Crystal Data


Crystal data for $p$-bromochlorobenzene and $p$-dichlorobenzene/$p$-bromochlorobenzene mixed crystals at 293 K. Erratum.* By M. LABRADOR and E. TAUER, Departament de Cristallografia, Universitat de Barcelona, Gran Via 585, 08007 Barcelona, Spain, Y. HAGET, Laboratoire de Cristallographie et de Physique Cristalline LA 144, Université de Bordeaux I, 351, Cours de la Libération, 33405 Talence CEDEX, France, T. CALVET and M. A. CUEVAS, Departament de Cristallografia, Universitat de Barcelona, Gran Via 585, 08007 Barcelona, Spain, and E. ESTOP, Departament de Cristallografia, Universitat Autònoma de Barcelona, Bellaterra, Spain

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Abstract

The data given in the Abstract published in J. Appl. Cryst. (1985), 18, 542 are in error. The correct data are given below:

The powder data for $p$-bromochlorobenzene (PBCB) and $p$-dichlorobenzene/$p$-bromochlorobenzene mixed crystals $[pDCB]_x[pBCB]_{1-x}$ at 293 K are reported; their thermal stability at 293 K is given. Vertical diffractometer, graphite monochromator, Cu Ka, $\lambda = 1.5405$ Å. They are all iso- morphous, monoclinic, $P2_1/a$ with $Z = 2$. $a = 15.134(4)$, $b = 5.843(2)$, $c = 4.073(1)$ Å, $\beta = 112.53(1)^\circ$, $V = 332.7$ Å$^3$, $D_x = 1.911$ Mg m$^{-3}$ for PBCB. $a = 14.808(8)$, $b = 5.838(3)$, $c = 4.038(1)$ Å, $\beta = 112.52(3)^\circ$, $V = 322.5$ Å$^3$, $D_x = 1.675$ Mg m$^{-3}$ for $[pDCB]_{0.90}[pBCB]_{0.10}$. $a = 15.033(5)$, $b = 5.844(3)$, $c = 4.062(2)$ Å, $\beta = 112.48(3)^\circ$, $V = 326.6$ Å$^3$, $D_x = 1.797$ Mg m$^{-3}$ for $[pDCB]_{0.30}[pBCB]_{0.70}$. The JCPDS Nos. are: 36-1995 for PBCB; 36-1992 for $[pDCB]_{0.90}[pBCB]_{0.10}$; 36-1993 for $[pDCB]_{0.60}[pBCB]_{0.40}$; 36-1994 for $[pDCB]_{0.30}[pBCB]_{0.70}$. Data for $[pDCB]_{0.80}[pBCB]_{0.20}$, $[pDCB]_{0.70}[pBCB]_{0.30}$, $[pDCB]_{0.60}[pBCB]_{0.40}$ and $[pDCB]_{0.50}[pBCB]_{0.50}$ have also been measured and are available from the authors or as part of the Supplementary Publication.

Computer Programs


PITMOS—a system of interactive computer programs for visualization of crystal packing. By SERGE PÉREZ and RAYMOND P. SCARINGE, Centre de Recherches sur les Macromolécules Végétales, BP 68, 38042 Saint-Martin d’Hères, France, and Research Laboratories, Eastman Kodak Company, Rochester, New York 14650, USA

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Abstract

A system of computer programs for interactive representation of crystalline architecture and organization is presented. This program allows the unit cell and its contents to be rotated with respect to any selected reference frame. Molecular representations such as the stick model or the solid ball-and-stick model can be selected. Two graphic modes are available. The first is the conventional projection, in which color may be used extensively to differentiate different atomic species and distinct molecules. The second mode makes use of a stereoscopic representation and yields a three-dimensional view of the structure, which can be interactively modified. Several other user-friendly features are available, including a selective erase/restore procedure and an interactive change of the representation parameters. The program also offers the possibility of calculating and displaying specific intermolecular bonds such as hydrogen bonds or metal–ligand bonds.

Introduction

For an acceptable representation of crystal packing, an iterative approach generally must be used. Ordinarily, the illustration must be computed and plotted several times before an optimal representation is obtained. To avoid tedious procedures, the initial stage of the work can be done on a graphics terminal. This paper describes an interactive...
system of computer programs for plotting molecules and crystal structures (PITMOS). This is a highly modified version of the originally reported program (Dheu & Pérez, 1981). When the PITMOS system was designed, priority was given to a high level of interactivity and ease of use. Several features were not taken into account: the representation of thermal ellipsoids, the drawing of chemical symbols and bond-distance labels, and overlap.

Description

The basic input data are the unit-cell parameters, the atomic labels, coordinates and species codes. A dialog program (ENTPIT) interactively sets up the input file to PITMOS. Starting from the atomic coordinates in the asymmetric unit, the program allows the user to assign radius and a color code to each atomic species. Provision is also made to generate a complete molecule when this species is located on a crystallographic symmetry element. The program determines the interatomic bonds as a function of the atomic species and distance range. PITMOS allows the user quickly to find the best way to visualize a complex arrangement. To do so, two kinds of interactive rotations are possible; both refer to the reference system, which is set to the screen X and Y axes. In the first option, the rotation matrix is applied to the crystal axes: a, b and c. The second option allows the user to define his own reference system, which may be an atomic group. Rotations about the reference system axes can be done in any order. Interactive access to two types of molecular representation (the stick model and the solid ball-and-stick model) is possible. For the latter option, variable radii for atoms and colors associated with the atomic species are available. Also, noncovalent bonds can be drawn as dashed lines. The drawing program PITMOS is to be run on a color CRT graphics terminal. Two basic graphic modes are available. In the first mode, the conventional projection, color may be used extensively to differentiate different atomic species and distinct molecules. In the second mode, which makes use of stereoscopic representation (the stick model and the solid ball-and-stick model) is possible. For the latter option, variable radii for atoms and colors associated with the atomic species are available. Also, noncovalent bonds can be drawn as dashed lines. The drawing program PITMOS is to be run on a color CRT graphics terminal. Two basic graphic modes are available. In the first mode, the conventional projection, color may be used extensively to differentiate different atomic species and distinct molecules. In the second mode, which makes use of stereoscopic representation, every molecule displayed on the screen is automatically drawn in green and red, after rotations of −3 and +3° about the Y axis of the screen. Green and red stereo glasses are required to see the three-dimensional image on the screen. Either mode can be selected, alternately, while the program is being run. PITMOS takes into account the symmetry-related molecules in the unit cell and those derived from pure translations along the crystallographic axes. Input data describing crystallographic symmetries and translations are given one by one, in the form of a single rotation matrix and translation vectors. When a molecule is drawn on the screen, it can be either discarded or saved and added to the set of molecules already displayed. Upon request, a selective erase procedure eliminates the last displayed molecule from the drawing. Otherwise, the last displayed molecule is given a sequential number. At any step of the procedure, the packing representation can be subjected to several changes, such as scale factor, type of representation (mono or stereoscopic views), style (stick or ball-and-stick model) and rotations. When rotations are made, it may be convenient to erase a particular molecule or set of molecules. This is done by specifying the sequential number (apparent on the screen) of these molecules and by calling the selective erase procedure. Conversely, it is also possible to restore any erased molecule or set of molecules. PITMOS offers the possibility of calculating and drawing specific intermolecular bonds, such as hydrogen bonds or metal–ligand bonds, between the molecules displayed on the screen. A simple algorithm based on distance criteria and on the type of potentially interacting atoms (e.g. acceptor and/or donor species for hydrogen bonding) is used. These intermolecular bonds are shown as dashed lines. When a session is ended, an ASCII output file is created, which can be used as an input file either to the program PITMOS for a further session or to the computer program PITBEN. PITBEN creates a binary file such that the drawing can be plotted on a plotter or a dot-matrix printer; several drawing options can be handled through PITBEN.

PITMOS can handle a maximum of 150 atoms and 200 bonds per molecule. Up to 50 different symmetry-related molecules can be displayed on the screen, and up to 250 intermolecular bonds, such as hydrogen bonds, can be searched for and subsequently displayed. The present version has been written for use with a PDP 11/23 mini-computer equipped with 512 K of RAM and operating under the Digital Equipment Corporation RSX-11M operating system. The video terminal used to display the drawing is a C. Itoh CIT 161 color video alphanumeric character attribute display terminal and therefore would be compatible with a number of Tektronix graphics terminals. The dialog program (ENTPIT) used to set up the input file to PITMOS is written in interactive standard Basic. Both PITMOS and PITBEN are written in Fortran IV. The drawing routines of PITMOS utilize the TEKTRONIX PLOT 10 library. The drawing program PITBEN, used to produce the hardcopy, creates a binary file that uses the TEXRAY graphics library, which is compatible with CALCOMP/VERSAPLOT-07. Its adaptation to other plotters is straightforward. A small program is also available for compatibility with the Nonius SDP system.

Reference