

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

## 2.2 (cont.)

- Rogers, D. & Wilson, A. J. C. (1953). *The probability distribution of X-ray intensities. V. A note on some hypersymmetric distributions.* *Acta Cryst.* **6**, 439–449.
- Rossmann, M. G., Blow, D. M., Harding, M. M. & Collier, E. (1964). *The relative positions of independent molecules within the same asymmetric unit.* *Acta Cryst.* **17**, 338–342.
- Sayre, D. (1952). *The squaring method: a new method for phase determination.* *Acta Cryst.* **5**, 60–65.
- Sayre, D. (1953). *Double Patterson function.* *Acta Cryst.* **6**, 430–431.
- Sayre, D. (1972). *On least-squares refinement of the phases of crystallographic structure factors.* *Acta Cryst.* **A28**, 210–212.
- Sayre, D. & Toupin, R. (1975). *Major increase in speed of least-squares phase refinement.* *Acta Cryst.* **A31**, S20.
- Schenk, H. (1973a). *Direct structure determination in P1 and other non-centrosymmetric symmorphic space groups.* *Acta Cryst.* **A29**, 480–481.
- Schenk, H. (1973b). *The use of phase relationships between quartets of reflexions.* *Acta Cryst.* **A29**, 77–82.
- Sheldrick, G. M. (1990). *Phase annealing in SHELX-90: direct methods for larger structures.* *Acta Cryst.* **A46**, 467–473.
- Sheldrick, G. M. (1997). In *Direct methods for solving macromolecular structures.* NATO Advanced Study Institute, Erice, Italy.
- Sheldrick, G. M. (2000a). *The SHELX home page.* <http://shelx.uni-ac.gwdg.de/SHELX/>.
- Sheldrick, G. M. (2000b). *SHELX.* <http://www.ucg.ie/cryst/shelx.htm>.
- Sheldrick, G. M. & Gould, R. O. (1995). *Structure solution by iterative peaklist optimization and tangent expansion in space group P1.* *Acta Cryst.* **B51**, 423–431.
- Sim, G. A. (1959). *The distribution of phase angles for structures containing heavy atoms. II. A modification of the normal heavy-atoms method for non-centrosymmetrical structures.* *Acta Cryst.* **12**, 813–815.
- Simerska, M. (1956). *Czech. J. Phys.* **6**, 1.
- Simonov, V. I. & Weissberg, A. M. (1970). *Calculation of the signs of structure amplitudes by a binary function section of interatomic vectors.* *Sov. Phys. Dokl.* **15**, 321–323. [Translated from *Dokl. Akad. Nauk SSSR*, **191**, 1050–1052.]
- Sint, L. & Schenk, H. (1975). *Phase extension and refinement in non-centrosymmetric structures containing large molecules.* *Acta Cryst.* **A31**, S22.
- Smith, J. L. (1998). *Multiwavelength anomalous diffraction in macromolecular crystallography.* In *Direct methods for solving macromolecular structures*, edited by S. Fortier, pp. 221–225. Dordrecht: Kluwer Academic Publishers.
- Srinivasan, R. & Parthasarathy, S. (1976). *Some statistical applications in X-ray crystallography.* Oxford: Pergamon Press.
- Taylor, D. J., Woolfson, M. M. & Main, P. (1978). *On the application of phase relationships to complex structures. XV. Magic determinants.* *Acta Cryst.* **A34**, 870–883.
- Tsoucaris, G. (1970). *A new method for phase determination. The maximum determinant rule.* *Acta Cryst.* **A26**, 492–499.
- Van der Putten, N. & Schenk, H. (1977). *On the conditional probability of quintets.* *Acta Cryst.* **A33**, 856–858.
- Vaughan, P. A. (1958). *A phase-determining procedure related to the vector-coincidence method.* *Acta Cryst.* **11**, 111–115.
- Vermin, W. J. & de Graaff, R. A. G. (1978). *The use of Karle–Hauptman determinants in small-structure determinations.* *Acta Cryst.* **A34**, 892–894.
- Vicković, I. & Viterbo, D. (1979). *A simple statistical treatment of unobserved reflexions. Application to two organic substances.* *Acta Cryst.* **A35**, 500–501.
- Weeks, C. M., DeTitta, G. T., Hauptman, H. A., Thuman, P. & Miller, R. (1994). *Structure solution by minimal-function phase refinement and Fourier filtering. II. Implementation and applications.* *Acta Cryst.* **A50**, 210–220.
- Weeks, C. M. & Miller, R. (1999). *The design and implementation of SnB version 2.0.* *J. Appl. Cryst.* **32**, 120–124.
- Weinzierl, J. E., Eisenberg, D. & Dickerson, R. E. (1969). *Refinement of protein phases with the Karle–Hauptman tangent formula.* *Acta Cryst.* **B25**, 380–387.
- White, P. & Woolfson, M. M. (1975). *The application of phase relationships to complex structures. VII. Magic integers.* *Acta Cryst.* **A31**, 53–56.
- Wilkins, S. W., Varghese, J. N. & Lehmann, M. S. (1983). *Statistical geometry. I. A self-consistent approach to the crystallographic inversion problem based on information theory.* *Acta Cryst.* **A39**, 47–60.
- Wilson, A. J. C. (1942). *Determination of absolute from relative X-ray intensity data.* *Nature (London)*, **150**, 151–152.
- Wilson, K. S. (1978). *The application of MULTAN to the analysis of isomorphous derivatives in protein crystallography.* *Acta Cryst.* **B34**, 1599–1608.
- Wolff, P. M. de & Bouman, J. (1954). *A fundamental set of structure factor inequalities.* *Acta Cryst.* **7**, 328–333.
- Woolfson, M. M. (1958). *Crystal and molecular structure of p,p'-dimethoxybenzophenone by the direct probability method.* *Acta Cryst.* **11**, 277–283.
- Woolfson, M. M. (1977). *On the application of phase relationships to complex structures. X. MAGLIN – a successor to MULTAN.* *Acta Cryst.* **A33**, 219–225.
- Woolfson, M. & Fan, H.-F. (1995). *Physical and non-physical methods of solving crystal structures.* Cambridge University Press.
- Yao, J.-X. (1981). *On the application of phase relationships to complex structures. XVIII. RANTAN – random MULTAN.* *Acta Cryst.* **A37**, 642–664.

## 2.3

- Abad-Zapatero, C., Abdel-Meguid, S. S., Johnson, J. E., Leslie, A. G. W., Rayment, I., Rossmann, M. G., Suck, D. & Tsukihara, T. (1980). *Structure of southern bean mosaic virus at 2.8 Å resolution.* *Nature (London)*, **286**, 33–39.
- Acharya, R., Fry, E., Stuart, D., Fox, G., Rowlands, D. & Brown, F. (1989). *The three-dimensional structure of foot-and-mouth disease virus at 2.9 Å resolution.* *Nature (London)*, **337**, 709–716.
- Adams, M. J., Blundell, T. L., Dodson, E. J., Dodson, G. G., Vijayan, M., Baker, E. N., Harding, M. M., Hodgkin, D. C., Rimmer, B. & Sheat, S. (1969). *Structure of rhombohedral 2 zinc insulin crystals.* *Nature (London)*, **224**, 491–495.
- Åkervall, K., Strandberg, B., Rossmann, M. G., Bengtsson, U., Fridborg, K., Johannisen, H., Kannan, K. K., Lövgren, S., Petef, G., Öberg, B., Eaker, D., Hjertén, S., Rydén, L. & Moring, I. (1972). *X-ray diffraction studies of the structure of satellite tobacco necrosis virus.* *Cold Spring Harbor Symp. Quant. Biol.* **36**, 469–488.
- Argos, P., Ford, G. C. & Rossmann, M. G. (1975). *An application of the molecular replacement technique in direct space to a known protein structure.* *Acta Cryst.* **A31**, 499–506.
- Argos, P. & Rossmann, M. G. (1974). *Determining heavy-atom positions using non-crystallographic symmetry.* *Acta Cryst.* **A30**, 672–677.
- Argos, P. & Rossmann, M. G. (1976). *A method to determine heavy-atom positions for virus structures.* *Acta Cryst.* **B32**, 2975–2979.
- Argos, P. & Rossmann, M. G. (1980). *Molecular replacement methods.* In *Theory and practice of direct methods in crystallography*, edited by M. F. C. Ladd & R. A. Palmer, pp. 361–417. New York: Plenum.
- Arnold, E., Erickson, J. W., Fout, G. S., Frankenberger, E. A., Hecht, H. J., Luo, M., Rossmann, M. G. & Rueckert, R. R. (1984). *Virion orientation in cubic crystals of the human common cold virus HRV14.* *J. Mol. Biol.* **177**, 417–430.
- Arnold, E. & Rossmann, M. G. (1986). *Effect of errors, redundancy, and solvent content in the molecular replacement procedure for the structure determination of biological macromolecules.* *Proc. Natl Acad. Sci. USA*, **83**, 5489–5493.

## REFERENCES

## 2.3 (cont.)

- Arnold, E., Vriend, G., Luo, M., Griffith, J. P., Kamer, G., Erickson, J. W., Johnson, J. E. & Rossmann, M. G. (1987). *The structure determination of a common cold virus, human rhinovirus 14*. *Acta Cryst.* **A43**, 346–361.
- Beevers, C. A. & Robertson, J. M. (1950). *Interpretation of the Patterson synthesis*. *Acta Cryst.* **3**, 164.
- Beurskens, P. T. (1981). *A statistical interpretation of rotation and translation functions in reciprocal space*. *Acta Cryst.* **A37**, 426–430.
- Bhat, T. N. & Blow, D. M. (1982). *A density-modification method for the improvement of poorly resolved protein electron-density maps*. *Acta Cryst.* **A38**, 21–29.
- Bijvoet, J. M. (1954). *Structure of optically active compounds in the solid state*. *Nature (London)*, **173**, 888–891.
- Bijvoet, J. M., Peerdeman, A. F. & van Bommel, A. J. (1951). *Determination of the absolute configuration of optically active compounds by means of X-rays*. *Nature (London)*, **168**, 271–272.
- Bloomer, A. C., Champness, J. N., Bricogne, G., Staden, R. & Klug, A. (1978). *Protein disk of tobacco mosaic virus at 2.8 Å resolution showing the interactions within and between subunits*. *Nature (London)*, **276**, 362–368.
- Blow, D. M. (1958). *The structure of haemoglobin. VII. Determination of phase angles in the noncentrosymmetric [100] zone*. *Proc. R. Soc. London Ser. A*, **247**, 302–336.
- Blow, D. M. & Crick, F. H. C. (1959). *The treatment of errors in the isomorphous replacement method*. *Acta Cryst.* **12**, 794–802.
- Blow, D. M. & Rossmann, M. G. (1961). *The single isomorphous replacement method*. *Acta Cryst.* **14**, 1195–1202.
- Blow, D. M., Rossmann, M. G. & Jeffery, B. A. (1964). *The arrangement of  $\alpha$ -chymotrypsin molecules in the monoclinic crystal form*. *J. Mol. Biol.* **8**, 65–78.
- Bluhm, M. M., Bodo, G., Dintzis, H. M. & Kendrew, J. C. (1958). *The crystal structure of myoglobin. IV. A Fourier projection of sperm-whale myoglobin by the method of isomorphous replacement*. *Proc. R. Soc. London Ser. A*, **246**, 369–389.
- Blundell, T. L. & Johnson, L. N. (1976). *Protein crystallography*. New York: Academic Press.
- Bodo, G., Dintzis, H. M., Kendrew, J. C. & Wyckoff, H. W. (1959). *The crystal structure of myoglobin. V. A low-resolution three-dimensional Fourier synthesis of sperm-whale myoglobin crystals*. *Proc. R. Soc. London Ser. A*, **253**, 70–102.
- Bragg, W. L. (1958). *The determination of the coordinates of heavy atoms in protein crystals*. *Acta Cryst.* **11**, 70–75.
- Bragg, W. L. & Perutz, M. F. (1954). *The structure of haemoglobin. VI. Fourier projections on the 010 plane*. *Proc. R. Soc. London Ser. A*, **225**, 315–329.
- Braun, P. B., Hornstra, J. & Leenhouts, J. I. (1969). *Automated crystal-structure determination by Patterson search using a known part of the molecule*. *Philips Res. Rep.* **24**, 85–118.
- Bricogne, G. (1974). *Geometric sources of redundancy in intensity data and their use for phase determination*. *Acta Cryst.* **A30**, 395–405.
- Bricogne, G. (1976). *Methods and programs for the direct space exploitation of geometric redundancies*. *Acta Cryst.* **A32**, 832–847.
- Buehner, M., Ford, G. C., Moras, D., Olsen, K. W. & Rossmann, M. G. (1974). *Structure determination of crystalline lobster D-glyceraldehyde-3-phosphate dehydrogenase*. *J. Mol. Biol.* **82**, 563–585.
- Buerger, M. J. (1946). *The interpretation of Harker syntheses*. *J. Appl. Phys.* **17**, 579–595.
- Buerger, M. J. (1950a). *Some new functions of interest in X-ray crystallography*. *Proc. Natl Acad. Sci. USA*, **36**, 376–382.
- Buerger, M. J. (1950b). *Limitation of electron density by the Patterson function*. *Proc. Natl Acad. Sci. USA*, **36**, 738–742.
- Buerger, M. J. (1951). *A new approach to crystal-structure analysis*. *Acta Cryst.* **4**, 531–544.
- Buerger, M. J. (1953a). *Image theory of superposed vector sets*. *Proc. Natl Acad. Sci. USA*, **39**, 669–673.
- Buerger, M. J. (1953b). *Solution functions for solving superposed Patterson syntheses*. *Proc. Natl Acad. Sci. USA*, **39**, 674–678.
- Buerger, M. J. (1953c). *An intersection function and its relations to the minimum function of X-ray crystallography*. *Proc. Natl Acad. Sci. USA*, **39**, 678–680.
- Buerger, M. J. (1959). *Vector space and its application in crystal-structure investigation*. New York: John Wiley.
- Buerger, M. J. (1966). *Background for the use of image-seeking functions*. *Trans. Am. Crystallogr. Assoc.* **2**, 1–9.
- Bullough, R. K. (1961). *On homometric sets. I. Some general theorems*. *Acta Cryst.* **14**, 257–269.
- Bullough, R. K. (1964). *On homometric sets. II. Sets obtained by singular transformations*. *Acta Cryst.* **17**, 295–308.
- Burdina, V. I. (1970). *Symmetry of the rotation function*. *Kristallografiya*, **15**, 623–630.
- Burdina, V. I. (1971). *Symmetry of the rotation function*. *Sov. Phys. Crystallogr.* **15**, 545–550.
- Burdina, V. I. (1973). *Primitive rotation regions of two Patterson syntheses*. *Kristallografiya*, **18**, 694–700.
- Burnett, R. M. & Rossmann, M. G. (1971). *The determination of the crystal structure of trans-2,4-dihydroxy-2,4-dimethylcyclohexane-trans-1-acetic acid  $\gamma$ -lactone,  $C_{10}H_{16}O_3$ , using rotation and translation functions in reciprocal space*. *Acta Cryst.* **B27**, 1378–1387.
- Carlisle, C. H. & Crowfoot, D. (1945). *The crystal structure of cholesteryl iodide*. *Proc. R. Soc. London Ser. A*, **184**, 64–83.
- Caspar, D. L. D. & Klug, A. (1962). *Physical principles in the construction of regular viruses*. *Cold Spring Harbor Symp. Quant. Biol.* **27**, 1–24.
- Clastre, J. & Gay, R. (1950). *La détermination des structures cristallines à partir du diagramme de Patterson*. *Compt. Rend.* **230**, 1876–1877.
- Collins, D. M. (1975). *Efficiency in Fourier phase refinement for protein crystal structures*. *Acta Cryst.* **A31**, 388–389.
- Colman, P. M. (1974). *Noncrystallographic symmetry and the sampling theorem*. *Z. Kristallogr.* **140**, 344–349.
- Colman, P. M. & Fehlhammer, H. (1976). *Appendix: the use of rotation and translation functions in the interpretation of low resolution electron density maps*. *J. Mol. Biol.* **100**, 278–282.
- Colman, P. M., Fehlhammer, H. & Bartels, K. (1976). *Patterson search methods in protein structure determination:  $\beta$ -trypsin and immunoglobulin fragments*. In *Crystallographic computing techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 248–258. Copenhagen: Munksgaard.
- Corfield, P. W. R. & Rosenstein, R. D. (1966). *Maximum information from the minimum function*. *Trans. Am. Crystallogr. Assoc.* **2**, 17–28.
- Crick, F. H. C. & Magdoff, B. S. (1956). *The theory of the method of isomorphous replacement for protein crystals. I*. *Acta Cryst.* **9**, 901–908.
- Cromer, D. T. (1974). *Dispersion corrections for X-ray atomic scattering factors*. In *International tables for X-ray crystallography*, Vol. IV, edited by J. A. Ibers & W. C. Hamilton, pp. 148–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- Crowther, R. A. (1967). *A linear analysis of the non-crystallographic symmetry problem*. *Acta Cryst.* **22**, 758–764.
- Crowther, R. A. (1969). *The use of non-crystallographic symmetry for phase determination*. *Acta Cryst.* **B25**, 2571–2580.
- Crowther, R. A. (1972). *The fast rotation function*. In *The molecular replacement method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon & Breach.
- Crowther, R. A. & Blow, D. M. (1967). *A method of positioning a known molecule in an unknown crystal structure*. *Acta Cryst.* **23**, 544–548.
- Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1962). *The structure of haemoglobin. IX. A three-dimensional Fourier synthesis at 5.5 Å resolution: description of the structure*. *Proc. R. Soc. London Ser. A*, **265**, 161–187.

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

### 2.3 (cont.)

- Dickerson, R. E., Kendrew, J. C. & Strandberg, B. E. (1961). *The crystal structure of myoglobin: phase determination to a resolution of 2 Å by the method of isomorphous replacement*. *Acta Cryst.* **14**, 1188–1195.
- Dickerson, R. E., Kopka, M. L., Varnum, J. C. & Weinzierl, J. E. (1967). *Bias, feedback and reliability in isomorphous phase analysis*. *Acta Cryst.* **23**, 511–522.
- Dickerson, R. E., Weinzierl, J. E. & Palmer, R. A. (1968). *A least-squares refinement method for isomorphous replacement*. *Acta Cryst.* **B24**, 997–1003.
- Dodson, E., Harding, M. M., Hodgkin, D. C. & Rossmann, M. G. (1966). *The crystal structure of insulin. III. Evidence for a 2-fold axis in rhombohedral zinc insulin*. *J. Mol. Biol.* **16**, 227–241.
- Egert, E. (1983). *Patterson search – an alternative to direct methods*. *Acta Cryst.* **A39**, 936–940.
- Egert, E. & Sheldrick, G. M. (1985). *Search for a fragment of known geometry by integrated Patterson and direct methods*. *Acta Cryst.* **A41**, 262–268.
- Eisenberg, D. (1970). *X-ray crystallography and enzyme structure*. In *The enzymes*, edited by P. D. Boyer, Vol. I, 3rd ed., pp. 1–89. New York: Academic Press.
- Fitzgerald, P. M. D. (1988). *MERLOT, an integrated package of computer programs for the determination of crystal structures by molecular replacement*. *J. Appl. Cryst.* **21**, 273–278.
- Fletcher, R. J. & Steitz, T. A. (1976). *The combination of independent phase information obtained from separate protein structure determinations of yeast hexokinase*. *Acta Cryst.* **A32**, 125–132.
- Fridrichsons, J. & Mathieson, A. McL. (1962). *Image-seeking. A brief study of its scope and comments on certain limitations*. *Acta Cryst.* **15**, 1065–1074.
- Fujinaga, M. & Read, R. J. (1987). *Experiences with a new translation-function program*. *J. Appl. Cryst.* **20**, 517–521.
- Fukuyama, K., Abdel-Meguid, S. S., Johnson, J. E. & Rossmann, M. G. (1983). *Structure of a  $T = 1$  aggregate of alfalfa mosaic virus coat protein seen at 4.5 Å resolution*. *J. Mol. Biol.* **167**, 873–894.
- Garrido, J. (1950a). *Sur la détermination des structures cristallines au moyen de la transformée de Patterson*. *Compt. Rend.* **230**, 1878–1879.
- Garrido, J. (1950b). *Les coïncidences fortuites dans la méthode des différences vectorielles*. *Compt. Rend.* **231**, 297–298.
- Gaykema, W. P. J., Hol, W. G. J., Vereijken, J. M., Soeter, N. M., Bak, H. J. & Beintema, J. J. (1984). *3.2 Å structure of the copper-containing, oxygen-carrying protein Panulirus interruptus haemocyanin*. *Nature (London)*, **309**, 23–29.
- Gibbs, J. W. (1898). *Remarks regarding Michelson's letter*. *Nature (London)*, **59**, 200.
- Grau, U. M., Rossmann, M. G. & Trommer, W. E. (1981). *The crystallization and structure determination of an active ternary complex of pig heart lactate dehydrogenase*. *Acta Cryst.* **B37**, 2019–2026.
- Green, D. W., Ingram, V. M. & Perutz, M. F. (1954). *The structure of haemoglobin. IV. Sign determination by the isomorphous replacement method*. *Proc. R. Soc. London Ser. A*, **225**, 287–307.
- Hamilton, W. C. (1965). *The crystal structure of orthorhombic acetamide*. *Acta Cryst.* **18**, 866–870.
- Harada, Y., Lifchitz, A., Berthou, J. & Jolles, P. (1981). *A translation function combining packing and diffraction information: an application to lysozyme (high-temperature form)*. *Acta Cryst.* **A37**, 398–406.
- Harker, D. (1936). *The application of the three-dimensional Patterson method and the crystal structures of proustite,  $Ag_3AsS_3$ , and pyrargyrite,  $Ag_3SbS_3$* . *J. Chem. Phys.* **4**, 381–390.
- Harker, D. (1956). *The determination of the phases of the structure factors of non-centrosymmetric crystals by the method of double isomorphous replacement*. *Acta Cryst.* **9**, 1–9.
- Harrison, S. C., Olson, A. J., Schutt, C. E., Winkler, F. K. & Bricogne, G. (1978). *Tomato bushy stunt virus at 2.9 Å resolution*. *Nature (London)*, **276**, 368–373.
- Hendrickson, W. A. & Lattman, E. E. (1970). *Representation of phase probability distributions for simplified combination of independent phase information*. *Acta Cryst.* **B26**, 136–143.
- Hendrickson, W. A. & Teeter, M. M. (1981). *Structure of the hydrophobic protein crambin determined directly from the anomalous scattering of sulphur*. *Nature (London)*, **290**, 107–113.
- Hendrickson, W. A. & Ward, K. B. (1976). *A packing function for delimiting the allowable locations of crystallized macromolecules*. *Acta Cryst.* **A32**, 778–780.
- High, D. F. & Kraut, J. (1966). *The crystal structure of androsterone*. *Acta Cryst.* **21**, 88–96.
- Hirshfeld, F. L. (1968). *Symmetry in the generation of trial structures*. *Acta Cryst.* **A24**, 301–311.
- Hodgkin, D. C., Kamper, J., Lindsey, J., MacKay, M., Pickworth, J., Robertson, J. H., Shoemaker, C. B., White, J. G., Prosen, R. J. & Trueblood, K. N. (1957). *The structure of vitamin B<sub>12</sub>. I. An outline of the crystallographic investigation of vitamin B<sub>12</sub>*. *Proc. R. Soc. London Ser. A*, **242**, 228–263.
- Hogle, J. M., Chow, M. & Filman, D. J. (1985). *Three-dimensional structure of poliovirus at 2.9 Å resolution*. *Science*, **229**, 1358–1365.
- Hoppe, W. (1957a). *Die Faltmolekülmethode und ihre anwendung in der Röntgenographischen Konstitutionsanalyse von Biflorin ( $C_{20}H_{20}O_4$ )*. *Z. Elektrochem.* **61**, 1076–1083.
- Hoppe, W. (1957b). *Die 'Faltmolekülmethode' – eine neue Methode zur Bestimmung der Kristallstruktur bei ganz oder teilweise bekannter Molekülstruktur*. *Acta Cryst.* **10**, 750–751.
- Hoppe, W. (1959). *Die Bestimmung genauer Schweratom-parameter in isomorphen azentrischen Kristallen*. *Acta Cryst.* **12**, 665–674.
- Hoppe, W. (1962). *'Nahezu-Homometrische Lösungen' und Faltmolekülmethode*. *Z. Kristallogr.* **117**, 249–258.
- Hoppe, W. & Gassmann, J. (1968). *Phase correction, a new method to solve partially known structures*. *Acta Cryst.* **B24**, 97–107.
- Hosemann, R. & Bagchi, S. N. (1954). *On homometric structures*. *Acta Cryst.* **7**, 237–241.
- Hosur, M. V., Schmidt, T., Tucker, R. C., Johnson, J. E., Gallagher, T. M., Selling, B. H. & Rueckert, R. R. (1987). *Structure of an insect virus at 3.0 Å resolution*. *Proteins*, **2**, 167–176.
- Huber, R. (1965). *Die automatisierte Faltmolekülmethode*. *Acta Cryst.* **19**, 353–356.
- Hughes, E. W. (1940). *The crystal structure of dicyandiamide*. *J. Am. Chem. Soc.* **62**, 1258–1267.
- International Tables for Crystallography* (1983). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.
- Jacobson, R. A., Wunderlich, J. A. & Lipscomb, W. N. (1961). *The crystal and molecular structure of cellobiose*. *Acta Cryst.* **14**, 598–607.
- James, R. W. (1965). *The optical principles of the diffraction of X-rays*. Ithaca: Cornell University Press.
- Johnson, J. E. (1978). *Appendix II. Averaging of electron density maps*. *Acta Cryst.* **B34**, 576–577.
- Johnson, J. E., Akimoto, T., Suck, D., Rayment, I. & Rossmann, M. G. (1976). *The structure of southern bean mosaic virus at 22.5 Å resolution*. *Virology*, **75**, 394–400.
- Johnson, J. E., Argos, P. & Rossmann, M. G. (1975). *Rotation function studies of southern bean mosaic virus at 22 Å resolution*. *Acta Cryst.* **B31**, 2577–2583.
- Karle, J. (1976). *Partial structures and use of the tangent formula and translation functions*. In *Crystallographic computing techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 155–164. Copenhagen: Munksgaard.
- Karle, J. & Hauptman, H. (1964). *Positivity, point atoms, and Pattersons*. *Acta Cryst.* **17**, 392–396.
- Kartha, G. (1961). *Isomorphous replacement method in non-centrosymmetric structures*. *Acta Cryst.* **14**, 680–686.
- Kartha, G. & Parthasarathy, R. (1965). *Combination of multiple isomorphous replacement and anomalous dispersion data for protein structure determination. I. Determination of heavy-atom positions in protein derivatives*. *Acta Cryst.* **18**, 745–749.

## REFERENCES

## 2.3 (cont.)

- Ketelaar, J. A. A. & de Vries, T. A. (1939). *The crystal structure of tetra phosphonitrile chloride, P<sub>4</sub>N<sub>4</sub>Cl<sub>8</sub>*. *Recl Trav. Chim.* **58**, 1081–1099.
- Kraut, J. (1961). *The crystal structure of 2-amino-ethanol phosphate*. *Acta Cryst.* **14**, 1146–1152.
- Lattman, E. E. (1972). *Optimal sampling of the rotation function*. *Acta Cryst.* **B28**, 1065–1068.
- Lattman, E. E. & Love, W. E. (1970). *A rotational search procedure for detecting a known molecule in a crystal*. *Acta Cryst.* **B26**, 1854–1857.
- Lentz, P. J. Jr, Strandberg, B., Unge, T., Vaara, I., Borell, A., Fridborg, K. & Petef, G. (1976). *The determination of the heavy-atom substitution sites in the satellite tobacco necrosis virus*. *Acta Cryst.* **B32**, 2979–2983.
- Lifchitz, A. (1983). *On the choice of the model cell and the integration volume in the use of the rotation function*. *Acta Cryst.* **A39**, 130–139.
- Liljas, L., Unge, T., Jones, T. A., Fridborg, K., Lövgren, S., Skoglund, U. & Strandberg, B. (1982). *Structure of satellite tobacco necrosis virus at 3.0 Å resolution*. *J. Mol. Biol.* **159**, 93–108.
- Lipson, H. & Cochran, W. (1966). *The determination of crystal structures*. Ithaca: Cornell University Press.
- Litvin, D. B. (1975). *The molecular replacement method. I. The rotation function problem, application to bovine liver catalase and STNV*. *Acta Cryst.* **A31**, 407–416.
- Luo, M., Vriend, G., Kamer, G., Minor, I., Arnold, E., Rossmann, M. G., Boege, U., Scraba, D. G., Duke, G. M. & Palmenberg, A. C. (1987). *The atomic structure of Mengo virus at 3.0 Å resolution*. *Science*, **235**, 182–191.
- Luzzati, V. (1953). *Résolution d'une structure cristalline lorsque les positions d'une partie des atomes sont connues: traitement statistique*. *Acta Cryst.* **6**, 142–152.
- McLachlan, D. Jr & Harker, D. (1951). *Finding the signs of the F's from the shifted Patterson product*. *Proc. Natl Acad. Sci. USA*, **37**, 846–849.
- Main, P. (1967). *Phase determination using non-crystallographic symmetry*. *Acta Cryst.* **23**, 50–54.
- Main, P. & Rossmann, M. G. (1966). *Relationships among structure factors due to identical molecules in different crystallographic environments*. *Acta Cryst.* **21**, 67–72.
- Matthews, B. W. (1966). *The determination of the position of anomalously scattering heavy atom groups in protein crystals*. *Acta Cryst.* **20**, 230–239.
- Matthews, B. W. & Czerwinski, E. W. (1975). *Local scaling: a method to reduce systematic errors in isomorphous replacement and anomalous scattering measurements*. *Acta Cryst.* **A31**, 480–487.
- Matthews, B. W., Sigler, P. B., Henderson, R. & Blow, D. M. (1967). *Three-dimensional structure of tosyl- $\alpha$ -chymotrypsin*. *Nature (London)*, **214**, 652–656.
- Menzer, G. (1949). *Über die mehrdeutigkeit der Kristallstrukturbestimmung*. *Z. Naturforsch. Teil A*, **4**, 11–21.
- Mighell, A. D. & Jacobson, R. A. (1963). *Analysis of three-dimensional Patterson maps using vector verification*. *Acta Cryst.* **16**, 443–445.
- Moncrief, J. W. & Lipscomb, W. N. (1966). *Structure of leurocristine methiodide dihydrate by anomalous scattering methods; relation to leurocristine (vincristine) and vincalkeb-lastine (vinblastine)*. *Acta Cryst.* **21**, 322–331.
- Moras, D., Comarmond, M. B., Fischer, J., Weiss, R., Thierry, J. C., Ebel, J. P. & Giegé, R. (1980). *Crystal structure of yeast tRNA<sup>Asp</sup>*. *Nature (London)*, **288**, 669–674.
- Muirhead, H., Cox, J. M., Mazzarella, L. & Perutz, M. F. (1967). *Structure and function of haemoglobin. III. A three-dimensional Fourier synthesis of human deoxyhaemoglobin at 5.5 Å resolution*. *J. Mol. Biol.* **28**, 117–156.
- Murthy, M. R. N., Reid, T. J. III, Sicignano, A., Tanaka, N. & Rossmann, M. G. (1981). *Structure of beef liver catalase*. *J. Mol. Biol.* **152**, 465–499.
- Nixon, P. E. (1978). *Overlapping Patterson peaks and direct methods: the structure of prostratin*. *Acta Cryst.* **A34**, 450–453.
- Nordman, C. E. (1966). *Vector space search and refinement procedures*. *Trans. Am. Crystallogr. Assoc.* **2**, 29–38.
- Nordman, C. E. (1972). *An application of vector space search methods to the Patterson function of myoglobin*. *Acta Cryst.* **A28**, 134–143.
- Nordman, C. E. (1980a). *Vector-space Patterson search and other stored-function sampling procedures*. In *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 5.01–5.13. Bangalore: Indian Academy of Sciences.
- Nordman, C. E. (1980b). *Procedures for detection and idealization of non-crystallographic symmetry with application to phase refinement of the satellite tobacco necrosis virus structure*. *Acta Cryst.* **A36**, 747–754.
- Nordman, C. E. & Nakatsu, K. (1963). *Interpretation of the Patterson function of crystals containing a known molecular fragment. The structure of an Alstonia alkaloid*. *J. Am. Chem. Soc.* **85**, 353–354.
- Nordman, C. E. & Schilling, J. W. (1970). *Calculation and use of vector overlap weights in Patterson search and refinement*. In *Crystallographic computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 110–114. Copenhagen: Munksgaard.
- North, A. C. T. (1965). *The combination of isomorphous replacement and anomalous scattering data in phase determination of non-centrosymmetric reflexions*. *Acta Cryst.* **18**, 212–216.
- Okaya, Y., Saito, Y. & Pepinsky, R. (1955). *New method in X-ray crystal structure determination involving the use of anomalous dispersion*. *Phys. Rev.* **98**, 1857–1858.
- Patterson, A. L. (1934a). *A Fourier series representation of the average distribution of scattering power in crystals*. *Phys. Rev.* **45**, 763.
- Patterson, A. L. (1934b). *A Fourier series method for the determination of the components of interatomic distances in crystals*. *Phys. Rev.* **46**, 372–376.
- Patterson, A. L. (1935). *A direct method for the determination of the components of interatomic distances in crystals*. *Z. Kristallogr.* **90**, 517–542.
- Patterson, A. L. (1939). *Homometric structures*. *Nature (London)*, **143**, 939–940.
- Patterson, A. L. (1944). *Ambiguities in the X-ray analysis of crystal structures*. *Phys. Rev.* **65**, 195–201.
- Patterson, A. L. (1949). *An alternative interpretation for vector maps*. *Acta Cryst.* **2**, 339–340.
- Pauling, L. & Shappell, M. D. (1930). *The crystal structure of bixbyite and the C-modification of the sesquioxides*. *Z. Kristallogr.* **75**, 128–142.
- Pepinsky, R., Okaya, Y. & Takeuchi, Y. (1957). *Theory and application of the P<sub>s</sub>(u) function and anomalous dispersion in direct determination of structures and absolute configuration in non-centric crystals*. *Acta Cryst.* **10**, 756.
- Perutz, M. F. (1954). *The structure of haemoglobin. III. Direct determination of the molecular transform*. *Proc. R. Soc. London Ser. A*, **225**, 264–286.
- Perutz, M. F. (1956). *Isomorphous replacement and phase determination in non-centrosymmetric space groups*. *Acta Cryst.* **9**, 867–873.
- Phillips, D. C. (1966). *Advances in protein crystallography*. In *Advances in structure research by diffraction methods*, Vol. 2, edited by R. Brill & R. Mason, pp. 75–140. New York: John Wiley.
- Poljak, R. J. (1963). *Heavy-atom attachment to crystalline lysozyme*. *J. Mol. Biol.* **6**, 244–246.
- Rabinovich, D. & Shakked, Z. (1984). *A new approach to structure determination of large molecules by multi-dimensional search methods*. *Acta Cryst.* **A40**, 195–200.
- Ramachandran, G. N. & Raman, S. (1959). *Syntheses for the deconvolution of the Patterson function. Part I. General principles*. *Acta Cryst.* **12**, 957–964.
- Raman, S. (1966). *Patterson functions and vector sets*. *Trans. Am. Crystallogr. Assoc.* **2**, 10–16.

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

### 2.3 (cont.)

- Raman, S. & Lipscomb, W. N. (1961). *Two classes of functions for the location of heavy atoms and for solution of crystal structures*. *Z. Kristallogr.* **116**, 314–327.
- Ramaseshan, S. & Abrahams, S. C. (1975). Editors. *Anomalous scattering*. Copenhagen: Munksgaard.
- Rao, S. N., Jih, J. H. & Hartsuck, J. A. (1980). *Rotation-function space groups*. *Acta Cryst.* **A36**, 878–884.
- Rayment, I. (1983). *Molecular replacement method at low resolution: optimum strategy and intrinsic limitations as determined by calculations on icosahedral virus models*. *Acta Cryst.* **A39**, 102–116.
- Rayment, I., Baker, T. S. & Caspar, D. L. D. (1983). *A description of the techniques and application of molecular replacement used to determine the structure of polyoma virus capsid at 22.5 Å resolution*. *Acta Cryst.* **B39**, 505–516.
- Rayment, I., Baker, T. S., Caspar, D. L. D. & Murakami, W. T. (1982). *Polyoma virus capsid structure at 22.5 Å resolution*. *Nature (London)*, **295**, 110–115.
- Rayment, I., Johnson, J. E., Suck, D., Akimoto, T. & Rossmann, M. G. (1978). *An 11 Å resolution electron density map of southern bean mosaic virus*. *Acta Cryst.* **B34**, 567–578.
- Robertson, J. M. (1935). *An X-ray study of the structure of phthalocyanines. Part I. The metal-free, nickel, copper, and platinum compounds*. *J. Chem. Soc.* pp. 615–621.
- Robertson, J. M. (1936). *An X-ray study of the phthalocyanines. Part II. Quantitative structure determination of the metal-free compound*. *J. Chem. Soc.* pp. 1195–1209.
- Robertson, J. M. (1951). *Interpretation of the Patterson synthesis: rubidium benzyl penicillin*. *Acta Cryst.* **4**, 63–66.
- Robertson, J. M. & Woodward, I. (1937). *An X-ray study of the phthalocyanines. Part III. Quantitative structure determination of nickel phthalocyanine*. *J. Chem. Soc.* pp. 219–230.
- Rogers, D. (1951). *New methods of direct structure determination using modified Patterson maps*. *Research*, **4**, 295–296.
- Rossmann, M. G. (1960). *The accurate determination of the position and shape of heavy-atom replacement groups in proteins*. *Acta Cryst.* **13**, 221–226.
- Rossmann, M. G. (1961a). *The position of anomalous scatterers in protein crystals*. *Acta Cryst.* **14**, 383–388.
- Rossmann, M. G. (1961b). *Application of the Buerger minimum function to protein structures*. In *Computing methods and the phase problem in X-ray crystal analysis*, edited by R. Pepinsky, J. M. Robertson & J. C. Speakman, pp. 252–265. Oxford: Pergamon Press.
- Rossmann, M. G. (1972). *The molecular replacement method*. New York: Gordon & Breach.
- Rossmann, M. G. (1990). *The molecular replacement method*. *Acta Cryst.* **A46**, 73–82.
- Rossmann, M. G., Arnold, E., Erickson, J. W., Frankenberger, E. A., Griffith, J. P., Hecht, H. J., Johnson, J. E., Kamer, G., Luo, M., Mosser, A. G., Rueckert, R. R., Sherry, B. & Vriend, G. (1985). *Structure of a human common cold virus and functional relationship to other picornaviruses*. *Nature (London)*, **317**, 145–153.
- Rossmann, M. G. & Blow, D. M. (1961). *The refinement of structures partially determined by the isomorphous replacement method*. *Acta Cryst.* **14**, 641–647.
- Rossmann, M. G. & Blow, D. M. (1962). *The detection of sub-units within the crystallographic asymmetric unit*. *Acta Cryst.* **15**, 24–31.
- Rossmann, M. G. & Blow, D. M. (1963). *Determination of phases by the conditions of non-crystallographic symmetry*. *Acta Cryst.* **16**, 39–45.
- Rossmann, M. G., Blow, D. M., Harding, M. M. & Collier, E. (1964). *The relative positions of independent molecules within the same asymmetric unit*. *Acta Cryst.* **17**, 338–342.
- Rossmann, M. G., Ford, G. C., Watson, H. C. & Banaszak, L. J. (1972). *Molecular symmetry of glyceraldehyde-3-phosphate dehydrogenase*. *J. Mol. Biol.* **64**, 237–249.
- Rossmann, M. G. & Henderson, R. (1982). *Phasing electron diffraction amplitudes with the molecular replacement method*. *Acta Cryst.* **A38**, 13–20.
- Sasada, Y. (1964). *The differential rotation function*. *Acta Cryst.* **17**, 611–612.
- Schevitz, R. W., Podjarny, A. D., Zwick, M., Hughes, J. J. & Sigler, P. B. (1981). *Improving and extending the phases of medium- and low-resolution macromolecular structure factors by density modification*. *Acta Cryst.* **A37**, 669–677.
- Shoemaker, D. P., Donohue, J., Schomaker, V. & Corey, R. B. (1950). *The crystal structure of L<sub>8</sub>-threonine*. *J. Am. Chem. Soc.* **72**, 2328–2349.
- Sim, G. A. (1961). *Aspects of the heavy-atom method*. In *Computing methods and the phase problem in X-ray crystal analysis*, edited by R. Pepinsky, J. M. Robertson & J. C. Speakman, pp. 227–235. Oxford: Pergamon Press.
- Simonov, V. I. (1965). *Calculation of the phases of the structure amplitudes by Fourier transformation of the sum, product and minimum functions*. *Proc. Indian Acad. Sci.* **A62**, 213–223.
- Simpson, P. G., Dobrott, R. D. & Lipscomb, W. N. (1965). *The symmetry minimum function: high order image seeking functions in X-ray crystallography*. *Acta Cryst.* **18**, 169–179.
- Singh, A. K. & Ramaseshan, S. (1966). *The determination of heavy atom positions in protein derivatives*. *Acta Cryst.* **21**, 279–280.
- Smith, J. L., Hendrickson, W. A. & Addison, A. W. (1983). *Structure of trimeric haemerythrin*. *Nature (London)*, **303**, 86–88.
- Speakman, J. C. (1949). *The crystal structures of the acid salts of some monobasic acids. Part I. Potassium hydrogen bisphenylacetate*. *J. Chem. Soc.* pp. 3357–3365.
- Stauffer, C. V., Usha, R., Harrington, M., Schmidt, T., Hosur, M. V. & Johnson, J. E. (1987). *The structure of cowpea mosaic virus at 3.5 Å resolution*. In *Crystallography in molecular biology*, edited by D. Moras, J. Drenth, B. Strandberg, D. Suck & K. Wilson, pp. 293–308. New York, London: Plenum.
- Steinrauf, L. K. (1963). *Two Fourier functions for use in protein crystallography*. *Acta Cryst.* **16**, 317–319.
- Stout, G. H. & Jensen, L. H. (1968). *X-ray structure determination*. New York: Macmillan.
- Strahs, G. & Kraut, J. (1968). *Low-resolution electron-density and anomalous-scattering-density maps of Chromatium high-potential iron protein*. *J. Mol. Biol.* **35**, 503–512.
- Tanaka, N. (1977). *Representation of the fast-rotation function in a polar coordinate system*. *Acta Cryst.* **A33**, 191–193.
- Taylor, W. J. (1953). *Fourier representation of Buerger's image-seeking minimum function*. *J. Appl. Phys.* **24**, 662–663.
- Terwilliger, T. C. & Eisenberg, D. (1983). *Unbiased three-dimensional refinement of heavy-atom parameters by correlation of origin-removed Patterson functions*. *Acta Cryst.* **A39**, 813–817.
- Tollin, P. (1966). *On the determination of molecular location*. *Acta Cryst.* **21**, 613–614.
- Tollin, P. (1969). *A comparison of the Q-functions and the translation function of Crowther and Blow*. *Acta Cryst.* **A25**, 376–377.
- Tollin, P. & Cochran, W. (1964). *Patterson function interpretation for molecules containing planar groups*. *Acta Cryst.* **17**, 1322–1324.
- Tollin, P., Main, P. & Rossmann, M. G. (1966). *The symmetry of the rotation function*. *Acta Cryst.* **20**, 404–407.
- Tollin, P. & Rossmann, M. G. (1966). *A description of various rotation function programs*. *Acta Cryst.* **21**, 872–876.
- Tong, L. & Rossmann, M. G. (1990). *The locked rotation function*. *Acta Cryst.* **A46**, 783–792.
- Wang, B. C. (1985). *Resolution of phase ambiguity in macromolecular crystallography*. *Methods Enzymol.* **115**, 90–112.
- Wilson, A. J. C. (1942). *Determination of absolute from relative X-ray intensity data*. *Nature (London)*, **150**, 151–152.
- Wilson, I. A., Skehel, J. J. & Wiley, D. C. (1981). *Structure of the haemagglutinin membrane glycoprotein of influenza virus at 3 Å resolution*. *Nature (London)*, **289**, 366–373.
- Woolfson, M. M. (1956). *An improvement of the 'heavy-atom' method of solving crystal structures*. *Acta Cryst.* **9**, 804–810.

## REFERENCES

## 2.3 (cont.)

- Woolfson, M. M. (1970). *An introduction to X-ray crystallography*. London: Cambridge University Press.
- Wrinch, D. M. (1939). *The geometry of discrete vector maps*. *Philos. Mag.* **27**, 98–122.
- Wunderlich, J. A. (1965). *A new expression for sharpening Patterson functions*. *Acta Cryst.* **19**, 200–202.

## 2.4

- Adams, M. J. (1968). DPhil thesis, Oxford University, England.
- Agard, D. A. & Stroud, R. M. (1982).  $\alpha$ -Bungarotoxin structure revealed by a rapid method for averaging electron density of non-crystallographically translationally related molecules. *Acta Cryst.* **A38**, 186–194.
- Arndt, U. W. (1986). *X-ray position-sensitive detectors*. *J. Appl. Cryst.* **19**, 145–163.
- Arndt, U. W. & Wonacott, A. J. (1977). *The rotation method in crystallography*. Amsterdam: North-Holland.
- Ashida, T. (1976). *Some remarks on the phase angle determination by the isomorphous replacement method*. In *Crystallographic computing techniques*, edited by F. R. Ahmed, pp. 282–284. Copenhagen: Munksgaard.
- Bhat, T. N. & Blow, D. M. (1982). *A density-modification method for improvement of poorly resolved protein electron-density maps*. *Acta Cryst.* **A38**, 21–29.
- Bijvoet, J. M. (1949). *Phase determination in direct Fourier-synthesis of crystal structures*. *Proc. K. Ned. Akad. Wet. (B)*, **52**, 313–314.
- Bijvoet, J. M. (1954). *Structure of optically active compounds in the solid state*. *Nature (London)*, **173**, 888–891.
- Bijvoet, J. M., Peerdeman, A. F. & van Bommel, A. J. (1951). *Determination of the absolute configuration of optically active compounds by means of X-rays*. *Nature (London)*, **168**, 271–272.
- Blow, D. M. & Crick, F. H. C. (1959). *The treatment of errors in the isomorphous replacement method*. *Acta Cryst.* **12**, 794–802.
- Blow, D. M. & Matthews, B. W. (1973). *Parameter refinement in the multiple isomorphous-replacement method*. *Acta Cryst.* **A29**, 56–62.
- Blow, D. M. & Rossmann, M. G. (1961). *The single isomorphous replacement method*. *Acta Cryst.* **14**, 1195–1202.
- Blundell, T. L. & Johnson, L. N. (1976). *Protein crystallography*. London: Academic Press.
- Bokhoven, C., Schoone, J. C. & Bijvoet, J. M. (1951). *The Fourier synthesis of the crystal structure of strychnine sulphate pentahydrate*. *Acta Cryst.* **4**, 275–280.
- Bradley, A. J. & Rodgers, J. W. (1934). *The crystal structure of the Heusler alloys*. *Proc. R. Soc. London Ser. A*, **144**, 340–359.
- Cannillo, E., Oberti, R. & Ungaretti, L. (1983). *Phase extension and refinement by density modification in protein crystallography*. *Acta Cryst.* **A39**, 68–74.
- Chacko, K. K. & Srinivasan, R. (1970). *On the Fourier refinement of anomalous dispersion corrections in X-ray diffraction data*. *Z. Kristallogr.* **131**, 88–94.
- Collins, D. M. (1975). *Efficiency in Fourier phase refinement for protein crystal structures*. *Acta Cryst.* **A31**, 388–389.
- Cork, J. M. (1927). *The crystal structure of some of the alums*. *Philos. Mag.* **4**, 688–698.
- Coster, D., Knol, K. S. & Prins, J. A. (1930). *Unterschiede in der Intensität der Röntgenstrahlenreflexion an den beiden 111-Flächen der Zinkblende*. *Z. Phys.* **63**, 345–369.
- Cromer, D. T. (1965). *Anomalous dispersion corrections computed from self-consistent field relativistic Dirac-Slater wave functions*. *Acta Cryst.* **18**, 17–23.
- Cruickshank, D. W. J. & McDonald, W. S. (1967). *Parameter errors in polar space groups caused by neglect of anomalous scattering*. *Acta Cryst.* **23**, 9–11.
- Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961a). *The structure of haemoglobin. VIII. A three-dimensional Fourier synthesis at 5.5 Å resolution: determination of the phase angles*. *Proc. R. Soc. London Ser. A*, **265**, 15–38.
- Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961b). *The structure of haemoglobin. IX. A three-dimensional Fourier synthesis at 5.5 Å resolution: description of the structure*. *Proc. R. Soc. London Ser. A*, **265**, 161–187.
- Dale, D., Hodgkin, D. C. & Venkatesan, K. (1963). *The determination of the crystal structure of factor V Ia*. In *Crystallography and crystal perfection*, edited by G. N. Ramachandran, pp. 237–242. New York and London: Academic Press.
- Dickerson, R. E., Kendrew, J. C. & Strandberg, B. E. (1961). *The crystal structure of myoglobin: phase determination to a resolution of 2 Å by the method of isomorphous replacement*. *Acta Cryst.* **14**, 1188–1195.
- Dickerson, R. E., Weinzierl, J. E. & Palmer, R. A. (1968). *A least-squares refinement method for isomorphous replacement*. *Acta Cryst.* **B24**, 997–1003.
- Dodson, E., Evans, P. & French, S. (1975). *The use of anomalous scattering in refining heavy atom parameters in proteins*. In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abraham, pp. 423–436. Copenhagen: Munksgaard.
- Dodson, E. & Vijayan, M. (1971). *The determination and refinement of heavy-atom parameters in protein heavy-atom derivatives. Some model calculations using acentric reflexions*. *Acta Cryst.* **B27**, 2402–2411.
- Einstein, J. E. (1977). *An improved method for combining isomorphous replacement and anomalous scattering diffraction data for macromolecular crystals*. *Acta Cryst.* **A33**, 75–85.
- Flood, R. J., Freeman, H. C. & Scudder, M. L. (1977). *An X-ray and neutron diffraction study of aqua(L-glutamato) cadmium(II) hydrate*. *Acta Cryst.* **B33**, 801–809.
- Gilli, G. & Cruickshank, D. W. J. (1973). *Effect of neglect of dispersion in centrosymmetric structures: results for OsO<sub>4</sub>*. *Acta Cryst.* **B29**, 1983–1985.
- Green, D. W., Ingram, V. M. & Perutz, M. F. (1954). *The structure of haemoglobin. IV. Sign determination by the isomorphous replacement method*. *Proc. R. Soc. London Ser. A*, **225**, 287–307.
- Green, E. A. (1979). *A new statistical model for describing errors in isomorphous replacement data: the case of one derivative*. *Acta Cryst.* **A35**, 351–359.
- Harker, D. (1956). *The determination of the phases of the structure factors of non-centrosymmetric crystals by the method of double isomorphous replacement*. *Acta Cryst.* **9**, 1–9.
- Helliwell, J. R. (1984). *Synchrotron X-radiation protein crystallography: instrumentation, methods and applications*. *Rep. Prog. Phys.* **47**, 1403–1497.
- Helliwell, J. R. (1985). *Protein crystallography with synchrotron radiation*. *J. Mol. Struct.* **130**, 63–91.
- Hendrickson, W. A. (1979). *Phase information from anomalous-scattering measurements*. *Acta Cryst.* **A35**, 245–247.
- Hendrickson, W. A. & Karle, J. (1973). *Carp muscle calcium-binding protein. III. Phase refinement using the tangent formula*. *J. Biol. Chem.* **248**, 3327–3334.
- Hendrickson, W. A. & Konnert, J. H. (1980). *Incorporation of stereochemical information into crystallographic refinement*. In *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 13.01–13.23. Bangalore: Indian Academy of Sciences.
- Hendrickson, W. A. & Lattman, E. E. (1970). *Representation of phase probability distributions in simplified combinations of independent phase information*. *Acta Cryst.* **B26**, 136–143.
- Hendrickson, W. A. & Sheriff, S. (1987). *General density function corresponding to X-ray diffraction with anomalous scattering included*. *Acta Cryst.* **A43**, 121–125.
- Hendrickson, W. A. & Teeter, M. M. (1981). *Structure of the hydrophobic protein crambin determined directly from the anomalous scattering of sulphur*. *Nature (London)*, **290**, 107–113.
- Hoppe, W. & Gassmann, J. (1968). *Phase correction, a new method to solve partially known structures*. *Acta Cryst.* **B24**, 97–107.
- Huber, R., Kukla, D., Bode, W., Schwager, P., Bartels, K., Deisenhofer, J. & Steigemann, W. (1974). *Structure of the complex formed by bovine trypsin and bovine pancreatic trypsin inhibitor. II. Crystallographic refinement at 1.9 Å resolution*. *J. Mol. Biol.* **89**, 73–101.