Lattice Complexes and Limiting Complexes *Versus* Orbit Types and Non-characteristic Orbits: a Comparative Discussion

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Dedicated to Professor Dr H. Wondratschek on the occasion of this 60th birthday

Abstract

The concept of lattice complexes is compared with the concept of orbit types, and the correspondences and differences are worked out in some detail. For this, it turned out to be necessary to distinguish whether a set of symmetrically equivalent points is regarded as attached to or as detached from its generating space group. The terms 'crystallographic orbit' and 'point configuration' used as synonyms so far are applied here to discriminate between these distinct meanings. On this basis, the terminology within both concepts is redefined stressing the aspect of equivalence classes. After that, the relations between non-characteristic orbits and limiting complexes are carefully discussed for the first time.

1. Introduction

In the past the terms 'point configuration' (Fischer & Koch, 1974) and 'crystallographic orbit' (Matsumoto & Wondratschek, 1979) have been used as synonyms for sets of points in R^3 that are equivalent with respect to a space group. Such sets of points have been classified in two different ways: (1) according to the concept of lattice complexes (*Gitterkomplexe*) and of limiting complexes, which goes back to Hermann (1935) and has been defined more strictly by Fischer & Koch (1974); (2) according to the concept of types of crystallographic orbits and of non-characteristic orbits introduced by Wondratschek (1976).

Both aspects have been adopted in *International Tables for Crystallography* (1983) [for short: IT (1983)].* They are strongly related but not identical. Therefore, it seems worthwhile and necessary to compare the classes originating from both concepts and, especially, to work out the differences.

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* The following papers are also related to these topics: Burzlaff & Zimmermann (1974); Engel (1983); Engel, Matsumoto, Steinmann & Wondratschek (1984); Fischer, Burzlaff, Hellner & Donnay (1973); Fischer & Koch (1978, 1983); Koch (1974); Koch & Fischer (1975, 1978); Steinmann (1984); Wondratschek (1980).

When trying to perform such a comparison the authors noted that so far 'point configuration' as well as 'crystallographic orbit' have been used with two meanings: (1) for sets of points equivalent with respect to a given space group, *i.e.* in the mathematical sense of 'orbit'; (2) for such sets of points, but detached from their generating space groups. The second meaning is referred to, for example, if one just speaks of a primitive cubic point lattice. As within both concepts both meanings are required one has to distinguish between them and to use different terms for their designation. This is done here by restricting the term 'crystallographic orbit' to the first, the term 'point configuration' to the second meaning. On this basis all other terms from both concepts are redefined, and subsequently a detailed comparison is given.

2. Crystallographic orbits, Wyckoff positions, Wyckoff sets and types of Wyckoff sets

In mathematics, orbit is a very general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group. In fact orbits are always used in crystallography where equivalence classes are defined by means of group action (*e.g.* a space-group type as the orbit of a space group under the action of the affine group). In the present context, however, the term (crystallographic) orbit will be used in a much more restricted sense as proposed by Wondratschek (1976):

From any point of R^3 the symmetry operations of a given space group G generate an infinite set of points, called a *crystallographic orbit with respect to* G or, for short, a *crystallographic orbit*. The space group G is called the *generating space group* of the orbit.

Each point of a crystallographic orbit defines uniquely a largest subgroup of G, which maps that point onto itself, its *site-symmetry group*. The site-symmetry groups belonging to different points out of the same crystallographic orbit are conjugate subgroups of G.

The crystallographic orbits with respect to a given space group G are equivalence classes within the set of points of R^3. It is also possible, however, to define equivalence relations on the set of all crystallographic orbits of G:

Two crystallographic orbits of a space group G belong to the same *Wyckoff position* if and only if the site-symmetry groups of any two points from the first and the second orbit are conjugate subgroups of G (*i.e.* if the two site-symmetry groups are mapped onto each other by an inner automorphism of G).

The following definition results in a coarser classification of crystallographic orbits:

Two crystallographic orbits of a space group G belong to the same *Wyckoff set* if and only if the site-symmetry groups of any two points from the first and the second orbit are conjugate subgroups of the affine normalizer of G (*i.e.* if the two site-symmetry groups are mapped onto each other by an automorphism of G).

Accordingly, all orbits of the same Wyckoff position belong to one and the same Wyckoff set. Therefore, the assignment of orbits to Wyckoff sets also defines an equivalence relation on the Wyckoff positions of a space group. The relationship between Wyckoff positions and Wyckoff sets was first tabulated by Koch & Fischer (1975). Corresponding information is also given in IT (1983).

For the set of all space groups of a given type it seems desirable to transfer the terms 'Wyckoff position' and 'Wyckoff set' from a single space group to the whole type. For the following reason this is not possible for Wyckoff positions: two space groups of the same type can be mapped onto each other by infinitely many isomorphisms or affine mappings. Each isomorphism results in a unique relation between the Wyckoff positions of the two groups, but different isomorphisms may give rise to different relations, and then the Wyckoff positions of the same Wyckoff set may change their roles. Such difficulties cannot occur for Wyckoff sets, as all Wyckoff sets of a space group differ in their group-theoretical relations to the space group.

Therefore, the Wyckoff sets may be classified as follows: Two Wyckoff sets of space groups of the same type belong to the same *type of Wyckoff sets* if and only if they are related by an isomorphism (affine mapping) of the two space groups. The 219 types of space groups in R^3 give rise to 1128 types of Wyckoff sets. They define in addition equivalence classes within the set of Wyckoff positions and within the set of crystallographic orbits belonging to that space-group type.

3. Point configurations and lattice complexes

If Wyckoff positions or Wyckoff sets from space groups of different types are compared, another kind of equivalence relationship between crystallographic orbits has to be used:

Two crystallographic orbits are *configuration-equivalent* if and only if their sets of points are identical.

A *point configuration* is the set of all points that is common to a class of configuration-equivalent crystallographic orbits. This definition uniquely assigns crystallographic orbits to point configurations, but not *vice versa*, as illustrated by the following example: Any point configuration that forms a primitive cubic lattice refers to crystallographic orbits, for example, of the types of Wyckoff sets $Pm\bar{3}m$ $1(a, b)$, $Fm\bar{3}$ $8(c)$ and $P432$ $8(g)$ with $x = \frac{1}{4}$. The generating space group cannot be recognized by looking at the point configuration.

The *inherent symmetry* of a point configuration is the most comprehensive space group that maps the point configuration onto itself. Accordingly, one crystallographic orbit out of each class of configuration-equivalent ones stands out because its generating space group coincides with the inherent symmetry of its point configuration.

The concept of configuration-equivalence may also be applied to types of Wyckoff sets:

Two types of Wyckoff sets are *configuration-equivalent* if and only if for each crystallographic orbit out of one type of Wyckoff sets there exists a configuration-equivalent crystallographic orbit out of the other type of Wyckoff sets, and *vice versa*.

All types of Wyckoff sets differ with respect to their crystallographic orbits, but the sets of point configurations related to configuration-equivalent types of Wyckoff sets coincide:

A *lattice complex* is the set of all point configurations that is common to a class of configuration-equivalent types of Wyckoff sets.

For the space groups of R^3 these definitions lead to 402 classes of configuration-equivalent types of Wyckoff sets and to 402 lattice complexes.

One has to bear in mind that configuration-equivalent crystallographic orbits do not necessarily belong to configuration-equivalent types of Wyckoff sets. In the above example the types of Wyckoff sets $Pm\bar{3}m$ $1(a, b)$ and $Fm\bar{3}$ $8(c)$ are configuration-equivalent; the type of Wyckoff sets $P432$ $8(g)$, however, contains further crystallographic orbits (for $x \ne \frac{1}{4}$), which do not form cubic primitive lattices. Consequently, lattice complexes are not equivalence classes of point configurations, but a point configuration may belong to several lattice complexes.

It follows from the definitions that each type of Wyckoff sets is uniquely assigned to one lattice complex. Therefore, it makes sense to speak of the types of Wyckoff sets, the Wyckoff sets, the Wyckoff positions and the crystallographic orbits of a lattice complex. -

Among the different types of Wyckoff sets of a lattice complex, one stands out because its crystallographic orbits show the highest site symmetry. This one is called the *characteristic type of Wyckoff sets* of that lattice complex, the corresponding space-group type its *characteristic space-group type*. All other types of Wyckoff sets are referred to as non-characteristic. The term 'characteristic' may also be transferred to single Wyckoff sets out of the characteristic type.

Originating from Hermann [*Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), for short: IT (1935)], one Wyckoff position out of each characteristic Wyckoff set has arbitrarily been chosen to represent its lattice complex and, therefore, has also been called characteristic. The lattice complex of all cubic primitive point lattices, for example, has been designated by its 'characteristic Wyckoff position' $Pm\bar{3}m$ $1(a)$ (*cf.* IT, 1935, 1983). This arbitrariness is avoided by symbolizing a lattice complex by its characteristic (type of) Wyckoff set(s).

4. Limiting complexes and comprehensive complexes

As has been stated above lattice complexes define equivalence classes of orbits but not of point configurations. This property gave rise to the concept of limiting complexes and comprehensive complexes (Fischer & Koch, 1974; Koch, 1974; IT, 1983).

For morphological crystal forms an almost analogous situation exists. A certain tetragonal prism, for example, may be a general representative of the crystal form 'tetragonal prism' on the one hand or it may be a special representative of the crystal forms 'tetragonal pyramid' or 'tetragonal bisphenoid' on the other hand. In the first case the generating point group may belong to the types $4/mmm$, 422, $4/m$ or $\bar{4}2m$ (with site symmetry 2 for each face), in the second case the types of the generating point groups are $4mm$ or 4 and $\bar{4}2m$ (site symmetry m) or $\bar{4}$, respectively. The crystal form 'tetragonal prism' is a limiting form of the crystal forms 'tetragonal pyramid' and 'tetragonal bisphenoid'.

If a first lattice complex forms a true subset of a second one, *i.e.* if each point configuration of the first lattice complex also belongs to the second one, then the first one is called a *limiting complex* of the second one and the second complex is called a *comprehensive complex* of the first one.

Furthermore, two lattice complexes without a limiting-complex relationship between them may have a non-empty intersection. Then the point configurations of the intersection form another lattice complex or, in very exceptional cases, two other lattice complexes (for a proof see Koch, 1974).

For each point configuration of a given lattice complex its inherent symmetry may be compared with the generating space group of the corresponding crystallographic orbit from the characteristic type of Wyckoff sets. In general, these groups coincide. All point configurations belonging to a limiting complex, however, stand out by a more comprehensive inherent symmetry. Examples: (1) The cubic lattice complex with characteristic type of Wyckoff sets $I\bar{4}3d$ $16(c)$ xxx has the two limiting complexes $Im\bar{3}m$ $2(a)$ 000 and $Ia\bar{3}d$ $16(b)$ $\frac{1}{8}\frac{1}{8}\frac{1}{8}$. The crystallographic orbits from $Im\bar{3}m$ $2(a)$ and from $I\bar{4}3d$ $16(c)$ with $x = 0$ are configuration equivalent, and so are the orbits from $Ia\bar{3}d$ $16(b)$ and from $I\bar{4}3d$ $16(c)$ with $x = \frac{1}{8}$. (2) The tetragonal lattice complex with characteristic type of Wyckoff sets $I4_1/amd$ $4(a, b)$ is a comprehensive complex of the cubic complex $Fd\bar{3}m$ $8(a, b)$. Each crystallographic orbit of $Fd\bar{3}m$ $8(a, b)$ is configuration-equivalent to a crystallographic orbit of a special space group $I4_1/amd$ with axial ratio $c/a = \sqrt{2}$. (3) The intersection of the two lattice complexes $Im\bar{3}$ $24(g)$ and $I\bar{4}3m$ $24(g)$ consists of all point configurations belonging to $Im\bar{3}m$ $24(h)$, *i.e.* each point configuration out of this intersection refers to a crystallographic orbit from $Im\bar{3}m$ $24(h)$ $0xx$ and in addition to an orbit from $Im\bar{3}$ $24(g)$ $0yz$ with $y = z$ and to another one from $I\bar{4}3m$ $24(g)$ xxz with $z = 0$.

5. Characteristic and non-characteristic orbits, orbit types

The generating space group of any crystallographic orbit may be compared with the inherent symmetry of its point configuration. If both groups coincide, the orbit is called a *characteristic crystallographic orbit*, otherwise it is named a *non-characteristic crystallographic orbit* (Wondratschek, 1976). If the inherent symmetry group contains translations additional to those of the generating space group the term *extraordinary orbit* has been used. Each class of configuration-equivalent orbits contains exactly one characteristic crystallographic orbit.

The set of all point configurations in R^3 may be divided into equivalence classes by means of their inherent symmetry. Two point configurations belong to the same *symmetry type of point configurations* if and only if their characteristic crystallographic orbits belong to the same type of Wyckoff sets.

This equivalence relation results in 402 symmetry types of point configurations, which differ from the 402 lattice complexes because of the unique or non-unique assignment of point configurations (*cf.* below). As each crystallographic orbit is uniquely related to one point configuration, each equivalence relationship on the set of all point configurations implies an equivalence relationship on the set of all crystallographic orbits: Two crystallographic orbits are assigned to the same *orbit type* if and only if the corresponding point configurations belong to the same symmetry type.

In contrast to lattice complexes, symmetry types of point configurations and orbit types cannot be used

to define equivalence relations on Wyckoff positions, Wyckoff sets and types of Wyckoff sets. Two crystallographic orbits out of the same Wyckoff position belong to different orbit types, if – owing to special coordinate values – they differ in the inherent symmetry of their point configurations. In addition, two analogous crystallographic orbits from different space groups of the same type (*i.e.* two orbits with the same coordinate description) may differ in their orbit types owing to a specialization of the metrical parameters. Examples: (1) Crystallographic orbits from $P\bar{4}3m$ $4(e)$ xxx with $x = \frac{1}{4}$ or $x = \frac{3}{4}$ belong to another orbit type than those with $x \neq \frac{1}{4}, \frac{3}{4}$, because the inherent symmetry of their point configurations is $Fm\bar{3}m$ $4(a,b)$ instead of $P\bar{4}3m$ $4(e)$. (2) In general, the inherent symmetry of point configurations corresponding to the type of Wyckoff sets $I4/m$ $2(a, b)$ is $I4/mmm$ $2(a, b)$. For space groups with the special axial ratio $c/a = 1$ or $c/a = \sqrt{2}$, however, the inherent symmetry of the respective point configurations is $Im\bar{3}m$ $2(a)$ or $Fm\bar{3}m$ $4(a, b)$, respectively.

6. Comparison of the two concepts

The common intention of the lattice-complex concept as well as of the orbit-type concept is to subdivide the sets of all point configurations and of all crystallographic orbits of R^3 into subsets with certain common properties. Some of these subsets are identical in both concepts, but most of them are not. As similar but not identical symmetry considerations are used within both concepts, each lattice complex is uniquely related to a certain symmetry type of point configurations and to a certain orbit type, and *vice versa*. Therefore, both concepts result in the same number of subsets: there exist 402 lattice complexes, 402 symmetry types of point configurations and 402 orbit types. The differences between the subsets are caused by the different properties of the point configurations and crystallographic orbits used for the classifications.

The concept of orbit types is entirely based on the inherent symmetry of point configurations: crystallographic orbits are regarded as isolated entities, *i.e.* detached from their Wyckoff positions and their types of Wyckoff sets. On the contrary, lattice complexes result from a hierarchy of classifications of crystallographic orbits into Wyckoff positions, Wyckoff sets, types of Wyckoff sets and classes of configuration-equivalent types of Wyckoff sets, *i.e.* the crystallographic orbits are always considered as being embedded in their types of Wyckoff sets, and the inherent symmetry of their point configurations is disregarded. The differences between the two concepts become clear if limiting complexes are considered.

There exist 49 lattice complexes, which completely coincide with the corresponding symmetry types of point configurations. These are exactly those that contain neither limiting complexes due to special coordinates nor limiting complexes due to specialized metric. As tables of non-characteristic orbits by Engel, Matsumoto, Steinmann & Wondratschek (1984) show there exist 64 lattice complexes without limiting complexes due to specialized coordinates. These complexes have further been investigated with respect to limiting complexes due to metrical specialization. Among them there are 38 cubic lattice complexes and eight hexagonal ones, which – for principal reasons – do not allow any metrical specialization. The cubic ones have already been derived by Koch (1974) and may be found in that paper. For the hexagonal ones the characteristic types of Wyckoff sets are $P6_{2,4}22$ $3(c, d)$, $P6_{2,4}22$ $6(g, h)$, $P6/mmm$ $1(a, b)$, $P6/mmm$ $2(c, d)$, $P6/mmm$ $3(f, g)$, $P6/mmm$ $6(l, m)$, $P6/mmm$ $12(p, q)$, $P6_3/mmc$ $2(c, d)$.

15 of the remaining 18 lattice complexes are invariant ones. It is already known and easy to recognize that all 15 contain limiting complexes, at least *e.g.* hexagonal or cubic ones. Examples: (1) The lattice complex of all triclinic point lattices includes as limiting complexes the 13 other lattice complexes corresponding to Bravais lattices. (2) The lattice complex of all orthorhombic diamond patterns [$Fddd$ $8(a, b)$] includes as limiting complexes those of the tetragonal and the cubic diamond patterns [$I4_1/amd$ $4(a, b)$ and $Fd\bar{3}m$ $8(a, b)$, respectively].

The last three of the 64 lattice complexes mentioned above are $P4/mmm$ $4(l$-$o)$, $P4_2/mmc$ $4(j$-$m)$ and $I4/mmm$ $8(i, j)$. They complete the list of the 49 lattice complexes coinciding with their symmetry types of point configurations. This has been proved by inspecting the minimal cubic supergroups of $P4/mmm$, $P4_2/mmc$ and $I4/mmm$.*

353 lattice complexes are more comprehensive than the corresponding symmetry types of point configurations. In such a case each additional point configuration of the lattice complex belongs to a limiting complex. Examples: (1) $Im\bar{3}$ $24(g)$ $0yz$ with limiting complexes $Im\bar{3}m$ $24(h)$ for $y = z$, and $Pm\bar{3}m$ $3(c, d)$ for $y = z = \frac{1}{4}$; (2) $P4/mmm$ $8(r)$ xxz with limiting complexes $P4/mmm$ $4(j, k)$ for $z = \frac{1}{4}$, $P4/mmm$ $2(g, h)$ for $x = \frac{1}{4}$, $P4/mmm$ $1(a$-$d)$ for $x = z = \frac{1}{4}$, $Pm\bar{3}m$ $8(g)$ for $a = c$ and $x = z$, and $Pm\bar{3}m$ $1(a, b)$ for $a = c$ and $x = z = \frac{1}{4}$.

The comparison of an orbit type with the set of crystallographic orbits corresponding to its lattice complex, *i.e.* the set of orbits referring to the respective class of configuration-equivalent types of Wyckoff sets, is a little bit more complicated, because the orbit type may as well be more comprehensive as less

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* After the submission of our manuscript we received information on the thesis of Steinmann (1984), which contains similar considerations. The comparison with his results revealed an error in our original list.

comprehensive. Again the concept of limiting complexes and comprehensive complexes elucidates the interrelation.

Let A be a lattice complex with a limiting complex B and a comprehensive complex C. The respective orbit types will be designated A, B and C, too. [Example: $A = Im\bar{3}m$ 24(h) $0xx$; $B = Pm\bar{3}m$ 3(c, d) $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}00$; $C = Im\bar{3}$ 24(g) $0yz$.] Then a crystallographic orbit from any Wyckoff position of lattice complex A only belongs to orbit type A if it does not correspond to a point configuration of the limiting complex B. [Only crystallographic orbits of $Im\bar{3}m$ 24(h) with $x \neq \frac{1}{4}$ belong to orbit type $Im\bar{3}m$ 24(h).] Those crystallographic orbits of lattice complex A, however, that do correspond to the limiting complex B do not belong to orbit type A but to orbit type B. [All crystallographic orbits from $Im\bar{3}m$ 24(h) with $x = \frac{1}{4}$ refer to lattice complex $Im\bar{3}m$ 24(h) but belong to orbit type $Pm\bar{3}m$ 3(c, d).] On the contrary, those orbits of lattice complex C that also correspond to the limiting complex A of C belong to orbit type A, but not to orbit type C. [All crystallographic orbits of $Im\bar{3}$ 24(g) $0yz$ with $y = z$ refer to lattice complex $Im\bar{3}$ 24(g) but belong to orbit type $Im\bar{3}m$ 24(h) or, if $y = z = \frac{1}{4}$, to $Pm\bar{3}m$ 3(c, d).]

For the comparison of lattice complexes and orbit types the concept of non-characteristic orbits is less helpful than the concept of limiting complexes. In terms of lattice complexes, there exist two basically different reasons for a crystallographic orbit to be non-characteristic:

(1) The crystallographic orbit under consideration belongs to a non-characteristic type of Wyckoff sets of a lattice complex. Then this orbit – together with all other crystallographic orbits out of its type of Wyckoff sets – is non-characteristic. Characteristic crystallographic orbits always stem from characteristic Wyckoff sets of lattice complexes.

(2) The crystallographic orbit under consideration stands out with respect to the inherent symmetry of its point configuration compared with the other orbits out of its type of Wyckoff sets, i.e. it corresponds to a limiting complex. Then this orbit together with all other orbits of that limiting complex is non-characteristic.

As a consequence, three kinds of non-characteristic orbits may be distinguished: (1) those that belong to a non-characteristic Wyckoff set, but do not correspond to a limiting complex [example: all orbits from $Pm\bar{3}$ 6(e, h)]; (2) those that belong to a characteristic Wyckoff set, but correspond to a limiting complex [examples: $Pm\bar{3}m$ 8(g) xxx with $x = \frac{1}{4}$; $P4/mmm$ 1(a, b) with $a = c$]; (3) those that belong to a non-characteristic Wyckoff set and, in addition, correspond to a limiting complex [example: $Pm\bar{3}$ 8(i) xxx with $x = \frac{1}{4}$].

As these considerations prove, limiting complexes and non-characteristic orbits do not correspond to

each other. Therefore, a statement by Engel (1983) proposing this correspondence is not correct.*

The concept of lattice complexes and limiting complexes on the one hand and of orbit types and non-characteristic orbits on the other are complementary in a certain sense: it is possible to derive all orbit types and all non-characteristic orbits from the complete knowledge of lattice complexes and limiting complexes and vice versa. Unfortunately, however, full information is available neither on limiting complexes nor on non-characteristic orbits, as far as is known by the authors.

The assignment of all Wyckoff positions to lattice complexes has been done by Hermann in IT (1935). This information has also been given by Fischer, Burzlaff, Hellner & Donnay (1973) and in IT (1983). The limiting complexes of the cubic lattice complexes have been derived by Koch (1974). This information has been supplemented by Barth (1980) who tabulated the (cubic and non-cubic) comprehensive complexes of the cubic lattice complexes. Barth's tables also contain the corresponding conditions for the metrical and coordinate parameters. The determination of the other comprehensive complexes has not been done so far.

Extensive tables by Engel, Matsumoto, Steinmann & Wondratschek (1984) contain information on the orbit types for part of the non-characteristic orbits, i.e. for such non-characteristic orbits that refer to special coordinates only. The further non-characteristic orbits, which are based on specialized metrical parameters of their generating space groups or on the simultaneous specialization of metrical and coordinate parameters, have not been determined so far.

The special, but not exceptional, case that a non-characteristic orbit is only produced if both, coordinates and metric, are specialized deserves extra concern. The crystallographic orbits from $R\bar{3}$ 6(f) xyz with $x = \frac{1}{4}$, $y = 0$, $z = \frac{1}{2}$ or with $x = \frac{1}{4}$, $y = \frac{1}{2}$, $z = 0$ and with the rhombohedral angle $\alpha = 90°$ may be used as an example. The inherent symmetry of the corresponding point configurations is $Pm\bar{3}n$ 6(c, d) (the position of the Cr atoms in the crystal structure of Cr_3Si). Accordingly, the lattice complex $R\bar{3}$ 6(f) contains $Pm\bar{3}n$ 6(c, d) as limiting complex. $Pm\bar{3}n$ 6(c, d) shows special integral reflection conditions (hkl: $h + k + l = 2n$ or $h = 2n + 1$, $k = 4n$, $l = 4n + 2$; h, k, l permutable), which of course also hold for all non-characteristic orbits of that orbit type. As geometrical structure factors are independent of metrical parameters, these reflection conditions are even valid for crystallographic orbits from $R\bar{3}$ 6(f) with $\alpha \neq 90°$, if only the coordinates are specialized to $\frac{1}{4}$, 0, $\frac{1}{2}$ or $\frac{1}{4}$, $\frac{1}{2}$, 0.

In general, the following statement holds: If a lattice complex causes special reflection conditions then exactly these reflection conditions are also valid

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* The authors of the present paper never made such a statement.

for any crystallographic orbit that refers to a comprehensive complex of that lattice complex if, in addition, it may be described by the same coordinate triplets as an orbit of the regarded lattice complex.

References

BARTH, H.-U. (1980). *Über umfassende Komplexe kubischer Gitterkomplexe.* Diplomarbeit, Univ. Münster.
BURZLAFF, H. & ZIMMERMANN, H. (1974). *Z. Kristallogr.* **139**, 252–269.
ENGEL, P. (1983). *Z. Kristallogr.* **163**, 243–249.
ENGEL, P., MATSUMOTO, T., STEINMANN, G. & WONDRATSCHEK, H. (1984). *Z. Kristallogr.* Suppl. No. 1.
FISCHER, W., BURZLAFF, H., HELLNER, E. & DONNAY, J. D. H. (1973). *Space Groups and Lattice Complexes. Natl Bur. Stand.*

(*US*) *Monogr.* No. 134. Washington: National Bureau of Standards.
FISCHER, W. & KOCH, E. (1974). *Z. Kristallogr.* **139**, 268–278.
FISCHER, W. & KOCH, E. (1978). *Z. Kristallogr.* **147**, 255–273.
FISCHER, W. & KOCH, E. (1983). *Acta Cryst.* **A39**, 907–915.
HERMANN, C. (1935). *Gitterkomplexe.* In *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, Vol. I. Berlin: Bornträger.
International Tables for Crystallography (1983). Vol. A. Dordrecht, Boston: D. Reidel.
Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Vol. I. Berlin: Bornträger.
KOCH, E. (1974). *Z. Kristallogr.* **140**, 75–86.
KOCH, E. & FISCHER, W. (1975). *Acta Cryst.* **A31**, 88–95.
KOCH, E. & FISCHER, W. (1978). *Z. Kristallogr.* **147**, 21–38.
MATSUMOTO, T. & WONDRATSCHEK, H. (1979). *Z. Kristallogr.* **150**, 181–198.
STEINMANN, G. (1984). *Kristallographische Orbits im dreidimensionalen Raum.* Dissertation, Univ. Karlsruhe.
WONDRATSCHEK, H. (1976). *Z. Kristallogr.* **143**, 460–470.
WONDRATSCHEK, H. (1980). *Commun. Math. Chem.* **9**, 121–125.

Restrained Structure-Factor Least-Squares Refinement of Protein Structures Using a Vector Processing Computer

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Abstract

A least-squares refinement program *RESTRAIN* has been developed, which is capable of refining macromolecular structures using structure amplitudes, phases from isomorphous replacement or anomalous scattering and pseudo-energy restraints. In addition to positional parameters and isotropic temperature factors, anisotropic mean-square displacements may be refined either as individual atomic U tensors or as TLS tensors applied to groups of atoms. Anharmonic effects may be handled by coupling together occupancies to enable the electron density of an atomic group to be distributed over more than one subsite. A novel way of restraining groups of atoms to be planar has been developed that does not require dummy atoms and does not restrain the plane to lie in its current orientation.

Introduction

Techniques for the refinement of macromolecular structures from diffraction data using geometrical

restraints are now well established. Before 1976 most refinements of protein structures were undertaken using difference Fourier methods. Several techniques for automating this approach were developed (Diamond, 1971; Freer, Alden, Carter & Kraut, 1975) and real-space refinement has recently been applied to the protein component of a virus (Jones & Liljas, 1984).

Reciprocal-space least-squares refinement techniques followed later and imposed geometrical restraints on the positional parameters in terms of bond lengths, bond angles and non-bonded interactions. Systems that have minimized functions that contain both structure amplitude and restraint terms (Konnert, 1976; Sussman, Holbrook, Church & Kim, 1977; Moss & Morffew, 1982) have been widely used in the refinement of protein and RNA structures (see, for example, Borkakoti, Palmer, Haneef & Moss, 1983; Sielecki, Hendrickson, Broughton, Delbaere, Bryer & James, 1979; Girling, Houston, Schmidt & Amma, 1980). Other systems, which impose the restraints in a separate least-squares or energy-minimization step outside the structure-amplitude refinement (Agarwal, 1978; Jack & Levitt, 1978), have also been successfully employed (Baker, 1980).