Crystal symmetry

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This lecture [1,2] will focus on the description of a crystal, which relies on two fundamental symmetries: point group (i.e. orientation) symmetries and translation symmetry. The final aim will be to understand and use the information contained in the space group of a crystal, as given in the International Tables for Crystallography [3]. Throughout this lecture, the various concepts will be exemplified through a few selected examples of oxide compounds and some useful websites will be presented. This lecture will be organized in three parts, as described hereafter.

In a first part, the various elementary point group symmetries (inversion, rotation, reflection, and roto-inversion) are first recalled. Combining the point symmetries that are compatible with the translation symmetry yields the 32 crystallographic point groups, among which 11 (called the Laue classes) possess inversion. Their description and their Hermann-Mauguin symbol (international notation) are explained, and further illustrated through examples of molecules. Last, the relation between the knowledge of the point group and the prediction of physical properties is exemplified in the case of dielectric properties.

In a second part, the notion of lattice and motif, based on the translation symmetry, is recalled, together with important concepts such as that of the unit cell and its multiplicity. After a classification of the various unit cells into 6 conventional cells or 7 crystal systems, based on their point symmetry, the various manners to center a unit cell are depicted, and the associated symbol for the corresponding lattice type is given. In the end, this yields a classification into 14 Bravais lattices (6 primitive ones and 8 centered ones). Then, some concepts very useful for diffraction (topic of my second lecture) are briefly recalled: lattice directions and net planes, reciprocal lattice.

The last part is devoted to space group symmetries. In some cases, point symmetries alone do not allow to obtain the perfect coincidence of the crystalline edifice with itself, and one has to combine them with fractional translations, that is, translations acting inside the unit cell. After presenting the two kinds of such non symmorphic symmetries (glide planes and screw axes), all the existing ones and the symmorphic ones (i.e. the point group symmetries) are reviewed with the information on their graphical and printed symbols. These symmetries act inside the motif and, combined to the lattice translations, yield the space group of the crystal (there are 230 in total), for which the Hermann-Mauguin symbol is also explained. The example of space group $Pnma$ is then discussed, based on the information found in [3], with a particular focus on the asymmetric unit and the Wyckoff sites.

[1] See a transcript of a similar lecture given at the thematic school "Contribution of symmetries in condensed matter" (Giens peninsula, 2009) in: Chapter 6 of "Contribution of symmetries in condensed matter", Edited by B. Grenier, V. Simonet, and H. Schober, EPJ Web of Conferences, Volume 22 (2012), website: https://www.epj-conferences.org/articles/epjconf/abs/2012/04/contents/contents.html

[2] See slides and video of a similar lecture (lecture I) given at a school of GDR MEETICC (Banyuls, 2018) website: http://gdr-meeticc.cnrs.fr/ecole-du-gdr-meeticc-school_v3/

[3] International Tables For Crystallography, Volume A, Space-group symmetry (Kluwer Academic Press, 5th ed., 2002), website: http://it.iucr.org/