

## **Calculations/formulae referenced as 'crystallographic least squares with constraints'**

### **Contributors**

Arnott, Struther, b.1934

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<https://wellcomecollection.org/works/tre8ret3>

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$$\theta = \sum_1^M \omega_m \Delta F_m^2 + \sum_1^H \lambda_h G_h$$

$$\mathbf{U} = [\Delta u_1 \cdots \cdots \Delta u_N]$$

$$\mathbf{L} = [2\lambda_1 \cdots \cdots 2\lambda_H]$$

$$\mathbf{G} = [-G_1 \cdots \cdots -G_H]$$

$$\mathbf{D} = [\sqrt{\omega_1} \Delta F_1 \cdots \cdots \sqrt{\omega_M} \Delta F_M]$$

$$\mathbf{N} = \begin{bmatrix} \frac{\partial G_1}{\partial u_1} & \cdots & \frac{\partial G_H}{\partial u_1} \\ \vdots & & \vdots \\ \frac{\partial G_1}{\partial u_N} & \cdots & \frac{\partial G_H}{\partial u_N} \end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} \sqrt{\omega_1} \frac{\partial F_1}{\partial u_1} & \cdots & \sqrt{\omega_1} \frac{\partial F_1}{\partial u_N} \\ \vdots & & \vdots \\ \sqrt{\omega_M} \frac{\partial F_M}{\partial u_1} & \cdots & \sqrt{\omega_M} \frac{\partial F_M}{\partial u_N} \end{bmatrix}$$

$$[\mathbf{U} | \mathbf{L}] = [\mathbf{D} \mathbf{P} | \frac{1}{2} \mathbf{G}] \begin{bmatrix} \mathbf{P}^T \mathbf{P} & \frac{1}{2} \mathbf{N} \\ \hline \frac{1}{2} \mathbf{N}^T & \mathbf{0} \end{bmatrix}^{-1}$$