


## Space group tables

## International Tables for Crystallography, Vol. A

$P4bm$

No. 100




$C_{4v}^2$

$P4bm$

4 mm

Tetragonal

Point group symmetry  $P4/mmm$



Origin on 4/2

Generators and  $PC(2), PC(2), PC(2), C(4)$

Symmetry operations

$(x) = x$	$(y) = y$	$(z) = z$	$(x) = x$	$(y) = y$	$(z) = z$
$(x) = x, z$	$(y) = y, z$	$(z) = z$	$(x) = x, z$	$(y) = y, z$	$(z) = z$

Generators selected: (1), (11), (12), (13), (14), (15), (2), (3), (5)				
Positions		Coordinates		Reflection conditions
Asymmetric (standard) setting for symmetry				
General				
$h, k, l$	(1) $x, y, z$ (2) $x+1, y+1, z$	(3) $x, y, z$ (4) $x+1, y+1, z$	(5) $x, y, z$ (6) $x+1, y+1, z$	General hkl: $h \equiv 2n$ 0kl: $k \equiv 2n$
Special: as above, plus				
$h, k, l$	$x, y+1, z$	$x, y, z+1$	$x+1, y, z$	as extra conditions
$h, k, l$	$2, 0, 0$	$0, 0, 2$		hkl: $h+k \equiv 2n$
$h, k, l$	$0, 0, 2$	$2, 0, 0$		hkl: $h+k \equiv 2n$
Symmetry of special projections				
Along [001] $p \times q$ $a^* = a$ $b^* = b$ Origin at 0,0,0	Along [100] $p \times m$ $a^* = b$ $b^* = a$ Origin at 0,0,0		Along [110] $p \times m$ $a^* = (b+a)/2$ $b^* = a$ Origin at $x, x, 0$	
Maximal non-isomorphic subgroups				
1	(2) $P4 \times 1$ ( $P4$ )	1, 2, 3, 4		
	(2) $P2 \times 1$ ( $P2 \times 2$ )	1, 2, 3, 6		
	(2) $P2 \times 1$ ( $C_{2v} \times 2$ )	1, 2, 3, 8		
No more				
0k	(2) $P4_2/b$ ( $a^* = 2a$ )	(2) $P4_2/m$ ( $a^* = 2a$ )	(2) $P4_2/a$ ( $a^* = 2a$ )	

# Crystal Data Space Group Tables

**Theo Hahn**



## **Crystal Data Space Group Tables:**

**International Tables for Crystallography, Space-Group Symmetry** Theo Hahn, 2005-06-06 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Each of the eight volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials Emphasis is given to symmetry diffraction methods and techniques of crystal structure determination and the physical and chemical properties of crystals The data are accompanied by discussions of theory practical explanations and examples all of which are useful for teaching Volume A treats crystallographic symmetry in direct or physical space It contains extensive tabulations and illustrations of the 17 plane groups the 230 space groups and the 32 crystallographic point groups Parts 1-5 of the volume present introductory material including lists of symbols and terms a guide to the use of the space group tables and the determination of space groups Later parts discuss aspects of symmetry theory such as crystal lattices and normalizers of space groups Thoroughly updated and improved the latest edition of Volume A includes an additional chapter on further properties of lattices Crystal Data Space-group Tables Alan D. Mighell, Helen M. Ondik, Bettijoyce Breen Molino, 1977

NBS Technical Note , 1980-06 International Tables for Crystallography, Space-group Symmetry Mois I.

Aroyo, 2017-02-13 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume A of the series Space group symmetry contains diagrams and tables of data for the 17 plane groups the 230 space groups and the 32 crystallographic point groups This new edition is edited by M I Aroyo and has been extensively updated and revised Part 1 of the volume provides an introduction to space group symmetry It includes chapters on groups crystallographic and space group symmetry descriptions of space groups coordinate system transformations and methods of space group determination The final chapter provides a useful introduction to topics treated in more depth in Volumes A1 and E of the series The chapters in this part have been written with teaching in mind and will prove invaluable for undergraduates or graduates wishing to learn about symmetry in crystallography while providing a clear introduction to the topic for researchers from other disciplines Part 2 of the volume presents the diagrams and tables of plane and space group data The layout of the tables of data the symbols used in the diagrams and the classification of the space groups are explained in a useful guide Together these form an essential resource not only for professional crystallographers but also for chemists physicists mineralogists biologists and material scientists who employ crystallographic methods and who are concerned with the structure and the properties of crystalline materials Part 3 treats more advanced topics on space group symmetry and covers crystal lattices point groups and crystal classes space group symbols and their use lattice complexes normalizers of space groups and magnetic subperiodic groups and magnetic space groups There are eight new chapters in this 6th edition of Volume A and five chapters have been revised The layout of the space group tables has been simplified as

the sub and supergroup data are now available in Volume A1 and there are new general position diagrams for the cubic space groups Additional diagrams showing tilted perspective views of some of the more complex cubic space groups are also provided More information on the series can be found at <http://it.iucr.org> **International Tables for Crystallography, Volume G** Sydney Hall, Brian McMahon, 2005-10-07 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Each of the volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials Emphasis is given to symmetry diffraction methods and techniques of crystal structure determination and the physical and chemical properties of crystals The data are accompanied by discussions of theory practical explanations and examples all of which are useful for teaching Volume G deals with methods and tools for organizing archiving and retrieving crystallographic data The volume describes the Crystallographic Information File CIF the standard data exchange and archival file format used throughout crystallography The volume is divided into five parts Part 1 An introduction to the development of CIF Part 2 Details concepts and specifications of the files and languages Part 3 Discusses general considerations when defining a CIF data item and the classification and use of data Part 4 Defines all the data names for the core and other dictionaries Part 5 Describes CIF applications including general advice and considerations for programmers The accompanying software includes the CIF dictionaries in machine readable form and a collection of libraries and utility programs Volume G is an essential guide for programmers and data managers handling crystal structure information and provides in depth information vital for recording or using single crystal or powder diffraction data in small molecule inorganic and biological macromolecular structure science More information on the series can be found at <http://it.iucr.org> **International Tables for Crystallography** Mois I. Aroyo, 2021-07-06 This sixth edition of what was previously known as the Brief Teaching Edition of Volume A provides an introduction to the basic crystallographic data for space groups found in Volume A for symmetry relations between space groups in Volume A1 and for subperiodic groups in Volume E of International Tables for Crystallography to magnetic space groups and to the symmetry database that forms part of International Tables Online at <https://it.iucr.org> It is designed for graduate students and young researchers who are new to the field of crystallographic symmetry and includes many illustrative examples to help readers to understand and use these different kinds of information Selected tables of symmetry data from the full volumes in the series are also included making this a handy aid for classroom teaching References are also provided to further specialized sources for those who need to go deeper into the subject and to textbooks for those who need more background information **Publications of the National Bureau of Standards 1977 Catalog** United States. National Bureau of Standards, 1978 **Publications of the National Bureau of Standards** United States. National Bureau of Standards, 1977 [International Tables for Crystallography, Definition and Exchange of Crystallographic Data](#) Sydney R. Hall, Theo Hahn, Brian McMahon, 1984

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*International Tables for Crystallography, Volume A* Mois I. Aroyo, 2017-02-13

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume A of the series Space group symmetry contains diagrams and tables of data for the 17 plane groups the 230 space groups and the 32 crystallographic point groups This new edition is edited by M I Aroyo and has been extensively updated and revised Part 1 of the volume provides an introduction to space group symmetry It includes chapters on groups crystallographic and space group symmetry descriptions of space groups coordinate system transformations and methods of space group determination The final chapter provides a useful introduction to topics treated in more depth in Volumes A1 and E of the series The chapters in this part have been written with teaching in mind and will prove invaluable for undergraduates or graduates wishing to learn about symmetry in crystallography while providing a clear introduction to the topic for researchers from other disciplines Part 2 of the volume presents the diagrams and tables of plane and space group data The layout of the tables of data the symbols used in the diagrams and the classification of the space groups are explained in a useful guide Together these form an essential resource not only for professional crystallographers but also for chemists physicists mineralogists biologists and material scientists who employ crystallographic methods and who are concerned with the structure and the properties of crystalline materials Part 3 treats more advanced topics on space group symmetry and covers crystal lattices point groups and crystal classes space group symbols and their use lattice complexes normalizers of space groups and magnetic subperiodic groups and magnetic space groups There are eight new chapters in this 6th edition of Volume A and five chapters have been revised The layout of the space group tables has been simplified as the sub and supergroup data are now available in Volume A1 and there are new general position diagrams for the cubic space groups Additional diagrams showing tilted perspective views of some of the more complex cubic space groups are also provided More information on the series can be found at <http://it.iucr.org>

**Crystal Data: Organic compounds 1967-1974** Joseph Désiré Hubert Donnay, 1972

**International Critical Tables of Numerical Data, Physics, Chemistry and Technology** Edward Wight Washburn, 1926

**Crystallographic Databases**, 1987

**Publications** United States.

National Bureau of Standards,1978      *International Critical Tables of Numerical Data, Physics, Chemistry and Technology*  
National Research Council (U.S.),Callie Hull,1926      International Tables for Crystallography Theo Hahn,1987-06-30

**International Tables for Crystallography, Brief Teaching Edition of Volume A** Theo Hahn,2002-04-30

International Tables for Crystallography are no longer available for purchase from Springer For further information please contact Wiley Inc follow the link on the right hand side of this page This brief teaching edition is a condensed inexpensive version of Volume A of International Tables for Crystallography It consists of complete descriptions of the 17 plane groups useful for the teaching of symmetry 24 selected space group examples of varying complexity and distributed over all seven crystal systems those basic text sections of Volume A that are necessary for the understanding and handling of space groups Parts 1 2 3 and 5 The purpose of the teaching edition is threefold It should provide a handy and inexpensive tool for researchers and students wishing to familiarize themselves with the use of the space group tables in Volume A It is designed for use in classroom teaching and with this aim in mind the price has been kept as low as possible In order to achieve this the material has been reprinted from Volume A without any changes except for pagination It may serve as a laboratory handbook because the 24 examples include most of the frequently occurring space groups for both organic and inorganic crystals The fifth edition of the brief teaching edition has been reviewed by M Warren Mineral Mag 2003 67 826 827      **Bulletin of the Chemical Society of Japan** Nihon Kagakkai,1928      **Philosophical Magazine** ,1929      **Proceedings of the Royal Society of London** Royal Society (Great Britain),1928

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