

Generators selected

(1); $t(1,0,0)$; $t(0,1,0)'$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site Symmetry

Coordinates

(0,0,0) +

(0,1,0)' +

16 1 1

(1) x,y,z [u,v,w](2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ [u,v, \bar{w}](3) \bar{x}, y, \bar{z} [u, \bar{v}, w](4) $x + \frac{1}{2}, \bar{y}, \bar{z}$ [u, \bar{v}, \bar{w}](5) $\bar{x}, \bar{y}, \bar{z}$ [$\bar{u}, \bar{v}, \bar{w}$](6) $x + \frac{1}{2}, y, \bar{z}$ [\bar{u}, \bar{v}, w](7) x, \bar{y}, z [\bar{u}, v, \bar{w}](8) $\bar{x} + \frac{1}{2}, y, z$ [\bar{u}, v, w]8 k $m'..$ $\frac{1}{4}, y, z$ [$0,v,w$] $\frac{1}{4}, \bar{y}, z$ [$0,v, \bar{w}$] $\frac{3}{4}, y, \bar{z}$ [$0, \bar{v}, w$] $\frac{3}{4}, \bar{y}, \bar{z}$ [$0, \bar{v}, \bar{w}$]8 j $.m'$ $x, \frac{1}{2}, z$ [$u,0,w$] $\bar{x} + \frac{1}{2}, \frac{1}{2}, z$ [$\bar{u},0,w$] $\bar{x}, \frac{1}{2}, \bar{z}$ [$u,0,w$] $x + \frac{1}{2}, \frac{1}{2}, \bar{z}$ [$\bar{u},0,w$]8 i $.m$ $x,0,z$ [$0,v,0$] $\bar{x} + \frac{1}{2}, \frac{1}{2}, z$ [$0,v,0$] $\bar{x},0,\bar{z}$ [$0, \bar{v},0$] $x + \frac{1}{2},0,\bar{z}$ [$0, \bar{v},0$]8 h $.2'$ $0,y,\frac{1}{2}$ [$u,0,w$] $\frac{1}{2}, \bar{y}, \frac{1}{2}$ [$u,0, \bar{w}$] $0, \bar{y}, \frac{1}{2}$ [$\bar{u},0, \bar{w}$] $\frac{1}{2}, y, \frac{1}{2}$ [$\bar{u},0,w$]8 g $.2'$ $0,y,0$ [$u,0,w$] $\frac{1}{2}, \bar{y},0$ [$u,0, \bar{w}$] $0, \bar{y},0$ [$\bar{u},0, \bar{w}$] $\frac{1}{2}, y,0$ [$\bar{u},0,w$]4 f $m'm'2$ $\frac{1}{4}, \frac{1}{2}, z$ [$0,0,w$] $\frac{3}{4}, \frac{1}{2}, \bar{z}$ [$0,0,w$]4 e $m'm'2'$ $\frac{1}{4},0,z$ [$0,v,0$] $\frac{3}{4},0,\bar{z}$ [$0, \bar{v},0$]4 d $.2'/m'$ $0, \frac{1}{2}, \frac{1}{2}$ [$u,0,w$] $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ [$\bar{u},0,w$]4 c $.2'/m$ $0,0,\frac{1}{2}$ [$0,0,0$] $\frac{1}{2},0,\frac{1}{2}$ [$0,0,0$]4 b $.2'/m'$ $0, \frac{1}{2},0$ [$u,0,w$] $\frac{1}{2}, \frac{1}{2},0$ [$\bar{u},0,w$]4 a $.2'/m$ $0,0,0$ [$0,0,0$] $\frac{1}{2},0,0$ [$0,0,0$]

Symmetry of Special Projections

Along $[0,0,1]$ p_2-2mm $a^* = -a/2$ $b^* = b$ Origin at $0,0,z$ Along $[1,0,0]$ $p_{2h}-2mm$ $a^* = b$ $b^* = c$ Origin at $x,0,0$ Along $[0,1,0]$ $p2mg1'$ $a^* = -a$ $b^* = c$ Origin at $0,y,0$

International Tables For Crystallography

Mois I. Aroyo



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International Tables for Crystallography, 8 Volume Set C. P. Brock, 2017-03-20 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 International Tables for Crystallography provides access to the content of the full set 6000 pages of all the Volumes A to G including A1 in pdf format and also provides access to the International Tables Online site hosted by the International Union of Crystallography The International Tables Online site contains the full text of the series as both pdf and richly interlinked html along with many innovative features and additional resources The advanced search facility enables sophisticated searches to be performed across all the volumes across selected volumes and across International Tables Online and Crystallography Journals Online The International Tables for Crystallography includes nearly 2 000 pages of symmetry tables which are vital for the analysis of crystal structures and which feature extensive linking between sub and supergroups The contents can be browsed by volume across the 8 volumes below

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Volume A1 Symmetry relations between space groups
Volume B Reciprocal space 3e
Volume C Mathematical physical and chemical tables 3e
Volume D Physical properties of crystals
Volume E Subperiodic groups
Volume F Crystallography of biological macromolecules
Volume G Definition and exchange of crystallographic data

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treatment of the theory algorithms and crystallographic applications of Fourier methods and fundamental as well as advanced treatments of symmetry in reciprocal space In Part 2 these general accounts are followed by detailed expositions of crystallographic statistics the theory of direct methods Patterson techniques isomorphous replacement and anomalous scattering and treatments of the role of electron microscopy and diffraction in crystal structure determination including applications of direct methods to electron crystallography Part 3 deals with applications of reciprocal space to molecular geometry and best plane calculations and contains a treatment of the principles of molecular graphics and modelling and their applications A convergence acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method Part 4 contains treatments of various diffuse scattering phenomena arising from crystal dynamics disorder and low dimensionality liquid crystals and an exposition of the underlying theories and or experimental evidence Polymer crystallography and reciprocal space images of aperiodic crystals are also treated Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter dynamical theory as applied to X ray electron and neutron diffraction techniques The simplified trigonometric expressions for the structure factors in the 230 three dimensional space groups which appeared in Volume I of International Tables for X ray Crystallography are now given in Appendix 1 4 3 to Chapter 1 4 of this volume Volume B is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature **Space-group Symmetry** Theo Hahn,1992

International Tables for Crystallography, Volume B U. Shmueli,2008-08-25 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research This volume is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature New to this edition A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals Three new sections on electron diffraction and electron microscopy in structure determination describing point group and space group determination by convergent beam electron diffraction three dimensional reconstruction and single particle reconstruction Substantial revisions to the chapters on space group representations in reciprocal space direct methods Patterson and molecular replacement techniques and disorder diffuse scattering 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 *International Tables for Crystallography, Volume C* E. Prince, 2004-01-31 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 The purpose of Volume C is to provide the mathematical physical and chemical information needed for experimental studies in structural crystallography The volume covers all aspects of experimental techniques using all three principal radiation types from the selection and mounting of crystals and production of radiation through data collection and analysis to interpretation of results As such it is an essential source of information for all workers using crystallographic techniques in physics chemistry metallurgy earth sciences and molecular biology

International Tables for Crystallography Theo Hahn, 1984 **International Tables for X-ray Crystallography** International Union of Crystallography, 1962 [International Tables for Crystallography, Definition and Exchange of Crystallographic Data](#) Sydney Hall, Brian McMahon, 2005-10-17 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 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 **International Tables for**

Crystallography: Space-group symmetry Theo Hahn, 1987 **International Tables for Crystallography, Physical Properties of Crystals** A. Authier, 2004-02-13

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 D is concerned with the influence of symmetry on the physical and tensor properties of crystals and on their structural phase transitions. This role is very important in many different disciplines of the science of materials, such as crystallography, elasticity, solid state physics, magnetism, optics, ferroelectricity and mineralogy. Volume D deals with all these aspects in a unified way. The volume is divided into 3 parts. Part 1 introduces the mathematical properties of tensors and group representations and gives their independent components for each of the crystallographic groups. Part 2 is devoted to the symmetry aspects of excitations in reciprocal space: phonons, electrons, Raman scattering and Brillouin scattering. Part 3 deals with the symmetry aspects of structural phase transitions and twinning. A prominent feature is the joint description of twinning and domain structures, which are usually presented in completely separate ways in handbooks of physics and mineralogy. Supplementary software is provided to support and enhance Chapters 1.1 and 1.2 for the determination of irreducible group representations and tensor components and Part 3 on structural phase transitions.

International Tables for Crystallography, Subperiodic Groups V. Kopský, D. B. Litvin, 2010-03-01

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 E covers the standard nomenclature and representations for the 7 crystallographic frieze group types, the 75 crystallographic rod group types and the 80 crystallographic layer group types. The information tabulated for these groups is identical in format and content to that given for the 230 space groups in Volume A and is essential for the analysis of the structure and physical properties of crystalline materials that contain linear or planar substructures. In addition, scanning tables are given for each of the 230 space groups designed for use in the analysis of interfaces. This second edition of Volume E has been revised and includes additional information in the comparison tables of notations for the subperiodic group types to improve ease of use. The Seitz notation of each symmetry operation has also been included. More information on the series can be found at <http://it.iucr.org>

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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>

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