References

1.1

Arnold, H. (1983). *Transformations in crystallography*. In *International tables for crystallography,* Vol. A. *Space-group symmetry*, edited by Th. Hahn, pp. 70–79. Dordrecht: Kluwer Academic Publishers.

Ashcroft, N. W. & Mermin, N. D. (1975). *Solid state physics.* Philadelphia: Saunders College.

Bloch, F. (1928). *Über die Quantenmechanik der Elektronen in Kristallgittern. Z. Phys.* **52**, 555–600.

Buerger, M. J. (1941). *X-ray crystallography.* New York: John Wiley.

Buerger, M. J. (1959). *Crystal structure analysis.* New York: John Wiley.

Ewald, P. P. (1913). *Zur Theorie der Interferenzen der Röntgenstrahlen in Kristallen. Phys. Z.* **14**, 465–472.

Ewald, P. P. (1921). *Das reziproke Gitter in der Strukturtheorie. Z. Kristallogr.* **56**, 129–156.

International Tables for Crystallography (1995). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (1999). Vol. C. *Mathematical, physical and chemical tables*, edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.

Koch, E. (1999). In *International tables for crystallography*, Vol. C. *Mathematical, physical and chemical tables*, edited by A. J. C. Wilson & E. Prince, pp. 2–9. Dordrecht: Kluwer Academic Publishers.

Laue, M. (1914). *Die Interferenzerscheinungen an Röntgenstrahlen, hervorgerufen durch das Raumgitter der Kristalle. Jahrb. Radioakt. Elektron.* **11**, 308–345.

Lipson, H. & Cochran, W. (1966). *The determination of crystal structures.* London: Bell.

Patterson, A. L. (1967). In *International tables for X-ray crystallography*, Vol. II. *Mathematical tables*, edited by J. S. Kasper & K. Lonsdale, pp. 5–83. Birmingham: Kynoch Press.

Sands, D. E. (1982). *Vectors and tensors in crystallography.* New York: Addison-Wesley.

Schomaker, V. & Trueblood, K. N. (1968). *On the rigid-body motion of molecules in crystals. Acta Cryst.* B**24**, 63–76.

Wilson, E. B. (1901). *Vector analysis.* New Haven: Yale University Press.

Ziman, J. M. (1969). *Principles of the theory of solids.* Cambridge University Press.

1.2

Arfken, G. (1970). *Mathematical models for physicists*, 2nd ed. New York, London: Academic Press.

Avery, J. & Ørmen, P.-J. (1979). *Generalized scattering factors and generalized Fourier transforms. Acta Cryst.* A**35**, 849–851.

Avery, J. & Watson, K. J. (1977). *Generalized X-ray scattering factors. Simple closed-form expressions for the one-centre case with Slater-type orbitals. Acta Cryst.* A**33**, 679–680.

Bentley, J. & Stewart, R. F. (1973). *Two-centre calculations for X-ray scattering. J. Comput. Phys.* **11**, 127–145.

Born, M. (1926). *Quantenmechanik der Stoszvorgänge. Z. Phys.* **38**, 803.

Clementi, E. & Raimondi, D. L. (1963). *Atomic screening constants from SCF functions. J. Chem. Phys.* **38**, 2686–2689.

Clementi, E. & Roetti, C. (1974). *Roothaan–Hartree–Fock atomic wavefunctions. At. Data Nucl. Data Tables*, **14**, 177–478.

Cohen-Tannoudji, C., Diu, B. & Laloe, F. (1977). *Quantum mechanics.* New York: John Wiley and Paris: Hermann.

Condon, E. V. & Shortley, G. H. (1957). *The theory of atomic spectra.* London, New York: Cambridge University Press.

Coppens, P. (1980). *Thermal smearing and chemical bonding*. In *Electron and magnetization densities in molecules and solids*, edited by P. J. Becker, pp. 521–544. New York: Plenum.

Coppens, P., Guru Row, T. N., Leung, P., Stevens, E. D., Becker, P. J. & Yang, Y. W. (1979). *Net atomic charges and molecular dipole moments from spherical-atom X-ray refinements, and the relation between atomic charges and shape. Acta Cryst.* A**35**, 63–72.

Coulson, C. A. (1961). *Valence*. Oxford University Press.

Cruickshank, D. W. J. (1956). *The analysis of the anisotropic thermal motion of molecules in crystals. Acta Cryst.* **9**, 754–756.

Dawson, B. (1967). *A general structure factor formalism for interpreting accurate X-ray and neutron diffraction data. Proc. R. Soc. London Ser. A*, **248**, 235–288.

Dawson, B. (1975). *Studies of atomic charge density by X-ray and neutron diffraction – a perspective*. In *Advances in structure research by diffraction methods.* Vol. 6, edited by W. Hoppe & R. Mason. Oxford: Pergamon Press.

Dawson, B., Hurley, A. C. & Maslen, V. W. (1967). *Anharmonic vibration in fluorite-structures. Proc. R. Soc. London Ser. A*, **298**, 289–306.

Dunitz, J. D. (1979). *X-ray analysis and the structure of organic molecules.* Ithaca and London: Cornell University Press.

Feil, D. (1977). *Diffraction physics. Isr. J. Chem.* **16**, 103–110.

Hansen, N. K. & Coppens, P. (1978). *Testing aspherical atom refinements on small-molecule data sets. Acta Cryst.* A**34**, 909–921.

Hehre, W. J., Ditchfield, R., Stewart, R. F. & Pople, J. A. (1970). *Self-consistent molecular orbital methods. IV. Use of Gaussian expansions of Slater-type orbitals. Extension to second-row molecules. J. Chem. Phys.* **52**, 2769–2773.

Hehre, W. J., Stewart, R. F. & Pople, J. A. (1969). *Self-consistent molecular orbital methods. I. Use of Gaussian expansions of Slater-type atomic orbitals. J. Chem. Phys.* **51**, 2657–2664.

Hirshfeld, F. L. (1977). *A deformation density refinement program. Isr. J. Chem.* **16**, 226–229.

International Tables for Crystallography (1999). Vol. C. *Mathematical, physical and chemical tables*, edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

James, R. W. (1982). *The optical principles of the diffraction of X-rays*. Woodbridge, Connecticut: Oxbow Press.

Johnson, C. K. (1969). *Addition of higher cumulants to the crystallographic structure-factor equation: a generalized treatment for thermal-motion effects. Acta Cryst.* A**25**, 187–194.

Johnson, C. K. (1970*a*). *Series expansion models for thermal motion*. ACA Program and Abstracts, 1970 Winter Meeting, Tulane University, p. 60.

Johnson, C. K. (1970*b*). *An introduction to thermal-motion analysis*. In *Crystallographic computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 207–219. Copenhagen: Munksgaard.

Johnson, C. K. & Levy, H. A. (1974). *Thermal motion analysis using Bragg diffraction data*. In *International tables for X-ray crystallography* (1974), Vol. IV, pp. 311–336. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Kara, M. & Kurki-Suonio, K. (1981). *Symmetrized multipole analysis of orientational distributions. Acta Cryst.* A**37**, 201–210.

Kendall, M. G. & Stuart, A. (1958). *The advanced theory of statistics*. London: Griffin.

Kuhs, W. F. (1983). *Statistical description of multimodal atomic probability structures. Acta Cryst.* A**39**, 148–158.

Kurki-Suonio, K. (1977). *Symmetry and its implications. Isr. J. Chem.* **16**, 115–123.

Kutznetsov, P. I., Stratonovich, R. L. & Tikhonov, V. I. (1960). *Theory Probab. Its Appl. (USSR)*, **5**, 80–97.

Lipson, H. & Cochran, W. (1966). *The determination of crystal structures*. London: Bell.

McIntyre, G. J., Moss, G. & Barnea, Z. (1980). *Anharmonic temperature factors of zinc selenide determined by X-ray diffraction from an extended-face crystal. Acta Cryst.* A**36**, 482–490.