**, **b**, 3**c**) | 2 | | 0.00000, 0.15350, 0.33387 | 3.94901, 1.54970 | |
| | | | Ia | $I4_1/a$ | $I4_1/a$ (**a**, **b**, 3**c**) | 3 | | 0.00000, 0.15350, 0.33387 | 3.94901, 1.54970 | |
| | $o$-$m$ | | Ia | $Fddd$ | $Fddd$ (**a**, **b**, 3**c**) | 3 | | 0.07675, 0.07675, 0.33387 | 5.58474, 1.54970 | |
| $t[3/4/t2]^3$ | $t$-$m$ | | Ia | $I4_122$ | $I4_122$ (**a**, **b**, 3**c**) | 2 | 0.34147 | 0.13269, 0.04106, 0.23361 | 3.59986, 1.89320 | 1.11128 |
| $t[3/4/t3]^3$ | $t$-$m$ | | Ia | $I4_1/amd$ | $I4_1/amd$ (**a**, **b**, 3**c**) | 2 | 0.29812 | 0.18913, 0.08874, 0.16948 | 5.63440, 1.77035 | 1.24805 |
| $c[4/3/c6]^3$ | $c$-$l$ | | IIa | $I\bar{4}3d$ | $I\bar{4}2d$ (**a**, **b**, **c**; **b**, **c**, **a**; **c**, **a**, **b**) | 1 | 0.41609* | 0.00000, 0.12257, 0.28489 | 3.92358 | 1.20920 |
| $t[4/3/c6]^3$ | $t$-$m$ | | Ia | $I4_1/amd$ – $.m.$ | $I4_1/amd$ – $.m.$ (**a**, **b**, 3**c**) | 1 | 0.37062 | 0.00000, 0.13763, 0.29356 | 3.63299, 1.71261 | 1.22924 |
| | | | Ia | $I\bar{4}2d$ | $I\bar{4}2d$ (**a**, **b**, 3**c**) | 2 | | 0.00000, 0.13763, 0.29356 | 3.63299, 1.71261 | |

**Table 1 (continued)**

| Sphere-packing type | Pattern of interpenetr. Symbol | Min. surf. | Interp. class | Group $G$ | Subgroup $H$ | $df$ | $\rho$ | $x, y, z$ | $a$ or $a = b, c$ | $d$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Ia | $I4_122$ | $I4_122$ (**a**, **b**, 3**c**) | 1 | | 0.00000, 0.13763, 0.29356 | 3.63299, 1.71261 | |
| | | | Ia | $I4_1/a$ | $I4_1/a$ (**a**, **b**, 3**c**) | 2 | | 0.00000, 0.13763, 0.29356 | 3.63299, 1.71261 | |
| | *o-m* | | Ia | *Fddd* | *Fddd* (**a**, **b**, 3**c**) | 2 | | 0.06882, 0.06882, 0.29356 | 5.13783, 1.71261 | |
| $c[3/3/c1]^4{}_{\mathrm{I}}$ | *c-g* | | IIIa | $Ia\bar{3}d$ | $P4_{1,3}32$ | 2 | 0.28823* | −0.01434, 0.11000, 0.11434 | 5.58699 | 1.19697 |
| $c[3/3/c1]^4{}_{\mathrm{II}}$ | *c-h* | | IIb | $Ia\bar{3}d$ | $I2_13$ | 2 | 0.38563* | 0.01000, 0.01712, 0.15288 | 5.07029 | 1.20163 |
| $c[3/3/c1]^4{}_{\mathrm{III}}$ | *c-i* | | Ib | $P4_232$ – ..2 | $I4_132$ – ..2 (2**a**, 2**b**, 2**c**) | 0 | 0.22206 | 0.25000, 0.11603, 0.38397 | 3.04721 | 1.67969 |
| | | | Ib | $F4_132$ | $P4_332$ | 2 | | 0.12500, 0.05801, 0.30801 | 6.09441 | |
| | | | Ib | | $P4_132$ | | | 0.12500, 0.30801, 0.05801 | | |
| | | | Ib | *P*23 | $I2_13$ (2**a**, 2**b**, 2**c**) | 2 | | 0.25000, 0.11603, 0.38397 | 3.04721 | |
| $t[3/4/t1]^4$ | *t-p* | | IIIa | $P4/nnc$ | *Fddd* (2**a**, 2**b**, 2**c**) | 2 | 0.51643* | 0.31689, 0.12500, 0.12947 | 2.25526, 3.18942 | 1.02796 |
| $t[3/4/t2]^4$ | *t-p* | | IIIa | $P4_2/nbc$ | $I4_122$ (**a**−**b**, **a**+**b**, 2**c**) | 2 | 0.48865* | 0.19092, 0.10452, 0.11500 | 2.29722, 3.24876 | 1.02875 |
| $t[3/4/t1]^5$ | *t-r* | | Ia | $I4_1/a$ | $I4_1/a$ (2**a**−**b**, **a**+2**b**, **c**) | 3 | 0.60249* | 0.22158, 0.18750, 0.19000 | 1.81924, 4.20135 | 1.05612 |
| $c[3/3/c1]^8{}_{\mathrm{I}}$ | *c-j* | | Ib | *I*23 | $I2_13$ (2**a**, 2**b**, 2**c**) | 2 | 0.48940* | 0.35397, 0.16000, 0.08603 | 2.95018 | 1.01576 |
| $c[3/3/c1]^8{}_{\mathrm{II}}$ | *c-k* | | IIIb | $Fd\bar{3}c$ | $P4_{1,3}32$ | 2 | 0.49775* | 0.13739, −0.10000, 0.00261 | 5.86717 | 1.04176 |

† Igor A. Baburin and Davide M. Proserpio (private communication) pointed out that the sphere packings of types 4/3/*c*25 and 4/3/*c*26 have a special property not previously observed: although these sphere packings cannot be deformed into one another without opening sphere contacts their graphs are isomorphic. The pairs 4/3/*h*9*a* – 4/3/*h*9*b*, 3/4/*h*1*a* – 3/4/*h*1*b*, 3/4/*h*2*a* – 3/4/*h*2*b* (Koch & Sowa, 2004) and 4/3/*c*32*a* – 4/3/*c*32*b* (Fischer, 2005) show the same behaviour. In contrast to these cases, however, the sphere packings of the new pair are generated with different symmetry operations. This unusual property is transferred also to $c[4/3/c25]^2$ and $c[4/3/c26]^2$.

*Example:* Two sphere packings of type 3/4/*t*1 can interpenetrate in two different ways (*cf.* Fig. 2 and Table 1). The tetragonal axes of the two individual packings run parallel in the case of $t[3/4/t1]^2{}_{\mathrm{I}}$ and perpendicular to each other in the case of $t[3/4/t1]^2{}_{\mathrm{II}}$.

*Example:* Two sphere packings of type 3/4/*t*2 can also interpenetrate in two different ways (*cf.* Fig. 3 and Table 1). Each such sphere packing contains two kinds of screw parallel to **c**, namely with eight and with twelve spheres per translation period. In $t[3/4/t2]^2{}_{\mathrm{I}}$, the axes of the screws of the same kind coincide for both individual packings, whereas in $t[3/4/t2]^2{}_{\mathrm{II}}$ the axes of different kinds of screw coincide.

The *density* $\rho$ *of a sphere packing* is defined as the volume of all spheres within one unit cell divided by the unit-cell volume. This definition can be transferred to interpenetrating sphere packings without problems. The *density* $\rho$ *of a system of interpenetrating sphere packings* is defined as the volume of all spheres within one unit cell divided by the unit-cell volume.

The rings within an individual sphere packing may be subdivided into contractable and non-contractable ones. Any ring of another individual packing does not thread a contractable ring in a system of interpenetrating sphere packings. All other rings are *non-contractable*. For simple geometrical reasons, all three-membered or four-membered rings in sphere packings are necessarily contractable.

## 3. Derivation of interpenetrating sphere packings

The enumeration of the types of interpenetrating sphere packings with cubic (*cf.* Fischer & Koch, 1976) and with

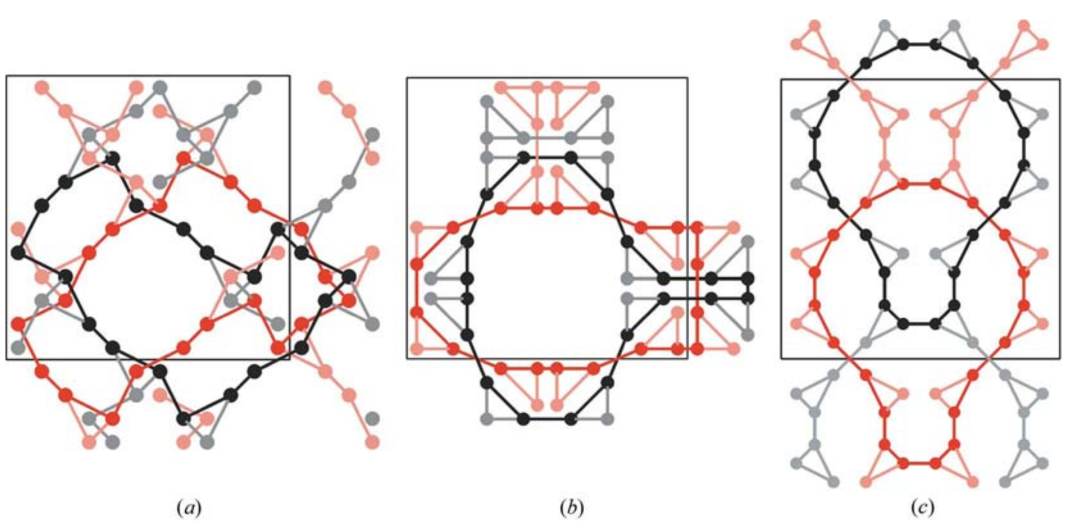


**Figure 1**
Interpenetrating sphere packings belonging to types (*a*) $c[3/3/c1]^2{}_{\mathrm{I}}$, (*b*) $c[3/3/c1]^2{}_{\mathrm{II}}$ and (*c*) $c[3/3/c1]^2{}_{\mathrm{III}}$. Interpenetration patterns *c-e*, *c-f* and *c-a*, respectively.

tetragonal (*cf.* Fischer & Koch, 1990) symmetry was done in an analogous way as described in previous papers for the derivation of all sphere packings with cubic (Fischer, 1973, 1974) and tetragonal (Fischer, 1991*a*,*b*, 1993) symmetry. For this, the already existing material has been reconsidered: each set of symmetry operations referring to equal shortest distances between points that are symmetrically equivalent with respect to a certain space group $G$ corresponds to a system of interpenetrating sphere packings if and only if the set generates a space group $H$ that is a subgroup of $G$ with index $i \geq 2$.

The types of interpenetrating sphere packings with hexagonal and trigonal symmetry were derived together with the sphere packings with the respective symmetry (Sowa *et al.*, 2003; Sowa & Koch, 2004, 2005, 2006).

All possible systems of interpenetrating sphere layers were derived in an analogous way.

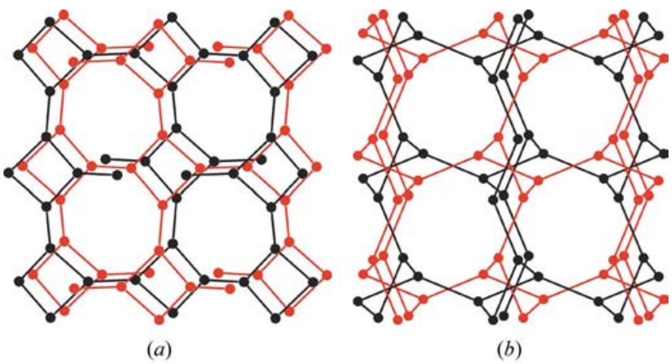

**Figure 2**
Interpenetrating sphere packings belonging to types (*a*) $t[3/4/t1]^2{}_{\rm I}$ and (*b*) $t[3/4/t1]^2{}_{\rm II}$. Interpenetration patterns *t-b*.

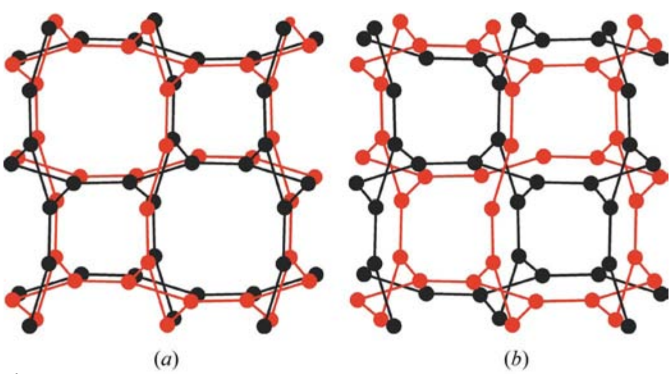

**Figure 3**
Interpenetrating sphere packings belonging to types (*a*) $t[3/4/t2]^2{}_{\rm I}$ and (*b*) $t[3/4/t2]^2{}_{\rm II}$. Interpenetration patterns *t-b* and *t-a*, respectively.

## 4. Results

### 4.1. Interpenetrating sphere packings

Table 1 contains a complete list of all types of interpenetrating sphere packings (column 1) except those that occur only with orthorhombic or lower symmetry. The next two columns describe for each type the pattern of the interpenetration (details in §5.6) by a symbol similar to those introduced by Fischer & Koch (1976) and – if possible – by the symbol of a three-periodic minimal surface. The fourth column shows the so-called interpenetration class as defined by Blatov *et al.* (2004).

Columns 5 and 6, respectively, display the symmetry group $G$ of the system of interpenetrating sphere packings and the subgroup $H$ of $G$ that refers to one individual sphere packing. It has to be noticed that in many cases $H$ does not describe the full symmetry group of such a sphere packing. $H$ is only that subgroup of $G$ with index $i$ that can be generated as described in §2. The parameter regions that belong to the various types of interpenetrating sphere packings may have up to four degrees of freedom. The number $df$ of degrees of freedom, *i.e.* the dimension of the parameter region, is given in the next column.

Most sphere-packing types encompass a packing with minimal density (for details compare the paper by Koch *et al.*, 2005). This is also true for the types of interpenetrating sphere packings. Therefore, the last four columns of Table 1 refer to interpenetrating sphere packings with minimal density, if possible: column 8 shows the minimal density $\rho$, columns 9 and 10 the corresponding coordinates and lattice parameters, respectively (normalized to a shortest distance of 1 between sphere centres of an individual packing). The last column gives the shortest distance $d$ between sphere centres from different individual packings. In the case of a

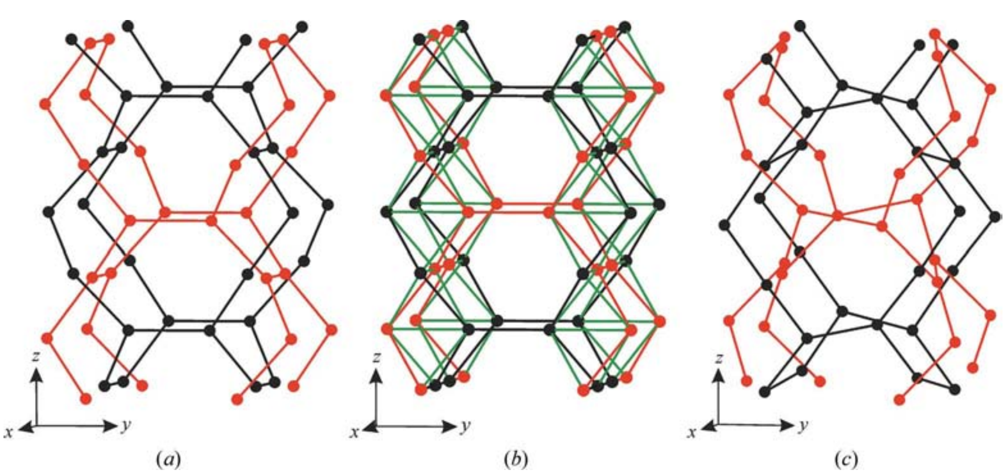


**Figure 4**
Interpenetrating sphere packings belonging to type $t[3/8/t1]^2{}_{\rm I}$ with symmetries (*a*) $I4_1/amd$ – $I4_1md$ and (*c*) $I4_1/acd$ – $I4_1/a$. Interpenetration pattern *t-b*. (*b*) Type 6/3/*t*5 refers to the common limiting complex $P4_2/mmc$ 4*j* of $I4_1/amd$ 32*i* and $I4_1/acd$ 32*g*. The green lines show the additional sphere contacts.

**Table 2**
Interpenetrating sphere layers occurring with highest symmetry in the hexagonal or tetragonal crystal family.

For all corresponding lattice complexes the parameters are tabulated. $\beta$ is 90° in the case of $I12/a(1)$.

| Type | Space group | Subgroup | *df* | $\rho$ | *x*, *y*, *z* | *a*, *c* or *a*, *b*, *c* | *d* |
|---|---|---|---|---|---|---|---|
| $\mathbf{t[6^3]^2}$ | $I4/mcm$ – $m.2m$ | $Cmm(m)$ – $2mm$ (**a**+**b**, **c**, **a**−**b**) | 1 | 0.50579 | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | 1.02740 |
| | $P4/nbm$ – $..m$ | $Pma(m)$ – $..m$ (**a**+**b**, **c**, **a**−**b**) | 1 | | 0.15000, 0.65000, 0.25000 | 2.35702, 1.49071 | |
| | $P4_2/ncm$ – $..m$ | $Pma(m)$ – $..m$ (**a**+**b**, **c**, **a**−**b**) | 1 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $P4/mcc$ – $m..$ | $Pbm(b)$ – $.m.$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $P4_2/mbc$ – $m..$ | $Pbm(b)$ – $.m.$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.15000, 0.00000 | 2.35702, 1.49071 | |
| | $I\bar{4}2m$ – $..m$ | $C2m(m)$ – $..m$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.15000, 0.25000 | 2.35702, 1.49071 | |
| | $I4/m$ – $m..$ | $C12/m(1)$ – $.m.$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $Ibam$ – $..m$ | $C12/m(1)$ – $.m.$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.15000, 0.65000, 0.00000 | 2.35702, 2.35702, 1.49071 | |
| | $P4/nnc$ | $P11(2/n)$ (**b**, **c**, **a**) | 2 | | 0.10000, 0.25000, 0.25000 | 3.33333, 1.49071 | |
| | $P4/nnc$ | $Pba(b)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.12500 | 2.35702, 2.98142 | |
| | $P4_2/nbc$ | $Pba(b)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.15000, 0.12500 | 2.35702, 2.98142 | |
| | $P4/ncc$ | $Pb2(b)$ (**b**, **c**, **a**) | 3 | | 0.10000, 0.25000, 0.00000 | 3.33333, 1.49071 | |
| | $P\bar{4}c2$ | $P2_12(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $P\bar{4}b2$ | $P2_12(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.15000, 0.25000 | 2.35702, 1.49071 | |
| | $P\bar{4}2c$ | $Pn2(b)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $P\bar{4}2_1c$ | $Pn2(b)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.15000, 0.15000, 0.25000 | 2.35702, 1.49071 | |
| | $P422$ | $P2_12(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.25000 | 2.35702, 1.49071 | |
| | $P4_22_12$ | $P2_12(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.25000 | 2.35702, 1.49071 | |
| | $P4_2/n$ | $P12/a(1)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.65000, 0.00000 | 2.35702, 1.49071 | |
| | $P4/n$ | $P12/a(1)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.15000, 0.15000, 0.25000 | 2.35702, 1.49071 | |
| | $I\bar{4}$ | $C12(1)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.15000, 0.15000, 0.25000 | 2.35702, 1.49071 | |
| | $Pccn$ | $P12/a(1)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.10000, 0.10000, 0.25000 | 2.35702, 2.35702, 1.49071 | |
| | $Pban$ | $P12/a(1)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.15000, 0.15000, 0.25000 | 2.35702, 2.35702, 1.49071 | |
| | $Pbcn$ | $P12_1/a(1)$ (**a**+**b**, **c**, **a**−**b**) | 4 | | 0.15000, 0.15000, 0.00000 | 2.35702, 2.35702, 1.49071 | |
| | $I222$ | $C12(1)$ (**a**+**b**, **c**, **a**−**b**) | 4 | | 0.15000, 0.15000, 0.25000 | 2.35702, 2.35702, 1.49071 | |
| | $I12/a1$ | $P12_1/a(1)$ (**c**, −**b**, **a**) | 4 | | 0.00000, 0.15000, 0.65000 | 1.49071, 2.35702, 2.35702 | |
| $\mathbf{t[48^2]^2}$ | $I4/mcm$ – $..m$ | $Cmm(m)$ – $..m$ (**a**+**b**, **c**, **a**−**b**) | 1 | 0.48190* | 0.16289, 0.66289, 0.13550 | 2.17055, 3.68994 | 1.10181 |
| | $I4/m$ | $C12/m(1)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.66289, 0.13550 | 2.17055, 3.68994 | |
| | $I422$ | $C22(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.66289, 0.11450 | 2.17055, 3.68994 | |
| | $I\bar{4}c2$ | $C22(2)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.66289, 0.13550 | 2.17055, 3.68994 | |
| | $P4/mcc$ | $Pbm(n)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.66289, 0.13550 | 2.17055, 3.68994 | |
| | $P4_2/mbc$ | $Pbm(n)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.16289, 0.13550 | 2.17055, 3.68994 | |
| | $P4/ncc$ | $Pba(n)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.16289, 0.38550 | 2.17055, 3.68994 | |
| | $P4_2/nbc$ | $Pba(n)$ (**a**+**b**, **c**, **a**−**b**) | 2 | | 0.16289, 0.66289, 0.13550 | 2.17055, 3.68994 | |
| | $Ibam$ | $C12/m(1)$ (**a**+**b**, **c**, **a**−**b**) | 3 | | 0.16289, 0.16289, 0.13550 | 2.17055, 2.17055, 3.68994 | |
| $\mathbf{h[6^3]^3}$ | $P6/mcc$ – $..m$ | $Pbm(n)$ – $m..$ (**b**, **c**, 2**a**+**b**) | 2 | 0.47176* | 0.45145, 0.13500, 0.00000 | 3.03521, 1.66937 | 1.08977 |
| | $P622$ | $P2_12(2)$ (**b**, **c**, 2**a**+**b**) | 2 | | 0.45145, 0.13500, 0.25000 | 3.03521, 1.66937 | |
| | $P\bar{3}c1$ | $P2_1/b1(1)$ (**b**, **c**, 2**a**+**b**) | 3 | | 0.45145, 0.13500, 0.00000 | 3.03521, 1.66937 | |
| | $P\bar{3}1c$ | $P11(2/n)$ (**b**, **c**, 2**a**+**b**) | 2 | | 0.45145, 0.13500, 0.00000 | 3.03521, 1.66937 | |
| $\mathbf{h[48^2]^3}$ | $P6/mcc$ | $Pbm(n)$ (**b**, **c**, 2**a**+**b**) | 2 | 0.42590* | 0.45264, 0.13500, 0.13658 | 3.05067, 3.66081 | 1.08662 |

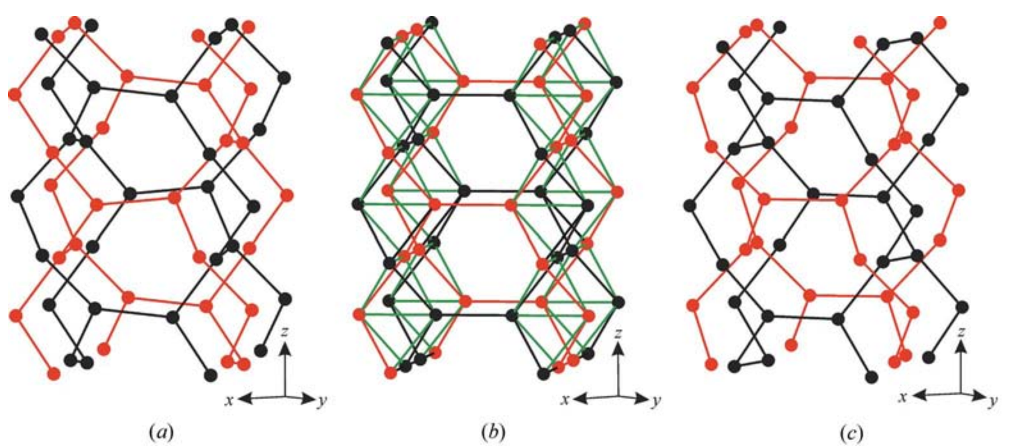


**Figure 5**
Interpenetrating sphere packings belonging to type $t[3/10/c1]^2_{\mathrm{II}}$ with symmetries (*a*) $P4_322$ – $P4_32_12$ and (*c*) $I4_122$ – $I4_1$. Interpenetration pattern *t-b*. (*b*) Type 6/3/*t*5 refers to the common limiting complex $P4_2/mmc$ 4*j* of $P4_322$ 8*d* and $I4_122$ 16*g*. The green lines show the additional sphere contacts.

type of interpenetrating sphere packings without a minimal density, the information in columns 8 to 12 refers to an arbitrarily chosen point of the respective parameter region. An asterisk in column 8 marks these instances.

For certain types, the interpenetrating sphere packings can be generated with different symmetry. Then, information is given in Table 1 for all corresponding group–subgroup pairs $G - H$. For all but three of these types, a uniquely defined pair $G - H$ exists where the interpenetrating sphere packings occur with highest site symmetry. All other pairs $G - H$ may then be derived by subgroup degradation.

The three exceptional cases are $h[3/10/h1]^2$ (Sowa & Koch, 2006), $t[3/8/t1]^2{}_{\rm I}$ and $t[3/10/c1]^2{}_{\rm II}$. Each of these three types exists in two parameter regions that belong to two different lattice complexes with three degrees of freedom having a common limiting complex. The point configurations referring to this limiting complex, however, do not belong to the interior of the two parameter regions but only to their boundaries. As a consequence, it is impossible to deform a system of interpenetrating sphere packings from the first parameter range into another system from the second range without allowing additional contacts between spheres during the deformation process. An analogous behaviour has been described before for sphere-packing types 4/4/*t*29 and 4/6/*t*4 (*cf.* Fischer, 2005; Koch *et al.*, 2005).

Interpenetrating sphere packings of type $t[3/8/t1]^2{}_{\rm I}$ may be generated either in $I4_1/amd$ 32*i* (Fig. 4*a*) or in $I4_1/acd$ 32*g* (Fig. 4*c*). Sphere-packing type 6/3/*t*5 refers to the common limiting complex ($P4_2/mmc$ 4*j*). Removal of three contacts per sphere from such a packing and subsequent deformation results in interpenetrating sphere packings either with symmetry $I4_1/amd$ or $I4_1/acd$. Consequently, three kinds of contacts between spheres may be distinguished in a sphere packing of type 6/3/*t*5: contacts that are preserved in the two interpenetrating sphere packings of type 3/8/*t*1 (red or black lines in Fig. 4*b*) and the additional contacts in sphere-packing type 6/3/*t*5 (green lines in Fig. 4*b*).

Interpenetrating sphere packings of type $t[3/10/c1]^2{}_{\rm II}$ occur in $P4_322$ 8*d* (Fig. 5*a*) and in $I4_122$ 16*g* (Fig. 5*c*). They are also related to a sphere packing of type 6/3/*t*5 (Fig. 5*b*), and again $P4_2/mmc$ 4*j* is the common limiting complex of both lattice complexes.

### 4.2. Interpenetrating two-periodic layers of spheres

Two-periodic layers of spheres in mutual contact can interpenetrate only if the layers do not run parallel to each other. As a consequence, each infinite set of interpenetrating layers consists of two or three subsets of layers with the following properties: all layers of the same subset run parallel and are not interwoven; each layer is entangled with all layers from the other (two) subset(s). No such interpenetrating layers exist with cubic symmetry. Two sets of such layers perpendicular to each other are found with tetragonal symmetry and three sets running perpendicular to $2\mathbf{a} + \mathbf{b}$, $\mathbf{a} + 2\mathbf{b}$ and $\mathbf{a} - \mathbf{b}$ with hexagonal symmetry.

Table 2 describes all types of interpenetrating two-periodic layers of spheres. In column 1, these types are designated by the symbols $6^3$ or $48^2$ of the corresponding vertex-transitive plane nets (Shubnikov, 1916) in square brackets. These symbols are preceded by the letter *t* or *h* depending on the crystal system where the type of interpenetrating sphere layers occurs with highest symmetry. A superscript 2 or 3 gives the number of subsets of parallel sphere layers. The symmetry group of the entire sphere configuration is shown in column 2, whereas column 3 describes the layer group[4] that corresponds to one individual sphere layer. All other columns are analogous to those in Table 1.

## 5. Discussion

Sphere packings of 49 types may interpenetrate. In total, they lead to 74 types of interpenetrating sphere packings. Table 3 shows a list of these 49 types. Their sphere-packing symbols in columns 1 are compared with the net symbols in column 2 used in the database RCSR (Reticular Chemistry Structure Resource at http://okeeffe-ws1.la.asu.edu/RCSR/home.htm, *cf.* also Delgado Friedrichs *et al.*, 2003, 2005; Blatov *et al.*, 2004). For certain types of sphere packing, several possibilities exist to fit *i* such packings into each other, where *i* may be equal to 2, 3, 4, 5 or even 8. The numbers of types of *i* interpenetrating sphere packings are given in the last five columns.

If two sphere packings interpenetrate, both of them have necessarily the same symmetry group *H* because *H* is a normal subgroup of *G*, the symmetry group of the entire system. Then, each symmetry operation from the coset of *H* in *G* maps *H* onto itself and the two individual packings onto one another. In the case of more than two interpenetrating sphere packings, the situation is more complex depending on the normalizer of *H* with respect to *G*, *i.e.* on $N_G(H)$ (*cf. e.g.* Koch *et al.*, 2002). Three cases may be distinguished.

1. $N_G(H) = G$. As for $i = 2$, *H* is a normal subgroup of *G* and is common, therefore, to all individual sphere packings. An arbitrarily chosen set of representatives of the cosets of *H* in *G* maps any first individual packing onto the other ones.

2. $N_G(H) = H$. Each of the *i* individual packings corresponds to its own subgroup $H_1, H_2, \ldots, H_i$. All *i* subgroups are conjugate in *G*. An arbitrarily chosen set of representatives of the left cosets of, for example, $H_1$ in *G* maps $H_1$ onto $H_2, \ldots, H_i$ and the first individual packing onto the other ones. It has to be noticed that, in general, such sets of representatives differ for the individual subgroups.

3. $N_G(H) \neq G$ and $N_G(H) \neq H$. This can occur only if *i* is not prime, *i.e.* if *i* equals 4 or 8 in the current context. Let $i_g$ be the index of $N_G(H)$ in *G* and $i_h$ the index of *H* in $N_G(H)$ with $i = i_g i_h$. Then $i_h$ individual packings share a common subgroup. They can be generated from an arbitrary first one by means of a set of representatives of the cosets of $H_j$ in $N_G(H_j)$. There exist $i_g$ different subgroups that are conjugate in *G*. As a consequence, the representatives of the cosets of $N_G(H_j)$ in *G* map the original subgroup $H_j$ onto the other $i_g - 1$ subgroups. In addition, they map each of the first $i_h$ individual packings onto $i_g - 1$ further ones, resulting in $i = i_g i_h$ different individual packings in total.

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

**Table 3**
The 49 types of sphere packings that give rise to interpenetrating sphere packings.

| Sphere-packing type | Net symbol | Types of interpenetrating sphere packings with $i = 2$ | $i = 3$ | $i = 4$ | $i = 5$ | $i = 8$ |
|---|---|---|---|---|---|---|
| 3/3/*c*1 | **srs-a** | 3 | | 3 | | 2 |
| 3/4/*c*1 | **nbo-a** | 1 | | | | |
| 3/4/*c*5 | | 1 | | | | |
| 3/4/*c*6 | **sin = lcv-g** | 1 | | | | |
| 3/4/*c*7 | **lcv-f** | 1 | | | | |
| 3/4/*h*1*a* | **qtz-f** | 1 | 1 | | | |
| 3/4/*h*2*a* | **qtz-g** | 1 | | | | |
| 3/4/*h*3 | **qtz-h** | 1 | 1 | | | |
| 3/4/*t*1 | **dia-f** | 2 | 2 | 1 | 1 | |
| 3/4/*t*2 | **dia-g** | 2 | 1 | 1 | | |
| 3/4/*t*3 | **lvt-a** | 1 | 1 | | | |
| 3/6/*c*3 | **crs-f** | 1 | | | | |
| 3/6/*c*5 | **pcu-g** | 1 | | | | |
| 3/6/*h*1 | **pcu-h** | 1 | | | | |
| 3/8/*c*2 | **utc** | 1 | | | | |
| 3/8/*t*1 | **lig** | 2 | | | | |
| 3/8/*t*5 | **utg** | 1 | | | | |
| 3/10/*c*1 | **srs** | 2 | | | | |
| 3/10/*h*1 | **bto** | 1 | | | | |
| 3/10/*t*4 | **ths** | 2 | | | | |
| 4/3/*c*1 | **lcv = srs-e** | 1 | | | | |
| 4/3/*c*4 | **uno** | 1 | | | | |
| 4/3/*c*6 | **dia-a** | 1 | 2 | | | |
| 4/3/*c*11 | **uku** | 1 | | | | |
| 4/3/*c*13 | **cbo** | 1 | | | | |
| 4/3/*c*14 | **ulh** | 1 | | | | |
| 4/3/*c*15 | **ulg** | 2 | | | | |
| 4/3/*c*20 | | 1 | | | | |
| 4/3/*c*22 | | 1 | | | | |
| 4/3/*c*23 | **ulf** | 1 | | | | |
| 4/3/*c*24 | | 1 | | | | |
| 4/3/*c*25 | **uld** | 1 | | | | |
| 4/3/*c*26 | **uld-z** | 1 | | | | |
| 4/3/*c*27 | **lcv-a** | 1 | | | | |
| 4/3/*h*1 | **afw** | 1 | | | | |
| 4/3/*h*5 | **unp** | 2 | | | | |
| 4/3/*h*9*a* | **qtz-a** | 1 | | | | |
| 4/4/*t*1 | **lvt** | 1 | | | | |
| 4/4/*t*3 | **gis** | 1 | | | | |
| 5/3/*c*3 | **cab = pcu-a** | 1 | | | | |
| 5/3/*c*10 | **crs-a** | 1 | | | | |
| 5/3/*c*19 | **fcf** | 1 | | | | |
| 5/3/*c*28 | **fcn** | 1 | | | | |
| 5/3/*c*29 | **fco** | 1 | | | | |
| 5/3/*c*30 | **srs-f** | 1 | | | | |
| 5/3/*c*31 | **srs-g** | 1 | | | | |
| 5/3/*t*1 | **xft** | 1 | | | | |
| 5/3/*t*22 | **yfi** | 1 | | | | |
| 6/3/*c*25 | **snb** | 1 | | | | |

### 5.1. Interpenetration of two sphere packings

Intertwining of two congruent sphere packings gives rise to 58 types of systems of interpenetrating sphere packings (*cf.* Table 1). 42 of them are simple because they refer to only one type of group–subgroup pair $G - H$. In these cases, $H$ is either a class-equivalent or a translation-equivalent subgroup of $G$, and all corresponding interpenetrating sphere packings can be uniquely assigned to class Ia or IIa, respectively, as defined by Blatov *et al.* (2004).

Class Ia occurs 13 times. If $G$ and $H$ are class-equivalent rotation groups, two chiral sphere packings with the same handedness interpenetrate each other and the systems of interpenetrating sphere packings occur in enantiomorphic pairs. There are 10 such types: $c[3/3/c1]^2_{\rm I}$, $h[3/4/h1a]^2$, $h[3/4/h2a]^2$, $h[3/4/h3]^2$, $t[3/4/t2]^2_{\rm I}$, $t[3/10/t4]^2_{\rm I}$, $c[4/3/c11]^2$, $c[4/3/c15]^2_{\rm I}$, $h[4/3/h5]^2_{\rm I}$, $h[4/3/h9a]^2$. If $G$ as well as $H$ comprises symmetry operations other than rotations, the individual sphere packings are achiral: $h[3/4/c1]^2$, $t[3/4/t3]^2$, $c[4/3/c13]^2$.

The other 29 types belong to class IIa. If $H$ is that unique subgroup of $G$ that consists of all rotations of $G$, two chiral sphere packings of different handedness interpenetrate. 22 such types occur: $c[3/4/c5]^2$, $c[3/4/c6]^2$, $c[3/4/c7]^2$, $t[3/4/t2]^2_{\rm II}$, $c[3/8/c2]^2$, $t[3/8/t5]^2$, $c[4/3/c14]^2$, $c[4/3/c15]^2_{\rm II}$, $c[4/3/c20]^2$, $c[4/3/c22]^2$, $c[4/3/c23]^2$, $c[4/3/c24]^2$, $c[4/3/c25]^2$, $c[4/3/c26]^2$, $c[4/3/c27]^2$, $h[4/3/h5]^2_{\rm II}$, $c[5/3/c19]^2$, $c[5/3/c28]^2$, $c[5/3/c29]^2$, $c[5/3/c30]^2$, $c[5/3/c31]^2$, $c[6/3/c25]^2$. Two chiral sphere packings of the same handedness are combined if $G$ and $H$ are both pure rotation groups but belong to different crystal classes. This case occurs only once, namely in $c[3/3/c1]^2_{\rm II}$. If symmetry operations other than rotations exist in $G$ as well as in $H$, all individual sphere packings are achiral. Six such types are found: $t[3/4/t1]^2_{\rm II}$, $c[3/6/c5]^2$, $t[3/8/t1]^2_{\rm II}$, $t[3/10/t4]^2_{\rm II}$, $t[4/4/t3]^2$, $t[5/3/t22]^2$.

The systems of interpenetrating sphere packings belonging to the remaining 16 types can be generated with different symmetry. Their discussion, therefore, is more complicated. Four cases have to be distinguished.

(i) Let $G - H$ be that group–subgroup pair where the considered system of interpenetrating sphere packings is generated with highest site symmetry. If $H$ consists of all rotations of $G$ then all other corresponding group–subgroup pairs have the same property and two chiral sphere packings of different handedness interpenetrate. This is the case for the following five types: $c[3/3/c1]^2_{\rm III}$, $c[3/10/c1]^2_{\rm I}$, $c[4/3/c1]^2$, $c[4/3/c4]^2$, $h[4/3/h1]^2$. All of them belong to class IIa according to Blatov *et al.* (2004).

(ii) Types $t[4/4/t1]^2$ and $t[5/3/t1]^2$ occur with highest site symmetry in $I4_1/amd - I4_1md$. All other corresponding group–subgroup pairs are also translation-equivalent. Therefore, all interpenetrating sphere packings of both types belong to class IIa. Although the group–subgroup pairs $I4_1/a - I4_1$ and $I4_122 - I4_1$ would allow chiral individual sphere packings in principle, nevertheless all existing partial configurations are achiral because both space-group pairs do not permit additional deformations in comparison to $I4_1/amd - I4_1md$.

(iii) Let $G - H$ be that class-equivalent group–subgroup pair where the considered system of interpenetrating sphere packings is generated with highest site symmetry. If $H$ contains symmetry operations other than rotations, two achiral sphere packings interpenetrate. According to Blatov *et al.* (2004), they have to be assigned to class Ia. This concerns the following types: $t[3/4/t1]^2_{\rm I}$, $c[3/6/c3]^2$, $h[3/6/h1]^2$, $c[4/3/c6]^2$, $c[5/3/c3]^2$, $c[5/3/c10]^2$. Interpenetrating sphere packings of all six types occur also with lower symmetry and, in some cases, with additional degrees of freedom. The corresponding group–subgroup pairs may either be class-equivalent again or they may be translation-equivalent. Accordingly, the corresponding interpenetrating sphere packings have to be assigned to class Ia or to class IIa, respectively. Let us regard, for instance, type $c[5/3/c3]^2$. It refers to the following pairs of class-equivalent groups: $Im\bar{3}m$ – $Pm\bar{3}m$, $R\bar{3}m$ – $R\bar{3}m$ (2**c**), $R32$ – $R32$ (2**c**) and $R\bar{3}$ – $R\bar{3}$ (2**c**) (class Ia). The respective translation-equivalent group–subgroup pairs are $Ia\bar{3}d$ – $Ia\bar{3}$, $R\bar{3}c$ – $R32$ and $R\bar{3}c$ – $R\bar{3}$ (class IIa). Chiral individual packings with the same handedness occur in $R32$ – $R32$ (2**c**), enantiomorphic packings in $R\bar{3}c$ – $R32$.

(iv) The remaining types are the three exceptional cases described in §4. The individual sphere packings of types $t[3/10/c1]^2{}_{\rm II}$ and $h[3/10/h1]^2$ are chiral with the same handedness. Both types belong to one pair of class-equivalent and to a second pair of translation-equivalent groups and, therefore, either to class Ia or to class IIa, respectively. In contrast to that, both group–subgroup pairs of type $t[3/8/t1]^2{}_{\rm I}$ are translation-equivalent and lead to class IIa. The individual sphere packings are achiral.

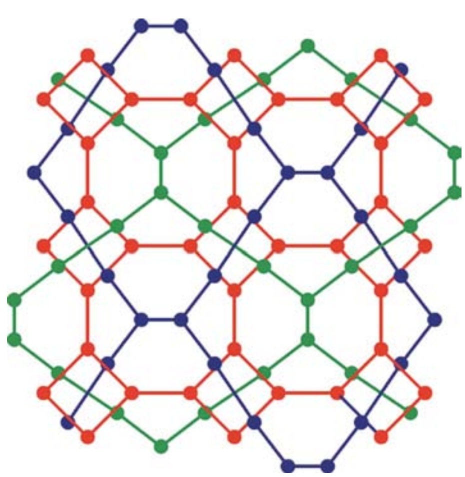

**Figure 6**
Interpenetrating sphere packings belonging to type $c[3/4/t1]^3$. Interpenetration pattern *c-l*.

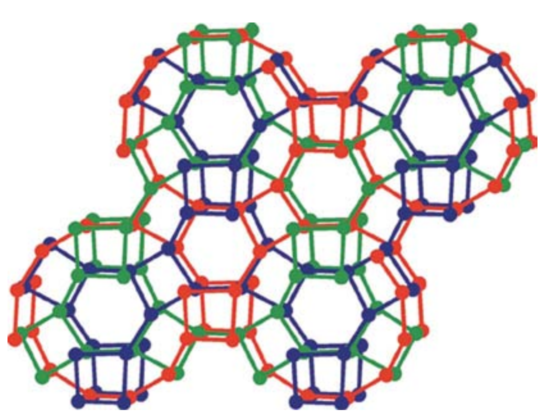

**Figure 7**
Interpenetrating sphere packings belonging to type $h[3/4/h1a]^3$. Interpenetration pattern *h-o*.

### 5.2. Interpenetration of three sphere packings

Three sphere packings of eight different types can be combined to systems of interpenetrating sphere packings belonging to eight different types (*cf.* Table 1). In all cases, $N_G(H) = H$ is fulfilled. Accordingly, each of the three individual packings belongs to a different subgroup $H_1$, $H_2$ and $H_3$ of $G$ with index 3.

For two of the eight cases, namely for $c[3/4/t1]^3$ and $c[4/3/c6]^3$, the pair $G$ – $H$ is translation-equivalent. The three tetragonal subgroups $H_1$, $H_2$ and $H_3$ (type $I\bar{4}2d$) of $G = I\bar{4}3d$ differ in the directions of their tetragonal axes. They can be mapped onto one another, for example, by a threefold rotation of $G$. This rotation interchanges also the three individual packings. Both types of interpenetrating sphere packings, therefore, have to be assigned to class IIa (Blatov *et al.*, 2004). In the first case, the three individual packings belong to the tetragonal type 3/4/*t*1 (*cf.* Fig. 6), whereas in the second case three tetragonally distorted packings of the cubic type 4/3/*c*6 are combined.

The other six types of interpenetrating sphere packings correspond to class-equivalent group–subgroup pairs $G$ – $H$. Then, the three subgroups $H_1$, $H_2$ and $H_3$ differ only in the positions of their origins and can be mapped onto one another by a translation from $G$ (class Ia). For $h[3/4/h1a]^3$ (Fig. 7) and $h[3/4/h3]^3$, this translation vector can be chosen as (110), in $t[3/4/t1]^3$ (Fig. 8) and in all other cases as (001).

Only types $h[3/4/h1a]^3$, $h[3/4/h3]^3$ and $t[3/4/t2]^3$ allow enantiomorphic systems of interpenetrating sphere packings.

### 5.3. Interpenetration of four sphere packings

Four sphere packings of three different types may be combined in five different ways (*cf.* Table 1). With respect to $N_G(H)$, all three cases discussed above really occur.

1. $N_G(H) = G$. This is true for only one type of interpenetrating sphere packing, namely for $c[3/3/c1]^4{}_{\rm II}$ (Fig. 9). The symmetry group $H = I2_13$ is a normal subgroup of $G = Ia\bar{3}d$ and is identical for all four individual packings,

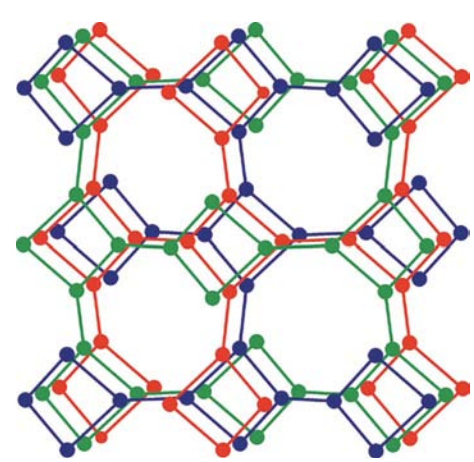

**Figure 8**
Interpenetrating sphere packings belonging to type $t[3/4/t1]^3$. Interpenetration pattern *t-m*.

therefore. $H$ is a translation-equivalent subgroup of $G$ with index 4. A first individual packing can be mapped onto the other three by three arbitrarily chosen symmetry operations, one from each of the three cosets of $H$ in $G$ (class IIb). The individual packings are chiral. Two packings with the same or with different handedness can be combined to a system of interpenetrating sphere packings of type $c[3/3/c1]^2{}_{\rm II}$ (red/blue or black/green in Fig. 9) or of type $c[3/3/c1]^2{}_{\rm III}$ (green/blue or black/red), respectively. A combination of two systems of the same kind results in interpenetrating sphere packings of type $c[3/3/c1]^4{}_{\rm II}$. In the first case, two systems with different handedness have to be combined.

2. $N_G(H) = H$. This applies only to type $c[3/3/c1]^4{}_{\rm III}$ (Fig. 10). Here, the highest symmetry group $G$ of the entire arrangement is $P4_232$. It has four maximal conjugate class-equivalent subgroups $H_j$ ($j = 1, 2, 3, 4$) with index 4 and doubled cell parameters (type $I4_132$). The four individual packings and their symmetry groups $H_j$ can be mapped onto one another, for example, by translations with vectors (100), (010) and (001) (class Ib). A similar relation exists for all other space-group pairs referring to $c[3/3/c1]^4{}_{\rm III}$. As the individual packings are chiral and only packings with the same handedness are combined, the systems of interpenetrating sphere packings occur in enantiomorphic pairs.

3. $N_G(H) \neq G$ and $N_G(H) \neq H$. Then, $H$ is a general subgroup of $G$ with index 4 and $i_g = i_h = 2$ holds. This applies to three types, namely to $c[3/3/c1]^4{}_{\rm I}$, $t[3/4/t1]^4$ and $t[3/4/t2]^4$. All three belong to class IIIa.

The four individual packings of $c[3/3/c1]^4{}_{\rm I}$ (Fig. 11) refer to the two conjugate subgroups $H_1 = P4_132$ and $H_2 = P4_332$ of $Ia\bar{3}d$ with index 4. The common normalizer of $H_1$ and $H_2$ with respect to $G$ is $N_G(H_{1,2}) = I4_132$. The centring translation of $I4_132$ combines two individual packings with symmetry $P4_132$ or $P4_332$ to pairs belonging to type $c[3/3/c1]^2{}_{\rm I}$. Each symmetry

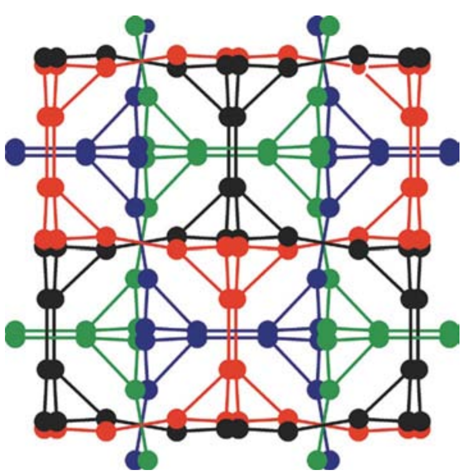

**Figure 9**
Interpenetrating sphere packings belonging to type $c[3/3/c1]^4{}_{\rm II}$. Interpenetration pattern *c-h*.

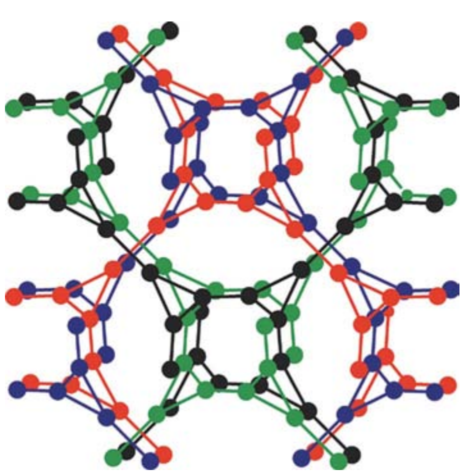

**Figure 10**
Interpenetrating sphere packings belonging to type $c[3/3/c1]^4{}_{\rm III}$. Interpenetration pattern *c-i*.

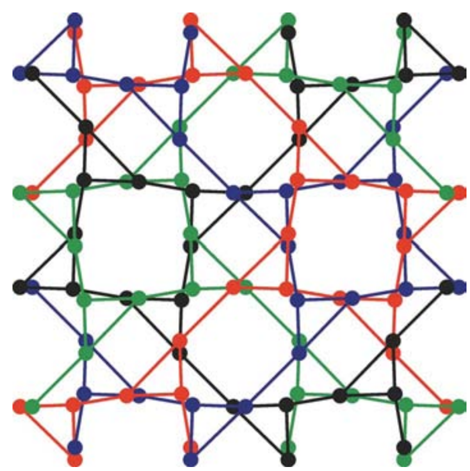

**Figure 11**
Interpenetrating sphere packings belonging to type $c[3/3/c1]^4{}_{\rm I}$. Interpenetration pattern *c-g*.

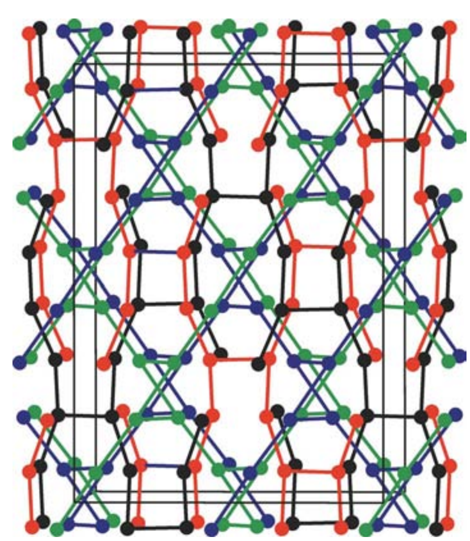

**Figure 12**
Interpenetrating sphere packings belonging to type $t[3/4/t1]^4$. Interpenetration pattern *t-p*.

operation from the coset of $I4_132$ in $Ia\bar{3}d$, *e.g.* an inversion, transforms one such pair into a second one with different handedness (red/blue or black/green in Fig. 11).

A system of interpenetrating sphere packings of type $t[3/4/t1]^4$ with symmetry $G = P4/nnc$ (Fig. 12) splits up into two sets of individual packings with symmetry $H_1$ and $H_2$. Both subgroups $H_1$ and $H_2$ of $G$ belong to type *Fddd*. They are parallel oriented and shifted against each other by a vector $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ referred to a basis of $G$. Their common normalizer with respect to $G$ is $N_G(H_1) = N_G(H_2) = Pnnn$. Each symmetry operation from the coset of $H_1$ (or $H_2$) in *Pnnn*, *e.g.* a translation with vector (001) referred to a basis of $G$, combines the corresponding two individual packings with the same symmetry (green/blue or black/red in Fig. 12) to a system of type $t[3/4/t1]^2{}_{\rm I}$. Any symmetry operation from the coset of *Pnnn* in *P*4/*nnc*, *e.g.* a fourfold rotation, maps the two systems $t[3/4/t1]^2{}_{\rm I}$ onto one another.

Type $t[3/4/t2]^4$ forms a similar case (Fig. 13). Each such system splits up into two enantiomorphic pairs of individual packings of type $t[3/4/t2]^2{}_{\rm I}$. The symmetry groups $H_1$ and $H_2$ of the two pairs belong to type $I4_122$ with basis vectors $\mathbf{a} - \mathbf{b}$, $\mathbf{a} + \mathbf{b}$, $2\mathbf{c}$. They are shifted against each other by a vector $(\frac{1}{2}\frac{1}{2}0)$ referred to $G = P4_2/nbc$. Each symmetry operation from the coset of $H_1$ (or $H_2$) in $N_G(H_1) = [N_G(H_2) =]$ $P4_222$, *e.g.* the translation with vector (001) referred to $P4_2/nbc$ combines the two individual packings with the same symmetry to a system of type $t[3/4/t2]^2{}_{\rm I}$ (green/blue or black/red in Fig. 13). Any symmetry operation from the coset of $P4_222$ in $P4_2/nbc$, *e.g.* an inversion, maps two such systems of type $t[3/4/t2]^2{}_{\rm I}$ onto another.

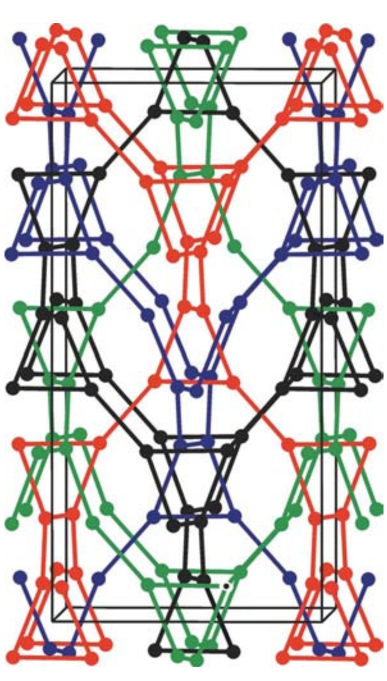

**Figure 13**
Interpenetrating sphere packings belonging to type $t[3/4/t2]^4$. Interpenetration pattern *t-p*.

### 5.4. Interpenetration of five sphere packings

Only one type of five interpenetrating sphere packings has been found, namely $t[3/4/t1]^5$ with symmetry $G = I4_1/a$ (*cf.* Table 1 and Fig. 14). All symmetry groups of the five individual packings are different. They belong also to type $I4_1/a$, but with enlarged lattice vectors $2\mathbf{a} - \mathbf{b}$, $\mathbf{a} + 2\mathbf{b}$, $\mathbf{c}$ in comparison to $G$. As $i = 5$ is prime, $N_G(H_j)$ equals $H_j$. Repeated application of a translation *e.g.* with vector (100), if referred to $G$, maps any of the subgroups together with its individual packing onto the other four subgroups and individual packings. Accordingly, type $t[3/4/t1]^5$ has to be assigned to class Ia.

### 5.5. Interpenetration of eight sphere packings

Eight sphere packings of type $3/3/c1$ can be combined in two different ways (*cf.* Table 1), namely to systems of types $c[3/3/c1]^8{}_{\rm I}$ (Fig. 15) and $c[3/3/c1]^8{}_{\rm II}$ (Fig. 16) with $G = I23$ and $G = Fd\bar{3}c$, respectively. $N_G(H) = H$ applies to both cases although the symmetries of the individual packings are different, namely $I2_13$ and $P4_132$ or $P4_332$, respectively. Eight different subgroups with index 8 correspond to the eight individual packings. Interpenetrating sphere packings of both types may be split up into two times four sphere packings that belong to type $c[3/3/c1]^4{}_{\rm III}$.

The eight class-equivalent subgroups $I2_13$ of $I23$ differ only in the positions of their origins. Translations by the basis vectors of $I23$ map each individual packing onto three others. The four packings form together a system of interpenetrating sphere packings of type $c[3/3/c1]^4{}_{\rm III}$ (*e.g.* black/red/light blue/light green in Fig. 15) with symmetry $P23$. The centring translations of $I23$ give rise to a second system with the same handedness. $c[3/3/c1]^8{}_{\rm I}$, therefore, belongs to class Ib. The same translations map also the eight subgroups of type $I2_13$ onto one another.

The two times four subgroups $P4_132$ and $P4_332$ of $Fd\bar{3}c$ are general ones with one common intermediate group $F4_132$. Therefore, $c[3/3/c1]^8{}_{\rm II}$ has to be assigned to class IIIb. Application of the centring translations of $Fd\bar{3}c$ to any of the individual packings results in a system of interpenetrating sphere

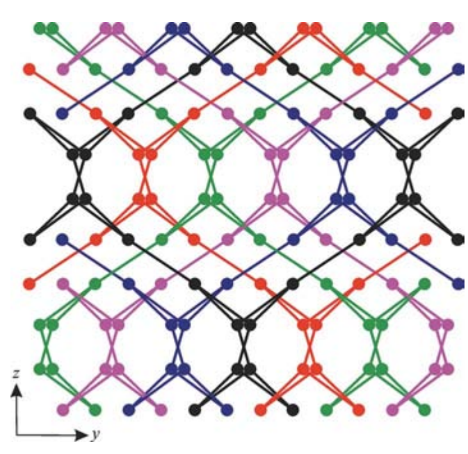


**Figure 14**
Interpenetrating sphere packings belonging to type $t[3/4/t1]^5$. Interpenetration pattern *t-r*.

packings of type $c[3/3/c1]^4_{\rm III}$ with symmetry $F4_132$ (*e.g.* black/red/blue/green in Fig. 16). These translations map also the four subgroups of type $P4_132$ (or $P4_332$) onto one another. Two enantiomorphic systems of that type can be combined with the aid of any symmetry operation from the coset of $F4_132$ in $Fd\bar{3}c$, *e.g.* an inversion. It interchanges in addition the four subgroups of type $P4_132$ with those four of type $P4_332$.

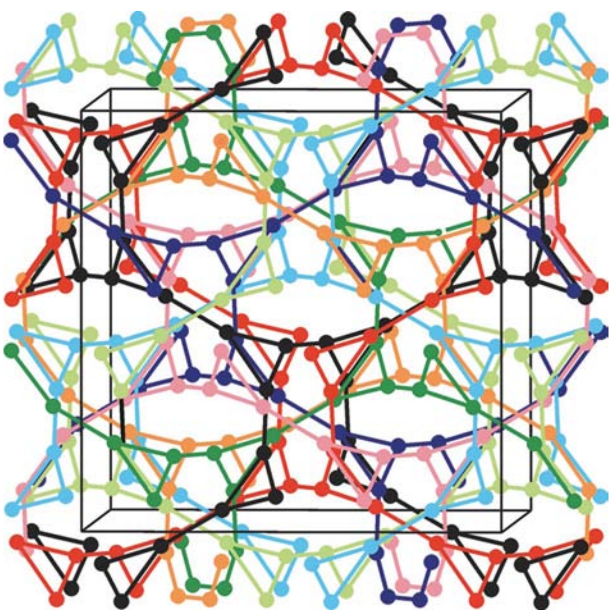

**Figure 15**
Interpenetrating sphere packings belonging to type $c[3/3/c1]^8_{\rm I}$. Interpenetration pattern *c-j*.

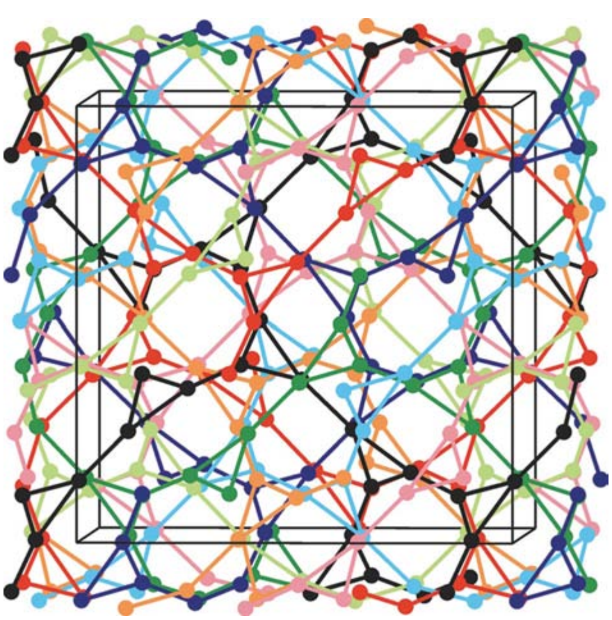

**Figure 16**
Interpenetrating sphere packings belonging to type $c[3/3/c1]^8_{\rm II}$. Interpenetration pattern *c-k*.

### 5.6. Patterns of interpenetration

The symbols of the so-called interpenetration classes (Blatov *et al.*, 2004, column 4 of Table 1) show immediately whether the individual sphere packings that interpenetrate are in parallel or in different orientation and whether more than one translation vector is needed to generate all packings in parallel orientation from a given one. Unfortunately, different orientations of the individual packings, enantiomorphic individual packings or enantiomorphic systems of interpenetrating sphere packings are not considered. Actually, these interpenetration classes do not really describe the geometrical or topological properties of the interpenetration of two (or more) three-periodic nets or sphere packings, but instead they only classify the corresponding group–subgroup pairs of space groups. The specific nets under consideration are completely irrelevant to this classification. Moreover, in some cases, exactly the same arrangement is assigned to different interpenetration classes if described with different symmetry (*cf. e.g.* Table 1, type $t[3/4/t1]^2_{\rm I}$).

In contrast to this, the different patterns of interpenetration for sphere packings (or also for interwoven three-periodic nets) are classified in columns 2 and 3 of Table 1. A first such attempt was made by Fischer & Koch (1976) for all types of interpenetrating sphere packings with cubic symmetry.

If one disregards the details of the individual sphere packings such as, for example, the contractable rings and looks only at their mutual catenation, the pattern of the interpenetration can be compared for sphere packings of different types. This will be demonstrated by the following examples.

(i) A sphere packing of type 4/6/*c*1 corresponds to an ideal cubic diamond configuration (lattice complex *cD*). When shifted against each other by the vector $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, two such sphere packings may be fitted into each other. Then, however, they do not result in a system of interpenetrating sphere packings but they form together a packing of type 8/4/*c*1 that corresponds to an ideal cubic body-centred lattice (lattice complex *cI*). Let us now replace each sphere in a packing of type 4/6/*c*1 either by a tetrahedron of four spheres or by a capped tetrahedron made up of 12 spheres.[5] The resulting sphere packings belong to the cubic types 4/3/*c*6 and 4/3/*c*14, respectively. In both cases, two sphere packings that are shifted against each other by the vector $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ may be intertwined. They result in systems of interpenetrating sphere packings of type $c[4/3/c6]^2$ and $c[4/3/c14]^2$, respectively. The differences between the two cases consist only in the existence of different contractable rings and in the different lengths of some non-contractable rings. As a consequence, the types $c[4/3/c6]^2$ and $c[4/3/c14]^2$ show the same *pattern of interpenetration*.

(ii) A sphere packing of type 3/3/*c*1 is built up from contractable triangles of spheres around the cubic threefold rotation axes. In addition, each sphere is in contact with one sphere from another triangle so that large 20-membered rings are formed. With symmetry $Ia\bar{3}d$, two enantiomorphic packings of this type may be intertwined, giving rise to inter-

[5] If applied to three-periodic nets instead of sphere packings, such a procedure has been called 'augmentation' or 'decoration' by O'Keeffe *et al.* (2000).

penetrating sphere packings of type $c[3/3/c1]^2_{\rm III}$ (*cf.* Fig. 1*c*). Only the large rings are essential for the interpenetration pattern, *i.e.* one can replace each triangle by only one sphere with three contacts without changing the interpenetration pattern. The resulting system of interpenetrating sphere packings belongs to type $c[3/10/c1]^2_{\rm I}$. The centres of the spheres form a point configuration of the invariant cubic lattice complex *cY***. If – on the other hand – each pair of contacting spheres from different triangles is replaced by one sphere, the interpenetration type does not change as well. In that case, two sphere packings of type 4/3/*c*1 are formed giving rise to interpenetrating sphere packings of type $c[4/3/c1]^2$. The corresponding point configuration belongs to the invariant cubic lattice complex *cV**. As a consequence, all three types of interpenetrating sphere packings $c[3/3/c1]^2_{\rm III}$, $c[3/10/c1]^2_{\rm I}$ and $c[4/3/c1]^2$ are assigned in Table 1 to the same pattern of interpenetration.

In a similar manner, all types of interpenetrating sphere packings are compared and assigned to interpenetration patterns. Fischer & Koch (1976) used small letters (*a* to *k*) to designate the different patterns of interpenetration with cubic symmetry. A modified version of these symbols is applied in the second column of Table 1. Another small letter indicating the Bravais system precedes each symbol: cubic *c*, hexagonal *h*, rhombohedral *r*, tetragonal *t* and orthorhombic *o*.

**5.6.1. Cubic patterns**. Within the cubic system, there are 33 different types of systems with two interpenetrating sphere packings. They correspond to only six patterns of interpenetration, labelled *c-a* to *c-f*. Three of them, namely *c-d*, *c-e* (Fig. 1*a*) and *c-f* (Fig. 1*b*), occur only once. The most frequent pattern *c-a* (*cf.* Fig. 1*c*) appears 19 times. It describes the well known interpenetration pattern of two sphere packings that refer to the lattice complex *cY*** or *cV** (*cf.* above). The interpenetration patterns *c-b* of two cubic diamond arrangements and *c-c* of two cubic primitive lattices are found eight times and three times, respectively.

Patterns *c-a*, *c-b* and *c-c* correspond to the labyrinth graphs of the three simplest cubic minimal surfaces without self-intersection (*cf. e.g.* Fischer & Koch, 1989), the *G* surface (gyroid), the *D* surface and the *P* surface. The two labyrinths of a self-intersecting $NO3^2$-*c*4 surface (*cf.* Koch, 2000) interpenetrate each other in a way analogous to the two sphere packings in a system of type $c[3/3/c1]^2_{\rm I}$. The symbols of such minimal surfaces, therefore, offer an alternative possibility of describing the interpenetration patterns. Column 3 of Table 1 contains such a symbol if a corresponding minimal surface could be identified.

The two cubic types of three interpenetrating sphere packings, $c[3/4/t1]^3$ (*cf.* Fig. 6) and $c[4/3/c6]^3$, show the same interpenetration pattern *c-l*. The three types of four (Figs. 9–11) and the two types of eight interpenetrating sphere packings (Figs. 15–16) differ in their interpenetration patterns.

**5.6.2. Hexagonal and rhombohedral patterns**. Hexagonal systems of two interpenetrating sphere packings may show two different patterns: *h-n* refers only to type $h[3/10/h1]^2$, whereas *h-q* occurs four times. It describes the interpenetration of two quartz-like arrangements with symmetry $H = P6_422$ in the supergroup $G = P6_222$ ($\frac{1}{2}\mathbf{c}$). The two labyrinths of an $NO3^2$-*h*10 minimal surface (*cf.* Koch, 2000) show an analogous pattern of interpenetration.

Both hexagonal types of three interpenetrating sphere packings refer to interpenetration pattern *h-o* (*cf.* Fig. 7). Three quartz-like arrangements are shifted against each other by a vector perpendicular to the hexagonal *c* direction.

The only interpenetration pattern with rhombohedral symmetry belongs to five types of interpenetration of two sphere packings. It is designated *r-bc* because it may be derived by rhombohedral deformation from the *c-b* pattern with maximal symmetry $Pn\bar{3}m$ – $Fd\bar{3}m$ (2**a**) as well as from the *c-c* pattern with maximal symmetry $Im\bar{3}m$ – $Pm\bar{3}m$. In both cases, the maximal rhombohedral symmetry is $R\bar{3}m$ – $R\bar{3}m$ (2**c**). This relation is also reflected by the rhombohedral family of minimal surfaces *rPD* (*cf. e.g.* Koch & Fischer, 1988) with symmetry $R\bar{3}m$ – $R\bar{3}m$ (2**c**) that encompasses both a cubic *P* surface ($c/a = \frac{1}{4}\surd 6$) and a cubic *D* surface ($c/a = \frac{1}{2}\surd 6$). Accordingly, a cubic *P* surface (together with its labyrinth graphs) can continuously be deformed into a cubic *D* surface (with its labyrinth graphs). As a consequence, it does not make sense to distinguish the corresponding two interpenetration patterns within the rhombohedral system.

**5.6.3. Tetragonal patterns**. Two different patterns with tetragonal symmetry for the interpenetration of two sphere packings have been found: *t-b* occurs 13 times and *t-a* twice.

The *t-b* pattern may be derived from the *c-b* pattern by tetragonal distortion. With maximal symmetry, it corresponds to the group–subgroup pair $P4_2/nnm$ – $I4_1/amd$ (*cf.* Figs. 2*a*, 2*b*, 3*a*, 4*a*, 4*c*, 5*a*, 5*c*). Accordingly, a tetragonal family *tD* of minimal surfaces exists that shows this symmetry. Such surfaces may be regarded as deformed cubic *D* surfaces.

In a similar way, the *t-a* pattern is related to the *c-a* pattern. Its maximal tetragonal symmetry is $I4_1/acd$ – $I4_122$ (*cf.* Fig. 3*b*). As Fogden & Hyde (1999) showed, a family *tG* of minimal surfaces with symmetry $I4_1/acd$ – $I4_122$ can be derived by tetragonal distortion from the cubic *G* surface. The family of *tD* surfaces, however, is also compatible with this symmetry because the pair $I4_1/acd$ – $I4_122$ can be derived from $P4_2/nnm$ – $I4_1/amd$ by subgroup degradation. As a consequence and in contrast to the situation in the rhombohedral system described above, there exist two minimal surfaces *tD*

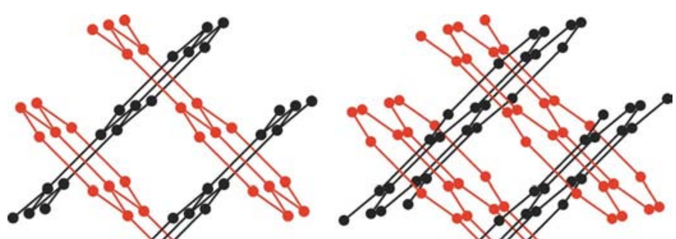


**Figure 17**
Interpenetrating sphere layers of types (*a*) $t[6^3]^2$ and (*b*) $t[48^2]^2$.

and $tG$ for small values of the axial ratio $c/a$ that differ in their inherent symmetry $P4_2/nnm$ – $I4_1/amd$ and $I4_1/acd$ – $I4_122$, respectively. The $tD$ surface contains straight lines corresponding to the twofold rotation axes of $P4_2/nnm$, whereas the respective lines in the $tG$ surface are screws. For $c/a = 1.1315$ (referred to $I4_1/acd$), these screws become straight lines (*cf.* Fogden & Hyde, 1999) and the two surfaces are identical, therefore. Cubic symmetry occurs for the $tG$ surface at $c/a = 1$ and for the $tD$ surface at $c/a = \surd 2$ (both referred to $I4_1/acd$). Above $c/a = 1.1315$, only $tD$ surfaces are possible. As a consequence, patterns *t-b* and *t-a* can be deformed into one another with symmetry $I4_1/acd$ – $I4_122$, whereas symmetry $P4_2/nnm$ – $I4_1/amd$ is compatible only with the *t-b* pattern. This feature sets the tetragonal case apart from the rhombohedral case described above and makes it plausible to distinguish between the patterns *t-b* and *t-a*.

Pattern *t-m* refers to the interpenetration of three diamond-like arrangements that are shifted against each other parallel to the tetragonal **c** direction. It corresponds to all three tetragonal types of three interpenetrating sphere packings (*cf.* Fig. 8).

There are two types of tetragonal systems of four interpenetrating sphere packings (Figs. 12, 13). For both cases, the interpenetration pattern is *t-p*. Diamond-like arrangements are shifted against each other parallel to **a**, **b** and **c**.

Pattern *t-r* corresponds to the only possibility of the interpenetration of five sphere packings (Fig. 14). Diamond-like arrangements are shifted against each other by a vector perpendicular to the tetragonal **c** direction.

### 5.7. Interpenetration of sphere layers

Only two of the eleven vertex-transitive plane nets (Shubnikov, 1916), namely the $6^3$ net and the $48^2$ net, allow analogous interpenetrating layers of spheres.

Only a sphere configuration of type $t[6^3]^2$ (Fig. 17*a*) can be realized with minimal density $\rho_{\min} = 0.50579$. Surprisingly, the respective sphere layers are flat but the hexagons are compressed parallel to the tetragonal **c** direction and the shortest normalized distance between centres of spheres from different layers is only $d = 1.02740$. For undistorted $6^3$ layers with $x = \frac{1}{6}$, $a = \frac{3}{2}\surd 2$ and $c = \surd 3$ (if referred to $I4/mcm$), the corresponding distance is increased to $d = 1.11803$ whereas $\rho = 0.53742$ is slightly larger. With hexagonal symmetry, even three sets of $6^3$ layers can interpenetrate. Then, the nets must necessarily be corrugated (*cf.* Sowa & Koch, 2004).

Analogous patterns of interpenetration exist also for $48^2$ sphere layers. The interpenetration of two sets of such layers with tetragonal symmetry (Fig. 17*b*) requires a deformation of the octagons. Again, three such sets can interpenetrate only if the layers are corrugated (*cf.* Sowa & Koch, 2005).

## 6. Conclusions

Although the present investigation does not comprise the orthorhombic, monoclinic and triclinic crystal systems, probably there exist no or at most very few additional types of interpenetrating sphere packings. This statement, however, may not be transferred to the interpenetration of three-periodic nets in general. It is noteworthy that only a relatively small number of different interpenetration patterns occur.

3/3/*c*1 is the sphere-packing type compatible with the largest number of different interpenetration patterns. All the corresponding eight types of interpenetrating sphere packings have two degrees of freedom. They allow or even require individual packings with different large deviations from the ideal configuration. Fischer (1976) presented projections of the parameter regions for the eight types of interpenetrating sphere packings.

Hyde & Oguey (2000) derived some of the more complicated interpenetration patterns in a completely different way, namely by embeddings of infinite families of trees in the hyperbolic plane and subsequent folding into three-periodic minimal surfaces. Patterns *c-a*, *c-e*, *c-f*, *c-i* and *c-k* could almost certainly be identified. In a recent paper, Baburin *et al.* (2005) relate a large number of inorganic crystal structures to interpenetrating three-periodic nets. The greater part of the corresponding interpenetration patterns agrees with the most common patterns from Table 1, namely with *c-a*, *c-b*, *c-c*, *t-b*, *r-bc* or *h-q*. It is noteworthy that the authors found four interpenetrating nets in eglestonite with interpenetration pattern *c-h* and three interpenetrating nets in $Ag_3CuS_2$ and in $CsCo(CO)_4$, both with interpenetration pattern *t-m*. On the other hand, the six interpenetrating nets in the crystal structures of $Zn[Au(CN)_2]_2$ and $Co[Au(CN)_2]_2$ do not correspond to any interpenetrating sphere packings. According to a private communication (Igor A. Baburin, 2006), there also exist examples of metal–organic crystal structures that can be related to cubic systems of three, four or eight interpenetrating sphere packings with interpenetration patterns *c-l*, *c-i*, *c-j* and *c-k*.

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