

References

- Aroyo, M. I. & Perez-Mato, J. M. (1998). *Symmetry-mode analysis of displacive phase transitions using International Tables for Crystallography*. *Acta Cryst.* **A54**, 19–30.
- Ascher, E. (1966). *Role of particular maximal subgroups in continuous phase transitions*. *Phys. Lett.* **20**, 352–354.
- Ascher, E. (1967). *Symmetry changes in continuous transitions. A simplified theory applied to V_3Si* . *Chem. Phys. Lett.* **1**, 69–72.
- Ascher, E. (1968). *Lattices of equi-translation subgroups of the space groups*. Geneva: Battelle Institute.
- Ascher, E., Gramlich, V. & Wondratschek, H. (1969). *Corrections to the sections 'Untergruppen' of the space groups in Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935) Vol. I*. *Acta Cryst.* **B25**, 2154–2156.
- Astbury, W. T. & Yardley, K. (1924). *Tabulated data for the examination of the 230 space-groups by homogeneous X-rays*. *Philos. Trans. R. Soc. London*, **224**, 221–257.
- Barlow, W. (1894). *Über die geometrischen Eigenschaften homogener starrer Strukturen*. *Z. Kristallogr. Mineral.* **23**, 1–63.
- Bärnighausen, H. (1975). *Group-subgroup relations between space groups as an ordering principle in crystal chemistry: the "family tree" of perovskite-like structures*. *Acta Cryst.* **A31**, part S3, S3, 01.1-9.
- Bärnighausen, H. (1980). *Group-subgroup relations between space groups: a useful tool in crystal chemistry*. *MATCH Comm. Math. Chem.* **9**, 139–175.
- Baur, W. H. (1994). *Rutile type derivatives*. *Z. Kristallogr.* **209**, 143–150.
- Baur, W. H. & Kassner, D. (1992). *The perils of Cc: comparing the frequencies of falsely assigned space groups with their general population*. *Acta Cryst.* **B48**, 356–369.
- Baur, W. H. & McLarnan, T. J. (1982). *Observed wurtzite derivatives and related tetrahedral structures*. *J. Solid State Chem.* **42**, 300–321.
- Bertaut, E. F. & Billiet, Y. (1979). *On equivalent subgroups and supergroups of the space groups*. *Acta Cryst.* **A35**, 733–745.
- Billiet, Y. (1973). *Les sous-groupes isosymboliques des groupes spatiaux*. *Bull. Soc. Fr. Minéral. Cristallogr.* **96**, 327–334.
- Billiet, Y. (1980). *The subgroups of finite index of the space groups: determination via conventional coordinate systems*. *MATCH Comm. Math. Chem.* **9**, 127–190.
- Billiet, Y. & Bertaut, E. F. (2002). *Isomorphic subgroups of space groups*. *International Tables for Crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 13. Dordrecht: Kluwer Academic Publishers.
- Billiet, Y. & Rolley Le Coz, M. (1980). *Le groupe P1 et ses sous-groupes. II. Tables des sous-groupes*. *Acta Cryst.* **A36**, 242–248.
- Billiet, Y. & Sayari, A. (1984). *Les sous-groupes isomorphes d'un group d'espace de type p4. I. Détermination univoque*. *Acta Cryst.* **A40**, 624–631.
- Billiet, Y., Sayari, A. & Zarrouk, H. (1978). *L'association des familles de Wyckoff dans les changements de repère conventionnel des groupes spatiaux et les passages aux sous-groupes spatiaux*. *Acta Cryst.* **A34**, 811–819.
- Biltz, W. (1934). *Raumchemie der festen Stoffe*. Leipzig: L. Voss.
- Birman, J. L. (1966a). *Full group and subgroup methods in crystal physics*. *Phys. Rev.* **150**, 771–782.
- Birman, J. L. (1966b). *Simplified theory of symmetry change in second-order phase transitions: application to V_3Si* . *Phys. Rev. Lett.* **17**, 1216–1219.
- Bock, O. & Müller, U. (2002a). *Symmetrieverwandtschaften bei Varianten des Perowskit-Typs*. *Acta Cryst.* **B58**, 594–606.
- Bock, O. & Müller, U. (2002b). *Symmetrieverwandtschaften bei Varianten des ReO_3 -Typs*. *Z. Anorg. Allg. Chem.* **628**, 987–992.
- Boyle, L. L. & Lawrenson, J. E. (1973). *The origin dependence of the Wyckoff site description of a crystal structure*. *Acta Cryst.* **A29**, 353–357.
- Bravais, A. (1850). *Mémoire sur les systèmes formés par les points distribués régulièrement sur un plan ou dans l'espace*. *J. Ecole Polytech.* **19**, 1–128. (English: Memoir 1, Crystallographic Society of America, 1949.)
- Brown, H., Bülow, R., Neubüser, J., Wondratschek, H. & Zassenhaus, H. (1978). *Crystallographic groups of four-dimensional space*. New York: John Wiley & Sons.
- Buerger, M. J. (1947). *Derivative crystal structures*. *J. Chem. Phys.* **15**, 1–16.
- Buerger, M. J. (1951). *Phase transformations in solids*, ch. 6. New York: Wiley.
- Burckhardt, J. J. (1988). *Die Symmetrie der Kristalle*. Basel: Birkhäuser.
- Byström, A., Hök, B. & Mason, B. (1941). *The crystal structure of zinc metaantimonate and similar compounds*. *Ark. Kemi Mineral. Geol.* **15B**, 1–8.
- Chapuis, G. C. (1992). *Symmetry relationships between crystal structures and their practical applications. Modern perspectives in inorganic chemistry*, edited by E. Parthé, pp. 1–16. Dordrecht: Kluwer Academic Publishers.
- Cracknell, A. P. (1975). *Group theory in solid state physics*. New York: Taylor and Francis Ltd. and Pergamon.
- Deonarine, S. & Birman, J. L. (1983). *Group-subgroup phase transitions, Hermann's space group decomposition theorem, and chain subduction criterion in crystals*. *Phys. Rev. B*, **27**, 4261–4273.
- Eick, B., Gähler, F. & Nickel, W. (1997). *Computing maximal subgroups and Wyckoff positions of space groups*. *Acta Cryst.* **A53**, 467–474.
- Eick, B., Gähler, F. & Nickel, W. (2001). *The 'Cryst' Package*. Version 4.1. <http://www.itap.physik.uni-stuttgart.de/~gaeler/gap/packages.html>.
- Fedorov, E. (1891). *Symmetry of regular systems and figures*. *Zap. Mineral. Obshch.* (2), **28**, 1–46. (In Russian.) (English: *Symmetry of crystals*, American Crystallographic Association, 1971.)
- Finken, H., Neubüser, J. & Plesken, W. (1980). *Space groups and groups of prime power order II*. *Arch. Math.* **35**, 203–209.
- Fischer, W. & Koch, E. (1983). *On the equivalence of point configurations due to Euclidean normalizers (Cheshire groups) of space groups*. *Acta Cryst.* **A39**, 907–915.
- Flack, H. D., Wondratschek, H., Hahn, Th. & Abrahams, S. C. (2000). *Symmetry elements in space groups and point groups. Addenda to two IUCr reports on the nomenclature of symmetry*. *Acta Cryst.* **A56**, 96–98.
- Goldschmidt, V. M. (1926). *Untersuchungen über den Bau und Eigenschaften von Kristallen*. *Skr. Nor. Vidensk. Akad. Oslo Mat.-Nat. Kl.* 1926 No. 2 and 1927 No. 8.
- Haag, F. (1887). *Die regulären Kristallkörper. Programm des Königlichen Gymnasiums in Rottweil zum Schlusse des Schuljahres 1886–1887*.
- Hahn, Th. & Wondratschek, H. (1994). *Symmetry of crystals. Introduction to International Tables for Crystallography*, Vol. A. Sofia: Heron Press.
- Heesch, H. (1930). *Zur systematischen Strukturtheorie. II*. *Z. Kristallogr.* **72**, 177–201.
- Hermann, C. (1929). *Zur systematischen Strukturtheorie. IV. Untergruppen*. *Z. Kristallogr.* **69**, 533–555.
- International Tables for Crystallography* (1983). Vol. A, *Space-group symmetry*, edited by Th. Hahn, 1st ed. Dordrecht: Kluwer Academic Publishers. (Abbreviated *IT A*.)
- International Tables for Crystallography* (2002). Vol. A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers. (Abbreviated *IT A*.)
- International Tables for Crystallography* (2002). Vol. E, *Subperiodic groups*, edited by V. Kopský & D. B. Litvin. Dordrecht: Kluwer Academic Publishers.
- International Tables for X-ray Crystallography* (1952, 1965, 1969). Vol. I, *Symmetry groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press.
- Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). 1. Bd. Edited by C. Hermann. Berlin: Borntraeger. (In German, English and French.) (Abbreviated *IT 35*.)
- Izumov, Y. A. & Syromyatnikov, V. N. (1990). *Phase transitions and crystal symmetry*. Dordrecht: Kluwer Academic Publishers.
- Janovec, V. (1976). *A symmetry approach to domain structures*. *Ferroelectrics*, **12**, 43–53.

REFERENCES

- Janovec, V. & Přívratská, J. (2003). *Domain structures. International tables for crystallography*, Vol. D, edited by A. Authier, *Physical properties of crystals*, ch. 3.4. Dordrecht: Kluwer Academic Publishers.
- Koch, E. (1984). *The implications of normalizers on group-subgroup relations between space groups*. *Acta Cryst.* **A40**, 593–600.
- Koch, E. & Fischer, W. (1975). *Automorphismengruppen von Raumgruppen und die Zuordnung von Punktlagen zu Konfigurationslagen*. *Acta Cryst.* **A31**, 88–95.
- Koch, E. & Fischer, W. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion*. *Acta Cryst.* **A41**, 421–426.
- Koch, E., Fischer, W. & Müller, U. (2002). *Normalizers of space groups and their use in crystallography. International tables for crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 15. Dordrecht: Kluwer Academic Publishers.
- Kroumova, E., Aroyo, M. I. & Pérez-Mato, J. M. (2002). *Prediction of new displacive ferroelectrics through systematic pseudosymmetry search. Results for materials with Pba2 and Pmc2₁ symmetry*. *Acta Cryst.* **B58**, 921–933.
- Kroumova, E., Perez-Mato, J. M. & Aroyo, M. I. (1998). *WYCKSPLIT. Computer program for the determination of the relations of Wyckoff positions for a group-subgroup pair*. *J. Appl. Cryst.* **31**, 646. Accessible at: <http://www.cryst.ehu.es/cryst/wpsplit.html>.
- Lampart, L. (1994). *A document preparation system*. 2nd ed. Reading, MA: Addison-Wesley.
- Landau, L. D. (1937). *Theory of phase transitions*. *Zh. Eksp. Teoret. Fiz.* **7**, pp. 19–32, 627–636. (In Russian.) (German: *Phys. Z. Sowjetunion*, **11**, pp. 20–47, 545–555.)
- Landau, L. D. & Lifshitz, E. M. (1980). *Statistical physics*, Part 1, 3rd ed., pp. 459–471. London: Pergamon. (Russian: *Statisticheskaya Fizika*, chast 1. Moskva: Nauka, 1976; German: *Lehrbuch der theoretischen Physik*, 6. Aufl., Bd. 5, Teil 1, S. 436–447. Berlin: Akademie-Verlag, 1984.)
- Lawrenson, J. E. (1972). *Theoretical studies in crystallography*. Dissertation, University of Kent at Canterbury.
- Ledermann, W. (1976). *Introduction to group theory*. London: Longman. (German: *Einführung in die Gruppentheorie*, Braunschweig: Vieweg, 1977.)
- Levanyuk, A. P. & Sannikov, D. G. (1971). *Phenomenological theory of dielectric anomalies in ferroelectric materials with several phase transitions at temperatures close together*. *Sov. Phys. JETP*, **11**, 600–604.
- McLarnan, T. J. (1981a). *Mathematical tools for counting polytypes*. *Z. Kristallogr.* **155**, 227–245.
- McLarnan, T. J. (1981b). *The numbers of polytypes in close packings and related structures*. *Z. Kristallogr.* **155**, 269–291.
- McLarnan, T. J. (1981c). *The combinatorics of cation-deficient close-packed structures*. *J. Solid State Chem.* **26**, 235–244.
- Marsh, R. E., Kapon, M., Hu, S. & Herbstein, F. H. (2002). *Some 60 new space-group corrections*. *Acta Cryst.* **B58**, 62–77.
- Megaw, H. D. (1973). *Crystal structures: A working approach*. Philadelphia: Saunders.
- Meyer, A. (1981). *Symmetriebeziehungen zwischen Kristallstrukturen des Formeltyps AX₂, ABX₄ und AB₂X₆ sowie deren Ordnungs- und Leerstellenvarianten*. Dissertation, Universität Karlsruhe.
- Müller, U. (1978). *Strukturmöglichkeiten für Pentahalogenide mit Doppeloktaeder-Molekülen (MX₅)₂ bei dichtester Packung der Halogenatome*. *Acta Cryst.* **A34**, 256–267.
- Müller, U. (1980). *Strukturverwandtschaften unter den EPh₄⁺-Salzen*. *Acta Cryst.* **B36**, 1075–1081.
- Müller, U. (1981). *MX₄-Ketten aus kantenverknüpften Oktaedern: mögliche Kettenkonfigurationen und mögliche Kristallstrukturen*. *Acta Cryst.* **B37**, 532–545.
- Müller, U. (1986). *MX₅-Ketten aus eckenverknüpften Oktaedern. Mögliche Kettenkonfigurationen und mögliche Kristallstrukturen bei dichtester Packung der X-Atome*. *Acta Cryst.* **B42**, 557–564.
- Müller, U. (1992). *Berechnung der Anzahl möglicher Strukturtypen für Verbindungen mit dichtest gepackter Anionenteilstruktur. I. Das Rechenverfahren*. *Acta Cryst.* **B48**, 172–178.
- Müller, U. (1993). *Inorganic structural chemistry*, pp. 233–246. Chichester, New York: Wiley. (German: *Anorganische Strukturchemie*, 3. Aufl., 1996, S. 296–309. Stuttgart: Teubner.)
- Müller, U. (1998). *Strukturverwandtschaften zwischen trigonalen Verbindungen mit hexagonal-dichtester Anionenteilstruktur und besetzten Oktaederlücken*. *Z. Anorg. Allg. Chem.* **624**, 529–532.
- Müller, U. (2002). *Kristallpackungen mit linear koordinierten Atomen*. *Z. Anorg. Allg. Chem.* **628**, 1269–1278.
- Müller, U. (2003). *Die Zahl der Substitutions- und Leerstellenvarianten des NaCl-Typs bei verdoppelter Elementarzelle (a, b, 2c)*. *Z. Anorg. Allg. Chem.* **629**, 487–492.
- Müller, U. & Brelle, A. (1995). *Über isomorphe Untergruppen von Raumgruppen der Kristallklassen 4, $\bar{4}$, 4/m, 3, $\bar{3}$, 6, $\bar{6}$ und 6/m*. *Acta Cryst.* **A51**, 300–304.
- Nespolo, M. & Ferraris, G. (2004). *Applied geminography – symmetry analysis of twinned crystals and definition of twinning by reticular polyhohedry*. *Acta Cryst.* **A60**, 89–95.
- Neubüser, J. & Wondratschek, H. (1966). *Untergruppen der Raumgruppen*. *Krist. Tech.* **1**, 529–543.
- Niggli, P. (1919). *Geometrische Kristallographie des Diskontinuums*. Leipzig: Gebrüder Borntraeger. Reprint (1973) Wiesbaden: Dr M. Saendig.
- Nolze, G. (1996). *POWDER CELL. Computer program for the calculation of X-ray powder diagrams*. Bundesanstalt für Materialforschung, Berlin.
- Pauling, L. (1928). *The coordination theory of the structure of ionic compounds – Probleme der modernen Physik (Sommerfeld-Festschrift)*, p. 11. Leipzig: S. Hirzel.
- Pauling, L. (1929). *The principles determining the structures of complex ionic crystals*. *J. Am. Chem. Soc.* **51**, 1010–1026.
- Plesken, W. & Schulz, T. (2000). *Counting crystallographic groups in low dimensions*. *Exp. Math.* **9**, 407–411.
- Pöttgen, R. & Hoffmann, R.-D. (2001). *AlB₂-related intermetallic compounds – a comprehensive view based on a group-subgroup scheme*. *Z. Kristallogr.* **216**, 127–145.
- Salje, E. K. H. (1990). *Phase transitions in ferroelastic and co-elastic crystals*. Cambridge University Press.
- Sayari, A. (1976). *Contribution à l'étude des groupes d'espace bidimensionnels, dérivation des sous-groupes et des surstructures*. Thesis, University of Tunis, Tunisia.
- Sayari, A. & Billiet, Y. (1977). *Subgroups and changes of standard settings of triclinic and monoclinic space groups*. *Acta Cryst.* **A33**, 985–986.
- Schoenflies, A. M. (1891). *Krystallsysteme und Krystallstruktur*. Leipzig: Teubner. Reprint 1984: Springer.
- Sohncke, L. (1879). *Entwicklung einer Theorie der Krystallstruktur*. Leipzig: Teubner.
- Sowa, H. (2001). *On the transition from the wurtzite to the NaCl type*. *Acta Cryst.* **A57**, 176–182.
- Stokes, H. T. & Hatch, D. M. (1988). *Isotropy subgroups of the 230 crystallographic space groups*. Singapore: World Scientific.
- Stokes, H. T. & Hatch, D. M. (2002). *Procedure for obtaining microscopic mechanisms of reconstructive phase transitions in crystalline solids*. *Phys. Rev. B*, **65**, 144114–144123.
- Strukturbericht 1913–1928* (1931). Edited by P. P. Ewald & C. Hermann. Leipzig: Akademische Verlagsgesellschaft. Continued by *Structure Reports*.
- Tendeloo, G. van & Amelinckx, S. (1974). *Group-theoretical considerations concerning domain formation in ordered alloys*. *Acta Cryst.* **A30**, 431–440.
- The GAP Group (2002). *GAP – Groups, Algorithms and Programming*. Version 4.3. <http://www.gap-system.org>.
- Tolédano, J.-C., Janovec, V., Kopský, V., Scott, J.-F. & Boček, P. (2003). *Structural phase transitions. International tables for crystallography*, Vol. D, *Physical properties of crystals*, edited by A. Authier, ch. 3.1. Dordrecht: Kluwer Academic Publishers.
- Tolédano, J.-C. & Tolédano, P. (1987). *The Landau theory of phase transitions*. Singapore: World Scientific.
- Wiener, C. (1863). *Grundzüge der Weltordnung. I. Atomlehre*, p. 82. Leipzig: Heidelberg.
- Wondratschek, H. (1976). *Extraordinary orbits of space groups. Theoretical considerations*. *Z. Kristallogr.* **143**, 460–470.
- Wondratschek, H. (1980). *Crystallographic orbits, lattice complexes, and orbit types*. *MATCH Comm. Math. Chem.* **9**, 121–125.

REFERENCES

- Wondratschek, H. (1993). *Splitting of Wyckoff positions (orbits)*. *Mineral. Petrol.* **48**, 87–96.
- Wondratschek, H. (2002). *Special topics on space groups*. *International tables for crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 8. Dordrecht: Kluwer Academic Publishers.
- Wondratschek, H. & Aroyo, M. I. (2001). *The application of Hermann's group \mathcal{M} in group–subgroup relations between space groups*. *Acta Cryst.* **A57**, 311–320.
- Wondratschek, H. & Jeitschko, W. (1976). *Twin domains and antiphase domains*. *Acta Cryst.* **A32**, 664–666.
- Wondratschek, H., Müller, U., Aroyo, M. I. & Sens, I. (1995). *Splitting of Wyckoff positions (orbits)*. II. *Group–subgroup chains of index 6*. *Z. Kristallogr.* **210**, 567–573.
- Wyckoff, R. W. G. (1922). *The analytical expression of the results of the theory of space groups*. Washington: Carnegie Institution.
- Wyckoff, R. W. G. (1965). *Crystal structures*, 2nd ed., Vol. 3, pp. 361–362. New York: Interscience.