

# A LITTLE DICTIONARY OF CRYSTALLOGRAPHY

Prepared by the Commission on Crystallographic  
Nomenclature of the International Union of Crystallog-  
raphy

Edited by ANDRÉ AUTHIER and GERVAIS CHAPUIS

INTERNATIONAL UNION OF  
CRYSTALLOGRAPHY

*Edition: July 2014*

## Foreword

The lack of a compendium of crystallographic terms and the many questions related to matters of definitions and nomenclature led the IUCr Commission on Crystallographic Nomenclature to put forward the idea of an *Online Dictionary of Crystallographic Terms* at the 20th IUCr Congress in Florence (August 2005). The idea was received enthusiastically by the Executive Committee of the Union and a Working Group was set up to provide guidance on the establishment and conduct of a project undertaken under the aegis of the Commission.

The first task of the Working Group was to define the nature and scope of the *Dictionary*. A Pilot Project was then prepared by the Research and Development Officer of the IUCr, Brian McMahon; it was based on the principle of Wikipedia and used *mediawiki* software. This pilot project was adopted by the Executive Committee in 2006 and a Board of Editors was appointed, with the Chairman of the Commission on Crystallographic Nomenclature as Chief Editor. The *Online Dictionary* was operational in 2007 and, by 2008, almost 200 substantial definitions had been entered and grouped into categories. In 2009, a new Editor in Chief, Gervais Chapuis, was appointed.

*André Authier*  
Chairman

*IUCr Commission on Crystallographic Nomenclature (2002–2014)*

## Preface

It is our hope that this pocket-sized edition of the *Online Dictionary of Crystallography* will convince the community of crystallographers to contribute directly to the project. I am sure that careful readers will find some errors, shortcomings or omissions. They might also find that some specific domains of crystallography are not currently covered in the present edition. The solution to this problem is quite straightforward, knowing that the *Online Dictionary of Crystallography* is published in the form of a Wiki. In other words, we have set up an open system where any *bona fide* crystallographers can correct or modify some definitions and also introduce some new ones after registering for an account. It is the task of the Editors to check that all the contributions are in line with the nomenclature maintained by the IUCr.

*Gervais Chapuis*  
Editor in Chief  
*Online Dictionary of Crystallography*

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## Introduction

As described above, the *Online Dictionary of Crystallography* was launched in 2007 using *mediawiki* (<http://www.mediawiki.org>) as the authoring and dissemination platform.

### *Scientific scope*

Broadly speaking, the project deals with the subject of crystallography, the area of science over which the IUCr has authority. Terms from related disciplines (physics, mathematics, chemistry, mineralogy, biology *etc.*) are included so long as they have a specific relevance to crystallography, *e.g.* crystallographic group. Names of chemical or biological substances or minerals are not generally included. References to specific computer programs are generally avoided. Names of people are only included if they relate to crystallographic concepts, *e.g.* Bragg's law, Ewald sphere. While not aimed specifically at an expert audience, equations, tables and figures are included where necessary to illustrate and explain the definitions.

Translations of terms in other languages than English are given, but in keeping with the current role of English as the international language of science, the definitions themselves are not translated into other languages. There has not been an editorial effort to collect a comprehensive set of translations, but an advantage of the Wiki approach is that volunteers may contribute to the translation project at any time.

### *The granularity of definitions*

This project has produced an online reference that is a blend between 'dictionary' and 'encyclopaedia': a list of terms with short definitions and cross-links to other entries in the work, with at times longer developments. Many references are provided to other online resources of the IUCr (*Teaching Pamphlets*, CIF dictionaries, *International Tables for Crystallography*, Journals). These of course are active hyperlinks on the web.

The general pattern of a typical page is:

- translation of the term in other languages,
- main definition
- examples or applications or special cases
- history
- list of links to other entries or to IUCr or other web pages

The primary goal of the dictionary is to be a reference for authors and referees of IUCr Journals and for research professionals in general: it will give the 'official' IUCr acceptance of terms. As such it will also be useful to students and to the general public.

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### *Hard-copy publication*

The current volume is a printed snapshot of the contents of the *Online Dictionary of Crystallography*. It was produced by the IUCr Commission on Crystallographic Nomenclature as a contribution to the educational outreach activities of the International Year of Crystallography, proclaimed by the United Nations for the year 2014.

Its dissemination in a handy pocket-sized format will encourage wide circulation and may be useful in classrooms and public libraries, as well as in laboratories and on individual scientists' book shelves.

The most up-to-date version of the definitions in this book can be found online at the web address <http://reference.iucr.org/dictionary>

*Brian McMahon  
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## Learning more

Cross references to other entries in the body of the dictionary are indicated by the double-arrow symbol (*e.g.* ⇒ **crystal structure**).

The *See also* sections refer to

- Other entries in the dictionary.
- Teaching Pamphlets prepared by the Commission on Crystallographic Teaching of the International Union of Crystallography (mostly during the 1980s). These pamphlets are freely available to download from the IUCr web site  
<http://www.iucr.org/education/pamphlets>
- *International Tables for Crystallography*, published for the International Union of Crystallography by John Wiley & Sons Ltd, and available online to subscribers at <http://it.iucr.org>
- Reports and other articles published in IUCr journals, available online at <http://journals.iucr.org>

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method of its specification are different. The table compares the two cases.

	<b>Absolute structure</b>	<b>Absolute configuration</b>
<i>Property</i>	spatial arrangement	spatial arrangement
<i>Content</i>	atoms	atoms
<i>Object</i>	crystal	molecule
<i>Symmetry</i>	non-centrosymmetric	chiral
<i>Specification</i>	crystallographic space group cell dimensions atomic coordinates	stereochemical CIP

Whereas absolute configuration distinguishes between and specifies enantiomers (chiral molecules of opposite hand), absolute structure does the same for inversion-related models of the crystal structure. In the same way that there is no absolute configuration for an achiral molecule, there is no absolute structure for a centrosymmetric crystal structure.

### *Determination of absolute configuration from absolute structure*

One must first have a valid absolute-structure determination (see ⇒ **Flack parameter**). The most stringent requirement in order to deduce the absolute configuration of the molecules composing a crystal from an absolute-structure determination is that the crystal structure be composed of enantiopure (chiral) molecules. Experimental evidence should be provided of the enantiopurity of the crystal or of the bulk. Some necessary but not-sufficient requirements are easier to apply. The crystal structure should be chiral. A chiral crystal structure displays a space group that only contains translations, pure rotations and screw rotations, and does not contain any reflections, inversions, rotoinversions or glide reflections. Another necessary but not-sufficient condition is that the crystal structure contains chiral molecules.

*See also*

- Flack parameter
- Friedel's law

## Absolute structure

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### *Related chemical terms*

The IUPAC *Basic Terminology of Stereochemistry* contains definitions of related chemical terms of use to the crystallographer, viz: *absolute configuration*, *chiral*, *chirality*, *chirality sense*, *enantiomer*, *enantiomerically pure*, *enantiomorph*, *racemate*, *racemic*, *racemic conglomerate* and *relative configuration*.

### *Reference*

- IUPAC (1996). *Basic Terminology of Stereochemistry*. <http://www.chem.qmul.ac.uk/iupac/stereo>
- 

## Absorption edge

*Arête d'absorption* (Fr). *Absorptionskante* (Ge). *Canto de absorción* (Sp). край поглощения (Ru). *Spigolo di assorbimento* (It).

### *Definition*

An absorption edge is a sharp discontinuity in the absorption spectrum of X-rays by an element that occurs when the energy of the photon corresponds to the energy of a shell of the atom (*K*, *L<sub>I</sub>*, *L<sub>II</sub>*, *L<sub>III</sub>*, etc.).

### *Examples*

For gallium:

$$\lambda_K = 1.1958 \text{ \AA}; \lambda_{L_I} = 9.5446 \text{ \AA}; \lambda_{L_{II}} = 10.8414 \text{ \AA}; \\ \lambda_{L_{III}} = 11.1038 \text{ \AA}.$$

For arsenic:

$$\lambda_K = 1.0448 \text{ \AA}; \lambda_{L_I} = 8.1195 \text{ \AA}; \lambda_{L_{II}} = 9.1187 \text{ \AA}; \\ \lambda_{L_{III}} = 9.3617 \text{ \AA}.$$

See also

- Chapter 4.2.3 of *International Tables for Crystallography, Volume C*
-

## Acceptance domain

Synonyms: window, atomic domain, atomic surfaces

*Domaine d'acceptation, fenêtre (Fr).*

### *Definition*

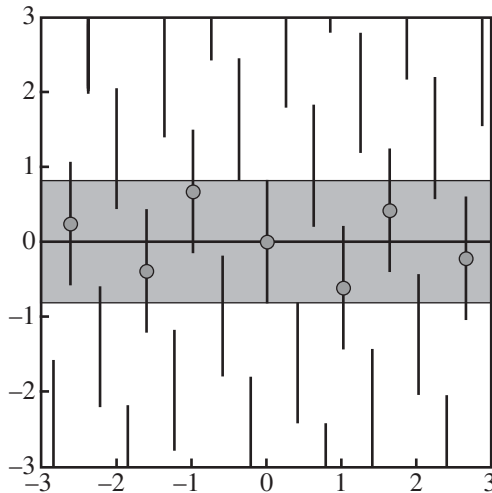
When an aperiodic crystalline point set is obtained by the intersection method, as the intersection of a periodic array of finite, disjoint components in superspace and the physical space, then there is, for each point, a component in the higher-dimensional unit cell. These components are called *acceptance domains*, *atomic surfaces*, *atomic domains*, or *windows* in the literature. The positions of atoms in aperiodic crystals (or vertices in the case of a tiling) are the intersection of the atomic surfaces with the physical space. This construction of the points is called the *intersection method*.

### *History*

The term *window* comes from an alternative construction. One considers a ‘tube’ in  $n$ -dimensional superspace that is the product of the  $m$ -dimensional physical space  $V$  and a transversal finite  $(n - m)$ -dimensional object  $O$ :  $V \otimes O$ . Then the points of the  $n$ -dimensional lattice, corresponding to the periodic embedding of the structure in  $V$ , that lie inside the tube are projected on  $V$  (see Fig. 1). These are the points of the aperiodic structure in  $V$ . The construction is called the *cut-and-project method*. The object  $O$  is the *window*, or *acceptance domain*. The latter expresses the fact that only lattice points inside the tube are projected. The result is the same as attaching a copy of  $O$  to each lattice point, and considering the intersection of this periodic array with  $V$ . Actually, the latter construction is more special, in the sense that the atomic surfaces in this are by definition flat, whereas the intersection method allows arbitrarily shaped ones.

## Acceptance domain

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**Figure 1**

The grey strip in superspace is the product of the (infinite) physical space (in this case the horizontal line) and a vertical finite line interval, the acceptance domain. The centres of the vertical lines form a lattice. When a lattice point falls inside the strip it is projected on the physical space. The projected points form an aperiodic crystal. These projected points are also the intersections of the array of vertical lines with the physical space.

See also

- Atomic surface

---

## Affine isomorphism

Each symmetry operation of a crystallographic group in  $E^3$  may be represented by a  $3 \times 3$  matrix  $\mathbf{W}$  (the *linear part*) and a vector  $\mathbf{w}$ . Two crystallographic groups  $G_1 = (\mathbf{W}_{1i}, \mathbf{w}_{1i})$  and  $G_2 = (\mathbf{W}_{2i}, \mathbf{w}_{2i})$  are called **affine isomorphic** if there exists a non-singular  $3 \times 3$  matrix  $\mathbf{A}$  and a vector  $\mathbf{a}$  such that:

$$G_2 = \{(\mathbf{A}, \mathbf{a})(\mathbf{W}_{1i}, \mathbf{w}_{1i})(\mathbf{A}, \mathbf{a})^{-1}\}.$$

Two crystallographic groups are affine isomorphic if and only if

their arrangement of symmetry elements may be mapped onto each other by an affine mapping of  $E^3$ . Two affine isomorphic groups are always isomorphic.

*See also*

- Automorphism
  - Group isomorphism
- 

## Affine mapping

*Transformation affine (Fr). Affine Abbildung (Ge). Trasformazione affine (It). アフィン写像 (Ja).*

*Definition*

An **affine mapping** is any mapping that preserves collinearity and ratios of distances: if three points belong to the same straight line, their images under an affine transformation also belong to a straight line. Moreover, the middle point is also conserved under the affine mapping. By contrast, angles and lengths in general are not kept constant by an affine mapping.

Under an affine mapping:

- parallel lines remain parallel;
- concurrent lines remain concurrent (images of intersecting lines intersect);
- the ratio of length of segments of a given line remains constant;
- the ratio of areas of two triangles remains constant;
- ellipses, parabolas and hyperbolas remain ellipses, parabolas and hyperbolas respectively;
- barycentres of polygons map into the corresponding barycentres.

Geometric contraction, expansion, dilation, reflection, rotation, shear, similarity transformations, spiral similarities, and translation are all affine transformations, as are their combinations.

## Affine mapping

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Affine mappings that keep also distances and angles are called Euclidean mappings or isometries.

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## Allotwin

*Allomacle* (Fr). *Allogeminato* (It). アロ双晶 (Ja).

### *Definition*

An **allotwin** is a twin whose individuals are oriented crystal associations of different polytypes of the same compound.

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## Anomalous absorption

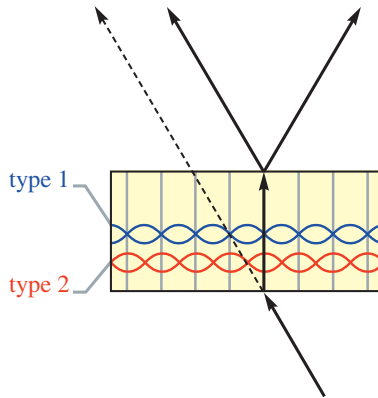
*Absorption anormale* (Fr). *Anomale Absorption* (Ge). *Absorción anómala* (Sp). *Assorbimento anomalo* (It).

### *Definition*

Anomalous absorption takes place when radiation is dynamically diffracted by a perfect or nearly perfect crystal. The optical field in the crystal is then made up of several components, called wavefields, two in the two-beam case (neglecting polarization in the X-ray case). One of them is absorbed more than normal and the other one less than normal. In the transmission, or Laue, geometry, both wavefields propagate inside the crystal; one then speaks of anomalous transmission for the less absorbed wavefield (Borrmann effect). In the reflection, or Bragg, geometry, one wavefield only propagates in the crystal, the more absorbed one for angles of incidence corresponding to one side of the total reflection rocking curve and the less absorbed one for the other side. This results in an asymmetry of the rocking curve that is calculated using dynamical theory.

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### *Physical interpretation*



**Figure 2**

Borrmann (1950) interpreted anomalous absorption by means of the standing waves that are formed by the interference of the incident and reflected waves (Laue, 1937, 1941). The nodes and antinodes of these standing waves have the periodicity of the lattice planes. In the transmission geometry (see Fig. 2), the nodes lie on the lattice planes for type 1 wavefields, which undergo therefore a quite small absorption, while it is the antinodes that lie on the lattice planes for type 2, which undergo a larger absorption.

In the reflection geometry, the nodes and antinodes shift by half a lattice distance as the crystal is rocked through the rocking curve. On the smaller angle side of the rocking curve it is type 1 wavefields that are excited, the nodes lie on the lattice planes and the absorption is small. On the higher angle side of the rocking curve, it is type 2 wavefields that are excited, the antinodes lie on the lattice planes and the absorption is large. This effect is used in the standing-wave technique for observing adsorbed atoms at the surface of crystals.

### *History*

Anomalous absorption was discovered by Borrmann on quartz [Borrmann G. (1941). *Physik Z.* **42**, 157–162. *Über Extinktions-*



## Anomalous absorption

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*diagramme der Röntgenstrahlen von Quarz*] and calcite crystals [Borrmann G. (1950). *Z. Phys.* **127**, 297–323. *Die Absorption von Röntgenstrahlen in Fall der Interferenz*] and first interpreted by Laue [Laue, M. von (1949). *Acta Cryst.*, **2**, 106–113. *Die Absorption der Röntgenstrahlen in Kristallen im Interferenzfall*].

See also

- Borrmann effect
  - Chapter 5.1 of *International Tables for Crystallography, Volume B* for X-rays
  - Chapter 5.2 of *International Tables for Crystallography, Volume B* for electrons
  - Chapter 5.3 of *International Tables for Crystallography, Volume B* for neutrons
- 

## Anomalous dispersion

*Dispersion anormale* (Fr). *Anomale Dispersion* (Ge). *Dispersion anómala* (Sp). *Dispersione anomala* (It).

*Definition*

The ‘anomalous’ dispersion corrections, which are not in fact anomalous, take into account the effect of absorption in the scattering of phonons by electrons. In the classic picture the electron is approximated by a damped harmonic oscillator. The scattering factor of the electron is then complex and the atomic scattering factor, or atomic form factor, is given by

$$f + f' + if''$$

where  $f'$  and  $f''$  are the real and imaginary parts of the anomalous dispersion correction. Their importance increases as one gets closer to an absorption edge ( $\Rightarrow$  **resonant scattering**). Numerical calculations usually follow the Hartree–Fock approximations. For details on the non-relativistic and relativistic approaches, see Chapter 4.2.6 of *International Tables of Crystallography, Volume C*.

### History

The dispersion of X-rays was theoretically predicted by Waller [Waller, I. (1928). *Z. Phys.* **51**, 213–231. *Über eine verallgemeinerte Streuungsformel*] and first calculated by Hönl [Hönl, H. (1933). *Z. Phys.* **84**, 1–16. *Zur Dispersionstheorie der Röntgenstrahlen*; Hönl, H. (1933). *Ann. Phys. (Leipzig)*, **18**, 625–657. *Atomfactor für Röntgenstrahlen als Problem der Dispersionstheorie (K-Schale)*].

### See also

- Anomalous scattering
  - Multiwavelength anomalous diffraction (MAD)
  - Chapter 4.2.6 of *International Tables for Crystallography, Volume C*
- 

## Anomalous scattering

*Diffusion anormale (Fr)*. *Anomale Streuung (Ge)*. *Difusión anómala (Sp)*. *Diffusione anomala (It)*.

### Definition

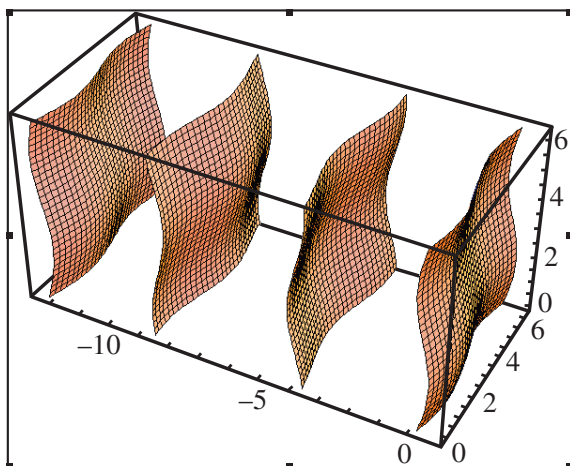
The history of the description of the scattering of an atom when illuminated with X-rays is that initially wavelength dependencies were ignored. This was initially referred to as ‘normal scattering’. The wavelength dependencies were then corrections to the normal scattering and also called anomalous. These had to describe changes in amplitude and phase, respectively initially given the symbols  $\Delta f'$  and  $\Delta f''$ . Thus the X-ray scattering factor of an atom is described by the equation

$$f = f_o + \Delta f' + i\Delta f''.$$

The nomenclature changed when tunable synchrotron sources became available and the  $\Delta$  prefixes were removed because changes between two wavelengths would then have required a double  $\Delta$  label, which is cumbersome. Thus the  $\Delta f'$  now means the change in  $f'$  between two wavelengths. The  $\Delta$  prefix to  $f''$  is dropped for consistency even though its use is based on its value at a single

## Atomic surface

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**Figure 4**

A one-dimensional incommensurate phase with a two-dimensional modulation is the intersection of the one-dimensional physical space with a periodic array of two-dimensional surfaces, with three-dimensional lattice periodicity.

See also

- Superspace
- Acceptance domain

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## Automorphism

*Automorphisme (Fr). Automorphismus (Ge). Automorfismo (Sp). Automorfismo (It). 自己同形 (Ja).*

*Definition*

An isomorphism from a group  $(G, *)$  to itself is called an **automorphism** of this group. It is a bijection  $f : G \rightarrow G$  such that

$$f(g) * f(h) = f(g * h)$$

## Bravais–Miller indices

*Indices de Bravais–Miller (Fr). Indices de Bravais–Miller (Sp).  
Indici di Bravais–Miller (It). ブラベー・ミラー指数 (Ja).*

### Definition

The Bravais–Miller indices are used in the case of hexagonal lattices. In that case, one uses four axes,  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$ ,  $\mathbf{c}$  and four Miller indices,  $(hkl)$ , where  $h$ ,  $k$ ,  $l$  are prime integers inversely proportional to the intercepts  $OP$ ,  $OQ$ ,  $OS$ ,  $OR$  of a plane of the family with the four axes. The indices  $h$ ,  $k$ ,  $l$  are cyclically permutable and related by

$$h + k + l = 0.$$

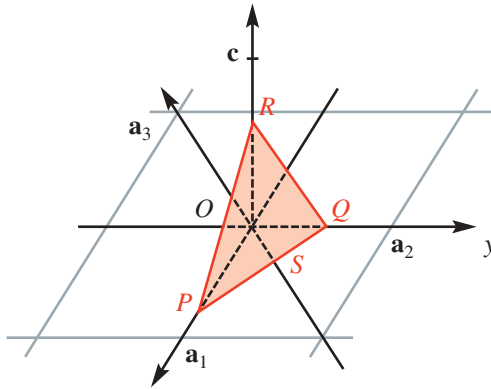


Figure 7

See also

- Miller indices

## Conventional cell

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Crystals having the same type of conventional cell belong to the same crystal family.

*See also*

- Primitive cell
- Unit cell
- Chapter 2.1.3 of *International Tables for Crystallography, Volume A*

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## Corresponding twins

*Macles correspondantes (Fr). Geminati corrispondenti (It).*

*Definition*

In the case of twinning by merohedry, when the twin element is twofold and the crystal is centrosymmetric, the twin operation can be described either as a rotation or as a reflection (the two operations being equivalent under the action of the centre).

In the case of twinning by pseudomerohedry, instead, the two twin operations are no longer equivalent even in centrosymmetric crystals but produce different twins, which are called **reciprocal twins** (Mügge, 1898) or **corresponding twins** (Friedel, 1904, 1926). One of the most classical examples is that of albite vs pericline twins in feldspars.

Pairs of corresponding twins normally do not have the same frequency of occurrence, as one would be tempted to assume from the identical value of their twin obliquity.

*History*

- Friedel, G. (1904). *Étude sur les groupements cristallins*. Extrait du *Bulletin de la Société de l'Industrie minière*, Quatrième série, Tomes III et IV. Saint-Étienne, Société de l'imprimerie Théolier J. Thomas et C., 485 pp.
- Friedel, G. (1926). *Leçons de Cristallographie*. Berger-Levrault, Nancy, Paris, Strasbourg, XIX+602 pp.

## Crystallographic Information File

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See also

- CIF
  - Hall, S. R. (1991). *J. Chem. Inf. Comput. Sci.* **31**, 326–333. *The STAR file: a new format for electronic data transfer and archiving*
  - Hall, S. R., Allen, F. H. and Brown, I. D. (1991). *Acta Cryst.* **A47**, 655–685. *The Crystallographic Information File (CIF): a new standard archive file for crystallography* (see also HTML version at <http://www.iucr.org/iucr-top/cif/standard/cifstd1.html>)
  - *International Tables for Crystallography, Volume G*
- 

## Crystallographic Information Framework

*Definition*

A system of standards and specifications for the standardized exchange and archiving of crystallographic data built upon, but not restricted to, the ⇒ **Crystallographic Information File**.

In addition to file formats, the framework includes formal relations between specific data items expressed in a machine-readable dictionary definition language (⇒ **DDL**), controlled vocabularies, constraints on allowable values of certain numeric data, and procedures for validating the self-consistency of a crystal structure model.

Responsibility for the maintenance of the standard is vested in COMCIFS, a Committee of the International Union of Crystallography.

See also

- Brown, I. D. and McMahon, B. (2002). *Acta Cryst.* **B58**, 317–324. *CIF: the computer language of crystallography*
- *International Tables for Crystallography, Volume G*

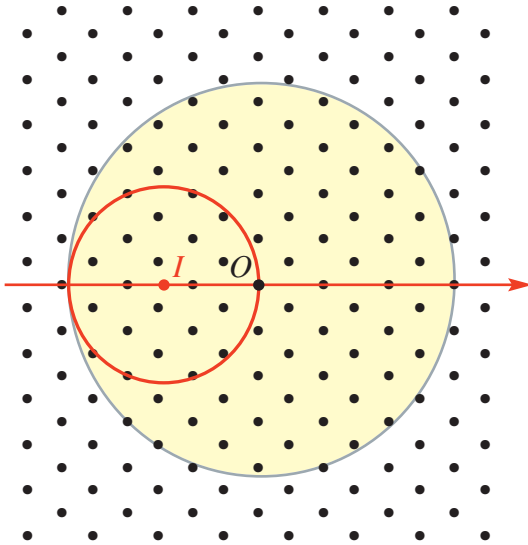


Figure 13

### History

The Ewald sphere was introduced by Ewald in 1913 under the name *Ausbreitungskugel* or sphere of reflection. [Ewald, P. P. (1913). *Physik. Z.*, **14**, 465–472. *Zur Theorie der Interferenzen der Röntgenstrahlen in Kristallen*. An English translation is given in D. W. J. Cruickshank, H. J. Juretschke and N. Kato, 1992, *P. P. Ewald and his dynamical theory of X-ray diffraction*. Oxford University Press, IUCr/OUP Book series, Oxford, 114–123). See also P. P. Ewald (1962). IUCr, *50 Years of X-ray Diffraction*, Utrecht: IUCr/Oosthoek, Section 15.3, page 250.]

### See also

- Chapter 2.2 of *International Tables for Crystallography, Volume C*

## Form

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### *List of crystal (face) and point forms*

The list of face forms includes 47 or 48 forms, depending on whether the dihedron is separated into sphenoid and dome or not.

#### *Open face forms and their dual point forms*

<b>Face form</b>	<b>Point form</b>	<b>Inherent symmetry</b>
Pedion	Single point	$\infty m$
Pinacoid	Line segment through origin	$\infty m / m$
Dihedron	Line segment	$mm2$
Rhombic prism	Rectangle through origin	$mmm$
Rhombic pyramid	Rectangle	$mm2$
Trigonal pyramid	Trigon	$3m$
Tetragonal pyramid	Square	$4mm$
Hexagonal pyramid	Hexagon	$6mm$
Ditrigonal pyramid	Truncated trigon	$3m$
Ditetragonal pyramid	Truncated square	$4mm$
Dihexagonal pyramid	Truncated hexagon	$6mm$
Trigonal prism	Trigon through origin	$\bar{6}2m$
Tetragonal prism	Square through origin	$4/mmm$
Hexagonal prism	Hexagon through origin	$6/mmm$
Ditrigonal prism	Truncated trigon through origin	$\bar{6}2m$
Ditetragonal prism	Truncated square through origin	$4/mmm$
Dihexagonal prism	Truncated hexagon	$6/mmm$

#### *Closed face forms and their dual point forms*

<b>Face form</b>	<b>Point form</b>	<b>Inherent symmetry</b>
Rhombic disphenoid	Rhombic disphenoid	$222$
Rhombic bipyramid	Quad	$mmm$
Trigonal bipyramid	Trigonal prism	$\bar{6}2m$
Tetragonal bipyramid	Tetragonal prism	$4/mmm$
Hexagonal bipyramid	Hexagonal prism	$6/mmm$
Ditrigonal bipyramid	Edge-truncated trigonal prism	$\bar{6}2m$
Ditetragonal bipyramid	Edge-truncated tetragonal prism	$4/mmm$
Dihexagonal bipyramid	Edge-truncated hexagonal prism	$6/mmm$
Tetragonal disphenoid	Tetragonal disphenoid	$\bar{4}2m$
Rhombohedron	Trigonal antiprism	$\bar{3}m$
Tetragonal scalenohedron	Tetragonal disphenoid cut off by pinacoid	$\bar{4}2m$



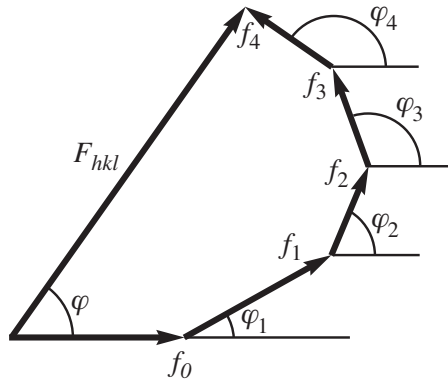


Figure 19

If the positions of known heavy atoms can be determined in this way, then the Patterson map, which describes interatomic vectors, allows nearby peaks to be assigned to other atoms in accordance with expected molecular geometry. These are then used in calculating phase angles for the next approximate electron density map.

A practical limitation is that a heavy atom that dominates the vector distribution is also likely to dominate the X-ray scattering as a whole, and overwhelm diffraction peaks from less strongly scattering species.

## Hemihedry

*Hémiédrie (Fr). Hemiedria (Sp). Emiedria (It). 半面像 (Ja).*

### Definition

The point group of a crystal is called hemihedry if it is a subgroup of index 2 of the point group of its lattice.

### See also

- Chapter 9.1 of *International Tables for Crystallography, Volume A*

Concretely, two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family. The 72 (in  $E^2$ ) or 1731 (in  $E^3$ ) Wyckoff positions are classified in 51 ( $E^2$ ) or 1128 ( $E^3$ ) types of Wyckoff sets. They are assigned to 30 ( $E^2$ ) or 402 ( $E^3$ ) lattice complexes.

The name *lattice complex* comes from the fact that an assemblage of points that are equivalent with respect to a group of symmetry operations including lattice translations can be visualized as a set of equivalent lattices.

### *Classification*

If a lattice complex can be generated in different space-group types, one of them stands out because its corresponding Wyckoff positions show the highest site symmetry. This is called the *characteristic space-group type of the lattice complex*. The characteristic space-group type and the corresponding oriented site symmetry express the common symmetry properties of all point configurations of a lattice complex. In the symbol of a lattice complex, however, instead of the site symmetry, the Wyckoff letter of one of the Wyckoff positions with that site symmetry is given. This Wyckoff position is called the *characteristic Wyckoff position of the lattice complex*.

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.

Lattice complexes are called *invariant* if they can occupy a parameterless position in a space group. The points in an invariant lattice complex can be split into different assemblages of equivalent points, the sum of which constitute a *variant* lattice complex (also termed a *lattice complex with degrees of freedom*). Variant lattice complexes are classified into *univariant*, *bivariant* and *trivariant* according to the number of parameters that can be varied independently.

### History

The first to introduce indices to denote a crystal plane was C. S. Weiss. His notation was modified independently by his student F. E. Neumann and W. Whewell whose indices are the inverse of the Weiss indices. These indices were systematically used by Whewell's student, and successor at the Chair of Mineralogy at Cambridge University, W. H. Miller, in his book *A treatise on Crystallography* (1839) – see *Historical Atlas of Crystallography* (1990), edited by J. Lima de Faria, published for the International Union of Crystallography by Kluwer Academic Publishers, Dordrecht, and A. Authier (2013), *The Early Days of X-ray Diffraction*, Oxford: IUCr/Oxford University Press.

### See also

- Law of rational indices
- Reciprocal lattice

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## Modulated crystal structure

*Structure cristalline modulée (Fr).* *Struttura cristallina modulata (It).* 変調構造 (*Ja*).

### Definition

A *modulated crystal structure* is a density (or atom arrangement) that may be obtained from a density (or atom arrangement) with space-group symmetry by a finite density change (or finite displacement of each atom, respectively) that is (quasi)periodic. A function or a displacement field is periodic if it is invariant under a lattice of translations. Then its Fourier transform consists of  $\delta$ -peaks on a reciprocal lattice that spans the space and is nowhere dense. A quasiperiodic function has a Fourier transform consisting of  $\delta$ -peaks on a vector module of finite rank. This means that the peaks may be indexed with integers using a finite number of basis vectors. If the modulation consists of deviations from the basic structure in the positions, the modulation is *displacive* ( $\Rightarrow$  **displacive modulation**),

## Normal subgroup

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In the special case that a subgroup  $H$  has only two cosets in  $G$  (namely  $H$  and  $gH$  for some  $g$  not contained in  $H$ ), the subgroup  $H$  is always normal in  $G$ .

### *Connection with homomorphisms*

If  $f$  is a  $\Rightarrow$ **homomorphism** from  $G$  to another group, then the kernel of  $f$  is a normal subgroup of  $G$ . Conversely, every normal subgroup  $H \triangleleft G$  arises as the kernel of a homomorphism, namely of the projection homomorphism  $G \rightarrow G/H$  defined by mapping  $g$  to its coset  $gH$ .

### *Example*

The group  $T$  containing all the translations of a space group  $G$  is a normal subgroup in  $G$  called the **translation subgroup** of  $G$ . The factor group  $G/T$  is isomorphic to the  $\Rightarrow$ **point group**  $P$  of  $G$ .

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## OD structure

*Structure OD (Fr). OD Struktur (Ge). Struttura OD (It). OD構造 (Ja).*

OD structures consist of slabs with their own symmetry, containing coincidence operations constituting a diperiodic group (layer group) only within individual slabs. For the entire structure these coincidence operations are only local (partial), *i.e.* they are valid only in a subspace of the crystal space. The ambiguity (= existence of more than one equivalent possibilities) in the stacking of slabs arises from the existence of this local symmetry, which does not appear in the space group of the structure. The resulting structure can be 'ordered' (*periodic*) or 'disordered' (*non-periodic*), depending on the sequence of local symmetry operations relating pairs of slabs. The set of all the operations valid in the whole crystal space constitutes a space group; by adding the set of all the operations valid in a subspace of it, one obtains a space groupoid.

In the OD theory, a central role is played by the **vicinity condition (VC)**, which states the geometrical equivalence of layer pairs. The

### *Definition*

Two crystallographic orbits are said to be *configuration-equivalent* if and only if their sets of points are identical. A **point configuration** is the set of all points that are common to a class of configuration-equivalent crystallographic orbits.

This definition uniquely assigns crystallographic orbits to point configurations but not *vice versa*.

The *inherent* symmetry of a point configuration is the most comprehensive space group that maps the point configuration onto itself. 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.

### *Synonyms*

Other terms used by different authors:

- regelmässiges Punktsystem
- regular system of points

### *See also*

- Chapter 14 of *International Tables for Crystallography, Volume A*

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## Point group

*Groupe ponctuel* (Fr). *Punktgruppe* (Ge). *Gruppo punto* (It). 点群 (Ja).

### *Definition*

A **point group** is a group of symmetry operations all of which leave at least one point unmoved. A *crystallographic* point group is a point group that maps a point lattice onto itself: in three dimensions rotations and rotoinversions are restricted to 1, 2, 3, 4, 6 and  $\bar{1}$ ,  $\bar{2}$  (=  $m$ ),  $\bar{3}$ ,  $\bar{4}$ ,  $\bar{6}$  respectively.

$(\mathbf{a}^*, \mathbf{b}^*)$ , are related to the corresponding lengths and angles for the direct basis vectors through the following relations:

$$\begin{aligned} a^* &= bc \sin \alpha / V; & b^* &= ca \sin \beta / V; & c^* &= ab \sin \gamma / V; \\ \cos \alpha^* &= (\cos \beta \cos \gamma - \cos \alpha) / (\sin \beta \sin \gamma); \\ \cos \beta^* &= (\cos \gamma \cos \alpha - \cos \beta) / (\sin \gamma \sin \alpha); \\ \cos \gamma^* &= (\cos \alpha \cos \beta - \cos \gamma) / (\sin \alpha \sin \beta). \end{aligned}$$

### History

The notion of reciprocal vectors was introduced in vector analysis by J. W. Gibbs [(1881). *Elements of Vector Analysis, arranged for the Use of Students in Physics*. Yale University, New Haven].

See also

- Reciprocal lattice
- *The Reciprocal Lattice* (Teaching Pamphlet No. 4 of the International Union of Crystallography)
- Chapter 5.1 of *International Tables for Crystallography, Volume A*
- Chapter 1.1 of *International Tables for Crystallography, Volume B*
- Chapter 1.1 of *International Tables for Crystallography, Volume C*
- Chapter 1.1.2 of *International Tables for Crystallography, Volume D*

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## Refinement

*Affinement* (Fr). *Affinamento* (It). 構造精密化 (Ja).

### Definition

In structure determination, the process of improving the parameters of an approximate (trial) structure until the best fit is achieved between an observed diffraction pattern and that calculated by Fourier transformation from the numerically parameterized trial structure.

### Least-squares refinement

The most common approach in the determination of inorganic or small-molecule structures is to minimize a function

## Serial reflection conditions

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### Definition

The serial reflection conditions are the general reflection conditions due to the presence of screw axes. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as  $h00$ ,  $0k0$ ,  $00l$ ). For instance, for a screw axis parallel to  $[001]$ , the reflection conditions are:

Type of reflection	Reflection condition	Screw vector	Screw axis
$00l$	$l = 2n$	$c/2$	$2_1; 4_2$
	$l = 4n$	$c/4$	$4_1; 4_3$
$000l$	$l = 2n$	$c/2$	$6_3$
	$l = 3n$	$c/3$	$4_1; 3_1; 3_2; 6_2; 6_4$
	$l = 6n$	$c/6$	$6_1; 6_5$

The serial reflection conditions are listed in Table 2.2.13.2 of *International Tables for Crystallography, Volume A*.

See also

- Reflection conditions
- Chapter 2.2.13 of *International Tables for Crystallography, Volume A*

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## Sharpened Patterson function

### Definition

Patterson methods of structure determination use the Patterson function

$$P(uvw) = (1/V) \sum_h \sum_k \sum_l \{|F(hkl)|^2 \cos[2\pi(hu + kv + lw)]\}$$

to generate a map of interatomic vectors within the unit cell. Better results can be obtained by artificially sharpening the peaks in the Patterson function, thereby enhancing the resolution of individual peaks.

One technique for doing so, introduced by Patterson in 1935, considers the effect of thermal motion on the broadening of electron-

## Twinning

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See also

- Twin index
  - Twin lattice
  - Twin law
  - Twin obliquity
  - Corresponding twins
  - Twinning (endemic conditions of)
  - Twinning (effects of)
  - Chapter 1.3 of *International Tables for Crystallography, Volume C*
  - Chapter 3.3 of *International Tables for Crystallography, Volume D*
- 

## Twinning (effects of)

*Maclage (effets de) (Fr). Geminazione (effetti della) (It).*

### *Morphological and optical effects*

At the morphological level, twinning introduces re-entrant angles that, in principle, are specific marks.

Except for twins by merohedry, the orientation of the optical indicatrix changes through the interface between adjacent crystals (individuals). Thus, apart from particular orientations, if observed by a polarizing microscope between crossed polars, a twin never can be brought by rotation to a position of complete extinctions (dark field).

### *Overlap of lattices*

By effect of a  $\Rightarrow$ **twin operation**, both the direct and reciprocal lattice of the individuals forming a twin are overlapped. Overlapping (restoration) of nodes belonging to different individuals can be: (i) exact and total (twinning by merohedry); (ii) exact but partial (*i.e.* only a fraction of the nodes of an individual lattice is restored; twinning by reticular merohedry); (iii) total but approximate (twinning by pseudomerohedry), approximate and partial (twinning by reticular pseudomerohedry).  $\Rightarrow$ **Twin lattice**,  $\Rightarrow$ **twin index** and  $\Rightarrow$ **twin obliquity** are entries related to the overlap of lattices.