

## 2.1. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

file, which essentially contains routines, called macros, that control the typographical layout of the data. Thus, the main principle of L<sup>A</sup>T<sub>E</sub>X – that of keeping content and presentation separate – was followed as closely as possible.

The final typesetting of all the plane- and space-group tables was done by running a single computer job. References in the tables from one page to another are automatically computed. The result is a PostScript file which can be fed to a laser printer or other printing or typesetting equipment. It can also be easily converted to a PDF file. It is also possible to generate the output for just one group, as accessed in the online edition, or a series of groups.

The different types of data in the L<sup>A</sup>T<sub>E</sub>X files were either keyed by hand or computer generated, and were additionally checked by specially written programs. The preparation of the data files can be summarized as follows:

*Headline, Origin, Asymmetric unit:* hand keyed.

*Symmetry operations:* partly created by a computer program. The algorithm for the derivation of symmetry operations from their matrix representation is similar to that described in the literature (*cf.* Section 1.2.2; see also Hahn & Wondratschek, 1994). The data were additionally checked by automatic comparison with the output of the computer program *SPACER* (Stróż, 1997).

*Generators:* transferred automatically from the data for Volume A1 of *International Tables for Crystallography* (2010), hereafter referred to as *IT A1*.

*General positions:* created by a program. The algorithm uses the well known generating process for space groups based on their solvability property (*cf.* Section 1.4.3).

*Special positions:* The first representatives of the Wyckoff positions were typed in by hand. The Wyckoff letters are assigned automatically by the T<sub>E</sub>X macros according to the order of appearance of the special positions in the data file. The multiplicity of the position, the oriented site-symmetry symbol and the rest of the representatives of the Wyckoff position were generated by a program. Again, the data were compared with the results of the program *SPACER*.

*Reflection conditions:* hand keyed. A program for automatic checking of the special-position coordinates and the corresponding reflection conditions with  $h, k, l$  ranging from  $-20$  to  $20$  was developed.

*Symmetry of special projections:* hand keyed.

*Maximal subgroups and minimal supergroups:* this information appeared in the fifth revised edition of Volume A, as in the previous editions. Most of the data were automatically transferred from the data files used for the production of *IT A1*. The macros for typesetting these data were re-implemented to obtain exactly the layout of Volume A. For the current edition these data have been omitted by redefining the macros to ignore the content, which is still present in the data files.

The symmetry-element diagrams were scanned and processed in the IUCr Editorial Office in Chester.

In the first edition of *IT A* published in 1983, the general-position diagrams of the cubic groups presented in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* were replaced by small stereodiagrams. At that time, such stereodiagrams were probably the easiest way to allow three-dimensional visualization, and the same stereodiagrams were reproduced in the following editions. However, the sizes of the stereodiagrams were limited by the page size, so they were very small, and they also lacked any indication of general-position ‘enantiomorph’ points. The situation has changed a lot

since then and three-dimensional visualization of the general positions is easily achieved with structure-drawing programs. Therefore, in this sixth edition, new general-position diagrams of the cubic groups, which are similar to those of the non-cubic groups, were created with a focus on better two-dimensional representation in print.

The new diagrams were created by K. Momma using the computer program *VESTA* (Momma & Izumi, 2011), which was extended for this purpose. The diagrams that were generated were carefully checked by comparing them with the original diagrams in the 1935 edition. The coordinates of general positions are slightly different from those used in the original diagrams and were chosen so that the general positions overlap as little as possible in the two-dimensional orthogonal projection of the diagrams. The coordinates of general positions used are:

- (i) 0.0375, 0.1125, 0.098 for space-group Nos. 198, 199, 205, 206, 212, 213, 214, 220 and 230;
- (ii) 0.065, 0.12, 0.048 for the second diagrams of space-group Nos. 212, 214 and 230;
- (iii) 0.435, 0.38, 0.452 for the second diagram of space-group No. 213;
- (iv) 0.31, 0.095, 0.21 for the second diagram of space-group No. 220; and
- (v) 0.048 $x$ , 0.12 $y$ , 0.089 $z$  for the remaining space groups, where  $x, y, z$  is the first coordinate triplet of the highest symmetry Wyckoff position of the space group.

In addition, three-dimensional-style tilted general-position diagrams were created by *VESTA* for each of the ten space groups of the  $m\bar{3}m$  crystal class. These diagrams can be reproduced and visualized in three dimensions using *VESTA*. They were provided in the form of Portable Network Graphics (PNG) raster images and were included in the page layout of the space-group tables with some scaling and cropping.

The preparation of the plane- and space-group tables was carried out on various computer platforms in Sofia, Bilbao, Karlsruhe, Tsukuba and Chester. The development of the computer programs and the layout macros in the L<sup>A</sup>T<sub>E</sub>X package file, and the preparation of the diagrams were done in parallel by different members of the team, which included Asen Kirov (Sofia), Eli Kroumova (Bilbao), Koichi Momma, Preslav Konstantinov and Mois Aroyo, and staff at the Editorial Office in Chester.

## References

- 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 Ser. A*, **224**, 221–257.
- Belov, N. V., Zagal'skaja, Ju. G., Litvinskaja, G. P. & Egorov-Tismenko, Ju. K. (1980). *Atlas of the Space Groups of the Cubic System*. Moscow: Nauka. (In Russian.)
- Biedl, A. W. (1966). *The projection of a crystal structure*. *Z. Kristallogr.* **123**, 21–26.
- Buerger, M. J. (1949). *Fourier summations for symmetrical crystals*. *Am. Mineral.* **34**, 771–788.
- Buerger, M. J. (1956). *Elementary Crystallography*. New York: Wiley.
- Buerger, M. J. (1960). *Crystal-Structure Analysis*, ch. 17. New York: Wiley.
- Buerger, M. J. (1965). *The geometry of projections*. *Tschermaks Mineral. Petrogr. Mitt.* **10**, 595–607.
- Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *The non-characteristic orbits of the space groups*. *Z. Kristallogr.*, Supplement Issue No. 1.
- Fedorov, E. S. (1895). *Theorie der Kristallstruktur. Einleitung. Regelmässige Punktsysteme (mit übersichtlicher graphischer Darstellung)*. *Z. Kristallogr.* **24**, 209–252, Tafel V, VI. [English translation by D. & K.

## 2. THE SPACE-GROUP TABLES

- Harker (1971). *Symmetry of Crystals*, esp. pp. 206–213. Am. Crystallogr. Assoc., ACA Monograph No. 7.]
- Fischer, K. F. & Knof, W. E. (1987). *Space groups for imaginary Patterson and for difference Patterson functions used in the lambda technique*. *Z. Kristallogr.* **180**, 237–242.
- Fischer, W., Burzlaff, H., Hellner, E. & Donnay, J. D. H. (1973). *Space Groups and Lattice Complexes*. NBS Monograph No. 134. Washington, DC: National Bureau of Standards.
- Flack, H. D. (2015). *Patterson functions*. *Z. Kristallogr.* **230**, 743–748.
- 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.
- Fokkema, D. S. (1983). *Computer production of Volume A. In International Tables for Crystallography, Vol. A, Space-Group Symmetry*, 1st ed., edited by Th. Hahn. Dordrecht: D. Reidel Publishing Company.
- Friedel, G. (1926). *Leçons de Cristallographie*. Nancy/Paris/Strasbourg: Berger-Levrault. [Reprinted: Paris: Blanchard (1964).]
- Hahn, Th. & Wondratschek, H. (1994). *Symmetry of Crystals*. Sofia: Heron Press.
- Heesch, H. (1929). *Zur systematischen Strukturtheorie. II*. *Z. Kristallogr.* **72**, 177–201.
- Hilton, H. (1903). *Mathematical Crystallography*. Oxford: Clarendon Press. [Reprint: New York: Dover (1963).]
- International Tables for Crystallography* (2002). Vol. A, 5th ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers. [Abbreviated as *IT A* (2002).]
- International Tables for Crystallography* (2004). Vol. C, 3rd ed., edited by E. Prince. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (2010). Vol. A1, 2nd ed., edited by H. Wondratschek & U. Müller. Chichester: Wiley. [Abbreviated as *IT A1* (2010).]
- International Tables for X-ray Crystallography* (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Revised editions: 1965, 1969 and 1977. Abbreviated as *IT* (1952).]
- Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Revised edition: Ann Arbor: Edwards (1944). Abbreviated as *IT* (1935).]
- Koch, E. & Fischer, W. (1974). *Zur Bestimmung asymmetrischer Einheiten kubischer Raumgruppen mit Hilfe von Wirkungsbereichen*. *Acta Cryst.* **A30**, 490–496.
- Lampport, L. (1994). *LaTeX: a Document Preparation System*, 2nd ed. Reading: Addison-Wesley.
- Momma, K. & Izumi, F. (2011). *VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data*. *J. Appl. Cryst.* **44**, 1272–1276.
- Müller, U. (2013). *Symmetry Relationships between Crystal Structures*. Oxford: IUCr/Oxford University Press.
- Niggli, P. (1919). *Geometrische Kristallographie des Diskontinuums*. Leipzig: Borntraeger. [Reprint: Wiesbaden: Sändig (1973).]
- Parthé, E., Gelato, L. M. & Chabot, B. (1988). *Structure description ambiguity depending upon which edition of International Tables for (X-ray) Crystallography is used*. *Acta Cryst.* **A44**, 999–1002.
- Sadanaga, R., Takeuchi, Y. & Morimoto, N. (1978). *Complex structures of minerals. Recent Prog. Nat. Sci. Jpn.*, **3**, 141–206, esp. pp. 149–151.
- Schiebold, E. (1929). *Über eine neue Herleitung und Nomenklatur der 230 kristallographischen Raumgruppen mit Atlas der 230 Raumgruppen-Projektionen*. Text, Atlas. In *Abhandlungen der Mathematisch-Physikalischen Klasse der Sächsischen Akademie der Wissenschaften*, Band 40, Heft 5. Leipzig: Hirzel.
- Shubnikov, A. V. & Belov, N. V. (1964). *Coloured Symmetry*, pp. 198–210. Oxford: Pergamon Press.
- Stróž, K. (1997). *SPACER: a program to display space-group information for a conventional and nonconventional coordinate system*. *J. Appl. Cryst.* **30**, 178–181.
- Templeton, D. H. (1956). *Systematic absences corresponding to false symmetry*. *Acta Cryst.* **9**, 199–200.
- Wilson, A. J. C. (1993). *Laue and Patterson symmetry in the complex case*. *Z. Kristallogr.* **208**, 199–206.
- Wolff, P. M. de, Belov, N. V., Bertaut, E. F., Buerger, M. J., Donnay, J. D. H., Fischer, W., Hahn, Th., Koptsik, V. A., Mackay, A. L., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1985). *Nomenclature for crystal families, Bravais-lattice types and arithmetic classes. Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry*. *Acta Cryst.* **A41**, 278–280.
- Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Hahn, Th., Senechal, M., Shoemaker, D. P., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1992). *Symbols for symmetry elements and symmetry operations. Final Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry*. *Acta Cryst.* **A48**, 727–732.
- Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Senechal, M., Shoemaker, D. P., Wondratschek, H., Hahn, Th., Wilson, A. J. C. & Abrahams, S. C. (1989). *Definition of symmetry elements in space groups and point groups. Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry*. *Acta Cryst.* **A45**, 494–499.