

1. GENERAL RELATIONSHIPS AND TECHNIQUES

References

- Altermatt, U. D. & Brown, I. D. (1987). *A real-space computer-based symmetry algebra*. *Acta Cryst.* **A43**, 125–130.
- Aroyo, M. I., Kirov, A., Capillas, C., Perez-Mato, J. M. & Wondratschek, H. (2006). *Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups*. *Acta Cryst.* **A62**, 115–128.
- Authier, A. (1981). *The Reciprocal Lattice*. Edited by the IUCr Commission on Crystallographic Teaching. Cardiff: University College Cardiff Press.
- Bertaut, E. F. (1964). *On the symmetry of phases in the reciprocal lattice: a simple method*. *Acta Cryst.* **17**, 778–779.
- Bienenstock, A. & Ewald, P. P. (1962). *Symmetry of Fourier space*. *Acta Cryst.* **15**, 1253–1261.
- Bourne, P. E., Berman, H. M., McMahon, B., Watenpugh, K. D., Westbrook, J. D. & Fitzgerald, P. M. D. (1997). *mmCIF: macromolecular crystallographic information file*. *Methods Enzymol.* **277**, 571–590.
- Bragg, L. (1966). *The Crystalline State*, Vol. I, *A General Survey*. London: Bell.
- Buerger, M. J. (1942). *X-ray Crystallography*. New York: John Wiley.
- Buerger, M. J. (1949). *Crystallographic symmetry in reciprocal space*. *Proc. Natl Acad. Sci. USA*, **35**, 198–201.
- Buerger, M. J. (1960). *Crystal Structure Analysis*. New York: John Wiley.
- Computers in the New Laboratory – a Nature Survey* (1981). *Nature (London)*, **290**, 193–200.
- Dowty, E. (2000). *ATOMS: a program for the display of atomic structures*. Commercial software available from <http://www.shapesoftware.com>.
- Ewald, P. P. (1921). *Das 'reziproke Gitter' in der Strukturtheorie*. *Z. Kristallogr. Teil A*, **56**, 129–156.
- Grosse-Kunstleve, R. W. (1995). *SGINFO: a comprehensive collection of ANSI C routines for the handling of space-group symmetry*. Freely available from <http://cci.lbl.gov/sginfo/>.
- Grosse-Kunstleve, R. W. (1999). *Algorithms for deriving crystallographic space-group information*. *Acta Cryst.* **A55**, 383–395.
- Hall, S. R. (1981a). *Space-group notation with an explicit origin*. *Acta Cryst.* **A37**, 517–525.
- Hall, S. R. (1981b). *Space-group notation with an explicit origin: erratum*. *Acta Cryst.* **A37**, 921.
- Hall, S. R. (1997). *LoopX: a script used to loop Xtal*. Copyright University of Western Australia. Freely available from <http://www.crystal.uwa.edu.au/~syd/symmetry/>.
- Hall, S. R., du Boulay, D. J. & Olthof-Hazekamp, R. (2000). *Xtal: a system of crystallographic programs*. Copyright University of Western Australia. Freely available from <http://xtal.crystal.uwa.edu.au>.
- Hearn, A. C. (1973). *REDUCE 2.0 user's manual*. University of Utah, Salt Lake City, Utah, USA.
- Hovmöller, S. (1992). *CRISP: crystallographic image processing on a personal computer*. *Ultramicroscopy*, **41**, 121–135.
- International Tables for Crystallography* (1983). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn. Dordrecht: Reidel.
- International Tables for Crystallography* (1987). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 2nd ed. Dordrecht: Reidel.
- International Tables for Crystallography* (1992). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 3rd ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (1995). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 4th ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (2002). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (2005). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 5th ed., corrected reprint. Heidelberg: Springer.
- International Tables for Crystallography* (1993). Vol. B, *Reciprocal Space*, edited by U. Shmueli, 1st ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for X-ray Crystallography* (1952). Vol. I, *Symmetry Groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press.
- International Tables for X-ray Crystallography* (1965). Vol. I, *Symmetry Groups*, edited by N. F. M. Henry & K. Lonsdale, 2nd ed. Birmingham: Kynoch Press.
- Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). 1. Band. Edited by C. Hermann. Berlin: Borntraeger.
- Koch, E. & Fischer, W. (2005). In *International Tables for Crystallography*, Vol. A, Part 11, *Symmetry operations*. Heidelberg: Springer.
- Larine, M., Klimkovich, S., Farrants, G., Hovmöller, S. & Xiaodong, Z. (1995). *Space Group Explorer: a computer program for obtaining extensive information about any of the 230 space groups*. Freely available from <http://www.calidris-em.com/>.
- Lipson, H. & Cochran, W. (1966). *The Crystalline State*, Vol. II, *The Determination of Crystal Structures*. London: Bell.
- Lipson, H. & Taylor, C. A. (1958). *Fourier Transforms and X-ray Diffraction*. London: Bell.
- Seitz, F. (1935). *A matrix-algebraic development of crystallographic groups. III*. *Z. Kristallogr.* **90**, 289–313.
- Shmueli, U. (1984). *Space-group algorithms. I. The space group and its symmetry elements*. *Acta Cryst.* **A40**, 559–567.
- Waser, J. (1955). *Symmetry relations between structure factors*. *Acta Cryst.* **8**, 595.
- Wells, M. (1965). *Computational aspects of space-group symmetry*. *Acta Cryst.* **19**, 173–179.
- Zachariasen, W. H. (1945). *Theory of X-ray Diffraction in Crystals*. New York: John Wiley.