

REFERENCES

8.3

- Cruickshank, D. W. J. (1961). *Coordinate errors due to rotational oscillations of molecules*. *Acta Cryst.* **14**, 896–897.
- Finger, L. W. (1969). *The crystal structure and cation distribution of a grunerite*. *Mineral. Soc. Am. Spec. Pap.* **2**, 95–100.
- Gill, P. E., Murray, W. & Wright, M. M. (1981). *Practical optimization*. New York: Academic Press.
- Hamilton, W. C. (1964). *Statistics in physical science: estimation, hypothesis testing and least squares*. New York: Ronald Press.
- Hendrickson, W. A. (1985). *Stereochemically restrained refinement of macromolecular structures*. *Methods in enzymology*, Vol. 115. *Diffraction methods for biological macromolecules, Part B*, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 252–270. New York: Academic Press.
- Hendrickson, W. A. & Konnert, J. H. (1980). *Incorporation of stereochemical information into crystallographic refinement*. *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & D. Venkatesan, pp. 13.01–13.26. Bangalore: Indian Academy of Sciences.
- Hestenes, M. & Stiefel, E. (1952). *Methods of conjugate gradients for solving linear systems*. *J. Res. Natl Bur. Stand.* **49**, 409–436.
- Jack, A. & Levitt, M. (1978). *Refinement of large structures by simultaneous minimization of energy and R factor*. *Acta Cryst.* **A34**, 931–935.
- Johnson, C. K. (1970). *Generalized treatments for thermal motion*. *Thermal neutron diffraction*, edited by B. T. M. Willis, pp. 132–160. Oxford University Press.
- Konnert, J. H. (1976). *A restrained-parameter structure-factor least-squares refinement procedure for large asymmetric units*. *Acta Cryst.* **A32**, 614–617.
- Konnert, J. H. & Hendrickson, W. A. (1980). *A restrained-parameter thermal-factor refinement procedure*. *Acta Cryst.* **A36**, 344–350.
- Levy, H. A. (1956). *Symmetry relations among coefficients of anisotropic temperature factors*. *Acta Cryst.* **9**, 679.
- Prince, E. (1994). *Mathematical techniques in crystallography and materials science*, 2nd ed. Berlin/Heidelberg/New York/London/Paris/Tokyo/Hong Kong/Barcelona/Budapest: Springer-Verlag.
- Prince, E., Dickens, B. & Rush, J. J. (1974). *A study of one-dimensional hindered rotation in $\text{NH}_3\text{OHCIO}_4$* . *Acta Cryst.* **B30**, 1167–1172.
- Prince, E. & Finger, L. W. (1973). *Use of constraints on thermal motion in structure refinement of molecules with librating side groups*. *Acta Cryst.* **B29**, 179–183.
- Rae, A. D. (1978). *An optimized conjugate gradient solution for least-squares equations*. *Acta Cryst.* **A34**, 578–582.
- Ralph, R. L. & Finger, L. W. (1982). *A computer program for refinement of crystal orientation matrix and lattice constants from diffractometer data with lattice symmetry constraints*. *J. Appl. Cryst.* **15**, 537–539.
- Rietveld, H. M. (1969). *A profile refinement method for nuclear and magnetic structures*. *J. Appl. Cryst.* **2**, 65–71.
- Schomaker, V. & Trueblood, K. N. (1968). *On the rigid-body motion of molecules in crystals*. *Acta Cryst.* **B24**, 63–76.
- Schomaker, V., Waser, J., Marsh, R. E. & Bergman, G. (1959). *To fit a plane or a line to a set of points by least squares*. *Acta Cryst.* **12**, 600–604.

- Sygyusch, J. (1976). *Constrained thermal motion refinement for a rigid molecule with librating side groups*. *Acta Cryst.* **B32**, 3295–3298.
- Waser, J. (1963). *Least-squares refinement with subsidiary conditions*. *Acta Cryst.* **16**, 1091–1094.

8.4

- Cramér, H. (1951). *Mathematical methods of statistics*. Princeton, NJ: Princeton University Press.
- Draper, N. & Smith, H. (1981). *Applied regression analysis*. New York: John Wiley.
- Fedorov, V. V. (1972). *Theory of optimal experiments*, translated by W. J. Studden & E. M. Klimko. New York: Academic Press.
- Hamilton, W. C. (1964). *Statistics in physical science: estimation, hypothesis testing and least squares*. New York: Ronald Press.
- Himmelblau, D. M. (1970). *Process analysis by statistical methods*. New York: John Wiley.
- Prince, E. (1982). *Comparison of the fits of two models to the same data set*. *Acta Cryst.* **B38**, 1099–1100.
- Prince, E. (1994). *Mathematical techniques in crystallography and materials science*, 2nd ed. Berlin/Heidelberg/New York/London/Paris/Tokyo/Hong Kong/Barcelona/Budapest: Springer-Verlag.
- Prince, E. & Nicholson, W. L. (1985). *Influence of individual reflections on the precision of parameter estimates in least squares refinement*. *Structure and statistics in crystallography*, edited by A. J. C. Wilson, pp. 183–195. Guilderland, NY: Adenine Press.
- Shoemaker, D. P. (1968). *Optimization of counting time in computer controlled X-ray and neutron single-crystal diffractometry*. *Acta Cryst.* **A24**, 136–142.
- Williams, E. J. & Kloot, N. H. (1953). *Interpolation in a series of correlated observations*. *Aust. J. Appl. Sci.* **4**, 1–17.

8.5

- Abrahams, S. C. & Keve, E. T. (1971). *Normal probability plot analysis of error in measured and derived quantities and standard deviations*. *Acta Cryst.* **A27**, 157–165.
- Beckman, R. J. & Cook, R. D. (1983). *Outlier.....s*. *Technometrics*, **25**, 119–149.
- Belsley, D. A. (1991). *Conditioning diagnostics*. New York: John Wiley & Sons.
- Belsley, D. A., Kuh, E. & Welsch, R. E. (1980). *Regression diagnostics*. New York: John Wiley & Sons.
- Chatterjee, S. & Hadi, A. S. (1986). *Influential observations, high leverage points, and outliers in linear regression*. *Stat. Sci.* **1**, 379–393.
- Fedorov, V. V. (1972). *Theory of optimal experiments*, translated by W. J. Studden & E. M. Klimko. New York: Academic Press.
- ISO (1993). *Guide to the expression of uncertainty in measurement*. Geneva: International Organization for Standardization.
- Kafadar, K. & Spiegelman, C. H. (1986). *An alternative to ordinary Q-Q plots: conditional Q-Q plots*. *Comput. Stat. Data Anal.* **4**, 167–184.
- Prince, E. (1994). *Mathematical techniques in crystallography and materials science*, 2nd ed. Berlin/Heidelberg/New York/London/Paris/Tokyo/Hong Kong/Barcelona/Budapest: Springer-Verlag.