# Molecular graphics abstracts

This year's annual meeting of the Molecular Graphics Society was held at the University of Surrey in Guildford, UK, over the weekend of 10–12 April 1987. Below are the abstracts of some of the papers presented at the meeting, followed by an author index.

## 1

AI in conformational analysis

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We are investigating the use of applied artificial intelligence techniques in the development of an expert system, called Wizard, for performing conformational analysis. The utility of this approach has been demonstrated in the domain of acyclic molecules, and we are currently extending the program to include cyclic systems.

The system is used to estimate minimum energy conformations for a given molecule. These structures can then be minimized using a suitable program (such as MM2). Because an 'expert' is used to suggest the conformations for minimization, this combination can be up to $10^5$ times more efficient than purely numerical methods such as torsion angle driving or random search. Another, longer term, advantage is that the development of such a system enables an axiomatic theory of conformational analysis to be formalized and tested.

The program constructs a high-level description of a molecule by recognizing the presence of conformational units and the way in which these units are joined together. This high-level description is then used by the system to reason at an abstract level about the conformational possibilities available to the molecule. The system contains different levels of knowledge which can be used to control the generation of conformations. The utilization of systematic search techniques enables an exhaustive enumeration of the conformations available to the molecule to be performed.

The system has been used to analyse a variety of molecules, its success being gauged by comparing the conformations it suggests with those produced by minimization, and from sources such as the Cambridge Crystallographic Database. We are now extending the program to include the relief of strain in high-energy conformations, new classes of molecules and the uses of symmetry.

## 2

Dynamic modelling of reaction mechanisms in chemical education

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The construction and manipulation of 3D rigid molecular models are today essential components of molecular graphics applications to chemical education. When teaching physical chemistry, it is also important to display some other aspects of molecular structure, such as molecular orbitals, electron densities, interaction potentials, etc. Finally, dynamic modelling applications to chemical education are also becoming very popular, as computer graphics is an ideal tool for visualizing the changes of a system as a function of time. As such, molecular graphics can be advantageously used to represent real-time animations of chemical reactions and molecular vibrations or rearrangements. However, as compared with static modelling, these applications are more elaborate since (i) they generally take place on rather sophisticated graphics equipment and (ii) they require the calculation of a reasonable reaction path.

In the past few years, we have developed a series of dynamic modelling applications on a Vector General calligraphic system, aiming at representing the following unimolecular rearrangements:

- inversion of ammonia,
- interconversion of cyclohexane,
- internal rotation of groups around single bonds,
- dis- and conrotatory ring opening of cyclobutene,
- (1,3) shift of the methyl group in 1-butene,
- pseudorotation of heterocycles,
- rearrangement of polycyclic $C_8H_9$ cations.

In addition, recent applications have been developed on a GDP raster system for the visualization of Diels–Alder reactions, namely the classical [4+2] cycloaddition of s-cis butadiene to ethylene and the cycloaddition of bis(methylene)-2,3 bicyclo[2.2.1]heptane to ethylene.

In most of these applications, the rearranging (or reacting) species are displayed simultaneously with their associated energies and/or orbitals, which provides additional and valuable information when teaching these reaction mechanisms.

The major problems that arise when designing and developing these dynamic modelling applications will be discussed and a 16mm film illustrating some of these mechanisms will be presented.

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