

Calculations and formula referenced as 'crystallographic least squares'

Contributors

Arnott, Struther, b.1934

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$$A(hkl) = \sum_1^N f_i \cos 2\pi(hx_i + ky_i + lz_i)$$

$$B(hkl) = \sum_1^N f_i \sin 2\pi(hx_i + ky_i + lz_i)$$

$$F(hkl) = \{A^2(hkl) + B^2(hkl)\}^{1/2}$$

$$\Phi = \sum \omega_m (\sigma F_m - F_m)^2 = \sum \omega_m \Delta F_m^2$$

$$\mathbf{U} = [\Delta u_1, \Delta u_2, \dots, \Delta u_N]$$

$$\mathbf{P} = \begin{bmatrix} \sqrt{\omega_1} \frac{\partial F_1}{\partial u_1} & \dots & \sqrt{\omega_m} \frac{\partial F_m}{\partial u_1} \\ \vdots & & \vdots \\ \sqrt{\omega_1} \frac{\partial F_1}{\partial u_N} & \dots & \sqrt{\omega_m} \frac{\partial F_m}{\partial u_N} \end{bmatrix}$$

$$\mathbf{D} = [\sqrt{\omega_1} \Delta F_1, \dots, \sqrt{\omega_m} \Delta F_m]$$

$$\mathbf{U} = \mathbf{D} \mathbf{P}^T (\mathbf{P}^T \mathbf{P})^{-1}$$