

chemical structures to be fitted together by matching vectors as well as by superimposing atoms. Vectors that can be matched in this way include vectors normal to planes, dipoles, and vectors representing other properties set up using the ChemLib module of Chem-X. This allows structures to be fitted according to their vector properties rather than simply by aligning atoms, and can be used, for example, to fit together five- and six-membered rings, or two structurally dissimilar molecules. No other commercially available software package provides this facility. (Fitting is important because it allows the modeller to study the similarities and differences between molecules and their properties by superimposing them graphically.)

Another important new feature is the automatic identification of the local maxima and minima of any function plotted out as a contour map, including wavefunction, electrostatic potential and electron density maps. Dummy atoms are automatically placed at the maxima and minima of the mapped function and may be used to fit two or more maps together. Information on the volume inside each map contour, the surface area at each contour, and the position and value of the maxima and minima is then available to the modeller, and can be written directly to a database. This is valuable when comparing maps to derive structure-activity relationships or to develop pharmacophores.

The January release of the **ChemQM** module of Chem-X now provides a transparent interface to Version 4.0 of the quantum mechanical program *MOPAC*, which has also been implemented on Chemical Design's transputer-based MITIE super-workstation. Other programs already implemented on the MITIE include the molecular dynamics program *AMBER* and the *ab initio* program *GAMESS*, as well as the powerful rule-based Chem-X conformational analysis routines.

Chem-X runs on DEC VAX computers under VMS.

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Low-Cost Workstations for Molecular Modelling

Very competitively priced molecular modelling workstations based on Digital Equipment Corporation's recently announced VAXstation 3100 (the 'desktop VAX') are now available from Chemical Design. The new **P-GRAF 2 workstations** run Chemical Design's powerful Chem-X software and are available in a variety of configurations.

Prices range from only £8000 for a diskless system configured for addition to an existing Chem-X system, to £36 000 for a stand-alone P-GRAF 2 system with 8 Mbyte memory, 19" colour monitor, 912 Mbyte disk, tape drive, tailored VMS environment and Chem-X software. Discounts are available to academic institutions.

For this price, P-GRAF 2 systems offer outstanding computational performance combined with 1024×864 colour graphics running DECwindows. Systems may also be configured to include a high-performance 3D graphics terminal.

Tests have shown that the new P-GRAF 2 workstations run on average three times faster than MicroVAX II-based systems for a range of typical modelling applications. For tasks which involve considerable disk access (e.g. searching databases) the performance of the P-GRAF 2 is even more impressive.

Chemical Design believes that there is considerable demand for a cost-effective modelling workstation that can also be closely coupled with existing chemical information management systems and databases. The VAX/VMS

environment supplied with P-GRAF systems is uniquely well suited to this type of integration.

The P-GRAF 2 systems are the newest members of Chemical Design's growing family of molecular modelling workstations. Others include MicroGRAF systems (based on the MicroVAX 3000) and the top-of-the-range MITIE super-workstation, a transputer-based parallel processing system running at up to 360 MIPS.

All Chemical Design workstations are supplied as integrated packages with their own built-in system management procedures and are fully supported by Chemical Design. They are easy to use and are designed to be operated by chemists, not computer specialists.

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Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

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Thermotropic liquid crystals. (Critical reports on applied chemistry, Vol. 22.) Edited by G. W. Gray. Pp. xii+178. Chichester, England and New York, USA: John Wiley and Sons, 1987. Price £38.

Thermotropic liquid crystals, fundamentals. (Springer Series in Chemical Physics, Vol. 45.) By G. W. Vertogen and W. H. de Jeu. Pp. xi+324. Berlin: Springer-Verlag, 1987. Price DM 134.

A review of these books, by Patrick G. Barber, has been published in the May 1989 issue of *Acta Crystallographica*, Section A, pages 347-348.