18.5-2 ARTIFICIAL INTELLIGENCE IN CONFORMATIONAL ANALYSIS. A.R.Leach, D.P.Dolata, C.K.Prout. Chemical Crystallography Laboratory, 9 Parks Road, Oxford, OXI 3PD, U.K.

WIZARD is an expert system designed to estimate minimum energy conformations of a molecule. In contrast to numerical methods for generating such structures the program uses rules about conformational analysis to **reason** about the conformational properties of a molecule at an abstract level, in a fashion similar to that used by a human expert performing the same task.

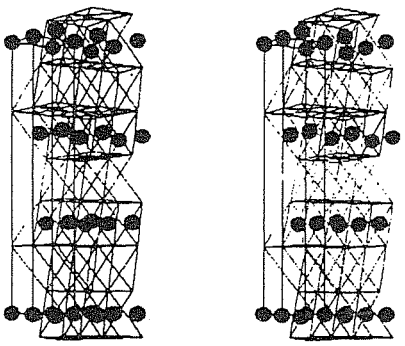
The program constructs a high-level description of a molecule by recognising the presence of **conformational units** and the way in which these units are joined together. A unit is a group of connected atoms (e.g. a cyclohexane ring) about which the system has some knowledge. This high-level description is then used by the system to reason at the abstract level about the conformational possibilities available to the molecule. An abstractly defined conformation is **suggested** by the system, and **criticised** to see if any problems exist. It is then constructed by the stepwise joining of conformational templates, with more criticism at each stage. When the conformation has been fully constructed it is possible to **resolve** any problems that may exist. By using systematic search techniques an exhaustive enumeration of the conformations available to the molecule can be performed; knowledge about the units and the way in which they can be joined together is used to ensure that this search is as efficient as possible.

The conformations generated by WIZARD may subsequently be submitted to an energy minimising program for further refinement; the combination of WIZARD plus the molecular mechanics program MM2 can be up to 10^5 times more efficient than purely numerical methods such as torsion angle driving. A further benefit is that by using techniques derived from research in Artificial Intelligence an **axiomatic theory** of conformational analysis can be easily formalised and tested for its validity. This is enhanced by our choice of Prolog, which is a computer language based upon the formal theories of logic, for the design of the reasoning and controlling parts of the system.

18.5-3 **INORGANIC GRAPHICS FOR MICROCOMPUTERS.** **By B.O. Loopstra, R.A.J. Driessen en H. Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.**

In many curricula inorganic crystal chemistry is the first time students are faced with the three dimensional results of crystallography. However, it is also the first time teaching does not always realise its goals entirely because to get the proper three dimensional impression of these simple structures is not easy. For instance to understand the difference between octahedral and tetrahedral holes is not trivial. Models are very essential in teaching crystal chemistry; mostly "hard-ware" models are used extensively. Another tool by means of which structures can be studied and manipulated quickly in stereo, is computer graphics. This technique can well assist in teaching crystal chemistry provided that an inexpensive solution can be realised.
Therefore we changed our molecular graphics programs for IBMPC and Commodore64 (Shareware of the Laboratory for Crystallography of the University of Amsterdam) such as to accomodate inorganic crystal structures rather than organic molecular structures. So the space group symmetry is given a very prominent place in the new program. Moreover, since in our department inorganic structures are studied regularly, it was also tried to make the interface between the user and the program such, that it could also assist easily in analysing research problems.
The interactive graphic program provides the following options: to display stick, ball and stick or ball models, in mono-, or stereo-view, with or without labels, and the model can be rotated. The user may vary the part of the crystal to be displayed in the picture as he/she wishes. There are no limitations on x, y and z, neither on search radii and plot radii. The view matrix is identical to that of PLUTO and can be displayed at any moment. Hard copy images can be made by the normal cheap printers in graphic mode, examples of which are shown on the next page.

Stereopair of $CdCL_2$.



For teaching the program is exellent; students very quickly get the main points of crystal chemistry. For this purpose an exensive library of essential structures accompanies the program. Also for research problems the program functions very nicely; it is well known that sometimes very many pictures of a structure have to be made before the underlying principles are clear. By means of the program a large number of them can be produced and studied in a relative short time. Even an error in a picture of a very well known textbook have been detected.

A O-Ca-O layer from $CaTe_2O_5$.