Other

PR03.08.01 CCP14 IN POWDER AND SINGLE-CRYSTAL DIFFRACTION. A. J. Holland - Daresbury Laboratory, U.K.

The aim of CCP14 is to develop an integrated and user-friendly suite of powder and single-crystal diffraction programs for data acquisition, data analysis and presentation of results. The CCP14 project commenced in 1994 and a project Steering Committee was formed. The first release of the CCP14 suite in March 1995 included a small number of good quality powder programs covering peak-fitting, autoindexing, Rietveld refinement, the GSAS package and the MOTPLOT program for profile manipulation and display. The CCP14 suite and the associated manual are available free of charge to academic users by means of anonymous FTP.

The EPDIC4 (Chester, U.K.) and SDPD (Oxford, U.K.) meetings in 1995 provided an opportunity to publicise CCP14 to a wide audience of potential users, whose comments have helped in the subsequent development of the suite. Work has begun to develop some of the "linking software" to allow programs to run smoothly in series, transforming CCP14 from a simple program library into a truly integrated suite. Two new releases of CCP14 are planned for 1996, and work has begun to build up the single-crystal element of the suite.

CCP14 exists to serve the academic powder and single-crystal communities and the Steering Committee is keen to hear from as many users as possible as to how exactly they think CCP14 can best serve their interests. Questions, suggestions and contributions of software to the CCP14 suite are very welcome and interested parties should contact the CCP14 secretary, Dr. A. J. Holland, by e-mail at "A.J.Holland@dl.ac.uk". Further information about CCP14 is available on the World Wide Web at "http://www.dl.ac.uk/CCP/CCP14".

PS03.08.02 PROGRAM HARDPACK: PREDICTION AND OPTIMIZATION OF CRYSTAL STRUCTURES USING ATOM-ATOM POTENTIALS AND POINT CHARGES. Rainer Rudert, Federal Institute for Materials Research and Testing, Rudower Chaussee 5, D-12489 Berlin (Germany), phone: (030) 6392 5858, fax: (030) 6392 5787, e-mail: rudert@chemie.fu-berlin.de or nwfrieden@gn.apc.org

A computer program is presented which is able to predict polymorphs of organic crystal structures. The program needs a 3-dimensional model of the molecule including the correct bond lengths, bond angles, and most of the torsional angles. The user may also supply atomic charges. The program varies cell constants, positions of molecules, orientations of molecules and selected torsional angles and calculates energies for each set of parameter values. There are several algorithms available to optimize the crystals structure with respect to the energy, including simulated annealing, grid search, steepest descent, Newton/Raphson, and Rosenbrock method.

The potential between two atoms i and j with distance r_{ij} is $V(r_{ij}) = A_{ij}\xi\exp(-B_{ij}\xi r_{ij})/r_{ij}^{D_{ij}} - C_{ij}/r_{ij}^6 + q_i\xi q_j/r_{ij}$, where A_{ij}, B_{ij}, C_{ij}, and D_{ij} are potential parameters depending on the atoms types, q_i and q_j are the atomic charges of atoms i and j. The user may also choose a "hard sphere" atomic model with $V(r_{ij} > 1.1\xi r_{vdw}) = 0$; $V(r_{vdw} < r_{ij} < 1.1\xi r_{vdw}) = 1$ kJ/mol; $V(r_{ij} < r_{vdw}) = 10^{10}$ kJ/mol, r_{vdw} is the van der Waals radius. It is possible to optimize Langmuir-Blodgett Monolayers with a flat surface substrate and an atom-surface potential $V(d_i) = E_i/d_i^9 - F_i/d_i^3$, where d_i is the distance atom-surface and E_i and F_i are material constants.

Constraints between parameters may be defined. The program is controlled by a user written input file, which has a SHELX-style format.

The program is written in FORTRAN77 and has been tested under MSDOS, UNIX, and VAX/VMS.

PR03.08.03 SPGR4D: A COMPUTER PROGRAM FOR DERIVING SYMMETRY OPERATIONS OF THE (3+1)-DIMENSIONAL SUPERSPACE GROUPS FROM THE TWO-LINE SYMBOLS. Zhengqing Fu* and Haifu Fan, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

A computer program was written for deriving the symmetry operations of the (3+1)-dimensional superspace groups from their two-line symbols. The (3+1)dimensional superspace groups, which are denoted by the two-line symbols, were first introduced by P.M.de Wolff (Acta Cryst. A30, 777-785,1974; A33, 493-497, 1977) and A. Janner & T. Janssen (Phys.Rev.B15,643-658, 1977) to describe the symmetry of one-dimensional incommensurate modulated structures. At present, the superspace-group formalism has been widely accepted and used in both classification and structure determination. Up to now, however, most structure-analusis program systems for incommensurate crystals require the input of multi-dimensional symmetry operations. This is much inconvenient and could easily bring errors. To avoid this disadvantage it is desirable to have a computer program providing the symmetry operations. In this paper, an approach is proposed for automatically deriving the (3+1)-dimensional superspace-group symmetric operations. The derivation is based on the concept of generators $\{R(i),e(i),s(i),t(i),q$ with $i=1,NG\}$, in which $\{R(i),s(i)\}$ denotes the set of generators of the basic space group represented by the upper line. The program, named SPGR4D, is written in Fortran77 and designed as a subroutine such that it can be easily used in further program systems. In SPGR4D, the program developed by H. Burzlaff & A. Hountas [J.Appl.Cryst. 15,464-467, 1982] is adopted for the derivation of symmetric operations of basic space groups. SPGR4D has been incorporated into a new version of the direct-method program DIMS (Z.Q. Fu & H.F. Fan, J.Appl.Cryst. 27,124-127, 1994) for solving incommensurate modulated structures. The detailed information about the approach and SPGR4D will be published elsewhere (Z.Q. Fu & H.F. Fan, to be published, 1996).