

REFERENCES

References

3.1

- Busing, W. R. & Levy, H. A. (1964). *Effect of thermal motion on the estimation of bond lengths*. *Acta Cryst.* **17**, 142–146.
- Hamilton, W. C. (1964). *Statistics in physical science*. New York: Ronald Press.
- Johnson, C. K. (1970). *The effect of thermal motion on interatomic distances and angles*. In *Crystallographic computing*, edited by F. R. Ahmed, pp. 220–226. Copenhagen: Munksgaard.
- Johnson, C. K. (1980). *Thermal motion analysis*. In *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 14.01–14.19. Bangalore: Indian Academy of Sciences.
- Sands, D. E. (1966). *Transformations of variance–covariance tensors*. *Acta Cryst.* **21**, 868–872.
- Sands, D. E. (1977). *Correlation and covariance*. *J. Chem. Educ.* **54**, 90–94.
- Sands, D. E. (1982a). *Vectors and tensors in crystallography*. Reading: Addison Wesley. Reprinted (1995) Dover Publications.
- Sands, D. E. (1982b). *Molecular geometry*. In *Computational crystallography*, edited by D. Sayre, pp. 421–429. Oxford: Clarendon Press.
- Shmueli, U. (1974). *On the standard deviation of a dihedral angle*. *Acta Cryst.* **A30**, 848–849.
- Taylor, R. & Kennard, O. (1983). *The estimation of average molecular dimensions from crystallographic data*. *Acta Cryst.* **B39**, 517–525.
- Taylor, R. & Kennard, O. (1985). *The estimation of average molecular dimensions. 2. Hypothesis testing with weighted and unweighted means*. *Acta Cryst.* **A41**, 85–89.
- Waser, J. (1973). *Dyadics and the variances and covariances of molecular parameters, including those of best planes*. *Acta Cryst.* **A29**, 621–631.

3.2

- Arley, N. & Buch, K. R. (1950). *Introduction to the theory of probability and statistics*. New York: John Wiley. London: Chapman & Hall.
- Clews, C. J. B. & Cochran, W. (1949). *The structures of pyrimidines and purines. III. An X-ray investigation of hydrogen bonding in aminopyrimidines*. *Acta Cryst.* **2**, 46–57.
- Deming, W. E. (1943). *Statistical adjustment of data*. New York: John Wiley. [First edition 1938.]
- Hamilton, W. C. (1961). *On the least-squares plane through a set of points*. *Acta Cryst.* **14**, 185–189.
- Hamilton, W. C. (1964). *Statistics in physical science*. New York: Ronald Press.
- Ito, T. (1981a). *Least-squares refinement of the best-plane parameters*. *Acta Cryst.* **A37**, 621–624.
- Ito, T. (1981b). *On the least-squares plane through a group of atoms*. *Sci. Pap. Inst. Phys. Chem. Res. Saitama*, **75**, 55–58.
- Ito, T. (1982). *On the estimated standard deviation of the atom-to-plane distance*. *Acta Cryst.* **A38**, 869–870.
- Kalantar, A. H. (1987). *Slopes of straight lines when neither axis is error-free*. *J. Chem. Educ.* **64**, 28–29.
- Lybanon, M. (1984). *A better least-squares method when both variables have uncertainties*. *Am. J. Phys.* **52**, 22–26.
- Robertson, J. M. (1948). *Bond-length variations in aromatic systems*. *Acta Cryst.* **1**, 101–109.
- Schomaker, V. & Marsh, R. E. (1983). *On evaluating the standard deviation of U_{eq}* . *Acta Cryst.* **A39**, 819–820.
- 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.
- Shmueli, U. (1981). *On the statistics of atomic deviations from the 'best' molecular plane*. *Acta Cryst.* **A37**, 249–251.

- Waser, J. (1973). *Dyadics and variances and covariances of molecular parameters, including those of best planes*. *Acta Cryst.* **A29**, 621–631.
- Waser, J., Marsh, R. E. & Cordes, A. W. (1973). *Variances and covariances for best-plane parameters including dihedral angles*. *Acta Cryst.* **B29**, 2703–2708.
- Whittaker, E. T. & Robinson, G. (1929). *The calculus of observations*. London: Blackie.

3.3

- 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.
- Abi-Ezzi, S. S. & Bunshaft, A. J. (1986). *An implementer's view of PHIGS*. *IEEE Comput. Graphics Appl.* Vol. 6, Part 2.
- Aharonov, Y., Farach, H. A. & Poole, C. P. (1977). *Non-linear vector product to describe rotations*. *Am. J. Phys.* **45**, 451–454.
- Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A., Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters, B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. & Watson, D. G. (1979). *The Cambridge Crystallographic Data Centre: computer-based search, retrieval, analysis and display of information*. *Acta Cryst.* **B35**, 2331–2339.
- Allinger, N. L. (1976). *Calculation of molecular structure and energy by force field methods*. *Adv. Phys. Org. Chem.* **13**, 1–82.
- Altona, C. & Sundaralingam, M. (1972). *Conformational analysis of the sugar ring in nucleosides and nucleotides. A new description using the concept of pseudorotation*. *J. Am. Chem. Soc.* **94**(23), 8205–8212.
- American National Standards Institute, *American National Standard for Information Processing Systems – Computer Graphics – Graphical Kernel System (GKS) Functional Description* (1985). ISO 7942, ISO Central Secretariat, Geneva, Switzerland.
- American National Standards Institute, *American National Standard for Information Processing Systems – Computer Graphics – Programmer's Hierarchical Graphics System (PHIGS) Functional Description, Archive File Format, Clear-Text Encoding of Archive File* (1988). ANSI X3.144-1988. ANSI, New York, USA.
- Anderson, S. (1984). *Graphical representation of molecules and substructure-search queries in MACCS*. *J. Mol. Graphics*, **2**, 83–90.
- Arnold, D. B. & Bono, P. R. (1988). *CGM and CGI: metafile and interface standards for computer graphics*. Berlin: Springer-Verlag.
- Barry, C. D. & North, A. C. T. (1971). *The use of a computer-controlled display system in the study of molecular conformations*. *Cold Spring Harbour Symp. Quant. Biol.* **36**, 577–584.
- Bash, P. A., Pattabiraman, N., Huang, C., Ferrin, T. E. & Langridge, R. (1983). *Van der Waals surfaces in molecular modelling: implementation with real-time computer graphics*. *Science*, **222**, 1325–1327.
- Beddell, C. J. (1970). *An X-ray crystallographic study of the activity of lysozyme*. DPhil thesis, University of Oxford, England.
- Bernstein, F. C., Koetzle, T. F., Williams, G. J. B., Meyer, E. F., Brice, M. D., Rodgers, J. R., Kennard, O., Shimanouchi, T. & Tasumi, M. (1977). *The Protein Data Bank: a computer-based archival file for macromolecular structures*. *J. Mol. Biol.* **112**, 535–542.
- 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.
- Boyd, D. B. & Lipkowitz, K. B. (1982). *Molecular mechanics, the method and its underlying philosophy*. *J. Chem. Educ.* **59**, 269–274.