routine starts with a few comment lines to facilitate the understanding of the program structure and help if modifications are required.

Availability: Copies of the *EDAUTOCAL* source code are available from the author on 9-track magnetic tape (format 1600 or 6250 b.p.i. ASCII or EBCDIC code) or by direct transmission through the network.

Keywords: Energy dispersive, detector calibration, detector resolution, non-linear least-squares fit.

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Crystallographers

J. Appl. Cryst. (1990). **23**, 223

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 Editoral 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 **Robin John Hawes Clark**, Professor of Chemistry at University College London, has been elected a Fellow of the Royal Society. Distinguished for his application of vibrational spectroscopy, particularly resonance Raman spectroscopy, to the determination of the structures of inorganic compounds. His work on the linear-chain complexes of palladium and platinum has been particularly notable.

Dr **Nicholas Charles Handy**, Reader in Quantum Chemistry in the University of Cambridge, has been elected a Fellow of the Royal Society. Distinguished for his development of very precise methods for the calculation of the structures and spectroscopic properties of molecules. Computer programs which he developed are now extensively used by the chemical community.

Dr **Louise Napier Johnson**, Lecturer in Molecular Biophysics in the University of Oxford, has been elected a Fellow of the Royal Society. Distinguished for her contributions to protein crystallography, in particular for her studies of the mechanism of action of the large complex enzyme glycogen phosphorylase b and its allosteric regulation.

Professor **Harold Walker Kroto**, Professor of Chemistry in the University of Sussex, has been elected a Fellow of the Royal Society. Distinguished for his spectroscopic studies of the structure of unstable molecules, notably leading to the discovery of cyanopolyacetylenes in space. Recent studies of carbon vapour led him to identify new structures, notably the 'carbon football' – C_{60}.

John Osbourne, former Director of the South London Science Centre, has been awarded the Bragg Medal and Prize of the British Institute of Physics for his contributions to the teaching of physics in schools.

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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ChemDBS-3D Links Molecular Modelling and 3D Database systems

Chemical Design is pleased to announce a new member of the Chem-X suite of programs for computer-aided molecular modelling. The new module, **ChemDBS-3D**, is designed to help research chemists indentify potentially active compounds in 3D databases of chemical structures, and is fully integrated with the rest of the Chem-X system.

Using Chem-X, chemists can not only build complex structures quickly and easily, but also calculate a wide range of molecular properties and identify structure–activity relationships. This information may be used to generate templates called pharmacophores which define the spatial arrangement of functional groups and properties common to active molecules of a particular class. Once a pharmacophore has been established, it can be compared with candidate molecules to test whether they are potentially active members of this class.

The most effective way of doing this is to compare the pharmacophore structure with the 3D structures of compounds stored in a database. 3D databases can store data specific to individual atoms, such as partial charges or coordinates, which makes it possible to search for pharmacophores defined by both geometric and electronic criteria.

ChemDBS-3D offers rapid automatic screening of a 3D database for compounds that can adopt the required 3D arrangement of key atoms, as defined by the pharmacophore, in any low-energy (stable) conformation. To save disk space, only one set of coordinates is stored for each molecule – the low-energy conformational space used in screening is generated automatically. The exceptionally efficient screening method enables searches to be performed very rapidly: preliminary tests suggest that a database containing 5500 compounds can be screened in 0·16 s of CPU time on a VAX 8600.

Only compounds which pass the initial screening test (ideally less than 10% of the molecules in the database) are considered in subsequent searches. The chemist may wish to select only compounds containing a particular substructure (a 2D atom connectivity search) and/or with a certain range of values in one or more predefined property fields. This reduces the size of the set of accepted molecules still further.

Preliminary results show that searching can be performed on any combination of 100 fields at approximately 150 compounds per second.

The low-energy conformations of the accepted compounds which actually match the given pharmacophore are then generated automatically.

The results of each phase of the search (a set of molecules or conformations) are stored in a database and can be listed or displayed. 'Hit lists' can be combined using logical operations (AND, OR, NOT *etc*), and may also be imported from or exported to other