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COMPUTERS AND CHEMISTRY

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Resource Related Research - Computers and Chemistry
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Research Highlights (1977-78)

1. Stereochemistry in Structure Elucidation.

The set of computer programs developed at Stanford as tools for molecular structure elucidation have been considerably enhanced by the addition of 3-dimensional structural information. The programs can now deal with some basic geometrical properties of molecules that are essential for understanding their biological significance. Research progress this year has resulted in extensions that allow computation of stereoisomers (alternative structures differing in 3 dimensions but having identical connections among atoms). Thus geometrical variations on structural hypotheses can be presented as well as topological variations.

2. Unified Package for Structure Elucidation.

Significant progress was made in unifying the computer programs for structure elucidation into a coherent package that is easily understood and used by chemists for complex biomolecular structure problems. Powerful tools are now well integrated for defining problem constraints, producing plausible solutions to structure problems, reducing the sets of alternative solutions with information about biosynthetic pathways, testing the alternatives, and suggesting new tests for further discrimination. New tools currently under development will be integrated into this same package.

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