

## 2.1. INTRODUCTION TO BASIC CRYSTALLOGRAPHY

map. For instance, the consequence of a twofold symmetry axis along  $\mathbf{b}$  is the presence of a large number of peaks in the  $(u0w)$  plane of the Patterson map. For a screw axis with translation  $\frac{1}{2}$  along  $\mathbf{b}$ , the peaks lie in the  $(u\frac{1}{2}w)$  plane. Such planes are called Harker planes (Harker, 1936). Peaks in Harker planes usually form the start of the interpretation of a Patterson map. Harker lines result from mirror planes, which do not occur in macromolecular crystal structures of biological origin.

Despite the improvements that can be made to the Patterson function, for structures containing atoms of nearly equal weight its complete interpretation can only be achieved for a restricted number of atoms per cell unless some extra information is available. Nowadays, most structure determinations of small compounds are based on direct methods for phase determination. However, these may fail for structures showing strong regularity. In these cases, Patterson interpretation is used as an alternative tool, sometimes in combination with direct methods. It is interesting to see that the value of the Patterson function has shifted from the small-compound field to macromolecular crystallography, where it plays an extremely useful role:

- (1) in the isomorphous replacement method, the positions of the very limited number of heavy atoms attached to the macromolecule can be derived from a difference Patterson map, as mentioned earlier in this section;
- (2) anomalous scatterers can be located by calculating a Patterson map with coefficients  $[|F_{PH}(\mathbf{h})| - |F_{PH}(-\mathbf{h})|]^2$ , in which  $|F_{PH}(\mathbf{h})|$  is the structure-factor amplitude of the protein containing the anomalous scatterer;
- (3) molecular replacement is based on the property that the Patterson map is a map of vectors between atoms in the real structure, combined with the fact that such a vector map is (apart from a rotation) similar for two homologous structures: the unknown and a known model structure.

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