Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to exisiting ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 *of the June* 1985 *issue of the Journal* [*J. Appl. Cryst.* (1985), **18**, 189–190].

J. Appl. Cryst. (1991). **24**, 263

SEXIE – a microcomputer program for the calculation of coordination shells and geometries.

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(*Received* 8 *August* 1990; *accepted* 29 *October* 1990)

The crystallographic problem: Phase shifts and amplitude functions, essential for the quantitative analysis of EXAFS data from new materials, are frequently extracted from model compounds with known crystallographic structure. Although many crystallographic programs can, in principle, provide the necessary data, the retrieval of relevant information may be cumbersome: grouping of atom distances into coordination shells is usually not provided; no attempts are made to determine coordination geometries; bond angles are not sorted; and the input of point-symmetry generators can be elaborate and error prone, especially for space groups of high symmetry.

We have designed a microcomputer program, *SEXIE* (Shells for EXAFS – InteractivE), which specifically satisfies the needs of the EXAFS experimentalist by providing the shell-by-shell atomic arrangement around a central atom in a form suitable for EXAFS data interpretation.

Method of solution: After reading a minimum of crystallographic input data (cell constants, the Hermann–Mauguin space-group symbol and the fractional atomic coordinate triples), the space group is decoded, equipoints generated and the unit-cell cluster expanded to required size. The atom distances are grouped in coordination shells and subshells and their coordination geometries suggested. A complete list of sorted distances, vertex coordinates and bond angles is provided. There is a detailed description of the program flow in the *User's Guide*.

Software environment:

Operating system: DOS 2.0 or higher; Digital Equipment VAX/VMS.

Language: ANSI X3.9-1978 standard Fortran (DOD MIL-1135 Standard). Source code (5000 lines) compatible with VAX Fortran.

Hardware environment:

Computers and installations: *SEXIE* runs on any iAP × 86-based IBM-compatible microcomputer under DOS (Version 2.0 and up) with at least 280 kbyte of available memory. A math coprocessor is strongly recommended. A version fully compatible with Digital Equipment VAX computers is distributed with the PC disks.

Program specifications:

Input description: *SEXIE* requires only a minimum of crystallographic input data: cell constants, the Hermann–Mauguin space-group symbol and the fractional coordinate triple of each nonequivalent atom in the asymmetric unit cell. Data input is simplified by a menu-driven preparation program *INSHELL* combined with a user-manageable input data base. At present, the data base includes structural data for most elements and for several model compounds.

Output features: Automatic space-group decoding and equipoint generation is followed by a tabulated output of structure information, densities and K-, $L_{I,II,III}$-edge energies. A compact listing of coordination shells, subcells and geometries is supplemented with a full sorted table of atom distances and angles.

Restrictions: At present, parameter statements within the program limit the unit cell to 20 nonequivalent atoms. The *User's Guide* shows how to expand the program limits and provides information about the associated memory requirements.

Unusual features: Both *SEXIE* and the associated input preparation program, *INSHELL*, provide internal checks on the consistency of the input. *INSHELL* warns of nonexistent space groups and incorrectly prepared input while *SEXIE* makes sure the generated equipoints have reasonable distances from one another and calculates the X-ray density of the material as a reference. Additionally, *INSHELL* automatically transfers rhombohedral space-group settings into hexagonal ones.

Run times: Entering the required input takes from 1 to 5 min depending on the complexity of the unit cell. Run times vary from 30 to 60 s depending on the maximum radius of coordination shells to be considered.

Test status: *SEXIE* and its associated utilities have been tested in over 100 crystal structures, including most elements and several model compounds.

Documentation: With the program disks, the authors distribute a 30 page *User's Guide*, complete with practical hints and a full sample session.

Availability: Copies are available from the authors on either 1.2 Mbyte $5\frac{1}{4}$" diskettes or on 720 kbyte 3.5" disks in IBM PC-DOS format.

Keywords: X-ray absorption spectroscopy, EXAFS, coordination shells, coordination geometries, bond angles, bond distances.

Crystallographers

J. Appl. Cryst. (1991). **24**, 263

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 *Abbey Square, Chester CH*1 2*HU, England).*

Dr **David Harker,** Research Scientist Emeritus at the Medical Foundation of Buffalo, New York State, USA, died on 27 February 1991 after a long illness. He was 84 years old. A memorial service was held in Buffalo on 7 March 1991. A full obituary will be published in *Acta Crystallographica* Section A in due course.

Dr **P. F. Fewster,** Senior Principal Scientist at Philips Research Laboratories, Redhill, England, has been awarded the Paterson medal and prize of the (UK) Institute of Physics for devising new techniques for analysing X-ray patterns from MBE-grown heterostructures of 3–5 compounds. Dr Fewster has developed the X-ray diffraction facility at the Philips site in Redhill into an international centre covering a range of materials, in particular semiconductors and multilayered structures.

Dr **Isabella L. Karle,** Naval Research Laboratory, Washington, DC, USA, has been awarded the Bijvoet Medal by the Bijvoet Centre for Biomolecular Research at Utrecht University, The Netherlands. Dr Karle was invited to give a lecture: 'Structural Chemistry of Peptides', and was then presented with this award in recognition of her outstanding contributions to X-ray crystallography.

0021-8898/91/030263-01$03.00