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Crystallographic orbits, lattice complexes, and orbit types

by

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In the description of crystal structures the concept of lattice complexes is useful, see, e.g., Internationale Tabellen (1935), Fischer, Burzlaff, Hellner, and Donnay (1973), Hellner (1979), and the literature cited in these papers. Two definitions of "lattice complex" have been given by Zimmermann and Burzlaff (1974) and Fischer and Koch (1974). The definition of lattice complexes given here follows closely that of Fischer and Koch (1974) but it avoids the introduction of automorphism groups and accentuates the relation of lattice complexes to orbit types.

A <u>crystallographic orbit</u> $O = R\,\underline{X} = \{r\,\underline{X} | r \in R\}$ is the orbit of a point $\underline{X}$ under the action of a space group R. The space group R is called the <u>generating space group</u> of the crystallographic orbit O. Such crystallographic orbits have been considered frequently in crystallography under different names, e.g. regelmäßiges Punktsystem, regelmäßiger Molekelhaufen, Gitterkomplex, (kristallographische)Punktkonfiguration, (crystallographic)point configuration, or discrete Euclidean universe. In most cases crystallographers consider a crystallographic orbit $O = R\,\underline{X}$ in connection with its generating space group R. If this connection is to be used the orbit will be denoted by O_R.

The set S of all $s \in R$, for which $s\,\underline{X} = \underline{X}$ holds, i.e. the stabilizer of $\underline{X}$ in R, is called the <u>site-symmetry group</u> of the point $\underline{X}$ with respect to R. (The term 'point symmetry' should be avoided in this context as it commonly refers to the crystal class of a crystal.) The site-symmetry groups of two points of the same crystallographic orbit under R are conjugate subgroups of R.

The site-symmetry groups may be used to classify points and orbits with respect to R. Let $\underline{X}_1$ be a point and S_1 its site-symmetry group with respect to R. The set of all points $\underline{X}_2$ such that the site-symmetry group S_2 of $\underline{X}_2$ with respect to R is conjugate to S_1, i.e. such that there exists an $r \in R$ with $r^{-1}S_1r = S_2$, is called the <u>Wyckoff position</u> $W_R(\underline{X}_1)$ <u>of the point</u> $\underline{X}_1$ <u>with respect to R</u>. A Wyckoff position $W_R(\underline{X})$ is a stratum of points under the action of R (the term 'stratum' being defined by Michel (1979) to be a complete set of points such that their stabilizers in R are conjugate under R). With each point $\underline{X}$ also the full orbit R $\underline{X}$ belongs to the Wyckoff position $W_R(\underline{X})$ with respect to R. Therefore, it is possible to speak of a Wyckoff position $W_R(R\ \underline{X})$ of orbits with respect to R.

A coarser classification of both, points and orbits with respect to R is used to define Wyckoff sets of points and orbits, respectively. Let $\underline{X}_1$ be a point and S_1 its site-symmetry group with respect to R. The set of all points $\underline{X}_2$ such that the site-symmetry group S_2 of $\underline{X}_2$ with respect to R is conjugate to S_1 under the normalizer N of R in the group A of all affine mappings, i.e. such that there exists an $n \in N$ with $n^{-1}\ S_1\ n = S_2$, is called the Wyckoff set of the point $\underline{X}_1$ with respect to R. Again with each point $\underline{X}$ also the full orbit R $\underline{X}$ belongs to the Wyckoff set of $\underline{X}$ with respect to R. Therefore, it is possible to speak of a Wyckoff set of orbits with respect to R. Moreover, a Wyckoff set contains full Wyckoff positions of points or orbits with respect to R.

Space groups are classified into finitely many space-group types by the following definition. Two space groups R_1 and R_2 belong to the same space-group type if there is an affine mapping $a \in A$, such that $R_2 = a\ R_1\ a^{-1}$, i.e. R_1 and R_2 are conjugate in the group A of all affine mappings. There are 219 such 'affine space-group types' in three-dimensional space and 17 plane-group types in the plane. 230 'crystallographic space-group types' do exist if conjugacy in A^+, the group of all proper affine mappings, is used instead of A in the definition of space-group type.

Affine classification may be transferred to the crystallographic orbits O_R with respect to space group R in the following way.

Let S be the site-symmetry group of a point Y of an orbit O_R of R, and S' the site-symmetry group of a point Y' of an orbit $O'_{R'}$ of R'. The two orbits are affinely related by their site symmetries with respect to their generating space groups or are affinely S_R-related if there exists an affine mapping $a \in A$ such that $R' = a\ R\ a^{-1}$ (R' and R belong to the same space-group type) and $S' = a\ S\ a^{-1}$ hold. The set of all orbits affinely S_R-related to an orbit O_R is called a _Wyckoff class of orbits with respect to the space-group type of R_. It has to be emphazised that the generating space groups play an essential rôle in this definition. The orbits as point sets per se are not sufficient to define Wyckoff classes. A Wyckoff class of orbits contains always full Wyckoff positions of orbits and full Wyckoff sets of orbits. By this, Wyckoff classes classify Wyckoff sets of orbits as well.

Let O_R and $O'_{R'}$ be two affinely S_R-related orbits with respect to the space groups R and R'. If R = R', then O_R and O'_R are elements of the same Wyckoff set with respect to R. They are not necessarily elements of the same Wyckoff position with respect to R nor does $O = O'$ hold in general. Analogously any two affinely S_R-related Wyckoff positions W_R $(R\underline{X})$ and W'_R $(R\underline{X}')$ with respect to R are contained in the same Wyckoff set with respect to R but are not necessarily identical. Two affinely S_R-related Wyckoff sets of orbits with respect to R, however, are always identical. Therefore, labelling the Wyckoff classes of orbits with respect to a space-group type may be transferred in a unique way to Wyckoff sets of orbits with respect to any space group of that type, but not to Wyckoff positions of orbits. The traditional labelling of Wyckoff positions of points or orbits with respect to a space group (Wyckoff notation, see International Tables 1952) is thus not unique but depends, in crystallographic terms, on the 'setting', i.e. the choice of the basis vectors and the origin for the description of the space group. The Wyckoff notations belonging to the same Wyckoff class are listed by Koch and Fischer (1975); changes in Wyckoff notation caused by changes of the coordinate system have been listed by Boyle and Lawrenson (1973), (1978).

One may consider crystallographic orbits also detached from their generating space groups. A _lattice complex_ (Gitterkomplex) is the set of all crystallographic orbits in a Wyckoff class, irrespective of the type of the generating space group. Different Wyckoff classes may contain exactly the same crystallographic orbits. In this case they define the same lattice complex.

Let $O = (R\underline{X})$ be a crystallographic orbit. The uniquely determined set E of all motions m with $m\,O = O$, i.e. leaving O invariant, is the Eigensymmetry space group E of the crystallographic orbit O or the stabilizer of O in the set M of all motions.

The generating space group R of O is not uniquely determined; a crystallographic orbit O may have been generated by different space groups which may belong to different space-group types. Therefore, the lattice complexes do not classify the set of all orbits but the intersection of two lattice complexes is not necessarily empty. A classification of all crystallographic orbits is possible, however, by the Eigensymmetry space groups E of the crystallographic orbits.

Let E be the Eigensymmetry space group of the crystallographic orbit O. Even if the crystallographic orbit O = $(R\underline{X})$ has not been generated by E, we can replace R by E in O = $(R\underline{X})$ without affecting O. Let S_E be the stabilizer of the point $\underline{Y} \in O$ in the space group E. The set of all crystallographic orbits affinely S_E-related to the orbit O is called the orbit type of the crystallographic orbit O.

In this way "orbit types" are defined closely related to the definition of "lattice complexes". It is well known that the orbits of a lattice complex may be elements of different orbit types. On the other hand orbits of the same orbit type may be elements of different lattices complexes. Both concepts may now be combined to describe crystal structures.

The way of defining lattice complexes and orbit types as given here has been used in a rather vague form by the author at the occasion of the Riederalp symposium, August 1979, for the first time. The present shape of definitions is considerably different from the initial one. Numerous colleagues have helped the author to improve and polish his original ideas. This essential aid, especially by W. Fischer, E. Koch, and J. Neubüser, as well as the financial support by the Deutsche Forschungsgemeinschaft, is gratefully acknowledged.

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