### Hexagonal space groups

| | | | |
|---|---|---|---|
| 168 $P6$<br>172 $P6_4$ | 169 $P6_1$<br>173 $P6_3$ | 170 $P6_5$ | 171 $P6_2$ |
| 174 $P\bar{6}$ | | | |
| 175 $P6/m$ | 176 $P6_3/m$ | | |
| 177 $P622$<br>181 $P6_422$ | 178 $P6_122$<br>182 $P6_322$ | 179 $P6_522$ | 180 $P6_222$ |
| 183 $P6mm$ | 184 $P6cc$ | 185 $P6_3cm$ | 186 $P6_3mc$ |
| 187 $P\bar{6}m2$ | 188 $P\bar{6}c2$ | 189 $P\bar{6}2m$ | 190 $P\bar{6}2c$ |
| 191 $P6/mmm$ | 192 $P6/mcc$ | 193 $P6_3/mcm$ | 194 $P6_3/mmc$ |

### Cubic space groups

| | | | |
|---|---|---|---|
| 195 $P23$<br>199 $I2_13$ | 196 $F23$ | 197 $I23$ | 198 $P2_13$ |
| 200 $Pm\bar{3}$<br>204 $Im\bar{3}$ | 201 $Pn\bar{3}$<br>205 $Pa\bar{3}$ | 202 $Fm\bar{3}$<br>206 $Ia\bar{3}$ | 203 $Fd\bar{3}$ |
| 207 $P432$<br>211 $I432$ | 208 $P4_232$<br>212 $P4_332$ | 209 $F432$<br>213 $P4_132$ | 210 $F4_132$<br>214 $I4_132$ |
| 215 $P\bar{4}3m$<br>219 $F\bar{4}3c$ | 216 $F\bar{4}3m$<br>220 $I\bar{4}3d$ | 217 $I\bar{4}3m$ | 218 $P\bar{4}3n$ |
| 221 $Pm\bar{3}m$<br>225 $Fm\bar{3}m$<br>229 $Im\bar{3}m$ | 222 $Pn\bar{3}n$<br>226 $Fm\bar{3}c$<br>230 $Ia\bar{3}d$ | 223 $Pm\bar{3}n$<br>227 $Fd\bar{3}m$ | 224 $Pn\bar{3}m$<br>228 $Fd\bar{3}c$ |

## BOOK LIST

Here is a short list of books mostly in English that we have found particularly useful. Some more-specialized books we have referred to in the text. References to all the crystal structure data given in this book are to be found in the various compilations listed in D (this is where they came from).

A. INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

These are: Volume A: Space-Group Symmetry, 3rd ed. 1992 [the indispensable reference]. Volume B: Reciprocal Space, 1993. Volume C: Mathematical, Physical and Chemical Tables, 1992. Kluwer Academic, Dordrecht.

B. Some books on crystallography and crystal chemistry

BLOSS, F. D.

*Crystallography and Crystal Chemistry*, reprinted by Mineral. Soc. Amer., Washington, D.C. (1994). Very clear exposition of the crystallographic point groups.

BURNS, G & GLAZER, A. M.

*Space Groups for Solid State Scientists* 2nd Ed., Academic Press, New York (1990). A good informal account of space groups with useful tables.

BOISEN, M. B. & GIBBS, G. V.

*Mathematical Crystallography*, Reviews in Mineralogy **15**, Mineral. Soc. of Amer., Washington, D.C. (Revised, 1990). A systematic account of how to do crystallographic calculations, and a derivation of the three-dimensional point and space groups.

DE JONG, W. F.

*General Crystallography*. Freeman, San Francisco (1959). Subtitled "A brief compendium" this useful little book contains a wide variety of information. Particularly useful for geometric aspects.

HYDE, B. G. & ANDERSSON, S.

*Inorganic Crystal Structures*, John Wiley & Sons, New York (1989). Systematic description of crystal structures with special emphasis on the development of "complex" structures from simpler ones using simple building principles. Numerous tables of data.

MEGAW, H. D.

*Crystal Structures: A Working Approach*, Saunders, Philadelphia (1973). Clear descriptions of symmetry and the crystallographic description of structures.

PEARSON, W. B.

*The Crystal Chemistry and Physics of Metals and Alloys*, John Wiley & Sons, New York (1972). A comprehensive account of the subject at the time and still very useful.

SMITH, J. V.

*Geometrical and Structural Crystallography*, John Wiley & Sons, New York (1982). A good introduction to formal crystallography. Intended for those who are prepared to *work* through a number of carefully considered examples.

WELLS, A. F.

*Structural Inorganic Chemistry*. 5th Ed., Clarendon Press, Oxford (1984). Contains a wealth of organized structural information with due attention to crystal structures. Introductory chapters discuss polyhedra, sphere packings *etc*. Every chemist should own a copy.

C. Some books on geometry

COXETER, H. S. M.
*Introduction to Geometry*, John Wiley & Sons, New York (1971). A classic that everyone should own and read. Includes a good account of two-dimensional symmetry groups.
CUNDY, H. M. & ROLLET, A. P.
*Mathematical Models*, 2nd Ed., Clarendon Press, Oxford (1961). Written for English sixth-formers, this book has, among other things, a lot of useful information on, and practical tips for making, polyhedra.
GRÜNBAUM, B. & SHEPHARD, G. C.
*Tilings and Patterns*, W. H. Freeman, New York (1986). An astonishing book, beautifully illustrated, that should dispel any illusions that two-dimensional patterns are boring. Heavy going in places.
HILBERT, D. & COHN-VOSSEN, S.
*Geometry and the Imagination*, Chelsea, New York (1952). Another classic, and one that is as fresh today as when it was written (originally published in 1932). 330 figures, some very beautiful. Every personal library should contain a copy.
SHUBNIKOV, A. V. & KOPSTIK, V. A.
*Symmetry in Science and Art*, Plenum Press, New York (1974). A readable guide to symmetry groups (including black-and-white and color groups) in different dimensions (*e.g.* rod and layer groups). Also material of general interest as suggested by the title.
WENNIGER, M. J.
*Polyhedron Models*, Cambridge University Press (1971). Illustrations of beautiful polyhedra and instructions for making them.

D. Reference books and data bases

STRUCTURE REPORTS
Originally *Strukturbericht* (Vols. 1-7), these are annual compendia of crystal structure data. The earlier volumes gave enough information to be a sufficient reference source, but later volumes have become mainly bibliographies (references without author's names!). The last volume was for 1990 and the series which started so auspiciously under P. P. Ewald and C. Hermann in 1931 seems to have died ignominiously without even a whimper. Hampered by a highly eccentric indexing system.
VILLARS, P. & CALVERT, L. D.
*Pearson's Handbook of Crystallographic Data for Intermetallic Phases*. 2nd edition, American Society of Metals, Metals Park, Ohio (1991). "Handbook" may not be the correct term for four volumes, each weighing more than 3 kg. Comprehensive and valuable reference source of structural data for compounds involving metallic elements, also includes data for pnictides and chalcogenides. Only *binary* oxides and no halides are included, and the price precludes personal ownership for most. The second edition omits some compounds reported in Volume I of the first edition, so one needs to have both. The assignments to structure types are not always reliable and one should check the original papers if unit cells and/or origins are changed. We have found a number of errors and misprints.
WYCKOFF, R. W. G.
*Crystal Structures*. John Wiley & Sons, New York. Vol 1 (1963), Vol 2 (1964), Vol 3 (1965), Vol 4 (1968). A convenient reference organized by structure type if one does not want the latest information.
INORGANIC CRYSTAL STRUCTURE DATA BASE - Gmelin Institut, Karlsruhe.
Contains 39,000 entries and growing at a rate of ≈ 1500 per year.
Criteria for inclusion are (a) no C-C and/or C-H bonds (these are in the Cambridge Structure Data Base) (b) contains at least one of H, He, B, C, N, O, F, Ne, Si, P, S, Cl, Ar, Se, Br, Te, I, Xe, At and Rn (*i.e.* elements right of the "Zintl line" on the periodic table). Neither perfect (we find errors) or comprehensive (some surprising omissions) but excellent value for money.

# Formula Index

This index lists chemical compounds for which some structural information appears in Chapters 1-7 or Appendix 5. If the page number is in bold face full crystallographic data are given. Look also for trivial names in the subject index (especially for minerals and zeolites).

# Subject Index

The Table of Contents should be consulted for major topics discussed in this book (space groups, polyhedra, sphere packings, etc.). The subject index serves mainly to guide the reader to definitions of terms, mineral names, etc. so only the principal (defining) occurrences of a term are indicated. Note also we normally use the "natural" order of words as in "clathrate hydrate" not "hydrate, clathrate" (but try different combinations). For chemical compounds, also consult the formula index.