SHORT COMMUNICATIONS

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Lattice complexes with at most one comprehensive complex.

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Abstract

Most lattice complexes with less than three degrees of freedom are contained as limiting complexes within several comprehensive complexes corresponding to general Wyckoff positions. There exist, however, 21 exceptional cases: 3 lattice complexes without any and 18 lattice complexes with exactly one such comprehensive complex each. They are listed together with their comprehensive complexes. This information may be used to restrict geometrical investigations of all point configurations to general positions of space groups.

For geometrical studies of individual *point configurations* (*i.e.* sets of points that are symmetrically equivalent with respect to a space group), it is not necessary to consider all Wyckoff positions of all space groups. Instead, it is sufficient to confine the investigation to the 402 lattice complexes (*cf. e.g.* Fischer & Koch, 1983). Such a procedure has been used before, *e.g.* for the derivation of sphere packings (Fischer, 1971) or of space partitions into Dirichlet domains (Koch, 1973). The effort may further be reduced by taking advantage of limiting-complex relationships between lattice complexes (*cf. e.g.* Fischer, 1991), a procedure first described by Fischer (1968): If all point configurations of a first lattice complex are contained in a second one, then the first one is called a *limiting complex* of the second one and the second one is called a *comprehensive complex* of the first one (*cf.* Fischer & Koch, 1983).

In general, each lattice complex has at least one comprehensive complex with the following property: its *characteristic Wyckoff position* (*i.e.* one of its Wyckoff positions with highest site symmetry) has three degrees of freedom and, therefore, corresponds to a general position of a space group (Fischer, 1980). There exist only three lattice complexes – not corresponding to the general position of a space group by themselves – without any comprehensive complex, namely $I\bar{4}3d$ 24(d), $Fd\bar{3}m$ 48(f) and $Ia\bar{3}d$ 48(f). Therefore, geometrical investigations of point configurations may be restricted to those general positions of space groups that form the characteristic Wyckoff position of a lattice complex (plus the three lattice complexes without any comprehensive complex). In addition, such a restriction has the following advantage: For a given starting point in general position, there exists a one-to-one correspondence between the symmetry operations of the space group and the points of the point configuration.

It may be desirable to transfer the results of such a study to all limiting complexes and thus make it available for all Wyckoff positions. This may give rise to problems, however, because until now the limiting-complex relationships between the lattice complexes are not completely tabulated. Nevertheless, the following considerations may be helpful: If a lattice complex has several comprehensive complexes corresponding to general positions then these general positions have part of their point configurations in common, *i.e.* there exist some identical point configurations within all the considered general positions of different space groups. Moreover, the inverse statement is also true: Whenever identical geometrical objects (*e.g.* sphere packings) are observed in two or more general positions, then the respective point configurations belong also to a further lattice complex that forms a common limiting complex of the considered ones. Its characteristic Wyckoff position necessarily shows site symmetry higher than 1. Therefore, the occurrence of identical point configurations or identical geometrical objects within different general positions is a sufficient, but not a necessary, condition for the presence of a limiting complex. Lattice complexes with only one comprehensive complex corresponding to a general position, however, cannot be identified as limiting complexes in this way. For this reason, it is useful to know how many and which lattice complexes have less than two such comprehensive complexes.

For each lattice complex for which the characteristic Wyckoff position is not a general one, it has been checked whether or not there exist at least two comprehensive complexes corresponding to general positions. The studies have been performed with the aid of subgroup relations between the corresponding space groups. For this, the tables of the limiting complexes of the cubic lattice complexes (Koch, 1974) and the tables of the non-characteristic orbits of the space groups (Engel, Matsumoto, Steinmann & Wondratschek, 1984), which, unfortunately, do not cover limiting complexes due to a specialized metric, were useful.

As a result, 18 lattice complexes have been found with only one comprehensive complex that corresponds to a general position. They are listed in Table 1 together with the three well known cubic complexes without any comprehensive complex. Except for the trivial case $P\bar{1}$ 1(a) (the lattice complex consisting of all point lattices), they all belong to the cubic system and most of them occur only in space groups that are subgroups of $Ia\bar{3}d$. Three of these lattice complexes are invariant and two have two degrees of freedom. All other complexes are univariant. Table 1 gives their characteristic Wyckoff positions, the corresponding site symmetries and the general coordinates of one point in the first four columns. The last two columns refer to the comprehensive complexes. They show the characteristic space groups and the resulting restrictions for the metrical parameters and for the coordinates of one point in general position. In case of lattice complexes corresponding to the enantiomorphic pair $P4_332-P4_132$, the information is given twice.

Table 1. *Lattice complexes with at most one comprehensive complex*

Lattice complex				Comprehensive complex	
$P\bar{1}$	1(*a*)	$\bar{1}$	0, 0, 0	$P\bar{1}$	$x = y = 0, z = \frac{1}{4}$
$I4_132$	12(*c*)	2.22	$\frac{1}{8}, 0, \frac{1}{4}$	$P2_13$	$x = \frac{1}{8}, y = 0, z = \frac{1}{4}$
$Ia\bar{3}d$	24(*c*)	2.22	$\frac{1}{8}, 0, \frac{1}{4}$	$Pa\bar{3}$	$x = \frac{1}{8}, y = 0, z = \frac{1}{4}$
$P2_13$	4(*a*)	.3.	x, x, x	$P2_12_12_1$	$x = y = z; a = b = c$
$I2_13$	8(*a*)	.3.	x, x, x	$I2_12_12_1$	$x = y = z; a = b = c$
$I2_13$	12(*b*)	2..	$x, 0, \frac{1}{4}$	$P2_13$	$y = 0, z = \frac{1}{4}$
$Pa\bar{3}$	8(*c*)	.3.	x, x, x	$Pbca$	$x = y = z; a = b = c$
$Ia\bar{3}$	16(*c*)	.3.	x, x, x	$Ibca$	$x = y = z; a = b = c$
$Ia\bar{3}$	24(*d*)	2..	$x, 0, \frac{1}{4}$	$Pa\bar{3}$	$y = 0, z = \frac{1}{4}$
$F4_132$	48(*g*)	..2	$\frac{1}{8}, y, \frac{1}{4} - y$	$F23$	$x = \frac{1}{8}, z = \frac{1}{4} - y$
$P4_332$	8(*c*)	.3.	x, x, x	$P4_32_12$	$y = \frac{1}{4} + x, z = -\frac{1}{8} + x; a = c$
$P4_132$	8(*c*)	.3.	x, x, x	$P4_12_12$	$y = -\frac{1}{4} + x, z = -\frac{3}{8} + x; a = c$
$P4_332$	12(*d*)	..2	$\frac{1}{8}, y, \frac{1}{4} - y$	$P2_13$	$x = \frac{1}{8}, z = \frac{1}{4} - y$
$P4_132$	12(*d*)	..2	$\frac{1}{8}, y, \frac{1}{4} + y$	$P2_13$	$x = \frac{1}{8}, z = \frac{1}{4} + y$
$I4_132$	16(*e*)	.3.	x, x, x	$I4_122$	$y = -\frac{1}{4} + x, z = -\frac{1}{8} + x; a = c$
$I4_132$	24(*f*)	2..	$x, 0, \frac{1}{4}$	$P4_332$	$y = 0, z = \frac{1}{4}$
				$P4_132$	$y = 0, z = \frac{1}{4}$
$I\bar{4}3d$	16(*c*)	.3.	x, x, x	$I\bar{4}2d$	$y = \frac{1}{4} + x, z = -\frac{1}{8} + x; a = c$
$I\bar{4}3d$	24(*d*)	2..	$x, 0, \frac{1}{4}$	–	
$Fm\bar{3}m$	48(*h*)	*m.m*2	$0, y, y$	$F23$	$x = 0, y = z$
$Fd\bar{3}m$	48(*f*)	2.*mm*	$x, 0, 0$	–	
$Ia\bar{3}d$	48(*f*)	2..	$x, 0, \frac{1}{4}$	–	
$Fm\bar{3}$	48(*h*)	*m*..	$0, y, z$	$F23$	$x = 0$
$F\bar{4}3m$	48(*h*)	..*m*	x, x, z	$F23$	$x = y$

This knowledge has been used for the complete derivation of all types of homogeneous sphere packings with three contacts per sphere (Koch & Fischer, 1995).

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Defective vertices in perfect icosahedral quasicrystals. By M. BAAKE, *Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle* 14, *D*-72076 *Tübingen, Germany*, S. I. BEN-ABRAHAM, *Department of Physics, Ben-Gurion University, POB* 653, *IL*-84105 *Beer-Sheba, Israel*, and D. JOSEPH, P. KRAMER and M. SCHLOTTMANN, *Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle* 14, *D*-72076 *Tübingen, Germany*

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Abstract

All combinatorially possible vertex configurations of the two rhombohedral prototiles of the primitive icosahedral tiling can be locally embedded into the perfect tiling. They can be created and relaxed by simpleton flips.

Recently, we have catalogued and discussed all combinatorially possible vertex configurations of the three-dimensional primitive icosahedral tiling in its random version (Baake, Ben-Abraham, Klitzing, Kramer & Schlottmann, 1994). The perfect primitive icosahedral tiling contains only 24 (32, if enantiomers are counted separately) non-congruent vertex configurations. In contrast, we find 5450 (10 527) different combinatorially possible vertices. Thus, the overwhelming majority is defective.

A very obvious and fundamental question imposes itself at once: Can all or some of these defective vertices be inserted without gaps and overlaps into an otherwise perfect structure? An affirmative answer immediately raises another question: Can some or all defective vertices be created from