

3.3 (cont.)

- Miller, J. R., Abdel-Meguid, S. S., Rossmann, M. G. & Anderson, D. C. (1981). A computer graphics system for the building of macromolecular models into electron density maps. *J. Appl. Cryst.* **14**, 94–100.
- Morffew, A. J. (1983). Bibliography for molecular graphics. *J. Mol. Graphics*, **1**, 17–23.
- Morffew, A. J. (1984). Bibliography for molecular graphics, 1983/84. *J. Mol. Graphics*, **2**, 124–128.
- Morimoto, C. N. & Meyer, E. F. (1976). Information retrieval, computer graphics, and remote computing. In *Crystallographic computing techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 488–496. Copenhagen: Munksgaard.
- Motherwell, W. D. S. (1978). *Pluto – a program for displaying molecular and crystal structures*. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England.
- Newman, W. M. & Sproull, R. F. (1973). *Principles of inter-active computer graphics*. New York: McGraw-Hill.
- North, A. C. T. (1982). Use of interactive computer graphics in studying molecular structures and interactions. *Chem. Ind.* pp. 221–225.
- North, A. C. T., Denson, A. K., Evans, A. C., Ford, L. O. & Willoughby, T. V. (1981). The use of an interactive computer graphics system in the study of protein conformations. In *Biomolecular structure, conformation, function and evolution*, Vol. 1, edited by R. Srinivasan, pp. 59–72. Oxford: Pergamon Press.
- O'Donnell, T. J. & Olson, A. J. (1981). GRAMPS – a graphics language interpreter for real-time, interactive, three-dimensional picture editing and animation. *Comput. Graphics*, **15**, 133–142.
- Olson, A. J. (1982). GRAMPS: a high level graphics interpreter for expanding graphics utilization. In *Computational crystallography*, edited by D. Sayre, pp. 326–336. Oxford University Press.
- Opdenbosch, N. van, Cramer, R. III & Giarrusso, F. F. (1985). Sybyl, the integrated molecular modelling system. *J. Mol. Graphics*, **3**, 110–111.
- Pearl, L. H. & Honegger, A. (1983). Generation of molecular surfaces for graphic display. *J. Mol. Graphics*, **1**, 9–12, C2.
- Phillips, S. E. V. (1980). Structure and refinement of oxymyoglobin at 1.6 Å resolution. *J. Mol. Biol.* **142**, 531–554.
- Phong, B. T. (1975). Illumination for computer generated images. *Commun. ACM*, **18**, 311–317.
- Porter, T. K. (1978). Spherical shading. *Comput. Graphics*, **12**, 282–285.
- Potenzzone, R., Cavicchi, E., Weintraub, H. J. R. & Hopfinger, A. J. (1977). Molecular mechanics and the CAMSEQ processor. *Comput. Chem.* **1**, 187–194.
- Potterton, E. A., Geddes, A. J. & North, A. C. T. (1983). Attempts to design inhibitors of dihydrofolate reductase using interactive computer graphics with real time energy calculations. In *Chemistry and biology of pteridines*, edited by J. A. Blair, pp. 299–303. Berlin, New York: Walter de Gruyter.
- Purisima, E. O. & Scheraga, H. A. (1986). An approach to the multiple-minima problem by relaxing dimensionality. *Proc. Natl Acad. Sci. USA*, **83**, 2782–2786.
- Richardson, J. S. (1977). β -Sheet topology and the relatedness of proteins. *Nature (London)*, **268**, 495–500.
- Richardson, J. S. (1981). The anatomy and taxonomy of protein structure. *Adv. Protein Chem.* **34**, 167–339.
- Richardson, J. S. (1985). Schematic drawings of protein structures. In *Methods in enzymology*, Vol. 115. Diffraction methods for biological molecules, Part B, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 359–380. Orlando, Florida: Academic Press.
- Sundaram, K. & Radhakrishnan, R. (1979). A computer program for topographic analysis of biomolecular systems. *Comput. Programs Biomed.* **10**, 34–42.
- Sutcliffe, D. C. (1980). Contouring over rectangular and skewed rectangular grids – an introduction. In *Mathematical methods in computer graphics and design*, edited by K. W. Brodie, pp. 39–62. London: Academic Press.
- Sutherland, I. E., Sproull, R. F. & Schumacker, R. A. (1974). A characterization of ten hidden surface algorithms. *Comput. Surv.* **6**, 1–55.
- Swanson, S. M., Wesolowski, T., Geller, M. & Meyer, E. F. (1989). Animation: a useful tool for protein molecular dynamicists, applied to hydrogen bonds in the active site of elastase. *J. Mol. Graphics*, **7**, 240–242, 223–224.
- Takenaka, A. & Sasada, Y. (1980). Computer manipulation of crystal and molecular models. *J. Crystallogr. Soc. Jpn.* **22**, 214–225. [In Japanese.]
- Thomas, D. J. (1993). Toward more reliable printed stereo. *J. Mol. Graphics*, **11**, 15–22.
- Tsernoglou, D., Petsko, G. A., McQueen, J. E. & Hermans, J. (1977). Molecular graphics: application to the structure determination of a snake venom neurotoxin. *Science*, **197**, 1378–1381.
- Vedani, A. & Meyer, E. F. (1984). Structure–activity relationships of sulfonamide drugs and human carbonic anhydrase C: modelling of inhibitor molecules into receptor site of the enzyme with an interactive computer graphics display. *J. Pharm. Sci.* **73**, 352–358.
- Walsh, G. R. (1975). *Methods of optimization*. London: John Wiley.
- Warne, P. K., Go, N. & Scheraga, H. A. (1972). Refinement of X-ray data of proteins. I. Adjustment of atomic coordinates to conform to a specified geometry. *J. Comput. Phys.* **9**, 303–317.
- Williams, T. V. (1982). Thesis. University of North Carolina at Chapel Hill, NC, USA.
- Willoughby, T. V., Morimoto, C. N., Sparks, R. A. & Meyer, E. F. (1974). Mini-computer control of a stereo graphics display. *J. Appl. Cryst.* **7**, 430–434.
- Wipke, W. T. (1974). Computer assisted three-dimensional synthetic analysis. In *Computer representation and manipulation of chemical information*, edited by W. T. Wipke, S. R. Heller, R. J. Feldmann & E. Hyde, pp. 147–174. New York: John Wiley.
- Wipke, W. T., Braun, H., Smith, G., Choplin, F. & Sieber, W. (1977). SECS – simulation and evaluation of chemical synthesis: strategy and planning. *ACS Symp. Ser.* **61**, 97–125.
- Wipke, W. T. & Dyott, T. M. (1974). Simulation and evaluation of chemical synthesis. Computer representation and manipulation of stereochemistry. *J. Am. Chem. Soc.* **96**, 4825–4834.

3.4

- Arfken, G. (1970). *Mathematical methods for physicists*, 2nd ed. New York: Academic Press.
- Bertaut, E. F. (1952). L'énergie électrostatique de réseaux ioniques. *J. Phys. (Paris)*, **13**, 499–505.
- Bertaut, E. F. (1978). The equivalent charge concept and its application to the electrostatic energy of charges and multipoles. *J. Phys. (Paris)*, **39**, 1331–1348.
- Busing, W. R. (1981). WMIN, a computer program to model molecules and crystals in terms of potential energy functions. Oak Ridge National Laboratory Report ORNL-5747. Oak Ridge, Tennessee 37830, USA.
- Cummins, P. G., Dunmur, D. A., Munn, R. W. & Newham, R. J. (1976). Applications of the Ewald method. I. Calculation of multipole lattice sums. *Acta Cryst.* **A32**, 847–853.
- Davis, P. J. (1972). Gamma function and related functions. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, edited by M. Abramowitz & I. A. Stegun, pp. 260–262. London, New York: John Wiley. [Reprint, with corrections of 1964 Natl Bur. Stand. publication.]
- DeWette, F. W. & Schacher, G. E. (1964). Internal field in general dipole lattices. *Phys. Rev.* **137**, A78–A91.
- Evjen, H. M. (1932). The stability of certain heteropolar crystals. *Phys. Rev.* **39**, 675–694.
- Ewald, P. P. (1921). Die Berechnung optischer und elektrostatischer Gitterpotentiale. *Ann. Phys. (Leipzig)*, **64**, 253–287.

3.4 (cont.)

- Fortuin, C. M. (1977). *Note on the calculation of electrostatic lattice potentials. Physica (Utrecht)*, **86A**, 574–586.
- Glasser, M. L. & Zucker, I. J. (1980). *Lattice sums. Theor. Chem. Adv. Perspect.* **5**, 67–139.
- Hastings, C. Jr (1955). *Approximations for digital computers*. New Jersey: Princeton University Press.
- Madelung, E. (1918). *Das elektrische Feld in Systemen von regelmässig angeordneten Punktladungen. Phys. Z.* **19**, 524–532.
- Massidda, V. (1978). *Electrostatic energy in ionic crystals by the planewise summation method. Physica (Utrecht)*, **95B**, 317–334.
- Nijboer, B. R. A. & DeWette, F. W. (1957). *On the calculation of lattice sums. Physica (Utrecht)*, **23**, 309–321.
- Pietila, L.-O. & Rasmussen, K. (1984). *A program for calculation of crystal conformations of flexible molecules using convergence acceleration. J. Comput. Chem.* **5**, 252–260.
- Widder, D. V. (1961). *Advanced calculus*, 2nd ed. New York: Prentice-Hall.
- Williams, D. E. (1971). *Accelerated convergence of crystal lattice potential sums. Acta Cryst.* **A27**, 452–455.
- Williams, D. E. (1984). *PCK83, a crystal molecular packing analysis program*. Quantum Chemistry Program Exchange, Department of Chemistry, Indiana University, Bloomington, Indiana 47405, USA.
- Williams, D. E. (1989). *Accelerated convergence treatment of R^{-n} lattice sums. Crystallogr. Rev.* **2**, 3–23. Corrections: *Crystallogr. Rev.* **2**, 163–166.