

1079-20-16

Massmo Nespolo* (massimo.nespolo@crm2.uhp-nancy.fr), BP 70239, Boulevard des Aiguillettes, 54506 Vandoeuvre-les-Nancy, France. *Analysis of crystal structures in terms of the eigensymmetry of crystallographic orbits and its application to twinned crystals.*

The infinite set of atoms generated by the action of the space group on each atom in the asymmetric unit (fundamental region) of a crystal structure is called a crystallographic orbit. The eigensymmetry E of each orbit is at least equal to the space group G (characteristic orbit). When E is a supergroup of G , the orbit is called non-characteristic. If $T(E)$ coincides $T(G)$, E/T is necessarily a supergroup of G/T . If instead $T(E)$ is supergroup of $T(G)$, the orbit is called extraordinary: E/T may coincide with G/T or be a supergroup of it. When heavy atoms occupy non-characteristic orbits, the diffraction pattern shows pseudo-symmetry or systematic weak diffractions, which can be exploited to build the initial model of the crystal structure. A promising application of crystallographic orbits is in the study of twins. These are oriented associations of crystals of the same compound whose respective orientations are mapped by an operation that does not belong to G/T . The crystal structures do not match at the interface. However, a substructure can be more or less continuous, if the atoms forming this substructure are on non-characteristic orbits, because the operation mapping the orientations of the crystals in the twin may be an operation of E/T without being an operation of G/T . (Received October 12, 2011)