Glossary

Symmetry

Property of physical and mathematical objects. After a symmetry operation, a symmetrical object and its transformed copy are indistinguishable. Proper symmetry involves pure rotation. Improper symmetry combines rotation with reflection; in particular, improper symmetry elements include center of inversion, mirror plane, and four-fold inversion axis.

Crystal system

All crystals are divided into seven groups, called crystal systems, according to their principal symmetry. In another definition, this principal symmetry itself may be identified with the crystal system. From the lowest to the highest symmetry, the crystal systems are: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, cubic.

Point group

Symmetry usually comes in bunches, i.e. a symmetrical object usually has more than one symmetry element. Those symmetry elements must form consistent sets, called groups. For finite objects, those groups are called point groups (or crystal classes with reference to crystals). The term "group" is used in strict mathematical sense, i.e. it means that (i) combination of any two symmetry elements is another element of the group, (ii) for each symmetry transformation there is an inverse operation, (iii) the group includes a null (or identity) element.

Lattice

A collection of nodes, i.e. points with integral coordinates. In crystallography, a lattice is an abstract representation of a crystal structure: it is periodic and infinite, and the real structure can be reconstructed by associating with each lattice point the concrete structural motif (molecule, cluster of ions, cluster of molecules) which it symbolically represents. Strictly speaking, lattices with points at integral coordinates are called primitive (P) lattices.

To preserve the maximal internal crystal symmetry, crystallography allows in some cases nodes with special combinations of “half-integral” (i.e. ½) coordinates, resulting in the so-called centered lattices. Each lattice point has exactly the same environment.

Bravais lattice

In some cases, non-primitive unit cells have to be chosen in order to make the symmetry of the unit cell compatible with the symmetry of the entire lattice. Non-primitive lattices, derived mathematically by AugusteBravais, can have the following centering nodes: ½ ½ ½ (I), ½ ½ 0 (C), or 0 ½ ½, ½ 0 ½, ½ ½ 0 (F). Convention and symmetry considerations lead to 14 Bravais lattices: triclinic P; monoclinic P, C; orthorhombic P, I, C, F; tetragonal P, I; trigonal R; hexagonal and trigonal P; cubic P, I, F.

Miller indices

A set of lattice planes is a family of parallel and equidistant planes which pass through lattice points. The number of divisions into which a plane set cuts the axial vectors a (h), b (k), and c (l) is known as Miller indices (hkl) of this set of lattice planes. The characteristic interplanar spacing is denoted d_{hkl}.

Bragg’s Law

In Bragg’s interpretation, the phenomenon of diffraction is viewed as reflection from the lattice planes (hkl). The incident and reflected beams make the same angle (θ) with the reflecting plane, and the two beams and the plane normal are coplanar, as in geometrical optics. The difference, however, is that this is selective reflection, which can occur only at θ angles selected by the Bragg’s Law: $n\lambda=2d_{hkl}\sin\theta$. This is because the rays reflected from consecutive planes of a plane-set must be in phase, i.e. must form an optical-path-difference equal to nλ. n is the order of reflection from the set of lattice planes (hkl) with interplanar spacing d_{hkl}

Fourier Transform

In Fourier Theory, a function defined as $F(h)=\Sigma f(x).\exp[2\pi i(hx)]$ has its nearly-identical twin companion, $f(x)=\Sigma F(h).\exp[-2\pi i(hx)]$ (scale neglected). In simple applications, these formulas (or Fourier transforms) can be interpreted as trigonometric Fourier series. The existence of this pair of Fourier transforms means, that if we have a recipe (+i transform) for calculating F expressed as a Fourier series in f, then automatically f can be calculated as a Fourier series in F (-i transform).

Electron density

Distribution of electrons, in the form of electron density ($e/Å^3$), usually drawn as a map, represents the chemical constituents of the crystal interior. Electron density maps are the primary product of crystal structure determination by X-ray crystallography, and atomic models represent their chemical interpretation. This is so because the X-rays, which are used to “probe” the crystal structure by diffraction, are scattered by electrons.