5.12: Sharpened Patterson function

Patterson methods of structure determination use the Patterson function

$P(uvw) = (1 / V)$	$\sum$	$\sum$	$\sum$	$\{ \mid F(hkl) \mid ^2 \cos[2\pi(hu + kv + lw)]\}$
	h	k	l	

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-density peaks and consequently their Patterson peaks. The F^2 coefficients can be corrected for thermal effects by simulating the atoms as point scatterers and using a modified set of coefficients $|\mathbf{F}_{\mathbf{h},\mathrm{sharp}}|^2 = |\mathbf{F}_{\mathbf{h}}|^2 / \bar{f}^{\,2}$, where $\bar{f}$, the average scattering factor per electron, is given by

$$\bar{f} = \sum_{i=1}^{N} f_i / \sum_{i=1}^{N} Z_i .$$

A common formulation for this type of sharpening expresses the atomic scattering factors at a given angle in terms of an overall isotropic thermal parameter B as $f(s) = f_0 \exp(-Bs^2)$. The Patterson coefficients then become

\(\mathbf{F}_{\mathbf{h}, \, \mathrm{sharp}} =

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More often nowadays normalized structure factors $\mid E^2 \mid - 1$ are used in place of $\mid F^2 \mid$. Normalized structure factors are used in direct methods techniques of structure solution. They are defined as

$$|E_{\mathbf{h}}|^2 = |F_{\mathbf{h}}|^2 / \langle |F_{\mathbf{h}}|^2 \rangle ,$$

where the squared observed structure-factor magnitudes on an absolute scale are divided by their expected values. Their use gives much greater weight to higher-resolution data and resolves some peaks in the vector map that would otherwise be continuous. On the other hand, they are less accurately known and are adjacent to data that have not been measured; they may therefore introduce spurious definition into the map.

A compromise that is often helpful is to use $\mid EF \mid$ as the Patterson coefficients.