# Orthorhombic sphere packings. IV. Trivariant lattice complexes of space groups without mirror planes belonging to crystal class *mmm*

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All homogeneous sphere packings and all interpenetrating layers of spheres were derived that can be realized in the ten orthorhombic trivariant lattice complexes belonging to the space groups of crystal class *mmm* without mirror symmetry. Altogether, sphere packings of 186 different types have been found; the maximal inherent symmetry is orthorhombic for 124 of these types. In addition, ten types of interpenetrating sphere packings were detected, and in three lattice complexes interpenetrating $6^3$ nets occur.

## 1. Introduction

In the fourth part of a series of publications on homogeneous sphere packings with orthorhombic symmetry, all types of sphere packing and of interpenetrating sphere packings and layers are tabulated that can be generated in the ten trivariant orthorhombic lattice complexes of space groups without mirror planes belonging to crystal class *mmm*. The three previous papers list the sphere-packing types belonging to orthorhombic lattice complexes with less than three degrees of freedom (*cf.* Fischer *et al.*, 2006; Sowa *et al.*, 2007) and those belonging to trivariant lattice complexes with mirror symmetry (Sowa & Fischer, 2010). The sphere packings with symmetry *Pnna* 8e have been derived earlier (Sowa & Koch, 2001).

The procedure of derivation of the sphere has been described elsewhere (Sowa *et al.*, 2003; Fischer *et al.*, 2006) and all definitions have already been given by Fischer *et al.* (2006). As mentioned by Fischer *et al.* (2006), the range of lattice parameters that has to be investigated could be restricted if the affine normalizer of the space group under consideration interchanges two or three lattice directions.

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 realized in the ten examined trivariant orthorhombic lattice complexes. For each lattice complex, the characteristic Wyckoff position and the investigated range of coordinate and lattice parameters are given. All space groups are treated with origin choice 1.

In a 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 coordinates $x, y, z$. The same letter may symbolize two neighbouring spheres if they are equidistant for symmetry reasons.

The third block lists the types of sphere packing, interpenetrating sphere packing or layer that can be realized 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 $i$ or $n$ indicates a type of interpenetrating sphere packing or layer, respectively. 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. Interpenetrating sphere packings are symbolized by $g[k/m/fn]^l$, where $l$ is the number of intertwined packings of type $k/m/fn$ and $g$ indicates the highest inherent symmetry of this type of interpenetrating sphere packing. In the symbol of interpenetrating sphere layers the sphere-packing symbol is replaced by the symbol of the Shubnikov net (Shubnikov, 1916). The string of capital letters in the third column describes the centres of spheres with contact to the original sphere. If the parameter region of the regarded type – owing to the choice of the asymmetric unit – disintegrates into two or more disconnected parts, then each part refers to another string of capital letters. In cases in which 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, the symbol in the first column is modified by a prime. If the two parts are related by a symmetry operation of the space group the symbol is given in parentheses.

The last two columns refer to the configuration 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. Some types of sphere packing or interpenetrating sphere packings do not include an arrangement with minimal density. In these cases, parameters for any other packing of that type are given in square brackets.

## 3. Discussion

In total, the ten orthorhombic trivariant lattice complexes belonging to space groups of crystal class $mmm$ without mirror symmetry give rise to sphere packings of 186 different types with contact numbers 3 to 12. For 124 of them the maximal inherent symmetry is orthorhombic. It is cubic for the sphere packings of seven types, hexagonal for those of seven types and tetragonal for those of 48 types as is indicated by the letter $c$, $h$ or $t$, respectively, in the sphere-packing symbol.

Sphere packings of 30 of the 124 orthorhombic types occur also in lattice complexes with less than three degrees of freedom (cf. Fischer et al., 2006; Sowa et al., 2007), whereas sphere packings of the other 94 types can exclusively be generated with site symmetry 1 in one of the ten examined trivariant orthorhombic lattice complexes. These are two types with contact number 3, 17 types with contact number 4, 27 types with contact number 5, 28 types with contact number 6, 12 types with contact number 7, six types with contact number 8 and two types with contact number 9. Types 5/3/o1, 5/4/o2, 5/4/o3 and 7/3/o4 with symmetry $Pnna$ 8e have been mentioned by Sowa & Koch (2001) and type 3/10/o1 has already been derived by Koch & Fischer (1995). A second orthorhombic type with three contacts per sphere 3/10/o2 which occurs in $Fddd$ 16e was overlooked in that paper. In order to derive new types of sphere packing, Blatov (2007) used net–subnet relations. He mentioned 3/10/o2 as **uke**-3-$Fddd$ and he found also most of the sphere packings derived in the present paper (Blatov, 2006, TTD database). Some of the newly described types are already included in the Reticular Chemistry Structure Resource (RCSR) database (O'Keeffe et al., 2008). For instance, 3/10/o2 is symbolized there by **utq**.[1] Ten of the sphere packings have never been described before.

In addition, ten types of interpenetrating sphere packings were found. For three of them, $o[3/10/o1]^2$ (Ccce 16i), $o[3/10/t4]^2$ and $o[3/4/t1]^3$ (Fddd 32h), the maximal symmetry is orthorhombic. These types have already been described in detail by Sowa (2009). All other types may also be generated with higher symmetry (Koch et al., 2006). Fig. 1 shows the
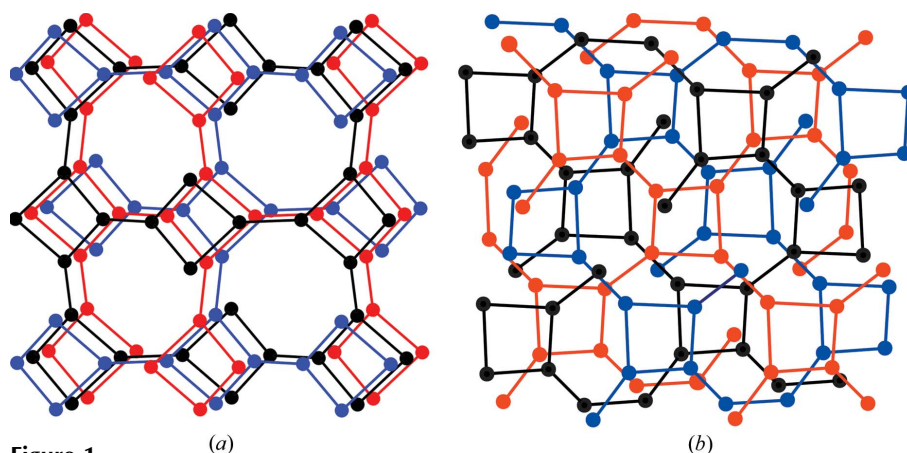


**Figure 1**
Interpenetrating sphere packings of types (a) $o[3/4/t1]^3$ and (b) $t[3/4/t1]^3$ (Fddd 32h).

types $t[3/4/t1]^3$ and $o[3/4/t1]^3$. Both types occur in $Fddd$ 32h and consist of three interpenetrating sphere packings of type 3/4/t1 which are intertwined in different ways (Sowa, 2009). Two sets of interpenetrating $6^3$ nets $t[6^3]^2$ may be realized in the general positions of $Pccn$, $Pban$ and $Pbcn$ (cf. Koch et al., 2006).

Among the sphere packings there are several types that show unusual properties. The appropriate graphs of sphere packings of types 5/4/o22 and 5/4/t49 (Fischer, 1993) are isomorphic. Packings of these types may be generated with site symmetry 1 in $Fddd$ 32h as well as in $I4_1/a$ 16f, but there is no common supergroup allowing one to obtain such a packing with higher site symmetry. The minimal density in each case is $\rho = 0.52360$. However, with this density an additional contact is formed resulting in a sphere packing of type 6/4/c1 that can be generated in the common supergroup $I4_1/amd$ 16f. Since the individual distortions of the packings are either tetragonal or orthorhombic a special symbol is introduced: 5/4/o22/t49. Special symbols are also used for further sphere-packing types; their graphs are isomorphic to those of tetragonal types. This concerns the pairs 6/3/o25–6/3/t44, 5/3/o6–5/3/t24, 5/4/o29–5/4/t48 and 4/4/o19–4/4/t39. 6/3/o25/t44 and 5/3/o6/t24 include sphere packings with minimal densities $\rho = 0.56286$ in $I4_1/a$ 16f, whereas in $Fddd$ 32h the obtained sphere packings have densities $\rho > 0.65226$. 5/4/o29/t48 and 4/4/o19/t39 can be realized in $I4_1/a$ 16f with densities $\rho > 0.56286$ and in $Fddd$ 32h with densities $\rho > 0.65226$. In each of these cases the topologies of the orthorhombic and tetragonal sphere packings belonging to a pair are identical. However, they cannot be deformed into each other without forming additional contacts resulting in type 12/3/c1. None of these couples involve two different variants a and b of sphere packings as has been observed for three hexagonal (Koch & Sowa, 2004) and one cubic (Fischer, 2004) sphere-packing pairs with isomorphic graphs. Therefore, the observed sphere-packing pairs are not couples of non-ambient isotopic embedding of the same net (cf. Hyde & Delgado Friedrichs, 2011).

It is worth noting that the two-dimensional parameter regions of the sphere-packing types 6/4/t11 and 5/4/o25 at the general position of $Fddd$ are each divided into two parts by the

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[1] A file which is readable with the programs Systre (Delgado-Friedrichs & O'Keeffe, 2003) and TOPOS (Blatov, 2006) and containing the RCSR symbols (other known names can be obtained from TOPOS databases) is available as supplementary material from the IUCr electronic archives (Reference: EO5017). Services for accessing these data are described at the back of the journal.

**Table 1**
The sphere packings corresponding to the ten orthorhombic trivariant lattice complexes belonging to the space groups without mirror symmetry of crystal class *mmm*.

**Pnnn 8m 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 | $-x, -y, z$ | G | $-x+\frac{1}{2}, -y+\frac{1}{2}, -z-\frac{1}{2}$ | | L | $-x-\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$ | |
| B | $x, -y, -z$ | H | $-x+1, -y, z$ | | M | $x, -y, -z+1$ | |
| C | $-x, y, -z$ | I | $x+1, y, z$ | | N | $-x+\frac{1}{2}, -y-\frac{1}{2}, -z+\frac{1}{2}$ | |
| D | $-x+1, y, -z$ | | $x-1, y, z$ | | O | $-x, y, 1-z$ | |
| E | $x, -y+1, -z$ | J | $-x+1, -y+1, z$ | | | | |
| F | $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$ | K | $-x, -y+1, z$ | | | | |
| 0.1 | 9/3/o1 | ACDFHIJK | $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}; \frac{1}{3}(3)^{1/2}, 1 + \frac{2}{3}(3)^{1/2}$ | | | | 0.64801 |
| 0.2 | 9/3/t2 | ABCDEFHJK | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}; 1, 1 + (2)^{1/2}$ | | | | 0.61343 |
| 0.3 | 7/3/o1 | ACFIKL | $0, \frac{1}{4}, 1 - \frac{1}{2}(3)^{1/2}; \frac{1}{2}, 1 + \frac{1}{2}(3)^{1/2}$ | | | | 0.56119 |
| 0.4 | 6/4/c1 | BCDEFG | $\frac{1}{4}, \frac{1}{4}, 0; 1, 1$ | | | | 0.52360 |
| 0.4' | | ABFHMN | $\frac{1}{4}, 0, \frac{1}{4}; 1, 1$ | | | | |
| 0.4' | | ACFKLO | $0, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | | |
| 1.1 | 7/3/t4 | ACDFHI | $\frac{1}{4}, \frac{3}{4} - \frac{1}{4}(6)^{1/2}, \frac{3}{4} - \frac{1}{4}(6)^{1/2}; (3)^{1/2} - (2)^{1/2}, 1$ | | | | 0.42315 |
| 1.2 | 7/4/o1 | ACDFHJK | $\frac{1}{4}, \frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}; \frac{1}{2}[10-2(13)^{1/2}]^{1/2}, \frac{1}{2} + \frac{1}{2}(13)^{1/2}$ | | | | 0.60210 |
| 1.3 | 6/3/t5 | ABCDFH | $\frac{1}{4}, \frac{1}{8}, \frac{1}{8}; \frac{1}{2}, 1$ | | | | 0.37024 |
| 1.4 | 6/3/t7 | ACFIL | $0, \frac{2}{5} - \frac{1}{10}(6)^{1/2}, \frac{2}{5} - \frac{1}{10}(6)^{1/2}; \frac{4}{5} - \frac{1}{5}(6)^{1/2}, 1$ | | | | 0.40281 |
| 1.5 | 6/4/o2 | ACFIK | $0.06652, \frac{1}{4}, 0.12896; 0.50448, 1.93858$ | | | | 0.54992 |
| 1.6 | 5/4/t6 | BCDEF | $\frac{1}{4}, \frac{1}{4}, \frac{1}{16}; 1, (2)^{1/2}$ | | | | 0.44179 |
| 1.7 | 5/4/h5 | ACFKL | $0, \frac{1}{4}, \frac{1}{6}; \frac{1}{2}(3)^{1/2}, \frac{3}{2}$ | | | | 0.40307 |
| 2.1 | 5/4/t5 | ACDFH | $[\frac{1}{4}, 0.145, 0.11743; 0.51845, 1.23482]$ | | | | >0.37024 |
| 2.2 | 5/4/t13 | ACFI | $0.10846, 0.14775, 0.14775; 0.30222, 1$ | | | | 0.38259 |
| 2.3 | 4/4/o2 | ABFH | $\frac{1}{4}, 0.08793, 0.14827; 0.74855, 1.26217$ | | | | 0.31354 |
| 2.3' | | BCDF, ACFK | | | | | |
| 2.4 | 4/4/t5 | ACFL | $0, \frac{5}{8} - \frac{1}{8}(13)^{1/2}, \frac{5}{8} - \frac{1}{8}(13)^{1/2}; [\frac{5}{6} - \frac{1}{6}(13)^{1/2}][2 + (13)^{1/2}]^{1/2}, 1$ | | | | 0.32252 |
| i2.1 | $c[4/3/c6]^2$ | ABCF | $\frac{3}{4} - \frac{1}{4}(6)^{1/2}, \frac{3}{4} - \frac{1}{4}(6)^{1/2}, \frac{3}{4} - \frac{1}{4}(6)^{1/2}; 1, 1$ | | | | 0.24708 |
| i3.1 | $t[3/4/t1]_I^2$ | ACF | $0.11075, \frac{11}{16} - \frac{1}{16}(73)^{1/2}, \frac{11}{16} - \frac{1}{16}(73)^{1/2}; 0.83247, 1$ | | | | 0.23110 |
| i3.1' | | BCF, ABF | | | | | |

**Pban 8m x, y, z**

| | | | | $0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b$ | | | |
|---|---|---|---|---|---|---|---|
| A | $-x, -y, z$ | G | $-x+1, -y, z$ | | K | $x, -y, -z+1$ | |
| B | $x, -y, -z$ | H | $x+1, y, z$ | | L | $-x, y, -z+1$ | |
| C | $-x, y, -z$ | | $x-1, y, z$ | | M | $-x+1, y, -z+1$ | |
| D | $-x+1, y, -z$ | I | $x+\frac{1}{2}, -y+\frac{1}{2}, z$ | | N | $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$ | |
| E | $x, y, z+1$ | | $x-\frac{1}{2}, -y+\frac{1}{2}, z$ | | O | $-x, -y+1, z$ | |
| | $x, y, z-1$ | J | $-x+\frac{1}{2}, y+\frac{1}{2}, z$ | | | | |
| F | $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$ | | $-x+\frac{1}{2}, y-\frac{1}{2}, z$ | | | | |
| 0.1 | 12/3/c1 | ABCDFGIKLMN | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}$ | | | | 0.74048 |
| 0.2 | 10/3/t1 | ACDGHILM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{6}(3)^{1/2}, \frac{1}{2}$ | | | | 0.69813 |
| 0.3 | 10/3/t1 | BCDEFKLMN | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{6}(3)^{1/2}$ | | | | 0.69813 |
| 0.4 | 10/3/t1 | ABFGIJKN | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(3)^{1/2}, \frac{1}{2}(3)^{1/2}$ | | | | 0.69813 |
| 1.1 | 8/3/t4 | BCEFKLN | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}; 1, \frac{2}{3}(3)^{1/2} - \frac{1}{3}(6)^{1/2}$ | | | | 0.47912 |
| 1.2 | 8/4/c1 | ACDGILM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}(2)^{1/2}; \frac{1}{2}, \frac{1}{2}$ | | | | 0.68017 |
| 1.3 | 8/4/c1 | BCDFKLMN | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{4}(2)^{1/2}$ | | | | 0.68017 |
| 1.4 | 8/4/c1 | ABFGIKN | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}(2)^{1/2}; \frac{1}{2}(2)^{1/2}$ | | | | 0.68017 |
| 1.5 | 7/3/o1 | ACHIL | $0, 1 - \frac{1}{2}(3)^{1/2}, \frac{1}{4}; 2 - (3)^{1/2}, 4 - 2(3)^{1/2}$ | | | | 0.56119 |
| 1.6 | 7/3/o13 | ACFILN | $0.14855, 0.16950, \frac{1}{4}; 0.74185, 0.67802$ | | | | 0.55058 |
| 1.6' | | ABFJKN | | | | | |
| 1.7 | 7/3/t6 | ABCFKLN | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}; 1, 2-(2)^{1/2}$ | | | | 0.50819 |
| 1.8 | 7/3/t8 | AFIJN | $\frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{4}; 1, [4(3)^{1/2} - 6]^{1/2}$ | | | | 0.60304 |
| 1.9 | 6/4/c1 | BCDEF | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{4}$ | | | | 0.52360 |
| 1.10 | 6/4/c1 | ABGJK | $\frac{1}{4}, 0, \frac{1}{4}; 1, 1$ | | | | 0.52360 |
| 1.10' | | ACILO | $0, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | | |
| 2.1 | 6/4/t6 | BCFKLN | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}; 1, (2)^{1/2} - 1$ | | | | 0.46680 |
| 2.2 | 6/4/c1 | FIJN | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | | 0.52360 |
| 2.3 | 5/4/o10 | ACFLN | $0.14555, 0.15165, \frac{1}{4}; 0.97034, 0.60660$ | | | | 0.50664 |
| 2.3' | | ABFKN | | | | | |
| 2.4 | 5/4/o11 | AFIN | $0.14882, 0.16949, \frac{1}{4}; 0.74248, 0.67895$ | | | | 0.55058 |
| 2.4' | | AFJN | | | | | |
| 2.5 | 5/4/t4 | BCEF | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0; 1, 1 - \frac{1}{2}(2)^{1/2}$ | | | | 0.35934 |
| 2.6 | 5/4/h5 | ACIL | $0, \frac{1}{6}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}$ | | | | 0.40307 |
| 2.6' | | ABJK | | | | | |
| n3.1 | $t[6^3]^2$ | AFN | $\frac{3}{20}, \frac{3}{20}, \frac{1}{4}; 1, \frac{1}{5}(10)^{1/2}$ | | | | 0.50579 |

**Table 1 (continued)**

**Pnna** 8e $x, y, z$ $\qquad$ $0 \leq x \leq \tfrac{1}{4},\ 0 \leq y \leq \tfrac{1}{4},\ 0 \leq z \leq \tfrac{1}{4}$

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

| No. | Type | Letters | Coordinates | Density |
|---|---|---|---|---|
| 0.1 | 10/3/h2 | ABCDIOP | $\tfrac{1}{12}, \tfrac{1}{4}(6)^{1/2} - \tfrac{1}{2}, \tfrac{1}{4}; \tfrac{3}{2}(3)^{1/2} - \tfrac{3}{2}(2)^{1/2}, \tfrac{3}{2} - \tfrac{1}{2}(6)^{1/2}$ | 0.66568 |
| 0.2 | 9/3/o1 | ABDHJKLN | $0, \tfrac{1}{4}, \tfrac{3}{4}(3)^{1/2} - \tfrac{3}{4}; (3)^{1/2}, 2 + (3)^{1/2}$ | 0.64801 |
| 0.3 | 9/3/o1 | BDIKLMN | $0, \tfrac{1}{4}, \tfrac{3}{4}(3)^{1/2} - \tfrac{3}{4}; \tfrac{1}{3}(3)^{1/2}, 1 + \tfrac{2}{3}(3)^{1/2}$ | 0.64801 |
| 0.4 | 9/3/o1 | BDILMP | $0, \tfrac{1}{2}(3)^{1/2} - \tfrac{3}{4}, \tfrac{1}{4}; 2 - (3)^{1/2}, 2(3)^{1/2} - 3$ | 0.64801 |
| 0.5 | 9/3/t2 | ABDIJKLN | $0, \tfrac{1}{4}, \tfrac{1}{4}(2)^{1/2} - \tfrac{1}{4}; 1, 1 + (2)^{1/2}$ | 0.61343 |
| 0.6 | 9/3/t2 | ABDILOP | $0, \tfrac{1}{4}(2)^{1/2} - \tfrac{1}{4}, \tfrac{1}{4}; (2)^{1/2} - 1, (2)^{1/2} - 1$ | 0.61343 |
| 0.7 | 8/3/t1 | ABCDEI | $\tfrac{1}{8}, \tfrac{1}{8}, 0; \tfrac{1}{3}(3)^{1/2}, \tfrac{1}{6}(3)^{1/2}$ | 0.60460 |
| 0.8 | 8/3/h4 | ABCDEFG | $\tfrac{1}{8}, 0, 0; \tfrac{4}{3}(3)^{1/2}, \tfrac{1}{3}(3)^{1/2}$ | 0.60460 |
| 0.9 | 8/3/h4 | ABDEFGH | $\tfrac{1}{8}, 0, 0; 4, (3)^{1/2}$ | 0.60460 |
| 0.10 | 8/3/h4 | ABDEIJK | $\tfrac{1}{8}, \tfrac{1}{4}, 0; \tfrac{2}{3}(3)^{1/2}, \tfrac{2}{3}(3)^{1/2}$ | 0.60460 |
| 0.11 | 8/3/h4 | ABDEHJK | $\tfrac{1}{8}, \tfrac{1}{4}, 0; 2(3)^{1/2}, 2$ | 0.60460 |
| 0.12 | 7/3/o1 | ABDFHL | $0, 0, 1 - \tfrac{1}{2}(3)^{1/2}; 2, 2 + (3)^{1/2}$ | 0.56119 |
| 0.13 | 7/3/o1 | ABCDFO | $\tfrac{1}{2}(3)^{1/2} - \tfrac{3}{4}, 0, \tfrac{1}{4}; 1 + \tfrac{1}{2}(3)^{1/2}, \tfrac{1}{2}$ | 0.56119 |
| 0.14 | 6/4/c1 | ABDFLO | $0, 0, \tfrac{1}{4}; 1, 1$ | 0.52360 |
| 1.1 | 9/3/o1 | ACDIOP | $0, \tfrac{1}{2}(3)^{1/2} - \tfrac{3}{4}, \tfrac{1}{4}; 2(3)^{1/2} - 3, 2 - (3)^{1/2}$ | 0.64801 |
| 1.2 | 8/3/o2 | ABDIOP | $\tfrac{1}{32}, \tfrac{3}{28}, \tfrac{1}{4}; \tfrac{8}{49}(7)^{1/2}, \tfrac{4}{49}(21)^{1/2}$ | 0.60460 |
| 1.3 | 8/3/h4 | BDIMP | $\tfrac{1}{4}, \tfrac{1}{8}, \tfrac{1}{4}; \tfrac{1}{4}(3)^{1/2}$ | 0.60460 |
| 1.4 | 8/3/h4 | BCDIP | $\tfrac{1}{4}, \tfrac{1}{8}, \tfrac{1}{4}; (3)^{1/2}, \tfrac{1}{4}$ | 0.60460 |
| 1.5 | 7/3/o1 | ACDEI | $0, 1 - \tfrac{1}{2}(3)^{1/2}, 0; 4 - 2(3)^{1/2}, 2 - (3)^{1/2}$ | 0.56119 |
| 1.6 | 7/3/o1 | BCDEI | $\tfrac{1}{4}, 1 - \tfrac{1}{2}(3)^{1/2}, 0; 4 - 2(3)^{1/2}, 2 - (3)^{1/2}$ | 0.56119 |
| 1.7 | 7/3/o1 | BDIKM | $\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{2}(3)^{1/2} - \tfrac{3}{4}; 2, 1 + \tfrac{1}{2}(3)^{1/2}$ | 0.56119 |
| 1.8 | 7/3/o2 | ABDHJK | $\tfrac{1}{64} + \tfrac{1}{64}(33)^{1/2}, \tfrac{1}{8}, \tfrac{1}{8}(33)^{1/2} - \tfrac{5}{8}; \tfrac{5}{8}(3)^{1/2} + \tfrac{1}{4}(11)^{1/2}, \tfrac{7}{4} + \tfrac{1}{4}(33)^{1/2}$ | 0.43908 |
| 1.9 | 7/3/o3 | ABDIJK | $\tfrac{4}{36}(7)^{1/2} - \tfrac{7}{36}, \tfrac{1}{4}, \tfrac{1}{2}(7)^{1/2} - \tfrac{5}{4}; \tfrac{17}{216}(7)^{1/2} + \tfrac{5}{3}, \tfrac{1}{12}[78(7)^{1/2} + 204]^{1/2}$ | 0.48680 |
| 1.10 | 7/3/o4 | ABCDI | $0.12151, 0.11945, 0.08235; 0.54672, 0.27715$ | 0.58849 |
| 1.11 | 7/3/t4 | BDILM | $0, \tfrac{3}{4} - \tfrac{1}{4}(6)^{1/2}, \tfrac{3}{4} - \tfrac{1}{4}(6)^{1/2}; (3)^{1/2} - (2)^{1/2}, 1$ | 0.42315 |
| 1.12 | 7/4/o1 | ABDJKLN | $0, \tfrac{1}{4}, \tfrac{1}{24}(13)^{1/2} - \tfrac{1}{24}; \tfrac{1}{6}[30 + 6(13)^{1/2}]^{1/2}, [4 + (13)^{1/2}]^{1/2}$ | 0.60210 |
| 1.13 | 7/4/o1 | BDIKLN | $0, \tfrac{1}{4}, \tfrac{1}{24}(13)^{1/2} - \tfrac{1}{24}; \tfrac{1}{2}[10 - 2(13)^{1/2}]^{1/2}, \tfrac{1}{2} + \tfrac{1}{2}(13)^{1/2}$ | 0.60210 |
| 1.14 | 7/4/o1 | BDILP | $0, \tfrac{1}{24}(13)^{1/2} - \tfrac{1}{24}, \tfrac{1}{4}; \tfrac{1}{3}[12 - 3(13)^{1/2}]^{1/2}, \tfrac{1}{6}(13)^{1/2} - \tfrac{1}{6}$ | 0.60210 |
| 1.15 | 6/3/o1 | ABCDE | $\tfrac{1}{8}, \tfrac{11}{8} - \tfrac{1}{8}(105)^{1/2}, 0; (15)^{1/2} - (7)^{1/2}, \tfrac{1}{2}(35)^{1/2} - \tfrac{3}{2}(3)^{1/2}$ | 0.44226 |
| 1.16 | 6/3/o1 | ABDEI | $\tfrac{1}{8}, \tfrac{1}{8}(105)^{1/2} - \tfrac{9}{8}, 0; (35)^{1/2} - 3(3)^{1/2}, \tfrac{1}{2}(15)^{1/2} - \tfrac{1}{2}(7)^{1/2}$ | 0.44226 |
| 1.17 | 6/3/o2 | ABCDO | $\tfrac{1}{64}(105)^{1/2} - \tfrac{3}{64}, \tfrac{1}{16}(105)^{1/2} - \tfrac{9}{16}, \tfrac{1}{4}; \tfrac{3}{8}(15)^{1/2} - \tfrac{1}{8}(7)^{1/2}, \tfrac{13}{8} - \tfrac{1}{8}(105)^{1/2}$ | 0.44226 |
| 1.18 | 6/3/o3 | ABDFH | $0.10178, 0, 0.11409; 3.37328, 3.18602$ | 0.38975 |
| 1.19 | 6/3/t5 | ABDIL | $0, \tfrac{1}{8}, \tfrac{1}{8}; \tfrac{1}{2}, 1$ | 0.37024 |
| 1.20 | 6/4/o1 | ABCDF | $0.12146, 0, 0.16363; 1.97462, 0.50763$ | 0.54664 |
| 1.21 | 6/4/o2 | ABDHL | $0, 0.06652, 0.12896; 1.98222, 3.84270$ | 0.54992 |
| 1.22 | 6/4/t2 | ABDEH | $\tfrac{1}{8}, \tfrac{1}{8}, 0; (15)^{1/2}, \tfrac{1}{2}(15)^{1/2}$ | 0.55805 |
| 1.23 | 6/4/c1 | ABDEFG | $\tfrac{1}{8}, 0, 0; 2(2)^{1/2}, 1$ | 0.52360 |
| 1.24 | 6/4/c1 | ADEIJ | $0, \tfrac{1}{4}, 0; 1, 1$ | 0.52360 |
| 1.25 | 6/4/c1 | BDEIK | $\tfrac{1}{4}, \tfrac{1}{4}, 0; 1, 1$ | 0.52360 |
| 1.26 | 6/4/c1 | ABDEJK | $\tfrac{1}{8}, \tfrac{1}{4}, 0; 2, (2)^{1/2}$ | 0.52360 |
| 1.27 | 5/4/t6 | ABDLO | $0, \tfrac{1}{16}, \tfrac{1}{4}; \tfrac{1}{2}(2)^{1/2}, \tfrac{1}{2}(2)^{1/2}$ | 0.44179 |
| 1.28 | 5/4/h5 | ABDFO | $\tfrac{1}{12}, 0, \tfrac{1}{4}; \tfrac{3}{2}, \tfrac{1}{2}(3)^{1/2}$ | 0.40307 |
| 1.29 | 5/4/h5 | ABDFL | $0, 0, \tfrac{1}{6}; \tfrac{2}{3}(3)^{1/2}, (3)^{1/2}$ | 0.40307 |
| 2.1 | 7/4/o1 | ADIOP | $0, \tfrac{1}{24}(13)^{1/2} - \tfrac{1}{24}, \tfrac{1}{4}; \tfrac{1}{6}(13)^{1/2} - \tfrac{1}{6}, \tfrac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$ | 0.60210 |
| 2.2 | 6/3/o3 | BDIM | $\tfrac{1}{4}, 0.14822, 0.13591; 0.29645, 0.94449$ | 0.38975 |
| 2.3 | 6/4/o1 | BCDI | $\tfrac{1}{4}, 0.12854, 0.08637; 0.50643, 0.25708,$ | 0.54664 |
| 2.4 | 6/4/o2 | ACDI | $0, 0.12896, 0.06652; 0.51584, 0.26023$ | 0.54992 |
| 2.5 | 6/4/c1 | BDIP | $\tfrac{1}{4}, \tfrac{1}{8}, \tfrac{1}{4}; \tfrac{1}{4}(2)^{1/2}, \tfrac{1}{2}(2)^{1/2}$ | 0.52360 |
| 2.6 | 5/3/o1 | ABDI | $0.08682, 0.13978, 0.09705; 0.59624, 0.848879$ | 0.32707 |
| 2.7 | 5/4/o1 | ABDJK | $\tfrac{3}{28}, \tfrac{1}{4}, \tfrac{1}{8}; \tfrac{7}{6}(3)^{1/2}, \tfrac{1}{2}(21)^{1/2}$ | 0.40307 |
| 2.8 | 5/4/o2 | ABCD | $0.12230, 3 - \tfrac{1}{2}(34)^{1/2}, \tfrac{1}{8}; 1.16319, \tfrac{2}{15}[3855 - 660(34)^{1/2}]^{1/2}$ | 0.42072 |
| 2.9 | 5/4/o3 | ABDH | $0.10290, 0.07674, 0.10737; 3.35885, 3.28830$ | 0.37925 |
| 2.10 | 5/4/t5 | BDIL | $[0, 0.15, \tfrac{1}{8}; 0.4, 1.2]$ | >0.37024 |
| 2.11 | 5/4/t6 | ADIJ | $0, \tfrac{1}{4}, \tfrac{1}{16}; 1, (2)^{1/2}$ | 0.44179 |
| 2.12 | 5/4/h5 | ADEI | $0, \tfrac{1}{6}, 0; \tfrac{2}{3}, \tfrac{1}{3}(3)^{1/2}$ | 0.40307 |
| 2.13 | 5/4/h5 | BDEI | $\tfrac{1}{4}, \tfrac{1}{6}, 0; \tfrac{2}{3}, \tfrac{1}{3}(3)^{1/2}$ | 0.40307 |
| 2.14 | 5/4/h5 | BDIK | $\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{12}; \tfrac{1}{2}(3)^{1/2}, \tfrac{3}{2}$ | 0.40307 |
| 2.15 | 4/4/o1 | ABDF | $\tfrac{1}{16}(73)^{1/2} - \tfrac{7}{16}, 0, 0.14767; 1.93348, 1.56301$ | 0.28988 |

**Table 1 (continued)**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 2.16 | 4/4/o2 | ABDL | | 0, 0.08793, 0.14827; 0.74855, 1.26217 | | | 0.31354 |
| 2.17 | 4/6/h2 | ABDO | | $\frac{1}{12}, \frac{1}{16}, \frac{1}{4}; \frac{3}{4}(2)^{1/2}, \frac{1}{4}(6)^{1/2}$ | | | 0.34009 |
| 2.18 | 4/6/c1 | ABDE | | $\frac{1}{8}, \frac{1}{8}, 0; (2)^{1/2}, \frac{2}{3}(2)^{1/2}$ | | | 0.34009 |
| 3.1 | 4/4/o1 | BDI | | $\frac{1}{4}, \frac{11}{16} - \frac{1}{16}(73)^{1/2}, 0.10233; 0.51720, 0.80839$ | | | 0.28988 |
| 3.2 | 4/4/o2 | ADI | | $0, 0.14827, 0.08793; \frac{1}{8}(33)^{1/2} - \frac{1}{8}, 0.79229$ | | | 0.31354 |
| 3.3 | 3/10/o1 | ABD | | $\frac{1}{10}, \frac{3}{32}, \frac{1}{8}; \frac{5}{2}, \frac{5}{2}(5)^{1/2}$ | | | 0.22089 |

**Pcca 8f x, y, z** $\qquad 0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}$

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

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.1 | 12/3/c1 | ABCEFGJKL | | $\frac{1}{8}, \frac{1}{4}, 0; 2, 1$ | | | 0.74048 |
| 0.2 | 11/3/o2 | ABCDEJKL | | $\frac{3}{2}(2)^{1/2} - 2, \frac{1}{4}, \frac{1}{12}; \frac{2}{3}(6)^{1/2} + (3)^{1/2}, (3)^{1/2}$ | | | 0.71868 |
| 0.3 | 10/3/t1 | ABEFGHKL | | $\frac{1}{8}, \frac{1}{4}, 0; \frac{2}{3}(3)^{1/2}, 1$ | | | 0.69813 |
| 0.4 | 10/3/t1 | CEFGIJ | | $\frac{1}{8}, \frac{1}{4}, 0; 2, \frac{1}{3}(3)^{1/2}$ | | | 0.69813 |
| 0.5 | 9/3/o1 | ABDEKLNO | | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}; (3)^{1/2}, 2 + (3)^{1/2}$ | | | 0.64801 |
| 0.6 | 9/3/o1 | BEHKMNO | | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}; \frac{1}{3}(3)^{1/2}, 1 + \frac{2}{3}(3)^{1/2}$ | | | 0.64801 |
| 0.7 | 9/3/t2 | ABEHKLNO | | $0, \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}; 1, 1 + (2)^{1/2}$ | | | 0.61343 |
| 0.8 | 8/3/h4 | BEHKMP | | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}, (3)^{1/2}$ | | | 0.60460 |
| 0.9 | 8/3/h4 | BEFHKP | | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$ | | | 0.60460 |
| 1.1 | 10/3/t1 | ABCDJKL | | $\frac{1}{8}, \frac{1}{4}, 0; 2(3)^{1/2}, (3)^{1/2}$ | | | 0.69813 |
| 1.2 | 9/3/o1 | BCDEJK | | $1 - \frac{1}{3}(3)^{1/2}, \frac{1}{4}, \frac{1}{4}; 2 + (3)^{1/2}, (3)^{1/2}$ | | | 0.64801 |
| 1.3 | 9/3/o1 | CEFIJ | | $1 - \frac{1}{3}(3)^{1/2}, \frac{1}{4}, \frac{1}{4}; 1 + \frac{2}{3}(3)^{1/2}, \frac{1}{3}(3)^{1/2}$ | | | 0.64801 |
| 1.4 | 9/3/o5 | ABCEJKL | | $0.12338, \frac{1}{4}, 0.05627; 2.66256, 1.34858$ | | | 0.69006 |
| 1.5 | 9/3/t2 | BCEFJK | | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{4}, \frac{1}{4}; 1 + (2)^{1/2}, 1$ | | | 0.61343 |
| 1.6 | 8/4/c1 | CEFGJ | | $\frac{1}{8}, \frac{1}{4}, 0; 2, \frac{1}{2}(2)^{1/2}$ | | | 0.68017 |
| 1.7 | 8/4/c1 | ABEFGKL | | $\frac{1}{8}, \frac{1}{4}, 0; (2)^{1/2}, 1$ | | | 0.68017 |
| 1.8 | 7/3/o1 | ABCDE | | $\frac{1}{2}(3)^{1/2} - \frac{3}{4}, 0, \frac{1}{8}; 2 + (3)^{1/2}, 2$ | | | 0.56119 |
| 1.9 | 7/3/o9 | ABEHKL | | $\frac{3}{4} - \frac{1}{4}(7)^{1/2}, \frac{1}{4}, \frac{1}{12}; \frac{1}{3}[2(7)^{1/2} + 5]^{1/2}, (3)^{1/2}$ | | | 0.50736 |
| 1.10 | 7/3/o10 | ABDEKL | | $\frac{3}{4} - \frac{1}{4}(7)^{1/2}, \frac{1}{4}, \frac{1}{3} - \frac{1}{12}(7)^{1/2}; \frac{1}{3}[12(7)^{1/2} + 33]^{1/2}, [2(7)^{1/2} + 5]^{1/2}$ | | | 0.48680 |
| 1.11 | 7/3/o11 | BEHKM | | $0.15994, \frac{1}{4}, 0.11939; 0.50831, 1.84364$ | | | 0.58705 |
| 1.12 | 7/3/o12 | BEFHK | | $0.20293, \frac{1}{4}, 0.08603; 0.95602, 1$ | | | 0.57451 |
| 1.13 | 7/4/o1 | ABELKNO | | $0, \frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}; \frac{1}{6}[30 + 6(13)^{1/2}]^{1/2}, [4 + (13)^{1/2}]^{1/2}$ | | | 0.60210 |
| 1.14 | 7/4/o1 | BEHKNO | | $0, \frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}; \frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}, \frac{1}{2} + \frac{1}{2}(13)^{1/2}$ | | | 0.60210 |
| 1.15 | 6/4/c1 | ABDEN | | $0, 0, \frac{1}{8}; 4, 2$ | | | 0.52360 |
| 1.16 | 6/4/c1 | AEGHL | | $0, \frac{1}{4}, 0; 1, 1$ | | | 0.52360 |
| 1.17 | 6/4/c1 | BEFKP | | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | | | 0.52360 |
| 1.18 | 6/4/c1 | BEHKP | | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, (2)^{1/2}$ | | | 0.52360 |
| 2.1 | 8/4/c1 | ABCJKL | | $\frac{1}{8}, \frac{1}{4}, 0; 2(2)^{1/2}, (2)^{1/2}$ | | | 0.68017 |
| 2.2 | 7/4/o1 | BCEJK | | $\frac{7}{24} - \frac{1}{24}(13)^{1/2}, \frac{1}{4}, \frac{1}{4}; [4 + (13)^{1/2}]^{1/2}, \frac{1}{6}[30 + 6(13)^{1/2}]^{1/2}$ | | | 0.60210 |
| 2.3 | 7/4/o1 | CEFJ | | $\frac{7}{24} - \frac{1}{24}(13)^{1/2}, \frac{1}{4}, \frac{1}{4}; \frac{1}{2} + \frac{1}{2}(13)^{1/2}, \frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}$ | | | 0.60210 |
| 2.4 | 6/4/c1 | ABCD | | $\frac{1}{8}, 0, 0; 2, 4$ | | | 0.52360 |
| 2.5 | 6/4/c1 | BCDE | | $\frac{1}{8}, 0, \frac{1}{4}; 4, 2$ | | | 0.52360 |
| 2.6 | 6/4/c1 | BFHK | | $\frac{1}{4}, \frac{1}{4}, 0; 1, 1$ | | | 0.52360 |
| 2.7 | 5/4/o7 | ABEKL | | $\frac{3}{32}, \frac{1}{4}, \frac{1}{10}; \frac{4}{5}(5)^{1/2}, (5)^{1/2}$ | | | 0.44179 |
| 2.8 | 5/4/o8 | BEHK | | $0.14839, \frac{1}{4}, 0.10161; 0.84322, 1.56860$ | | | 0.46761 |
| 2.9 | 5/4/t6 | AEHL | | $0, \frac{1}{4}, \frac{1}{16}; 1, (2)^{1/2}$ | | | 0.44179 |
| 2.10 | 5/4/t6 | BEFK | | $\frac{3}{16}, \frac{1}{4}, \frac{1}{4}; (2)^{1/2}, 1$ | | | 0.44179 |
| 2.11 | 5/4/h5 | ABDE | | $\frac{1}{12}, 0, \frac{1}{8}; 3, 2(3)^{1/2}$ | | | 0.40307 |

**Pccn 8e x, y, z** $\qquad 0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}; a \leq b$

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

## Table 1 (continued)

| | | | | |
|---|---|---|---|---|
| 0.1 | 12/3/c1 | ABDGHILO | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}$ | 0.74048 |
| 0.2 | 11/3/o2 | ABDFGHL | $0, \frac{3}{2}(2)^{1/2} - 2, \frac{1}{6}; 3(3)^{1/2} - 2(6)^{1/2}, 9 - 6(2)^{1/2}$ | 0.71868 |
| 0.3 | 10/3/t1 | ADHILNO | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(3)^{1/2}, \frac{1}{2}(3)^{1/2}$ | 0.69813 |
| 0.4 | 10/3/t1 | ABGIJO | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{6}(3)^{1/2}$ | 0.69813 |
| 0.5 | 9/3/o1 | ADEFHLM | $0, 0, 1 - \frac{1}{2}(3)^{1/2}; \frac{1}{3}(3)^{1/2}, 1 + \frac{2}{3}(3)^{1/2}$ | 0.64801 |
| 0.6 | 9/3/t2 | ADEHLMN | $0, 0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}; 1, 1 + (2)^{1/2}$ | 0.61343 |
| 0.7 | 9/3/t2 | ABCDFL | $\frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{8}; 1 - \frac{1}{2}(2)^{1/2}, 2 - (2)^{1/2}$ | 0.61343 |
| 0.8 | 8/3/h4 | ABCDEL | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$ | 0.60460 |
| 0.9 | 8/3/h4 | ACDEFL | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}, (3)^{1/2}$ | 0.60460 |
| 1.1 | 10/3/t1 | BDFGHL | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{6}(3)^{1/2}, \frac{1}{2}$ | 0.69813 |
| 1.2 | 9/3/o1 | ABDFGH | $0, 1 - \frac{1}{2}(3)^{1/2}, 0; 2 - (3)^{1/2}, 2(3)^{1/2} - 3$ | 0.64801 |
| 1.3 | 9/3/o1 | ABGIJ | $0, 1 - \frac{1}{2}(3)^{1/2}, 0; 2(3)^{1/2} - 3, 2 - (3)^{1/2}$ | 0.64801 |
| 1.4 | 9/3/o5 | ABDGHL | $0, 0.12338, 0.19373; 0.37558, 0.50650$ | 0.69006 |
| 1.5 | 9/3/t2 | ABDGHI | $0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0; (2)^{1/2} - 1, (2)^{1/2} - 1$ | 0.61343 |
| 1.6 | 8/3/o6 | ABDFL | $0.19940, 0.10654, 0.13649; 0.28839, 0.57382$ | 0.60712 |
| 1.7 | 8/3/t4 | ABIJO | $\frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}; 1, \frac{2}{3}(3)^{1/2} - \frac{1}{3}(6)^{1/2}$ | 0.47912 |
| 1.8 | 8/4/c1 | ADHILO | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.68017 |
| 1.9 | 8/4/c1 | ABGIO | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{4}(2)^{1/2}$ | 0.68017 |
| 1.10 | 7/3/o1 | ABCDF | $\frac{1}{4}, 1 - \frac{1}{2}(3)^{1/2}, 0; 2 - (3)^{1/2}, 4 - 2(3)^{1/2}$ | 0.56119 |
| 1.11 | 7/3/o5 | ABCDL | $\frac{1}{4}, \frac{1}{2}(7)^{1/2} - \frac{5}{4}, \frac{1}{8}; [2(7)^{1/2} - 5]^{1/2}, 6 - 2(7)^{1/2}$ | 0.48680 |
| 1.12 | 7/3/o5 | ACDFL | $\frac{1}{4}, \frac{1}{2}(7)^{1/2} - \frac{5}{4}, \frac{1}{8}; 3 - (7)^{1/2}, 2[2(7)^{1/2} - 5]^{1/2}$ | 0.48680 |
| 1.13 | 7/3/o9 | ADHLN | $0, \frac{3}{4} - \frac{1}{4}(7)^{1/2}, \frac{1}{6}; [6(7)^{1/2} - 15]^{1/2}, 3[2(7)^{1/2} - 5]^{1/2}$ | 0.50736 |
| 1.14 | 7/3/o10 | ADFHL | $0, \frac{3}{4} - \frac{1}{4}(7)^{1/2}, \frac{1}{12}(7)^{1/2} - \frac{1}{12}; \frac{1}{3}[33 - 12(7)^{1/2}]^{1/2}, \frac{1}{3}[6(7)^{1/2} - 3]^{1/2}$ | 0.48680 |
| 1.15 | 7/3/o11 | ADEFL | $0.15994, 0, 0.13061; 0.50831, 1.84364$ | 0.58705 |
| 1.16 | 7/3/o12 | ABDEL | $0.20293, 0, 0.16397; 0.95602, 1$ | 0.57451 |
| 1.16' | | ADHIN | | |
| 1.17 | 7/3/o13 | ABDLO | $0.10145, 0.08050, \frac{1}{4}; 0.74185, 0.67802$ | 0.55058 |
| 1.17' | | ADINO | | |
| 1.18 | 7/3/t6 | ABDIO | $\frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}; 1, 2 - (2)^{1/2}$ | 0.50819 |
| 1.19 | 7/3/t8 | ADLNO | $\frac{1}{2} - \frac{1}{4}(3)^{1/2}, \frac{1}{2} - \frac{1}{4}(3)^{1/2}, \frac{1}{4}; 1, [4(3)^{1/2} - 6]^{1/2}$ | 0.60304 |
| 1.20 | 7/4/o1 | ADEHLM | $0, 0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}; \frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}, \frac{1}{2} + \frac{1}{2}(13)^{1/2}$ | 0.60210 |
| 1.21 | 6/4/c1 | ABCDE | $\frac{1}{4}, 0, 0; 1, 1$ | 0.52360 |
| 1.21' | | ADHIK | $0, \frac{1}{4}, 0; 1, 1$ | |
| 1.22 | 6/4/c1 | ACDEL | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, (2)^{1/2}$ | 0.52360 |
| 2.1 | 8/4/c1 | BDGHL | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{4}(2)^{1/2}, \frac{1}{2}$ | 0.68017 |
| 2.2 | 7/3/o1 | BDFL | $\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{8}; 2 - (3)^{1/2}, 4 - 2(3)^{1/2}$ | 0.56119 |
| 2.3 | 7/3/t4 | ABIJ | $\frac{1}{4}(6)^{1/2} - \frac{1}{2}, \frac{1}{4}(6)^{1/2} - \frac{1}{2}, 0; 1, (3)^{1/2} - (2)^{1/2}$ | 0.42315 |
| 2.4 | 7/4/o1 | ABDGH | $0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}, \frac{1}{6}(13)^{1/2} - \frac{1}{6}$ | 0.60210 |
| 2.5 | 7/4/o1 | ABGI | $0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{6}(13)^{1/2} - \frac{1}{6}, \frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$ | 0.60210 |
| 2.6 | 6/3/o10 | ADFL | $\frac{1}{8}, 0.07916, 0.13417; 0.35289, 1.12843$ | 0.46228 |
| 2.7 | 6/3/o11 | ABDL | $0.18320, 0.07858, 0.16744; 0.58713, 0.68570$ | 0.45266 |
| 2.7' | | ADIN | | |
| 2.8 | 6/3/t5 | ABDI | $\frac{1}{8}, \frac{1}{8}, 0; 1, \frac{1}{2}$ | 0.37024 |
| 2.9 | 6/3/t8 | ADLN | $0.05243, 0.05243, 0.17602; 1, 1.53037$ | 0.47761 |
| 2.10 | 6/4/o2 | ABDF | $0.18348, 0.12104, 0; 0.26023, 0.51584$ | 0.54992 |
| 2.11 | 6/4/t6 | ABIO | $\frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}; 1, (2)^{1/2} - 1$ | 0.46680 |
| 2.12 | 6/4/c1 | BDEL | $\frac{1}{4}, 0, \frac{1}{4}; 1, 1$ | 0.52360 |
| 2.12' | | DHIN | $0, \frac{1}{4}, \frac{1}{4}; 1, 1$ | |
| 2.13 | 6/4/c1 | ALNO | $0, 0, \frac{1}{4}; 1, 1$ | 0.52360 |
| 2.14 | 5/4/o7 | ADHL | $0, \frac{3}{32}, \frac{3}{20}; \frac{1}{4}(5)^{1/2}, \frac{5}{4}$ | 0.44179 |
| 2.15 | 5/4/o8 | ADEL | $0.14839, 0, 0.14839; 0.84322, 1.56860$ | 0.46761 |
| 2.15' | | ADHN | | |
| 2.16 | 5/4/o10 | ABDO | $0.10445, 0.09835, \frac{1}{4}; 0.97034, 0.60660$ | 0.50664 |
| 2.16' | | ADIO | | |
| 2.17 | 5/4/o11 | ADLO | $0.10118, 0.08051, \frac{1}{4}; 0.74248, 0.67895$ | 0.55058 |
| 2.17' | | ADNO | | |
| 2.18 | 5/4/t6 | ADHI | $0, \frac{3}{16}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.44179 |
| 2.18' | | ABDE | | |
| 2.19 | 5/4/t6 | ACDL | $\frac{1}{4}, \frac{1}{16}, \frac{1}{8}; \frac{1}{2}, 1$ | 0.44179 |
| 2.20 | 5/4/h5 | ABCD | $\frac{1}{4}, \frac{1}{12}, 0; \frac{1}{3}(3)^{1/2}, \frac{2}{3}$ | 0.40307 |
| 3.1 | 5/4/t5 | ABI | $[0.11310, 0.12297, 0; 0.92787, 0.4]$ | >0.37024 |
| 3.2 | 5/4/t6 | ALN | $0, 0, \frac{3}{16}; 1, (2)^{1/2}$ | 0.44179 |
| 3.3 | 5/4/h5 | BDL | $\frac{1}{4}, \frac{1}{12}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}$ | 0.40307 |
| 3.3' | | DIN | | |
| 3.4 | 4/4/o2 | ABD | $0.16207, 0.10173, 0; 0.79229, \frac{1}{8}(33)^{1/2} - \frac{1}{8}$ | 0.31354 |
| 3.4' | | ADI | | |

## Table 1 (continued)

| | | | | |
|---|---|---|---|---|
| 3.5 | 4/6/o2 | ADL | $\frac{1}{8}$, 0.07005, 0.15268; 0.58986, 1.08564 | 0.38484 |
| 3.5′ | | ADN | | |
| n3.1 | $t[6^3]^2$ | ADO | $\frac{1}{10}, \frac{1}{10}, \frac{1}{4}; 1, \frac{1}{5}(10)^{1/2}$ | 0.50579 |

**Pbcn 8d x, y, z**  $\qquad\qquad\qquad\qquad$ $0 \leq \mathbf{x} \leq \frac{1}{4},\, 0 \leq \mathbf{y} \leq \frac{1}{4},\, 0 \leq \mathbf{z} \leq \frac{1}{4}$

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

| | | | | |
|---|---|---|---|---|
| 0.1 | 12/3/h1 | ABCDFJLM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{6}(6)^{1/2}, \frac{1}{2}(3)^{1/2}$ | 0.74048 |
| 0.2 | 12/3/c1 | ABCFGJKLM | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{2}$ | 0.74048 |
| 0.3 | 12/3/c1 | ABDFGMNO | $\frac{1}{8}, \frac{1}{4}, 0; 2, 1$ | 0.74048 |
| 0.4 | 11/3/o2 | ABDEFNO | $\frac{3}{2}(2)^{1/2}-2, \frac{1}{4}, \frac{1}{12}; \frac{2}{3}(6)^{1/2}+(3)^{1/2}, (3)^{1/2}$ | 0.71868 |
| 0.5 | 10/3/o2 | ACDFIJL | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}(6)^{1/2}-\frac{1}{2}; \frac{1}{2}, \frac{1}{2}(3)^{1/2}+\frac{1}{2}(2)^{1/2}$ | 0.66568 |
| 0.6 | 10/3/t1 | BFGHJKM | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{6}(3)^{1/2}$ | 0.69813 |
| 0.7 | 10/3/t1 | BFGHMN | $\frac{1}{8}, \frac{1}{4}, 0; 2, \frac{1}{3}(3)^{1/2}$ | 0.69813 |
| 0.8 | 10/3/t1 | ADFGLMO | $\frac{1}{4}, \frac{1}{8}, 0; \frac{2}{3}(3)^{1/2}, 1$ | 0.69813 |
| 0.9 | 10/3/t1 | ACFGIJKL | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{6}(3)^{1/2}, \frac{1}{2}$ | 0.69813 |
| 0.10 | 10/3/h2 | ADFILP | $0, \frac{1}{6}, \frac{1}{4}(6)^{1/2}-\frac{1}{2}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2}+\frac{2}{3}(2)^{1/2}$ | 0.66568 |
| 0.11 | 9/3/o1 | ADEFOP | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2}-\frac{3}{4}; (3)^{1/2}, 2+(3)^{1/2}$ | 0.64801 |
| 0.12 | 9/3/t2 | ADFLOP | $0, \frac{1}{4}, \frac{1}{4}(2)^{1/2}-\frac{1}{4}; 1, 1+(2)^{1/2}$ | 0.61343 |
| 1.1 | 10/3/o1 | ABCFJLM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{20}; \frac{1}{5}(10)^{1/2}, \frac{1}{6}(15)^{1/2}$ | 0.69813 |
| 1.2 | 10/3/t1 | ABCDLM | $\frac{1}{4}, \frac{1}{8}, 0; \frac{2}{3}(3)^{1/2}, \frac{1}{2}(3)^{1/2}$ | 0.69813 |
| 1.3 | 10/3/t1 | ABDENO | $\frac{1}{8}, \frac{1}{4}, 0; 2(3)^{1/2}, (3)^{1/2}$ | 0.69813 |
| 1.4 | 9/3/o1 | BFHMN | $1-\frac{1}{2}(3)^{1/2}, \frac{1}{4}, \frac{1}{4}; 1+\frac{2}{3}(3)^{1/2}, \frac{1}{3}(3)^{1/2}$ | 0.64801 |
| 1.5 | 9/3/o1 | BDEFN | $1-\frac{1}{2}(3)^{1/2}, \frac{1}{4}, \frac{1}{4}; 2+(3)^{1/2}, (3)^{1/2}$ | 0.64801 |
| 1.6 | 9/3/o1 | DFILP | $0, \frac{1}{4}, \frac{1}{2}(3)^{1/2}-\frac{3}{4}; \frac{1}{3}(3)^{1/2}, 1+\frac{2}{3}(3)^{1/2}$ | 0.64801 |
| 1.7 | 9/3/o5 | ABDFNO | $0.12338, \frac{1}{4}, 0.05627; 2.66256, 1.34858$ | 0.69006 |
| 1.8 | 9/3/t2 | BDFMN | $\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{4}, \frac{1}{4}; 1+(2)^{1/2}, 1$ | 0.61343 |
| 1.9 | 8/3/o1 | ACDFJL | $\frac{1}{4}, \frac{1}{8}, \frac{3}{28}; \frac{1}{7}(21)^{1/2}, \frac{1}{2}(7)^{1/2}$ | 0.60460 |
| 1.10 | 8/3/o2 | ADFLP | $0, \frac{7}{32}, \frac{3}{28}; \frac{2}{3}(3)^{1/2}, \frac{7}{8}(7)^{1/2}$ | 0.60460 |
| 1.11 | 8/3/o7 | ABDFM | $0.16378, 0.15199, 0.07041; 1.34741, 0.91995$ | 0.56637 |
| 1.12 | 8/3/o8 | ADFLM | $0.17344, 0.18988, .04847; 1.00030, 0.97065$ | 0.61693 |
| 1.13 | 8/3/o9 | ADFIL | $\frac{1}{8}, \frac{3}{20}, \frac{1}{9}; \frac{2}{15}(15)^{1/2}, \frac{9}{5}$ | 0.62056 |
| 1.14 | 8/3/t1 | ABDEF | $\frac{1}{8}, 0, \frac{1}{8}; 2(3)^{1/2}, 2$ | 0.60460 |
| 1.15 | 8/3/t4 | BFGHM | $\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, 0; 1, \frac{2}{3}(3)^{1/2}-\frac{1}{6}(6)^{1/2}$ | 0.47912 |
| 1.16 | 8/3/h3 | ACFIJL | $\frac{1}{4}, \frac{1}{8}, \frac{1}{12}; \frac{1}{3}, \frac{1}{2}(3)^{1/2}$ | 0.53742 |
| 1.17 | 8/3/h4 | BFHJM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{1}{6}(3)^{1/2}$ | 0.60460 |
| 1.18 | 8/3/h4 | DFIJL | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}, (3)^{1/2}$ | 0.60460 |
| 1.19 | 8/3/h4 | DFJLM | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$ | 0.60460 |
| 1.20 | 8/3/h4 | ABCDFJ | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$ | 0.60460 |
| 1.21 | 8/3/h4 | BDFJM | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{2}(3)^{1/2}$ | 0.60460 |
| 1.22 | 8/3/h4 | ADFIP | $0, 0, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, \frac{4}{3}(3)^{1/2}$ | 0.60460 |
| 1.23 | 8/3/h4 | ACDFIJ | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}, (3)^{1/2}$ | 0.60460 |
| 1.24 | 8/3/h4 | ADEFP | $0, 0, \frac{1}{8}; (3)^{1/2}, 4$ | 0.60460 |
| 1.25 | 8/4/c1 | ACFGJKL | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{4}(2)^{1/2}, \frac{1}{2}$ | 0.68017 |
| 1.26 | 8/4/c1 | ADFGMO | $\frac{1}{8}, \frac{1}{4}, 0; (2)^{1/2}, 1$ | 0.68017 |
| 1.27 | 8/4/c1 | BFGJKM | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{4}(2)^{1/2}$ | 0.68017 |
| 1.28 | 8/4/c1 | BFGMN | $\frac{1}{8}, \frac{1}{4}, 0; 2, \frac{1}{2}(2)^{1/2}$ | 0.68017 |
| 1.29 | 7/3/o1 | AFGIL | $0, 1-\frac{1}{3}(3)^{1/2}, 0; 2-(3)^{1/2}, 4-2(3)^{1/2}$ | 0.56119 |
| 1.30 | 7/3/o9 | ADFLO | $\frac{3}{4}-\frac{1}{4}(7)^{1/2}, \frac{1}{4}, \frac{1}{12}; \frac{1}{3}[5+2(7)^{1/2}]^{1/2}, (3)^{1/2}$ | 0.50736 |
| 1.31 | 7/3/o10 | ADEFO | $\frac{3}{4}-\frac{1}{4}(7)^{1/2}, \frac{1}{4}, \frac{1}{3}-\frac{1}{12}(7)^{1/2}; \frac{1}{3}[33+12(7)^{1/2}]^{1/2}, [5+2(7)^{1/2}]^{1/2}$ | 0.48680 |
| 1.32 | 7/3/o13 | AFGLM | $0.14855, 0.16950, 0; 0.74185, 0.67802$ | 0.55058 |
| 1.33 | 7/3/t6 | ABFGM | $\frac{1}{2}-\frac{1}{4}(2)^{1/2}, \frac{1}{2}-\frac{1}{4}(2)^{1/2}, 0; 1, 2-(2)^{1/2}$ | 0.50819 |
| 1.34 | 7/4/o1 | ADFOP | $0, \frac{1}{4}, \frac{1}{24}(13)^{1/2}-\frac{1}{24}; \frac{1}{6}[30+6(13)^{1/2}]^{1/2}, [4+(13)^{1/2}]^{1/2}$ | 0.60210 |
| 1.35 | 6/4/c1 | AFGLO | $0, \frac{1}{4}, 0; 1, 1$ | 0.52360 |
| 2.1 | 8/4/c1 | ABCLM | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.68017 |
| 2.2 | 8/4/c1 | ABDNO | $\frac{1}{8}, \frac{1}{4}, 0; 2(2)^{1/2}, (2)^{1/2}$ | 0.68017 |
| 2.3 | 7/3/o1 | ABDE | $1-\frac{1}{2}(3)^{1/2}, 0, 0; (3)^{1/2}+2, 2$ | 0.56119 |
| 2.4 | 7/3/o1 | BDEF | $1-\frac{1}{2}(3)^{1/2}, 0, \frac{1}{4}; (3)^{1/2}+2, 2$ | 0.56119 |
| 2.5 | 7/3/o2 | BFHM | $\frac{7}{8}-\frac{1}{8}(33)^{1/2}, \frac{15}{64}-\frac{1}{64}(3)^{1/2}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}+\frac{1}{8}(11)^{1/2}, \frac{5}{16}(3)^{1/2}-\frac{1}{16}(11)^{1/2}$ | 0.43908 |
| 2.6 | 7/3/o3 | BDFM | $\frac{3}{2}-\frac{1}{2}(7)^{1/2}, \frac{4}{9}-\frac{1}{9}(7)^{1/2}, \frac{1}{4}; \frac{1}{3}(7)^{1/2}+\frac{2}{3}, \frac{2}{9}[14(7)^{1/2}-20]^{1/2}$ | 0.48680 |

**Table 1** (continued)

| | | | | |
|---|---|---|---|---|
| 2.7 | 7/3/o11 | *DFIL* | 0.15994, $\frac{1}{4}$, 0.11939; 0.50831, 1.84364 | 0.58705 |
| 2.8 | 7/3/o12 | *DFLM* | 0.20293, $\frac{1}{4}$, 0.08603; 0.95602, 1 | 0.57451 |
| 2.9 | 7/3/o13 | *ABDM* | 0.16950, 0.14855, 0; 1.34798, 0.91396 | 0.55058 |
| 2.10 | 7/3/t8 | *ADLM* | $\frac{1}{4}(3)^{1/2} - \frac{1}{4}$, $\frac{1}{4}(3)^{1/2} - \frac{1}{4}$, 0; 1, $[4(3)^{1/2} - 6]^{1/2}$ | 0.60304 |
| 2.11 | 7/4/o1 | *BDFN* | $\frac{7}{24} - \frac{1}{24}(13)^{1/2}$, $\frac{1}{4}$, $\frac{1}{4}$, $[4 + (13)^{1/2}]^{1/2}$, $\frac{1}{6}[30 + 6(13)^{1/2}]^{1/2}$ | 0.60210 |
| 2.12 | 7/4/o1 | *BFMN* | $\frac{7}{24} - \frac{1}{24}(13)^{1/2}$, $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{2}(13)^{1/2} + \frac{1}{2}$, $\frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}$ | 0.60210 |
| 2.13 | 7/4/o1 | *DFLP* | $0$, $\frac{1}{4}$, $\frac{1}{24}(13)^{1/2} - \frac{1}{24}$; $\frac{1}{2}[10 - 2(13)^{1/2}]^{1/2}$, $\frac{1}{2}(13)^{1/2} + \frac{1}{2}$ | 0.60210 |
| 2.14 | 6/3/o1 | *ADEF* | $\frac{11}{8} - \frac{1}{8}(105)^{1/2}$, 0, $\frac{1}{8}$; $\frac{1}{4}[62 + 6(105)^{1/2}]^{1/2}$, $\frac{1}{2}[26 + 2(105)^{1/2}]^{1/2}$ | 0.44226 |
| 2.15 | 6/3/o1 | *ABDF* | $\frac{1}{8}(105)^{1/2} - \frac{9}{8}$, 0, $\frac{1}{8}$; $\frac{1}{4}[22 + 2(105)^{1/2}]^{1/2}$, $\frac{1}{2}[26 - 2(105)^{1/2}]^{1/2}$ | 0.44226 |
| 2.16 | 6/3/o2 | *AFIL* | $0$, $\frac{19}{64} - \frac{1}{64}(105)^{1/2}$, $\frac{1}{16}(105)^{1/2} - \frac{9}{16}$; $\frac{1}{4}(15)^{1/2} - \frac{1}{4}(7)^{1/2}$, $\frac{3}{16}(15)^{1/2} + \frac{1}{16}(7)^{1/2}$ | 0.50712 |
| 2.17 | 6/3/o12 | *ABFM* | 0.14999, 0.14584, 0.01179; 1.02056, 0.61297 | 0.50712 |
| 2.18 | 6/3/o13 | *ADFL* | $\frac{1}{8}$, $\frac{1}{5}$, $\frac{3}{32}$; $\frac{2}{5}(5)^{1/2}$, $\frac{8}{5}$ | 0.48096 |
| 2.19 | 6/3/o14 | *AFLM* | 0.14872, 0.16950, 0.00023; 0.74226, 0.67862 | 0.55058 |
| 2.20 | 6/4/o4 | *ADFM* | 0.16363, 0.15451, 0.06910; 1.33748, 0.92418 | 0.56628 |
| 2.21 | 6/4/t2 | *ADFI* | $\frac{1}{8}$, 0, $\frac{1}{8}$; $\frac{2}{15}(15)^{1/2}$, 2 | 0.55851 |
| 2.22 | 6/4/t6 | *BFGM* | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0; 1, $(2)^{1/2} - 1$ | 0.46680 |
| 2.23 | 6/4/h2 | *ACFJL* | $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{12}$; $\frac{1}{6}(6)^{1/2}$, $\frac{1}{2}(3)^{1/2}$ | 0.52360 |
| 2.24 | 6/4/c1 | *BFJM* | $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{4}$; $\frac{1}{2}(2)^{1/2}$, $\frac{1}{2}$ | 0.52360 |
| 2.25 | 6/4/c1 | *ABCD* | $\frac{1}{4}$, 0, 0; 1, 1 | 0.52360 |
| 2.26 | 6/4/c1 | *BDFJ* | $\frac{1}{4}$, 0, $\frac{1}{4}$; 1, 1 | 0.52360 |
| 2.27 | 6/4/c1 | *DFJM* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; 1, 1 | 0.52360 |
| 2.28 | 6/4/c1 | *ACDFJ* | $\frac{1}{4}$, 0, $\frac{1}{8}$; $\frac{1}{2}(2)^{1/2}$, $(2)^{1/2}$ | 0.52360 |
| 2.29 | 6/4/c1 | *ADFP* | 0, 0, $\frac{1}{8}$; 1, $2(2)^{1/2}$ | 0.52360 |
| 2.30 | 6/4/c1 | *DFJL* | $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{8}$; $\frac{1}{2}(2)^{1/2}$, $(2)^{1/2}$ | 0.52360 |
| 2.31 | 5/4/o7 | *ADFO* | $\frac{3}{32}$, $\frac{1}{4}$, $\frac{1}{10}$; $\frac{4}{5}(5)^{1/2}$, $(5)^{1/2}$ | 0.44179 |
| 2.32 | 5/4/o10 | *AFGM* | 0.14555, 0.15165, 0; 0.97034, 0.60660 | 0.50664 |
| 2.33 | 5/4/t6 | *AFLO* | 0, $\frac{1}{4}$, $\frac{1}{16}$; 1, $(2)^{1/2}$ | 0.44179 |
| 2.34 | 5/4/h5 | *AFGL* | 0, $\frac{1}{6}$, 0; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}$ | 0.40307 |
| 3.1 | 6/4/c1 | *DLM* | $\frac{1}{4}$, $\frac{1}{4}$, 0; 1, 1 | 0.52360 |
| 3.2 | 5/4/o1 | *BFM* | $\frac{1}{6}$, $\frac{1}{7}$, $\frac{1}{4}$; $\frac{3}{7}(7)^{1/2}$, $\frac{2}{7}(3)^{1/2}$ | 0.40307 |
| 3.3 | 5/4/o8 | *DFL* | 0.14839, $\frac{1}{4}$, 0.10161; 0.84322, 1.56860 | 0.46761 |
| 3.4 | 5/4/o10 | *ABM* | 0.15165, 0.14555, 0; 1.03056, 0.62514 | 0.50664 |
| 3.5 | 5/4/o11 | *ALM* | 0.14882, 0.16949, 0; 0.74248, 0.67895 | 0.55058 |
| 3.6 | 5/4/o11 | *ADM* | 0.16949, 0.14882, 0; 1.34684, 0.91443 | 0.55058 |
| 3.7 | 5/4/t6 | *DFM* | $\frac{3}{16}$, $\frac{1}{4}$, $\frac{1}{4}$; $(2)^{1/2}$, 1 | 0.44179 |
| 3.8 | 5/4/h5 | *BDF* | $\frac{1}{6}$, 0, $\frac{1}{4}$; $(3)^{1/2}$, $\frac{2}{3}(3)^{1/2}$ | 0.40307 |
| 3.9 | 5/4/h5 | *ABD* | $\frac{1}{6}$, 0, 0; $(3)^{1/2}$, $\frac{2}{3}(3)^{1/2}$ | 0.40307 |
| 3.10 | 4/6/o3 | *AFM* | 0.14849, 0.15056, 0.00847; 0.98975, 0.62374 | 0.50607 |
| 3.11 | 4/6/h2 | *AFL* | 0, $\frac{1}{6}$, $\frac{1}{16}$; $\frac{1}{3}(3)^{1/2}$, $\frac{2}{3}(2)^{1/2}$ | 0.34009 |
| 3.12 | 4/6/c1 | *ADF* | $\frac{1}{8}$, 0, $\frac{1}{8}$; $(2)^{1/2}$, 2 | 0.34009 |
| n4.1 | $t[6^3]^2$ | *AM* | $\frac{3}{20}$, $\frac{3}{20}$, 0; 1, $\frac{1}{5}(10)^{1/2}$ | 0.50579 |

***Pbca 8c x, y, z***   $0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}, a \leq b, c \leq b$

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

| | | | | |
|---|---|---|---|---|
| 0.1 | 12/3/h1 | *ABCEGIJ* | $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{12}$; $\frac{1}{6}(6)^{1/2}$, $\frac{1}{2}(3)^{1/2}$ | 0.74048 |
| 0.2 | 12/3/c1 | *ABCGHIJ* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{2}$ | 0.74048 |
| 0.3 | 11/3/o2 | *ABDGHI* | $\frac{1}{6}$, $\frac{1}{2}(2)^{1/2} - 2$, 0; $9 - 6(2)^{1/2}$, $3(3)^{1/2} - 2(6)^{1/2}$ | 0.71868 |
| 0.4 | 10/3/o2 | *ABDGIL* | $\frac{1}{8}$, $\frac{1}{4}(6)^{1/2} - \frac{1}{2}$, $\frac{1}{4}$; $2(3)^{1/2} - 2(2)^{1/2}$, $(3)^{1/2} - (2)^{1/2}$ | 0.66568 |
| 0.5 | 10/3/t1 | *ACFGHJ* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{6}(3)^{1/2}$, $\frac{1}{2}$ | 0.69813 |
| 1.1 | 10/3/o1 | *ABCGIJ* | $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{20}$; $\frac{1}{5}(10)^{1/2}$, $\frac{1}{6}(15)^{1/2}$ | 0.69813 |
| 1.2 | 10/3/t1 | *BDGHI* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}$, $\frac{1}{6}(3)^{1/2}$ | 0.69813 |
| 1.3 | 10/3/t1 | *ABCEIJ* | $\frac{1}{4}$, $\frac{1}{8}$, 0; $\frac{1}{2}(3)^{1/2}$, $\frac{1}{2}(3)^{1/2}$ | 0.69813 |
| 1.4 | 9/3/o1 | *ADGHI* | $0$, $1 - \frac{1}{2}(3)^{1/2}$, 0; $2(3)^{1/2} - 3$, $2 - (3)^{1/2}$ | 0.64801 |
| 1.5 | 9/3/o1 | *AFGHJ* | $0$, $1 - \frac{1}{2}(3)^{1/2}$, 0; $2 - (3)^{1/2}$, $2(3)^{1/2} - 3$ | 0.64801 |
| 1.6 | 9/3/o5 | *ABGHI* | 0.19373, 0.12338, 0; 0.50650, 0.37558 | 0.69006 |
| 1.7 | 9/3/o6 | *ABEGI* | 0.18166, 0.11583, 0.16458; 0.99079, 0.88619 | 0.66314 |
| 1.7' | | *AEGIJ* | | |
| 1.8 | 9/3/o7 | *ABDGI* | $\frac{7}{24} - \frac{1}{24}(13)^{1/2}$, $\frac{5}{12} - \frac{1}{12}(13)^{1/2}$, $\frac{5}{8} - \frac{1}{8}(13)^{1/2}$; $\frac{1}{6}[42(13)^{1/2} - 138]^{1/2}$, $\frac{1}{9}[51 - 12(13)^{1/2}]^{1/2}$ | 0.65469 |
| 1.9 | 9/3/t2 | *AGHIJ* | $0$, $\frac{1}{2} - \frac{1}{4}(2)^{1/2}$, 0; $(2)^{1/2} - 1$, $(2)^{1/2} - 1$ | 0.61343 |

**Table 1 (continued)**

| | | | | |
|---|---|---|---|---|
| 1.10 | 8/3/o1 | ABGIL | $\frac{1}{8}, \frac{3}{28}, \frac{1}{4}; \frac{2}{7}(7)^{1/2}, \frac{2}{7}(3)^{1/2}$ | 0.60460 |
| 1.10′ | | ACEGJ | | |
| 1.11 | 8/3/h3 | ACFGJ | $\frac{1}{4}, \frac{1}{8}, \frac{1}{12}; \frac{1}{3}, \frac{1}{2}(3)^{1/2}$ | 0.53742 |
| 1.11′ | | ABDIL | | |
| 1.12 | 8/3/h4 | ABCEG | $\frac{1}{4}, 0, \frac{1}{8}; \frac{1}{2}(3)^{1/2}, 1$ | 0.60460 |
| 1.12′ | | AGILM | $0, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{2}(3)^{1/2}$ | |
| 1.13 | 8/3/h4 | ADGIL | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{1}{6}(3)^{1/2}$ | 0.60460 |
| 1.14 | 8/4/c1 | ACGHJ | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{4}(2)^{1/2}, \frac{1}{2}$ | 0.68017 |
| 2.1 | 8/3/h4 | BDGI | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{1}{6}(3)^{1/2}$ | 0.60460 |
| 2.2 | 8/3/h4 | BEGI | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{2}(3)^{1/2}$ | 0.60460 |
| 2.2′ | | EGIJ | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(3)^{1/2}, 1$ | |
| 2.3 | 8/4/c1 | ABCIJ | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.68017 |
| 2.4 | 8/4/c1 | BGHI | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{4}(2)^{1/2}$ | 0.68017 |
| 2.5 | 7/3/o9 | AGIJ | $0, \frac{1}{6}, \frac{3}{4} - \frac{1}{4}(7)^{1/2}; \frac{1}{3}(3)^{1/2}, \frac{1}{9}[6(7)^{1/2} + 15]^{1/2}$ | 0.50736 |
| 2.5′ | | ABEI | | |
| 2.6 | 7/3/o10 | AFGJ | $0, \frac{1}{12}(7)^{1/2} - \frac{1}{12}, \frac{3}{4} - \frac{1}{4}(7)^{1/2}; \frac{1}{3}[6(7)^{1/2} - 15]^{1/2}, \frac{1}{3}[2(7)^{1/2} + 1]^{1/2}$ | 0.48680 |
| 2.6′ | | ABDI | | |
| 2.7 | 7/3/o11 | ADGI | $0, 0.13061, 0.15994; 0.54240, 0.27571$ | 0.58705 |
| 2.8 | 7/3/o12 | ABEG | $0.20293, 0, \frac{1}{32}(105)^{1/2} - \frac{5}{32}; 0.95602, 1$ | 0.57451 |
| 2.8′ | | AGIM | $0, \frac{1}{32}(105)^{1/2} - \frac{5}{32}, 0.20293; 1, 0.95602$ | |
| 2.8′ | | AEIJ | | |
| 2.9 | 7/3/o16 | ABGI | $0.16160, 0.11690, \frac{1}{32}(105)^{1/2} - \frac{5}{32}; 0.71980, 0.51594$ | 0.57451 |
| 2.9′ | | AEGJ | | |
| 2.10 | 7/4/o1 | AGHI | $0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{6}(13)^{1/2} - \frac{1}{6}, \frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}$ | 0.60210 |
| 2.11 | 7/4/o1 | AGHJ | $0, \frac{7}{24} - \frac{1}{24}(13)^{1/2}, 0; \frac{1}{3}[12 - 3(13)^{1/2}]^{1/2}, \frac{1}{6}(13)^{1/2} - \frac{1}{6}$ | 0.60210 |
| 2.12 | 7/4/c1 | AEGI | $0.15451, 0.15451, 0.15451; 1, 1$ | 0.64227 |
| 2.13 | 6/4/h2 | ACGJ | $\frac{1}{4}, \frac{1}{8}, \frac{1}{12}; \frac{1}{6}(6)^{1/2}, \frac{1}{2}(3)^{1/2}$ | 0.52360 |
| 2.13′ | | ABIL | | |
| 2.14 | 6/4/c1 | ABCE | $\frac{1}{4}, 0, 0; 1, 1$ | 0.52360 |
| 2.14′ | | AIJK | $0, \frac{1}{4}, 0; 1, 1$ | |
| 2.14′ | | AGLM | $0, 0, \frac{1}{4}; 1, 1$ | |
| 2.15 | 6/4/c1 | AGIL | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}$ | 0.52360 |
| 2.15′ | | ACEG | | |
| 3.1 | 6/4/c1 | EIJ | $\frac{1}{4}, \frac{1}{4}, 0; 1, 1$ | 0.52360 |
| 3.1′ | | BEG | $\frac{1}{4}, 0, \frac{1}{4}; 1, 1$ | |
| 3.1′ | | GIM | $0, \frac{1}{4}, \frac{1}{4}; 1, 1$ | |
| 3.2 | 6/4/c1 | BGI | $\frac{1}{4}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}$ | 0.52360 |
| 3.2′ | | EGJ | | |
| 3.3 | 6/4/c1 | EGI | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; 1, 1$ | 0.52360 |
| 3.4 | 5/4/o7 | AGJ | $0, \frac{3}{20}, \frac{3}{32}; \frac{1}{5}(5)^{1/2}, \frac{4}{5}$ | 0.44179 |
| 3.4′ | | ABI | | |
| 3.5 | 5/4/o8 | AGI | $0, 0.14840, 0.14840; 0.63751, 0.53756$ | 0.46761 |
| 3.5′ | | AEG, AEI | | |
| 3.6 | 5/4/t6 | AIJ | $0, \frac{3}{16}, 0; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2}$ | 0.44179 |
| 3.6′ | | ABE | | |

***Ccce* 16*i* *x*, *y*, *z***

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | $0 \le x \le \frac{1}{4}, 0 \le y \le \frac{1}{4}, 0 \le z \le \frac{1}{4}; a \le b$ | | | |
| A | $x, -y, -z$ | | G | $-x + \frac{1}{2}, -y + \frac{1}{2}, z$ | | M | $-x + \frac{1}{2}, -y - \frac{1}{2}, z$ |
| B | $-x, y, -z$ | | H | $x, -y + \frac{1}{2}, z + \frac{1}{2}$ | | N | $x + \frac{1}{2}, y, -z + \frac{1}{2}$ |
| C | $-x, -y, z$ | | | $x, -y + \frac{1}{2}, z - \frac{1}{2}$ | | | $x - \frac{1}{2}, y, -z + \frac{1}{2}$ |
| D | $-x + \frac{1}{2}, y, z + \frac{1}{2}$ | | I | $-x + 1, -y, z$ | | O | $-x, -y + \frac{1}{2}, -z + \frac{1}{2}$ |
| | $-x + \frac{1}{2}, y, z - \frac{1}{2}$ | | J | $x + 1, y, z$ | | P | $-x, y, -z + 1$ |
| E | $-x + 1, y, -z$ | | | $x - 1, y, z$ | | Q | $x, -y, -z + 1$ |
| F | $x, y, z + 1$ | | K | $-x - \frac{1}{2}, -y + \frac{1}{2}, z$ | | R | $-x, -y + 1, z$ |
| | $x, y, z - 1$ | | L | $-x + \frac{1}{2}, -y, -z + \frac{1}{2}$ | | | |
| 0.1 | 12/3/c1 | ABCDGHLOPQ | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{2}$ | 0.74048 |
| 0.2 | 10/3/t1 | BCDGLNOP | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; \frac{1}{3}(3)^{1/2}, \frac{1}{2}$ | 0.69813 |
| 0.3 | 10/3/t1 | ABDFHPQ | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{6}(3)^{1/2}$ | 0.69813 |
| 0.4 | 9/3/o1 | ABDEGLN | $\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{8}; 2(3)^{1/2} - 3, 4 - 2(3)^{1/2}$ | 0.64801 |
| 0.5 | 9/3/o1 | BCEGIJN | $\frac{1}{4}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{1}{8}; 2 - (3)^{1/2}, 4(3)^{1/2} - 6$ | 0.64801 |
| 0.6 | 9/3/t2 | ABCEGILN | $\frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{8}; (2)^{1/2} - 1, 2(2)^{1/2} - 2$ | 0.61343 |
| 0.7 | 8/3/t5 | BCGJKN | $0, 1 - \frac{1}{2}(3)^{1/2}, 1 - \frac{1}{2}(3)^{1/2}; 2 - (3)^{1/2}, 1$ | 0.60148 |
| 0.8 | 7/3/t7 | BCGKNO | $0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}; (2)^{1/2} - 1, 1$ | 0.50819 |
| 0.9 | 6/4/c1 | ACGILM | $\frac{1}{4}, 0, \frac{1}{8}; 1, 2$ | 0.52360 |
| 0.10 | 6/4/c1 | BCGKOR | $0, \frac{1}{4}, \frac{1}{8}; 1, 2$ | 0.52360 |
| 1.1 | 8/3/t5 | ABDFH | $1 - \frac{1}{2}(3)^{1/2}, 1 - \frac{1}{2}(3)^{1/2}, 0; 1, 2 - (3)^{1/2}$ | 0.60148 |

**Table 1 (continued)**

| | | | | |
|---|---|---|---|---|
| 1.2 | 8/4/c1 | BCDGLOP | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}$ | 0.68017 |
| 1.3 | 8/4/c1 | ABDHPQ | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; 1, \frac{1}{4}(2)^{1/2}$ | 0.68017 |
| 1.4 | 7/3/o17 | BDGLN | 0.19179, 0.12200, 0.17441; 0.50181, 0.51198 | 0.59030 |
| 1.5 | 7/3/o18 | BCGJN | 0.08460, 0.12771, 0.13307; 0.25916, 0.95974 | 0.58629 |
| 1.6 | 7/3/t7 | ABDGH | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0; 1, (2)^{1/2} - 1$ | 0.50819 |
| 1.7 | 7/4/o1 | ABEGLN | $\frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}, \frac{1}{8}; \frac{1}{6}(13)^{1/2} - \frac{1}{6}, \frac{2}{3}[12-3(13)^{1/2}]^{1/2}$ | 0.60210 |
| 1.8 | 7/4/o1 | BCEGIN | $\frac{1}{4}, \frac{1}{24}(13)^{1/2} - \frac{1}{24}, \frac{1}{8}; \frac{1}{3}[12-3(13)^{1/2}]^{1/2}, \frac{1}{3}(13)^{1/2} - \frac{1}{3}$ | 0.60210 |
| 1.9 | 6/3/o15 | ABDGL | 0.17511, 0.11878, 0.14373; 0.67829, 0.52489 | 0.52446 |
| 1.10 | 6/3/o16 | BCGLN | $\frac{1}{4}(7)^{1/2} - \frac{1}{2}, \frac{1}{2}(3)^{1/2} - \frac{3}{4}, \frac{3}{8} - \frac{1}{8}(3)^{1/2}; \frac{1}{3}[105 - 60(3)^{1/2} + 42(7)^{1/2} - 24(21)^{1/2}]^{1/2}, (3)^{1/2} - 1$ | 0.51712 |
| 1.11 | 6/3/o17 | BCGNO | 0.07047, 0.13708, 0.15954; 0.47075, 0.85926 | 0.46487 |
| 1.12 | 6/4/t7 | BCGKN | [0, 0.14, 0.14; 0.34641, 1] | >0.50819 |
| 1.13 | 6/4/c1 | ABDEG | $\frac{1}{4}, \frac{1}{8}, 0; \frac{1}{2}, \frac{1}{2}$ | 0.52360 |
| 1.14 | 6/4/c1 | BCNOP | $0, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}$ | 0.52360 |
| 1.15 | 5/3/o2 | ABCGL | 0.15612, 0.10965, 0.13897; 0.70236, 0.78903 | 0.45095 |
| 1.16 | 5/4/o9 | BCGKO | 0, 0.17812, 0.13055; 0.65186, 1.36432 | 0.42583 |
| 1.17 | 5/4/t6 | ACGIL | $\frac{1}{4}, \frac{1}{16}, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, (2)^{1/2}$ | 0.44179 |
| 2.1 | 6/4/t7 | ABDH | [0.14, 0.14, 0; 1, 0.34641] | >0.50819 |
| 2.2 | 6/4/c1 | DGLN | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}$ | 0.52360 |
| 2.3 | 5/4/o14 | BCGN | 0.08586, 0.13284, 0.15511; 0.44754, 0.85644 | 0.46239 |
| 2.4 | 5/4/o15 | BDGL | 0.15884, 0.12245, 0.18; 0.68053 0.51020 | >0.52446 |
| 2.5 | 5/4/o16 | BGLN | [0.23454, 0.10864, 0.13; 0.43539, 0.75374] | >0.51712 |
| 2.6 | 5/4/o9 | ABDG | 0.17812, 0.13055, 0; 0.73297, 0.47779 | 0.42583 |
| 2.7 | 5/4/o9 | BCNO | 0, 0.13055, 0.17812; 0.47779, 0.73297 | 0.42583 |
| 2.8 | 4/4/o7 | BCGO | 0.07388, 0.16794, 0.13351; 0.91649, 1.25784 | 0.34516 |
| 2.8′ | | ACGL | | |
| 2.9 | 4/4/o8 | BCGL | [0.14640, 0.11354, 0.15; 0.73184, 0.75694] | >0.45095 |
| 2.10 | 4/4/o9 | ABGL | [0.20218, 0.11629, 0.13; 0.57518, 0.55] | >0.45095 |
| i3.1 | o[3/10/o1]² | BGL | [0.14451, 0.12, 0.17195; 0.69883, 0.64065] | >0.45095 |

**Fddd 32h x, y, z**        $0 \leq x \leq \frac{1}{8}, 0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{2}; a \leq b \leq c$

| | | | | |
|---|---|---|---|---|
| A | $-x, y, -z$ | I | $-x + \frac{1}{2}, -y + \frac{1}{2}, z$ | P   $x, -y, -z$ |
| B | $-x, -y, z$ | J | $-x - \frac{1}{2}, -y + \frac{1}{2}, z$ | Q   $x, -y, -z + 1$ |
| C | $-x, y, -z + 1$ | K | $x, -y + \frac{1}{2}, -z + \frac{1}{2}$ | R   $-x + \frac{3}{4}, -y + \frac{1}{4}, -z + \frac{3}{4}$ |
| D | $-x + \frac{1}{4}, -y + \frac{1}{4}, -z + \frac{1}{4}$ | L | $x + \frac{1}{4}, y + \frac{1}{4}, -z + \frac{1}{4}$ | S   $-x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$ |
| E | $x + 1, y, z$ | | $x - \frac{1}{4}, y - \frac{1}{4}, -z + \frac{1}{4}$ |    $-x + \frac{1}{4}, y - \frac{1}{4}, z - \frac{1}{4}$ |
| | $x - 1, y, z$ | M | $-x - \frac{1}{4}, -y + \frac{3}{4}, -z + \frac{1}{4}$ | T   $x - \frac{1}{4}, -y + \frac{1}{4}, z - \frac{1}{4}$ |
| F | $-x + \frac{1}{2}, y, -z + \frac{1}{2}$ | N | $x + \frac{1}{4}, y - \frac{1}{4}, -z + \frac{3}{4}$ |    $x + \frac{1}{4}, -y + \frac{1}{4}, z + \frac{1}{4}$ |
| G | $-x - \frac{1}{2}, y, -z + \frac{1}{2}$ | | $x - \frac{1}{4}, y + \frac{1}{4}, -z + \frac{3}{4}$ | U   $-x, -y + 1, z$ |
| H | $-x - \frac{1}{4}, -y + \frac{1}{4}, -z + \frac{3}{4}$ | O | $-x + \frac{1}{4}, -y + \frac{3}{4}, -z + \frac{3}{4}$ | |

| | | | | |
|---|---|---|---|---|
| 0.1 | 12/3/c1 | BCFIKNQST | $\frac{1}{8}, \frac{1}{8}, \frac{3}{8}; 1, 1$ | 0.74048 |
| 0.2 | 10/3/t1 | BCFHINRT | $\frac{1}{8}, \frac{1}{8}, \frac{3}{8}; \frac{1}{3}(3)^{1/2}, 1$ | 0.69813 |
| 0.3 | 9/3/t2 | ABDIJLMU | $0, \frac{1}{4}, \frac{1}{4} - \frac{1}{8}(2)^{1/2}; 1, 2 + (2)^{1/2}$ | 0.61343 |
| (0.3) | | BCHIJNOU | $0, \frac{1}{4}, \frac{1}{4} + \frac{1}{8}(2)^{1/2}; 1, 2 + (2)^{1/2}$ | |
| 0.3′ | | BDIJKLMU | $0, \frac{1}{4}, \frac{1}{8}(2)^{1/2}; 1, 2 + (2)^{1/2}$ | 0.61343 |
| 0.3′ | | BHIJKNOU | $0, \frac{1}{4}, \frac{1}{2} - \frac{1}{8}(2)^{1/2}; 1, 2 + (2)^{1/2}$ | |
| 0.4 | 8/3/o10 | BDEFGIJ | $0, 1 - \frac{1}{2}(3)^{1/2}, 0.19091; 2 - (3)^{1/2}, -6 - (2)^{1/2} + (6)^{1/2} + 4(3)^{1/2}$ | 0.61267 |
| 0.4′ | | BEFGHIJ | $0, 1 - \frac{1}{2}(3)^{1/2}, 0.30909; 2 - (3)^{1/2}, -6 - (2)^{1/2} + (6)^{1/2} + 4(3)^{1/2}$ | |
| 0.5 | 8/3/o11 | BFHKNT | 0.09209, 0.13954, 0.35639; 0.69950, 1.00441 | 0.69256 |
| 0.6 | 8/3/t15 | FHIKNT | 0.09354, 0.14191, 0.35809; 0.69089, 1 | 0.69309 |
| 0.7 | 8/3/t16 | BCHKNT | 0.08885, 0.14079, 0.35921; 0.71462, 1 | 0.69103 |
| 0.8 | 8/3/h4 | ADIJKLM | $0, \frac{1}{4}, \frac{1}{8}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2}$ | 0.60460 |
| (0.8) | | CHIJKNO | $0, \frac{1}{4}, \frac{3}{8}; \frac{1}{3}(3)^{1/2}, \frac{2}{3}(3)^{1/2}$ | |
| 0.9 | 7/3/o19 | ABDEIJ | $0, 1 - \frac{1}{2}(3)^{1/2}, 0.06358; 2 - (3)^{1/2}, 8 - (2)^{1/2} - 4(3)^{1/2} + (6)^{1/2}$ | 0.57092 |
| 0.9′ | | BCEHIJ | $0, 1 - \frac{1}{2}(3)^{1/2}, 0.43242; 2 - (3)^{1/2}, 8 - (2)^{1/2} - 4(3)^{1/2} + (6)^{1/2}$ | |
| 0.10 | 7/3/o20 | BDFGIJK | $0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0.19581; (2)^{1/2} - 1, 1.91082$ | 0.53190 |
| 0.10′ | | BFGHIJK | $0, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, 0.30419; (2)^{1/2} - 1, 1.91082$ | |
| 0.11 | 7/3/o21 | BFHIKN | 0.09274, 0.14061, 0.35001; 0.69562, 1.09380 | 0.65226 |
| 0.12 | 7/3/o22 | BCEHIR | $\frac{1}{8}, \frac{1}{8}, \frac{1}{4}(5)^{1/2} - \frac{1}{8}; \frac{1}{15}(5)^{1/2}, 1 + \frac{2}{5}(5)^{1/2}$ | 0.58963 |
| 0.12′ | | BEFHIR | $\frac{1}{8}, \frac{1}{8}, \frac{7}{8} - \frac{1}{4}(5)^{1/2}; \frac{1}{15}(5)^{1/2}, 1 + \frac{2}{5}(5)^{1/2}$ | |
| 1.1 | 8/4/c1 | BCFINT | $\frac{1}{8}, \frac{1}{8}, \frac{3}{8}; \frac{1}{2}(2)^{1/2}, 1$ | 0.68017 |
| 1.2 | 7/3/o5 | ADIJLM | $0, \frac{1}{4}, \frac{3}{4} - \frac{1}{4}(7)^{1/2}; \frac{1}{3}[6(7)^{1/2} - 12]^{1/2}, \frac{1}{3}[6(7)^{1/2} + 15]^{1/2}$ | 0.48680 |
| (1.2) | | CHIJNO | $0, \frac{1}{4}, \frac{1}{4}(7)^{1/2} - \frac{1}{4}; \frac{1}{3}[6(7)^{1/2} - 12]^{1/2}, \frac{1}{3}[6(7)^{1/2} + 15]^{1/2}$ | |
| 1.3 | 7/3/o5 | DIJKLM | $0, \frac{1}{4}, \frac{1}{4}(7)^{1/2} - \frac{1}{2}; \frac{1}{3}[6(7)^{1/2} - 12]^{1/2}, \frac{1}{3}[6(7)^{1/2} + 15]^{1/2}$ | 0.48680 |
| (1.3) | | HIJKNO | $0, \frac{1}{4}, 1 - \frac{1}{4}(7)^{1/2}; \frac{1}{3}[6(7)^{1/2} - 12]^{1/2}, \frac{1}{3}[6(7)^{1/2} + 15]^{1/2}$ | |
| 1.4 | 7/3/o23 | BHKNT | [0.09, 0.14033, 0.35818; 0.70918, 1.00155] | >0.69013 |

**Table 1 (continued)**

| | | | | |
|---|---|---|---|---|
| 1.5 | 7/3/o24 | BFHNT | 0.10400, 0.13323, 0.36529; 0.65003 1.00085 | 0.68710 |
| 1.6 | 7/3/o25 | FHKNT | [0.09289, 0.14084, 0.35733; 0.69477, 1.002] | >0.69256 |
| 1.7 | 7/3/o26 | BFKNT | 0.10010, 0.13786, 0.35944; 0.74812, 1.00249 | 0.69015 |
| 1.8 | 7/3/t25 | DEFGIJ | 0, 0.18019, 0.18019; 0.16122, 1 | 0.43550 |
| 1.8′ | | EFGHIJ | 0, 0.18019, 0.31981; 0.16122, 1 | |
| 1.9 | 7/3/t28 | BCHNT | 0.10163, 0.13421, 0.36579; 0.65944, 1 | 0.68623 |
| 1.10 | 7/3/t29 | FIKNT | 0.10161, 0.13925, 0.36075; 0.74632, 1 | 0.69006 |
| 1.11 | 7/3/t30 | BCKNT | 0.09607, 0.13925, 0.36075; 0.74632, 1 | 0.69006 |
| 1.12 | 7/4/t2 | FHINT | 0.10514, 0.13392, 0.36608; 0.64523, 1 | 0.68760 |
| 1.13 | 6/3/o18 | ADEIJ | 0, 0.18106, 0.07510; 0.15920, 1.05995 | 0.40066 |
| 1.13′ | | CEHIJ | 0, 0.18106, 0.42490; 0.15920, 1.05995 | |
| 1.13′ | | BDEFG, BEFGH | | |
| 1.14 | 6/3/o19 | BFHIN | 0.09504, 0.13909, 0.35207; 0.68587, 1.08659 | 0.65192 |
| 1.15 | 6/3/o20 | BCHIN | 0.05882, 0.17340, 0.41256; 0.85515, 1.98296 | 0.46521 |
| 1.16 | 6/3/o21 | CIKNO | 0.05770, 0.22221, 0.37693; 0.83414, 1.26371 | 0.54864 |
| 1.16′ | | BCHKN | | |
| 1.17 | 6/3/o22 | BFHKN | [0.09240, 0.14004, 0.35292; 0.69767, 1.05] | >0.65226 |
| 1.18 | 6/3/o23 | FHIKN | [0.09316, 0.14128, 0.35354; 0.69318, 1.05] | >0.65226 |
| 1.19 | 6/3/o24 | BHIKN | 0.05148, 0.18305, 0.33359; 0.88861, 2.11046 | 0.48012 |
| 1.20 | 6/3/o25/t44 | BFIKN | [0.10882, 0.13562, 0.35893; 0.81018, 1.05] | >0.65226 |
| 1.21 | 6/3/t4 | BEFHR | $\frac{1}{8}$, 0.07657, 0.32657; 0.15817, 1 | 0.41915 |
| 1.21′ | | CEHIR | $\frac{1}{8}$, 0.17343, 0.42343; 0.15817, 1 | |
| 1.22 | 6/3/t37 | BCEHR | $\frac{1}{8}$, 0.07657, 0.42343; 0.15817, 1 | 0.41915 |
| 1.22′ | | EFHIR | $\frac{1}{8}$, 0.17343, 0.32657; 0.15817, 1 | |
| 1.23 | 6/3/t39 | DFGIJK | 0, 0.18541, 0.18541; 0.25834, 1 | 0.39536 |
| 1.23′ | | FGHIJK | 0, 0.18541, 0.31459; 0.25834, 1 | |
| 1.24 | 6/4/o5 | ABDEI | 0.09573, 0.12696, 0.06197; 0.25870, 2.04860 | 0.54739 |
| (1.24) | | BDEFI | | |
| 1.25 | 6/4/o6 | BCEHI | 0.03713, 0.13107, 0.43581; 0.26287, 2.04205 | 0.56697 |
| 1.26 | 6/4/o7 | BDFGIJ | [0, 0.14, 0.19325; 0.34641, 1.93830] | >0.53190 |
| 1.26′ | | BFGHIJ | | |
| 1.27 | 6/4/o8 | BEFHI | 0.09156, 0.12724, 0.31410; 0.25886, 1.91517 | 0.58623 |
| 1.28 | 6/4/o9 | CHIKN | 0.04324, 0.21869, 0.37504; 0.73479, 1.21501 | 0.56036 |
| 1.28′ | | BFHKT | | |
| 1.29 | 6/4/c1 | ADKLM | 0, $\frac{1}{4}$, $\frac{1}{8}$; 1, $(2)^{1/2}$ | 0.52360 |
| (1.29) | | CHKNO | 0, $\frac{1}{4}$, $\frac{3}{8}$; 1, $(2)^{1/2}$ | |
| 1.30 | 5/3/o3 | BFHIK | 0.05798, 0.14503, 0.31166; 0.54668, 1.70252 | 0.47116 |
| 1.31 | 5/3/t25 | ABDIP | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{1}{8}(2)^{1/2} - \frac{1}{8}$; 1, $(2)^{1/2} + 1$ | 0.30672 |
| (1.31) | | BDIFK | $\frac{1}{8}$, $\frac{1}{8}$, $\frac{3}{8} - \frac{1}{8}(2)^{1/2}$; 1, $(2)^{1/2} + 1$ | |
| 1.32 | 5/4/o17 | ABDIJ | 0, 0.16104, 0.06645; 0.53695, 2.42336 | 0.43021 |
| 1.32′ | | BCHIJ | 0, 0.16104, 0.43355; 0.53695, 2.42336 | |
| 1.33 | 5/4/o18 | BDFGK | 0, 0.13203, 0.20818; 0.47189, 1.41746 | 0.46118 |
| 1.33′ | | BFGHK | 0, 0.13203, 0.29182; 0.47189, 1.41746 | |
| 1.33′ | | ADIJK, CHIJK | | |
| 1.34 | 5/4/o19 | BDIJK | 0, 0.17224, 0.18605; 0.61473, 2.40330 | 0.46358 |
| 1.34′ | | BHIJK | 0, 0.17224, 0.31395; 0.61473, 2.40330 | |
| 1.35 | 5/4/o20 | BFHIR | $\frac{1}{8}$, $\frac{1}{8}$, 0.32544; 0.43527, 1.65697 | 0.47089 |
| 1.35′ | | BCHIR | $\frac{1}{8}$, $\frac{1}{8}$, 0.42456; 0.43527, 1.65697 | |
| 2.1 | 6/3/o26 | BHNT | [0.1, 0.13510, 0.36346; 0.66597, 1.001] | >0.68623 |
| 2.2 | 6/3/o27 | FKNT | [0.10095, 0.13871, 0.36021; 0.74666, 1.001] | >0.69006 |
| 2.3 | 6/3/o28 | BKNT | [0.09763, 0.13871, 0.36021; 0.74666, 1.001] | >0.69006 |
| 2.4 | 6/3/t42 | HKNT | [0.09, 0.14107, 0.35893; 0.70864, 1.00000] | >0.69103 |
| 2.5 | 6/4/o10 | FHNT | [0.10100, 0.135, 0.36337; 0.66176, 1.00114] | >0.68710 |
| 2.6 | 6/4/o11 | BFNT | [0.10512, 0.13423, 0.36422; 0.70525, 1.001] | >0.68017 |
| 2.7 | 6/4/t11 | FINT | [0.11, 0.13280, 0.36720; 0.70020, 1] | >0.68017 |
| 2.7′ | | BCNT | [0.1, 0.13583, 0.36417; 0.69372, 1] | |
| 2.8 | 5/3/o4 | IKNO | 0.05802, 0.21593, 0.34241; 0.93211, 1.93651 | 0.44889 |
| 2.8′ | | BCHN | | |
| 2.9 | 5/3/o5 | CINO | 0.04768, 0.22355, 0.40921; 0.87071, 1.90808 | 0.45606 |
| 2.9′ | | BHKN | | |
| 2.10 | 5/3/o6/t24 | FIKN | [0.097, 0.14, 0.35391; 0.71895, 1.05862] | >0.65226 |
| 2.11 | 5/3/o7 | BFHN | [0.09332, 0.14, 0.35138; 0.69329, 1.08] | >0.65192 |
| 2.12 | 5/4/o21 | CEHI | 0.02764, 0.17932, 0.42466; 0.15783, 1.04585 | 0.39910 |
| 2.12′ | | BEFH | | |
| 2.13 | 5/4/o22/t49 | CHKN | [0.05, 0.19549, 0.37347; 0.84284, 1.24839] | >0.52360 |
| 2.13′ | | BHKT, CKNO | | |

**Table 1** (continued)

| | | | | |
|---|---|---|---|---|
| 2.14 | 5/4/o23 | CHIN | 0.04334, 0.20921, 0.40949; 0.81933, 1.88385 | 0.45883 |
| 2.14′ | | BFHT | | |
| 2.15 | 5/4/o24 | HIKN | 0.03774, 0.21837, 0.34070; 0.79762, 1.86669 | 0.45999 |
| 2.15′ | | FHKT | | |
| 2.16 | 5/4/o25 | BCIN | $\frac{1}{16}, \frac{7}{40}, \frac{33}{80}; \frac{2}{5}(5)^{1/2}, 2$ | 0.46459 |
| 2.16′ | | BIKN, BFIN | | |
| 2.17 | 5/4/o26 | CIKN | [0.075, 0.18, 0.37377; 0.84566, 1.19567] | >0.54864 |
| 2.17′ | | BCKN, BFKT | | |
| 2.18 | 5/4/o27 | FHIN | [0.1, 0.13640, 0.35791; 0.66537, 1.05272] | >0.65192 |
| 2.19 | 5/4/o28 | FHKN | [0.093, 0.14103, 0.35586; 0.69410, 1.02] | >0.65226 |
| 2.20 | 5/4/o29/t48 | BFKN | [0.095, 0.14, 0.35142; 0.70968, 1.08212] | >0.65226 |
| 2.21 | 5/4/t2 | ADEI | $\frac{1}{8}$, 0.17776, 0.07224; 0.14922, 1 | 0.37309 |
| (2.21) | | BDEF | $\frac{1}{8}$, 0.07224, 0.17776; 0.14922, 1 | |
| 2.22 | 5/4/t6 | ADLM | $0, \frac{1}{4}, \frac{3}{32}$; 1, 2 | 0.44179 |
| (2.22) | | CHNO | $0, \frac{1}{4}, \frac{13}{32}$; 1, 2 | |
| 2.22′ | | DKLM | $0, \frac{1}{4}, \frac{5}{32}$; 1, 2 | 0.44179 |
| 2.22′ | | HKNO | $0, \frac{1}{4}, \frac{11}{32}$; 1, 2 | |
| 2.23 | 5/4/t41 | ABDE | 0.05194, 0.07339, 0.07339; 0.14757, 1 | 0.36488 |
| 2.23′ | | BCEH | | |
| (2.23) | | DEFI | | |
| 2.24 | 5/4/t42 | EFHI | 0.09023, 0.17531, 0.32469; 0.15765, 1 | 0.41641 |
| 2.25 | 5/4/t43 | DFGIJ | 0, 0.18427, 0.18427; 0.24026, 1 | 0.39383 |
| 2.25′ | | FGHIJ | 0, 0.18427, 0.31573; 0.24026, 1 | |
| 2.26 | 4/3/c6 | ABDP | $\frac{3}{8} - \frac{1}{8}(6)^{1/2}, \frac{3}{8} - \frac{1}{8}(6)^{1/2}, \frac{3}{8} - \frac{1}{8}(6)^{1/2}$; 1, 1 | 0.12354 |
| (2.26) | | DFIK | | |
| 2.27 | 4/4/o10 | ADIJ | 0, 0.19275, 0.07898; 0.30745, 1.21341 | 0.31629 |
| 2.27′ | | CHIJ | 0, 0.19275, 0.42102; 0.30745, 1.21341 | |
| 2.27′ | | BFGH, BDFG | | |
| 2.28 | 4/4/o11 | DIJK | 0, 0.19914, 0.17403; 0.37364, 1.22961 | 0.35104 |
| 2.28′ | | HIJK | 0, 0.19914, 0.32597; 0.37364, 1.22961 | |
| 2.28′ | | DFGK, FGHK | | |
| 2.29 | 4/4/o12 | ABDI | 0.10754, 0.13788, 0.05694; 0.85897, 2.42130 | 0.29462 |
| (2.29) | | BDFI | | |
| 2.29′ | | BDIK | | |
| 2.30 | 4/4/o13 | BFHI | 0.08578, 0.13388, 0.31804; 0.47580, 1.70676 | 0.45255 |
| 2.31 | 4/4/o14 | BCHI | 0.05190, 0.14969, 0.42799; 0.58121, 2.07886 | 0.39501 |
| 2.32 | 4/4/o15 | BFHK | 0.03399, 0.13423, 0.30017; 0.53596, 1.40172 | 0.44346 |
| 2.32′ | | CHIK | | |
| 2.33 | 4/4/o16 | BHIK | 0.03813, 0.16523, 0.31862; 0.68046, 2.10107 | 0.43862 |
| 2.34 | 4/4/t40 | FHIR | $\frac{1}{8}$, 0.16757, 0.33243; 0.26012, 1 | 0.35858 |
| 2.34′ | | BCHR | $\frac{1}{8}$, 0.08243, 0.41757; 0.26012, 1 | |
| 2.35 | 4/4/t41 | BDFK | 0.11187, 0.11187, 0.20884; 1, 1.87409 | 0.28324 |
| 2.35′ | | ADIK, CIKO, BCHK | | |
| 2.36 | 4/6/t3 | BFHR | $\frac{1}{8}$, 0.08243, 0.33243; 0.26012, 1 | 0.35858 |
| 2.36′ | | CHIR | $\frac{1}{8}$, 0.16757, 0.41757; 0.26012, 1 | |
| i2.1 | $t[4/3/c6]^3$ | FHIK | $\frac{3}{8}(6)^{1/2} - \frac{7}{8}, \frac{1}{8}(6)^{1/2} - \frac{1}{8}, \frac{5}{8} - \frac{1}{8}(6)^{1/2}; \frac{1}{3}, 1$ | 0.37062 |
| 3.1 | 5/4/o30 | BNT | [0.1, 0.13607, 0.36340; 0.7, 1.00039] | >0.68017 |
| 3.1′ | | FNT | | |
| 3.2 | 5/4/t45 | HNT | [0.0934, 0.14, 0.36; 0.69293, 1] | >0.68623 |
| 3.3 | 4/4/o17 | HKN | [0.02, 0.22715, 0.34339; 0.98032, 1.97483] | >0.44179 |
| 3.3′ | | CNO, HKT, CHN, KNO, BHT | | |
| 3.4 | 4/4/o18 | BCN | [0.075, 0.15, 0.39086; 0.8, 1.37436] | >0.44889 |
| 3.4′ | | IKN, FKT, FIN | | |
| 3.5 | 4/4/o19/t39 | FKN | [0.1, 0.13900, 0.35901; 0.74, 1.01] | >0.65226 |
| 3.6 | 4/4/o20 | CIN | [0.05, 0.21, 0.40957; 0.86870, 1.91212] | >0.45606 |
| 3.6′ | | BKN, BFT, BFN | | |
| 3.7 | 4/4/o21 | FHN | [0.1, 0.13640, 0.36087; 0.66537, 1.02] | >0.65192 |
| 3.8 | 4/6/t4 | CKN | [0.05, 0.20894, 0.37584; 0.99238, 1.36091] | >0.52360 |
| 3.8′ | | BKT | | |
| 3.9 | 3/4/t1 | ABD | 0.05538, 0.7675, 0.7675; 0.83247, 1 | 0.11155 |
| 3.9′ | | BCH, DFI, DFK, DIK, IKO, BDP, ADP | | |
| 3.10 | 3/8/t1 | ADI | $\frac{1}{8}, \frac{3}{16}, \frac{1}{16}; \frac{1}{2}, 1$ | 0.18512 |
| (3.10) | | BDF | $\frac{1}{8}, \frac{1}{16}, \frac{3}{16}; \frac{1}{2}, 1$ | |
| (3.10) | | CIO | | |
| 3.10′ | | BDK, BHK, CHK, CKO | | |

**Table 1 (continued)**

| 3.11 | 3/10/o2 | CHI | 0.04096, 0.18419, 0.41878; 0.33047, 1.16280 | 0.30295 |
|---|---|---|---|---|
| 3.11′ | | BFH | | |
| i3.1 | $t[5/3/t1]^2$ | KNT | [0.094, 0.14, 0.36; 0.73103, 1] | >0.69006 |
| i3.2 | $o[3/4/t1]^3$ | HIK | 0.01975, 0.19462, 0.32675; 0.40042, 1.20125 | 0.34665 |
| i3.2′ | | FHK | | |
| i3.3 | $t[3/4/t1]^3$ | FHI | 0.08387, 0.17325, 0.32675; 0.27749, 1 | 0.34665 |
| i4.1 | $t[4/4/t1]^2$ | NT | [0.1, 0.1363, 0.36370; 0.7, 1] | >0.68017 |
| i4.2 | $o[3/10/t4]^2$ | FN | [0.1, 0.1364, 0.36071; 0.67, 1.02] | >0.44179 |
| i4.2′ | | KN, CN, KT, BT | | |

**Ibca 16f x, y, z**     $0 \leq x \leq \frac{1}{4}, 0 \leq y \leq \frac{1}{4}, 0 \leq z \leq \frac{1}{4}, a \leq b \leq c$

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

| 0.1 | 9/3/o1 | BCDFIJK | $\frac{1}{4}, \frac{1}{8}, 1 - \frac{1}{2}(3)^{1/2}; \frac{1}{2}(3)^{1/2}, 1 + \frac{1}{2}(3)^{1/2}$ | 0.64801 |
|---|---|---|---|---|
| 0.2 | 9/3/o1 | BDFGHK | $\frac{1}{4}, \frac{1}{8}, 1 - \frac{1}{2}(3)^{1/2}; \frac{1}{6}(3)^{1/2}, \frac{1}{3}(3)^{1/2} + \frac{1}{2}$ | 0.64801 |
| 0.3 | 9/3/t2 | BCDFGIK | $\frac{1}{4}, \frac{1}{8}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}; \frac{1}{2}(2)^{1/2}, \frac{1}{2}(2)^{1/2} + \frac{1}{2}$ | 0.61343 |
| 1.1 | 8/3/t3 | BDFGH | $\frac{1}{8}, \frac{1}{2}(5)^{1/2} - 1, \frac{5}{4} - \frac{1}{2}(5)^{1/2}; \frac{2}{3}[27 - 12(5)^{1/2}]^{1/2}, 1$ | 0.62249 |
| 1.2 | 7/3/t2 | BCDFG | $\frac{1}{8}, \frac{1}{6}(7)^{1/2} - \frac{1}{3}, \frac{7}{12} - \frac{1}{6}(7)^{1/2}; \frac{2}{3}(7)^{1/2} - \frac{4}{3}, 1$ | 0.54894 |
| 1.3 | 7/3/t3 | BCDFJ | $\frac{1}{4}(3)^{1/2} - \frac{1}{4}, \frac{1}{2} - \frac{1}{4}(3)^{1/2}, \frac{1}{8}; 1, 2$ | 0.58099 |
| 1.4 | 7/4/o1 | BCDFIK | $\frac{1}{4}, \frac{1}{8}, \frac{7}{24} - \frac{1}{24}(13)^{1/2}; \frac{1}{12}[30 + 6(13)^{1/2}]^{1/2}, \frac{1}{2}[4 + (13)^{1/2}]^{1/2}$ | 0.60210 |
| 1.5 | 7/4/o1 | BDFGK | $\frac{1}{4}, \frac{1}{8}, \frac{7}{24} - \frac{1}{24}(13)^{1/2}; \frac{1}{4}[10 - 2(13)^{1/2}]^{1/2}, \frac{1}{4} + \frac{1}{4}(13)^{1/2}$ | 0.60210 |
| 1.6 | 6/3/o29 | ABCDF | 0.09554, 0.07936, 0.12007; 0.65391, 1.25818 | 0.48883 |
| 1.6′ | | CDFGI, CDFIJ | | |
| 1.7 | 6/4/c1 | ABCDE | $0, 0, \frac{1}{8}; 1, 2$ | 0.52360 |
| 1.7′ | | DFIJK | $\frac{1}{4}, \frac{1}{4}, \frac{1}{8}; 1, 2$ | |
| 2.1 | 6/4/t5 | BDFG | $\frac{1}{8}, 0.10799, 0.14201; 0.42600, 1$ | 0.54889 |
| 2.2 | 6/4/c1 | BCFJ | $\frac{1}{4}, 0, \frac{1}{8}; 1, 2$ | 0.52360 |
| 2.3 | 5/4/o31 | BCDF | 0.11286, 0.08406, 0.12417; 0.64139, 1.27435 | 0.48658 |
| 2.3′ | | CDFG, CDFJ | | |
| 2.4 | 5/4/t6 | ABCD | $0, \frac{1}{16}, \frac{1}{8}; \frac{1}{2}(2)^{1/2}, (2)^{1/2}$ | 0.44179 |
| 2.4′ | | DFIJ, CFGI | | |
| 2.5 | 4/6/c4 | ACDF | $\frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}, \frac{1}{4}(2)^{1/2} - \frac{1}{4}; 1, 1$ | 0.38671 |
| 2.5′ | | CDFI | $\frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}, \frac{1}{2} - \frac{1}{4}(2)^{1/2}; 1, 1$ | |
| i3.1 | $c[3/10/c1]^2$ | CDF | $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}; 1, 1$ | 0.37024 |

one-dimensional region of the type 8/4/c1 (with endings referring to types 12/3/c1 and 10/3/t1). Each of the two sub-regions of type 6/4/t11 (maximal symmetry: $I4_1/amd$ 16h; Fischer, 1991) is bounded, in addition, by two further one-dimensional and one zero-dimensional parameter regions belonging to sphere-packing types with higher contact numbers (cf. Fig. 1 in Fischer, 1991, and Fig. 2). A sphere packing with parameters from one sub-region cannot be deformed into another one with parameters from the second sub-region without forming additional contacts. 6/4/t11 does not contain a sphere packing with minimal density. Within the examined parameter range of space group Fddd, sphere-packing type 6/4/t11 is generated with nearest neighbours symbolized by BCNT or FINT in Table 1. The three- and four-dimensional parameter regions belonging to subsets of these strings also disintegrate into two parts separated by the parameter region of 8/4/c1. This concerns the sphere-packing types 5/4/o30 (BNT, FNT) and 4/4/o18 (BCN, FIN, FKT, IKN – all are equivalent with respect either to the Euclidean or to



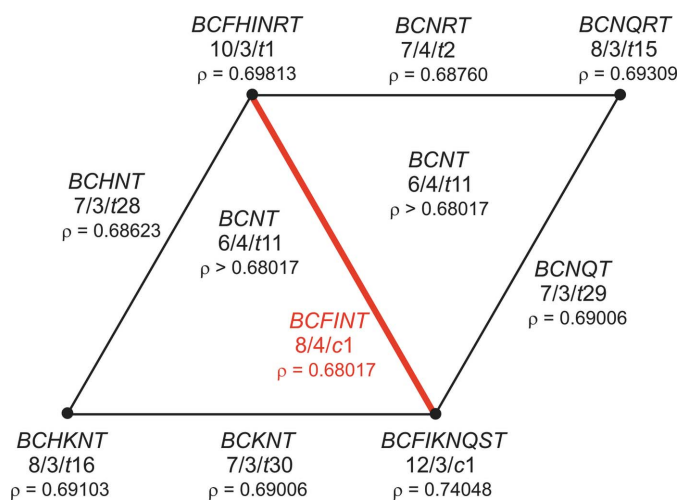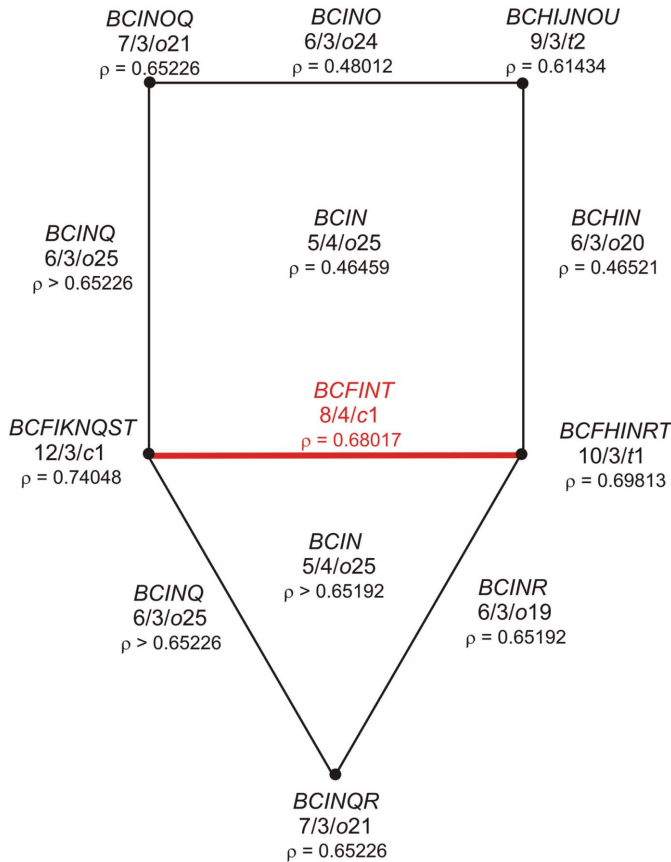| | | |
|---|---|---|
| BCFHINRT 10/3/t1 ρ = 0.69813 | BCNRT 7/4/t2 ρ = 0.68760 | BCNQRT 8/3/t15 ρ = 0.69309 |
| BCHNT 7/3/t28 ρ = 0.68623 | BCNT 6/4/t11 ρ > 0.68017 / BCNT 6/4/t11 ρ > 0.68017 / BCFINT 8/4/c1 ρ = 0.68017 | BCNQT 7/3/t29 ρ = 0.69006 |
| BCHKNT 8/3/t16 ρ = 0.69103 | BCKNT 7/3/t30 ρ = 0.69006 | BCFIKNQST 12/3/c1 ρ = 0.74048 |

**Figure 2**
Schematic representation of the two disconnected parameter regions of type 6/4/t11 (BCNT) with their boundaries (Fddd 32h).

**Figure 3**
Schematic representation of the two disconnected parameter regions of type 5/4/$o$25 (*BCIN*) with their boundaries (*Fddd* 32$h$).

the affine normalizer of *Fddd*), and the type of inter-penetrating sphere packing $o[3/10/t4]^2$ (*FN*, *CN*, *KN*, *KT*, *BT*). All three types do not comprise a configuration with a minimal density.

The two-dimensional parameter region of type 5/4/$o$25 is also divided into two parts by the one-dimensional region of 8/4/$c$1. One sub-region is bounded by a further two zero-dimensional and three one-dimensional, the other by one zero-dimensional and two one-dimensional parameter regions of sphere-packing types with higher contact numbers (*cf.* Fig. 3). Whereas the upper sub-region contains a sphere packing with minimal density, the lower sub-region does not. The string symbol of 5/4/$o$25 is *BCIN* (*BKIN*, *BFIN*) and configurations having a subset of these strings also show split parameter regions. These are again 4/4/$o$18 and $o[3/10/t4]^2$, and, in addition, 4/4/$o$20 (*CIN*, *BKN*, *BFN*, *BFT*).

The three-dimensional parameter region of 4/4/$o$17 (*HKN*, *CNO*, *HKT*, *CHN*, *KNO*, *BHT*) also shows an unusual behaviour (*cf.* Fig. 4). It is divided into two sub-regions by the two-dimensional parameter region of 5/4/$t$6 (*CHNO*, *HKNO*) that is bounded by three one-dimensional regions [belonging to type 6/4/$c$1 (*CHKNO*) and two times to type 7/3/$o$5 (*HIJKNO*, *CHIJNO*)] and three zero-dimensional regions [belonging to type 9/3/$t$2 (*BHIJKNOU*) and two times to type 8/3/$h$4 (*CHIJKNO*, *BCHKNOU*)]. The parameter regions of types 4/4/$o$17 and 5/4/$o$25 (*cf.* above) share a common vertex, namely 9/3/$t$2. There is no sphere packing of type 4/4/$o$17 with minimal density and, again, it is not possible to deform sphere packings generated within one sub-region into one of the other sub-region.
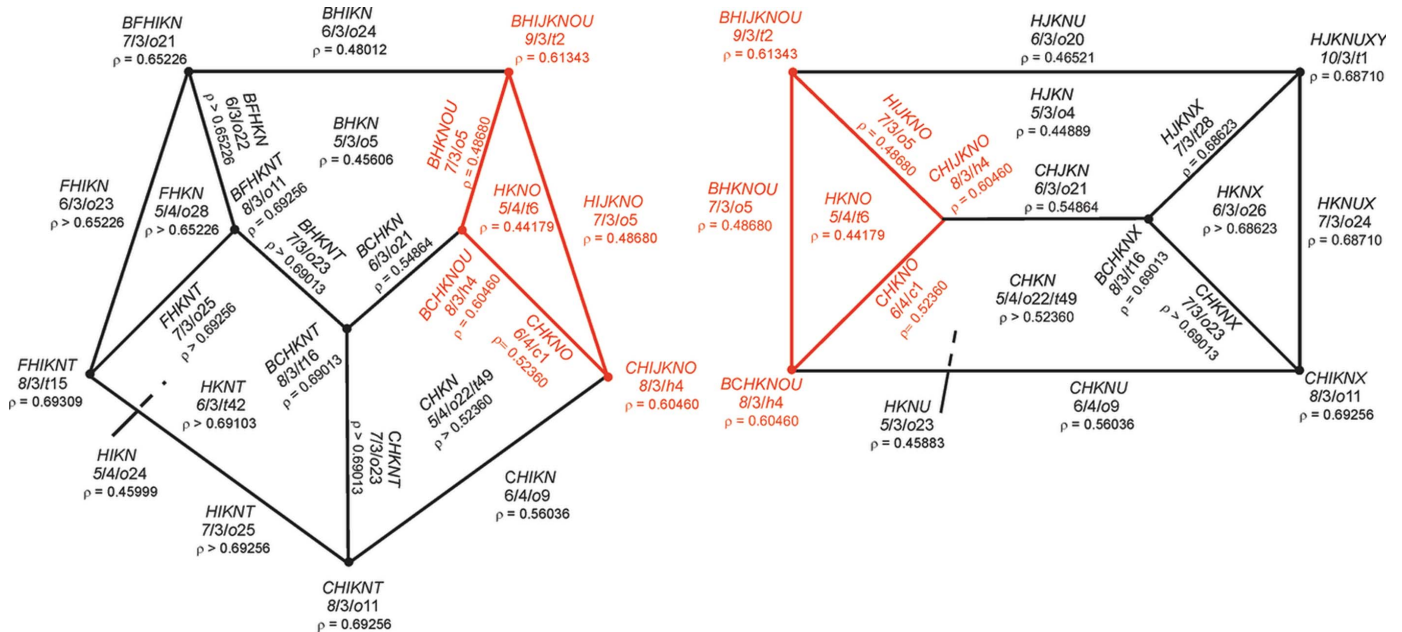


**Figure 4**
Schematic representation of the disconnected parameter regions of type 4/4/$o$17 symbolized by *HKN* and those of the adjoining sphere-packing types (*Fddd* 32$h$).
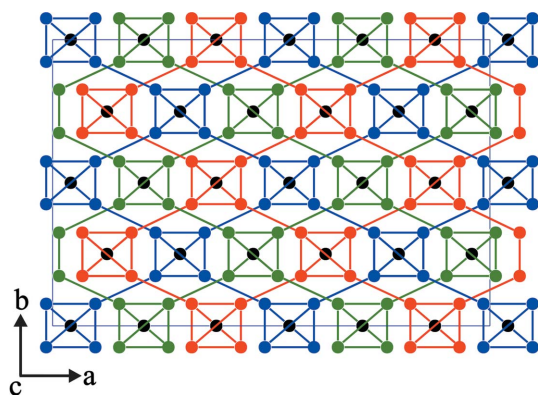
**Figure 5**
Oxygen arrangement in $Cr_2SiO_4$ forming triply interwined sphere packings of type 4/3/c6. Black dots: Cr atoms.

## 4. Examples of crystal structures

The following crystal structures show atomic arrangements that correspond to sphere packings in one of the trivariant orthorhombic lattice complexes described above.

(i) $Cr_2SiO_4$ crystallizes in space group *Fddd* (Miletich *et al.*, 1999). The O atoms occupy the general position. Their arrangement corresponds to three interpenetrating sphere packings of type $t[4/3/c6]^3$ (*cf.* Fig. 5). The Si atoms are tetrahedrally surrounded while the Cr atoms are located in strongly Jahn–Teller distorted octahedral voids.

(ii) The Bi atoms in $LiBiO_3$ occupy the general position in space group *Pccn* (Kumada *et al.*, 1996) and are arranged corresponding to a sphere packing of type 5/4o7. They are located in one third of the octahedral voids within the slightly distorted heterogeneous hexagonal closest packing formed by the O atoms.

(iii) An orthorhombically deformed sphere packing of the tetragonal type 6/3/t5 is formed by the Si atoms in ammonio-guanidinium hexafluorosilicate $(CH_8N_4)(SiF_6)$ that crystallizes in space group *Pccn* (Ross *et al.*, 1999).

(iv) $\alpha$-RbBiCrO$_4$ crystallizes in space group *Pnna* (Riou *et al.*, 1984). The arrangement of the Cr atoms at the general position corresponds to a slightly distorted sphere packing of type 4/6/h2.

(v) $Ba(H_2PO_4)_2$ has the symmetry *Pccn* (Gilbert *et al.*, 1977). The slightly distorted sphere packing formed by the P atoms at the general position belongs to type 4/6/o2 (Fig. 6).

Further examples for the occurrence of sphere packings can be found in the *TOPOS TTO* collection (Blatov, 2006). In particular, metal–organic framework materials (MOFs) can often be described by 3-periodic nets (*e.g.* Alexandrov *et al.*, 2011). Many of them correspond to sphere packings.
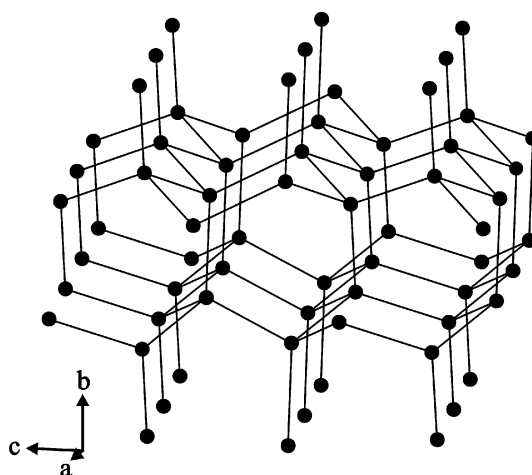
**Figure 6**
Sphere packing with minimal density of type 4/6/o2 (RCSR symbol **mmt**) (*Pccn* 8e) with corrugated $6^3$ nets perpendicular to **b** and **c**.

information that some tetragonal and orthorhombic sphere packings have isomorphic graphs.

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