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THE ROLE OF IMAGERY AND ANIMATION IN MOLECULAR GRAPHICS

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Abstract Molecular graphics (MG) is nowadays an essential component of the basic tools used in computer-assisted chemistry. As such, it is employed in numerous applications where its role consists not only in building and visualizing chemical models, but also in simulating complex situations resulting from the dynamic properties of chemical systems. By reviewing some of these applications developed in our laboratories, this paper presents several basic techniques used in MG, the emphasis being placed on the important role played by both imagery and animation.

INTRODUCTION

Molecular graphics (MG) may be defined as the use of computer graphics techniques to study molecular structure, function and interaction. In the last few years, MG has known a spectacular development mainly due (i) to considerable improvements in both hardware and software available in computer-assisted chemistry, and (ii) to recent progress in MG applications of increasing popularity such as drug design or protein crystallography. In these fields, MG techniques have evolved towards a tool complementary to experimental studies and, as such, they have become indispensable

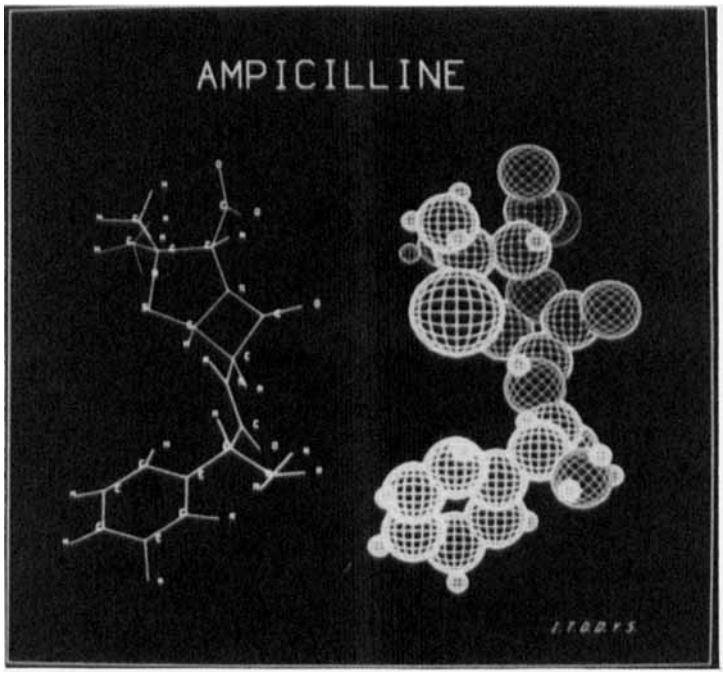

FIGURE 1. Stick (left) and space-filling (right) models of the ampicillin molecule as represented on the MPS calligraphic system.

in research activities.[1] The procedures of simulation and modelization on which MG is based have led to a veritable imagery centered on the interactive construction, visualization and manipulation of the multifaceted aspects of molecular structure, ranging from three-dimensional (3D) molecular models to solvent-accessible molecular surfaces and intermolecular interaction potentials.[2]

MG is also an ideal tool through which to visualize the changes in a system as a function of time: by means of dynamical simulation techniques, it is possible to carry out a real graphic animation of complex mechanisms such as dyna-

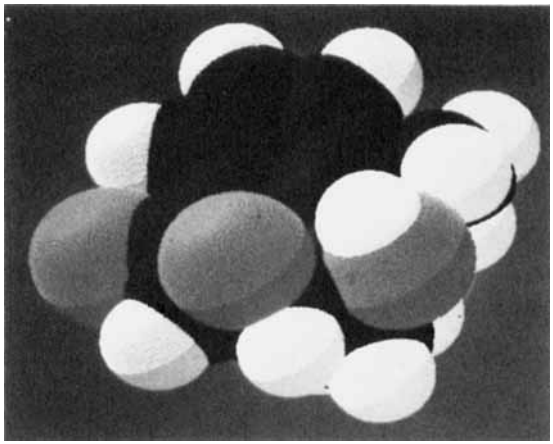

FIGURE 2. Space-filling model of a trioxane derivative as represented on the AED 512 raster system. See Color Plate XVII.

mics of activated processes in proteins[3] and molecular rearrangements [4] or reactions.[5] However, when compared with the modeling of rigid structures, these applications are more elaborate as they require solving the classical equations of motion for individual atoms, in the first case, and calculating using an adequate theoretical model for a chemical reaction path, in the second one.

In this paper, we would like to briefly review some applications recently developed in our laboratories and illustrated in a 16mm film[6] projected during the 8th International Conference on the Chemistry of the Organic Solid State held July 1987 in Lyon.

IMAGERY AND ANIMATION OF STRUCTURAL MODELS

Simple models of complex molecular architectures may be represented on graphic displays: in addition to stick models (Fig. 1), space-filling representations may also be synthe-

sized. They consist of intersecting atomic spheres, represented using solid modeling algorithms on raster systems (Fig. 2) and as mesh or "chicken-wire" spheres on calligraphic systems (Fig. 1). The advantages of using molecular models on a graphics display are obvious: accurate, reproducible representations of the geometrical structures are easily obtained and it is possible to manipulate them interactively so as to examine every detail. In addition, several structures may be simultaneously manipulated, which allows us to superimpose them and to rapidly evaluate their similarities and differences as well. Finally, interactive docking of inhibitor molecules into proteins such as enzymes may be nowadays simulated on sophisticated graphics systems, which may be used as an elegant tool for predicting the active sites of these species.[1]

However, because the assembly of atoms constituting a molecular skeleton never remains rigid under normal conditions, real time modeling is also of prime utility. Calligraphic and high quality raster systems as well have proved excellent for representing complex mechanisms such as structural fluctuations in large biological molecules and concerted deformations encountered in molecular vibrations and rearrangements. As examples, the rearrangement of the $C_8H_9^+$ polycyclic carbocation[7] (Fig. 3) and the conrotatory ring opening processes of the cyclobutene molecule[4] (Fig. 4) have been recently reported. In addition, the stereochemical aspects of the Diels-Alder reaction have been illustrated by computer graphics animated models[5] (Fig. 5), in an application enabling the user to visualize step by step the detailed features of the reaction mechanism, which also underlines the great potentials of MG for teaching

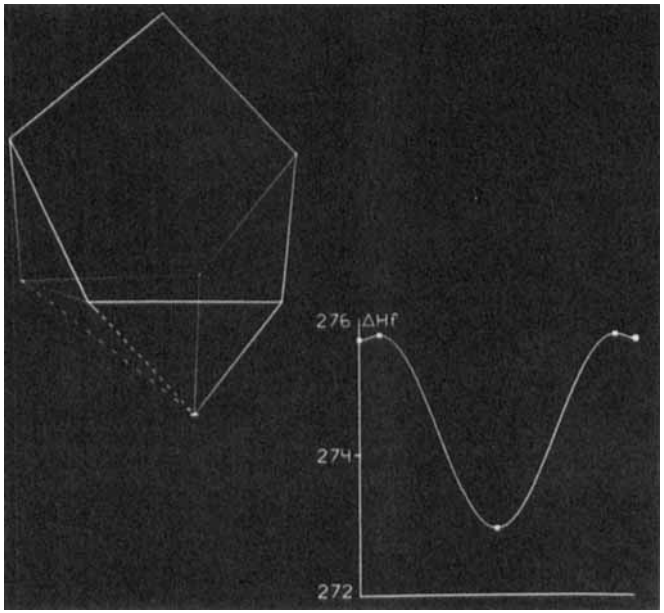

FIGURE 3. The $C_8H_9^+$ cation represented at a particular step of its rearrangement together with part of the minimum energy reaction path. Non-classical (longer) bonds are depicted by dotted lines.

chemistry. However, in most of the applications described so far, the indispensable role of theoretical chemistry should be stressed, as MG techniques are most of the time used merely for representing in an elegant way the results of theoretical models. As an example, when the actual geometry of a species is unknown, theoretical conformation searches have to be carried out before any further MG investigation.

IMAGERY AND ANIMATION OF ELECTRONIC PROPERTIES

As sophisticated as they might be, the different MG representations of structural models would be incomplete without

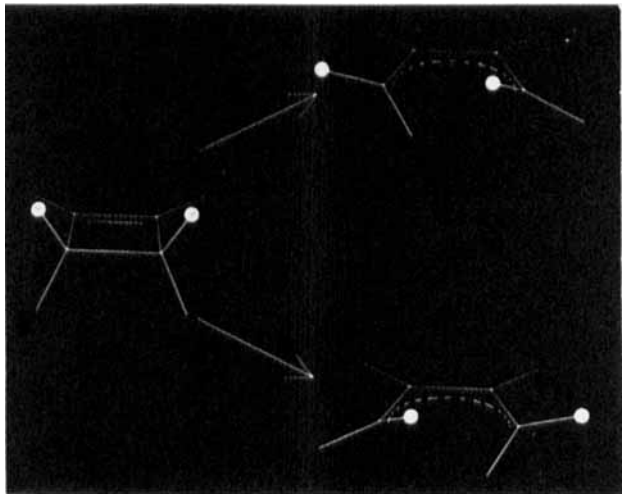

FIGURE 4. Snapshot of the sequence illustrating the two possible conrotatory ring opening processes of cyclobutene.

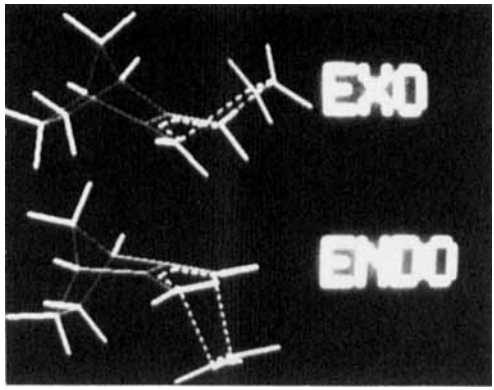

FIGURE 5. Transition states of the Diels-Alder cycloaddition (exo and endo modes) of bis(methylene)-2,3 bicyclo(2.2.1)heptane to ethylene. See Color Plate XVIII.

the capability to superimpose electronic properties such as electron densities, interaction potentials for possible associations with reagents, solvent-accessible surfaces, etc. To this end, computational quantum chemistry models have to be used for calculating the properties, in conjunction with graphics procedures and algorithms allowing us to generate 2D contour maps, 2D color-filled contour maps[8] or more sophisticated 3D graphics representations.[8-10] However, the MG imagery rapidly reaches a high level of complexity as several objects with different structures are now to be simultaneously displayed. The graphics facilities of modern modeling systems allow us to solve this problem by offering the possibility to represent interactively and manipulate complex images made of several hundreds of thousand vectors or dots. However, full animation of these images, in the manner described above for geometrical structures, is possible in a limited number of cases now, but there is no doubt that future progress in graphics hardware will make it possible.

Molecular electrostatic potentials (MEPs) are undoubtedly among the most useful properties employed routinely in MG applications. At large distances, i.e. beyond van der Waals radii, electrostatic interactions are indeed predominant and MEPs may be used as an approximate model for the prediction of the most reactive sites for electrophilic and, to a lesser extent, nucleophilic attack.[11] Indeed, MEP minima (i.e. the most negative regions) correspond to sites of electrophilic attack, the model electrophile being a bare proton, whereas the largest positive MEP values on the van der Waals surface may be considered as probable sites of nucleophilic attack, the model nucleophile being then a bare electron.[12] As examples, 2D contour levels of the MEP of γ

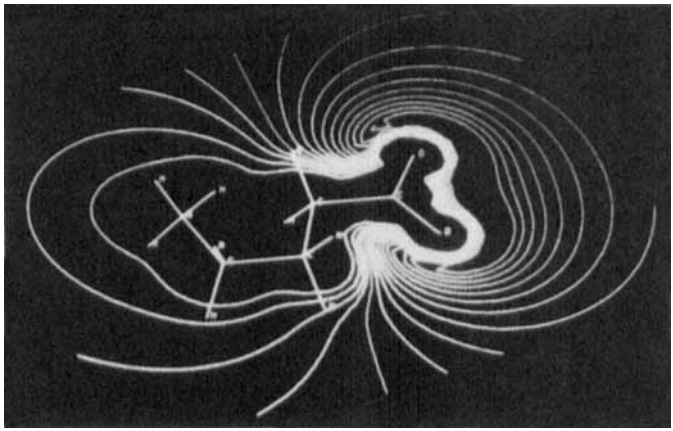

FIGURE 6. 2D contour levels of the MEP of γ-amino-butyric acid, assuming a planar geometry for this compound.

amino-butyric acid are presented in Figure 6, whereas an isometric 3D representation as a mesh surface of the repulsive (i.e. positive) part of the MEP of mescalin is displayed in Figure 7. In the latter case, it is seen that the clipping facility of the graphics system allows a simultaneous display of the molecular skeleton, which facilitates the interpretation by visualizing the MEP surface from inside. 3D solid models can also be obtained on raster systems as an alternative to mesh surfaces on calligraphic devices. In any case, whatever the type of representation to be chosen, the display and manipulation of both molecular properties and skeletons is of tremendous help for the design of new molecules, which allows us to conclude that the combined use of computational quantum chemistry and molecular graphics has opened new horizons in research strategies in chemistry and biology as well.

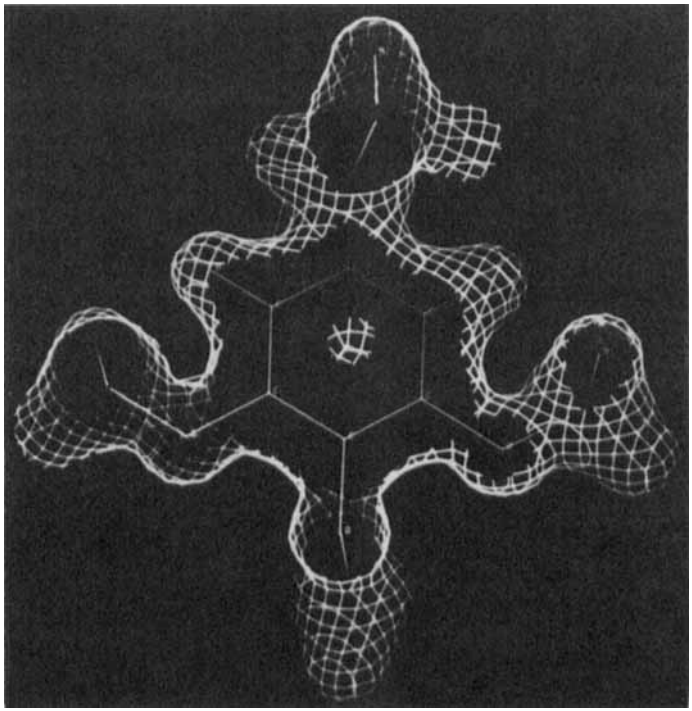

FIGURE 7. Isometric 3D representation of the repulsive MEP (+100 kcal/mol) of mescalin, with the clipping option allowing visualization of the molecular skeleton.

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