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 existing 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. (1986), 18, 189–190].

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MOLDRAW – program for the graphical manipulation of molecules on personal computers.

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The crystallographic problem: *MOLDRAW* provides a simple and quick way of analysing molecular geometry from known atomic coordinates. Graphical representations of the structure are displayed and, by means of user-friendly syntax, all possible views of the molecules are obtained and the most relevant stereochemical features are highlighted. The program not only provides the most relevant geometrical parameters, but also allows variation of the geometry by rotation around a selected bond; at the same time, simple energy calculations can be performed. Input to *MOLDRAW* has been conceived for easy use by both crystallographers and theoretical chemists.

Method of solution: The basic geometrical information together with title, cell parameters, space group and, when available, atomic charges are read from a free-format input file. All other operations are performed in an interactive mode by means of a selection of keyword commands. Geometry can be provided in two different forms: as crystallographic or orthogonal coordinates or as internal coordinates supplied in the form of a *Z* matrix as in *MOPAC* (Stewart, 1983). Initially, connectivity is automatically determined from covalent radii information and is written at the end of the input file for subsequent runs. Geometrical calculations are performed in a standard way. Molecules can be represented in three different ways: sticks, balls-and-sticks and solid-bond pseudo-tridimensional view with hidden line removal. Atom labelling is possible also by colour selection. Step and continuous rotation, step translation and zooming of the whole structure are possible. Rotation around a selected bond can be performed by step or continuous motion. The user can delete selected atoms in order to produce a molecular fragment, the coordinates of which are saved on a reusable disk file. In the energy calculations, non-bonded Buckingham model potentials are used and, when atomic charges are supplied, the electrostatic contributions can also be computed. The contents of the whole unit cell can be generated and displayed from the space-group symbol. At present, this utility can handle only the 17 most common space groups up to orthorhombic. The most important intermediate results are output on an ASCII file, which can be printed or edited for further use. Hard-copy of the screen can also be obtained.

Software environment: The program is written in Basic using Microsoft QuikBasic compiler 2.0 under MS-DOS 2.11 or later, without overlay structure. Dynamical memory is used and no external library is required.

Hardware environment: *MOLDRAW* runs on truly compatible IBM PC's equipped with at least 512 kilobytes of memory. It has been developed on a 6 MHz IBM AT but also tested on a B/W Olivetti M24 and on an AST equipped with an 8 MHz 80826 CPU. The mathematical coprocessor is not employed. Both the standard colour-graphics adapter and enhanced graphics adapter (EGA with 256K video memory) are supported. One floppy-disk drive is sufficient, but both hard and RAM disks are supported. The executable code occupies about 180K of memory. Hard-copy facility is implemented on a standard IBM graphics printer, but the use of printers with Epson emulation mode is equally possible.

Program specification: The present version of the program can include 500 atoms, but this number can easily be increased. All the elements are supported but uncommon elements have not been fully tested. Energy calculations based on the Buckingham potentials are restricted to molecules containing H, C, N, O, F, S, Cl, Br and I. The program listing contains about 3500 lines. *MOLDRAW* has been extensively used for almost one year and tested on tens of organic structures of different complexity.

Documentation: A user manual is available as a machine-readable file. On-line help facilities are also included.

Availability: The program, in the executable form only, is available on either 360 Kbytes or 1·2 Kbytes $5\frac{1}{4}$" floppy disks, together with user manual and input test examples.

Keywords: Molecular graphics, energy calculations.

References

STEWART, J. J. P. (1983). *MOPAC: A General Molecular Orbital Package, QCPE Bull.* No. 464, **3**, 101.

Crystallographers

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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 CH1 2HU, England).

Professor **Sir Charles Frank**, H. H. Wills Physics Laboratory, University of Bristol, England, has been awarded the 1987 Von Hippel Award of the Materials Research Society for 'his wide ranging impact on modern materials science through seminal contributions in areas of inorganic crystals, metals, polymers and liquid crystals; his outstanding research in crystallography, chemistry, physics and materials science exemplifies the interdisciplinary approach.'

Muttaiya Sundaralingam, Professor in the Biochemistry Department, University of Wisconsin, Madison, Wisconsin, USA, has been awarded the Steenbock Professorship in Biomolecular Structure in the department, in recognition of his pioneering contributions to biochemical structural principles.

The professorial chair honours Professor Harry Steenbock and was endowed by his wife, Evelyn. Professor Steenbock was born in Wisconsin, attended the University of Wisconsin and pursued his entire professional career there. He carried out research in, and wrote extensively on, human and animal nutrition with special emphasis on vitamins, dietary mineral elements and the effect of irradiation. He patented a process of ultraviolet food irradiation and vitamin D synthesis and was the founder of the Wisconsin Alumni Research Foundation.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

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Publish your Crystallographic Computer Programs

A large number of new crystallographic computer programs (or modifications to existing programs) presented at international and national conferences, summer schools, private demonstrations, or referred to only passingly in other publications remain unpublished. Consequently, potential users are deprived of valuable information and access to state-of-the-art computer code. The IUCr Commission on Crystallographic Computing is well aware of this problem and is particularly anxious to encourage authors of computer programs to publish their software. The journal of choice for crystallographic computer programs is:

Journal of Applied Crystallography – a publication of the IUCr – which provides two categories of publication concerned with crystallographic computer programs: *Computer Programs* is intended for complete articles giving in-depth information on the program and algorithm whereas *Computer Program Abstracts* provides a condensed format that contains only essential details.

In *Computer Programs*, a brief description of the purpose, strategy, computer language, machine requirement, input requirements and the type of results obtained should be included. Ordinarily, it is required also that the adequacy of the documentation shall have been proven by the successful use of the program by someone outside the authors' institution. Examples of *Computer Programs* are: *TREOR*, a semi-exhaustive trial-and-error powder indexing program for all symmetries [Werner, P.-E., Eriksson, L. & Westdahl, M. (1985). *J. Appl. Cryst.* **18**, 367–370]; *STRUPLO*84, a Fortran plot program for crystal structure illustrations in polyhedral representation [Fischer, R. X. (1985). *J. Appl. Cryst.* **18**, 258–262]. Notes for Authors may be found in *Acta Cryst.* (1983), A**39**, 174–186 and a checklist in *J. Appl. Cryst.* (1985), **18**, 1–2.

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New Commercial Products

Announcements of new commercial products are published by the Journal of Applied Crystallography *free of charge. The descriptions, up to* 300 *words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Professor M. Schlenker, Editor* Journal of Applied Crystallography, *Laboratoire Louis Néel du CNRS, BP*166, *F-*38042 *Grenoble CEDEX, France.*

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

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INRAD Forms New Optics Company

INRAD has formed a wholly owned subsidiary, **INRAD Optical Systems, Inc.**, that will specialize in the manufacture of precision optics and optical systems. Using INRAD's optical coating facility, the new company will provide finished optics for aerospace and defence applications. INRAD Optical Systems will complement and expand the parent company's present capabilities in these areas.

INRAD develops and manufactures crystals, crystal devices, and laser systems for the research, industry, and defence markets.

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INRAD'S Autotracker II now Available with BBB Crystals

INRAD now offers its **Autotracker II system with beta barium borate** (BBB). BBB produces the second and third harmonics of dye laser outputs more efficiently than most previously available materials. It also has a broad phase-matchable range, good ultraviolet transparency, and a high damage threshold.

INRAD's Autotracker II system extends the wavelength coverage of pulsed dye lasers using nonlinear frequency mixing to allow high-resolution spectroscopy in regions not easily reached by dye lasers alone.

INRAD, 181 *Legrand Ave*, *Northvale*, *NJ* 07647, *USA*.

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Philips 300 kV Transmission Electron Microscope

With the **transmission electron microscope CM30/STEM** Philips is completing their new generation of TEM/STEM instruments. Principal characteristics of this TEM/STEM are the 300 kV accelerating voltage, its further refined electron optics and the new operating concept – the **Microcontroller**.

The high acceleration voltage allows the investigation of specimens of greater thickness giving a deeper insight into the three-dimensional structure of the live-science or materials-science object. In high-resolution structure analysis the point resolution of 0·23 nm can be combined with local chemical analysis by X-rays or diffraction down to an area of 2 nm ∅.

The CM30/STEM is equipped with all necessary facilities to support the advanced technologies applied in fundamental and applied research. The list includes high-resolution imaging in TEM and STEM, small electron probes for local analyses in energy-dispersive X-ray spectroscopy, convergent-beam electron diffraction or electron energy loss spectroscopy.

Key to the operational concept of the CM30/STEM is the reduction of the number of control elements like knobs and buttons to the minimum of those required in a given operational condition. Control functions which vary between the different modes of operation are assigned to 'multifunction controls' while components which are standard in all modes like the focusing operation are firmly assigned to one input control. The concept ensures maximum flexibility for the experienced microscopist with highest degree of simplicity and effectiveness for the scientist using the instrument purely as tool in his activities.

Specific attention has been given to the on-line quantification of microscope data and images or diffraction patterns. An example is the facility for direct read out of lattice spacing from a diffraction pattern.

Chief component of the optical system is the patented **TWIN objective lens**, unsurpassed in its capability of providing the illumination and imaging conditions for high-resolution information.

Philips Industrial and Electro-acoustic Systems Division, Building HKF, PO Box 218, 5600 *MD Eindhoven, The Netherlands.*