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GENERATION AND MANAGEMENT OF THREE-DIMENSIONAL STRUCTURAL DIAGRAMS FOR ZEOLITES ON STANDARD GRAPHICAL SUPPORT OF AN IBM-PC

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The crystal structure of zeolites is a complex arrangement of alumino-silicate tetrahedra, characterized by the presence of peculiar channels and cavities. Computer aided molecular graphics can represent an advantageous and powerful alternative to the classic solid model for the three-dimensional representation of this kind of structure, with the great advantage of a possible software device which just requires as input file the space group symbol and the few atomic coordinates of the independent atoms of the framework. The commonly used molecular graphics computer programs are however mostly unsuitable and some are cumbersome to use, since they have been designed mainly for organic structures and therefore limited to stick and ball or space filling models.

The most significant representation of crystal structures of inorganic compounds is the idealized polyhedral drawing, with all the facilities of different colours or different shadowing. In an inorganic structure a polyhedron or a set of polyhedra can be considered as the equivalent of the unique-molecule in an organic lattice. Even when programs expressly written for inorganic structures are available, as far as the authors know, they are limited to the representation of simple fundamental polyhedra. Unfortunately zeolite polyhedral building blocks are much more complex than tetrahedra or octahedra, so that a convenient representation and manipulation of these models requires a more sophisticated approach.

The basic idea of the present work is the implementation of a molecular graphics package, expressly for inorganic structures and able to perform the two most significant representations of zeolite structures, i. e. framework model and polyhedral drawing.

Since nowadays micro and personal computers offer low cost independent workstations, with relatively high graphic and computing performances, they represent a convenient substrate for this purpose. Moreover they are spreadly diffused and, in comparison with mainframes, they allow an easy direct access to system resources.

VIDEOZEO is a completely original package of programs written and implemented for IBM-PC's or compatibles, running under MS-DOS operating system and able to represent zeolite structures as both polyhedral

blocks and framework models. In order to facilitate the access also to non crystallographers,which represent the major users of molecular graphics computing, the package has been made as much as possible user-friendly. It is characterized by a menu-aided processing and supplies an interactive run time user guide and error checking. The package include a card image (80 columns wide) full screen file editor and the most common MS-DOS commands allowing file management, leaving the knowledge of the operating system out of consideration. Nevertheless a full interfacing to MS-DOS is assured.

Peculiar features of the package are the possibility of perspective view with default or user defined vantage point setting, rotation around a user defined axis and removal or dashing of hidden lines in the polyhedral representation.

VIDEOZEO has been developed in a modular way: a functional diagram is shown in Fig. 1. The core of the package can be devided into four principal blocks, namely the coordinates generator, stick modelling, polyhedral modelling and picture display unit.

The first one is called when a new structure is considered. A limited user's crystallographic skill is required only the space group symbol and the independent coordinates are needed to generate the whole unit cell content. Options are provided to link adjacent unit cells.

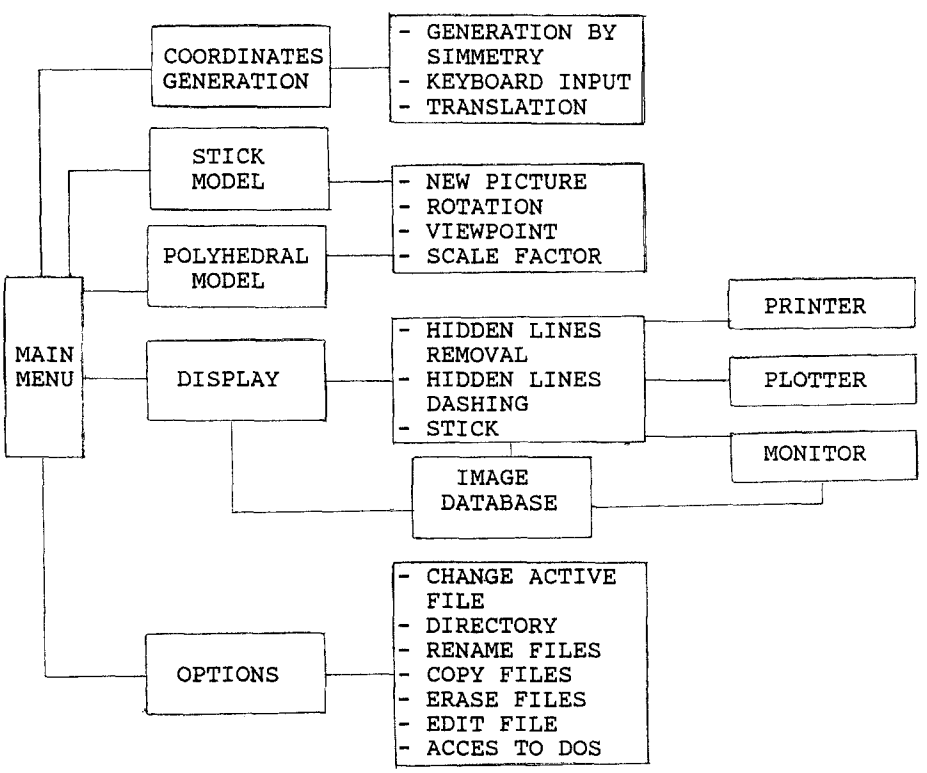

Figure 1. Functional diagram of the package

The second and third block provide respectively stick and polyhedral diagrams. In the latter case the program recognises automatically the faces of polyhedra, once the center are given. The algorithm is based only on the connectivity matrix and this permits the generation of non planar faces which are typical of some zeolite building blocks (e.g. the cancrinite 11-hedron, the chabazite 20-hedron and the gmelinite 14-hedron). The standard version of VIDEOZEO can recognize faces with up to eight edges and represent structures with up to 64 solids of up to 50 vertices. These limits can be however extended depending on the system memory configuration.

The fourth block performs output display for different graphic supports, such as IBM standard colour display, matrix printers (IBM-PC Graphic Printer or HP Laser Jet Plus) and plotters (CALCOMP M81 or M84). The pictures generated may be stored on hard or floppy disk forming an user's image data base, which can be managed inside the package. The high retrival and display rate of the stored figures allows to simulate animation. Some examples of zeolite framework as produced on a colour screen display are shown in Fig. 2.

The package is available on request from the Istituto di Strutturistica Chimica of the University of Parma.

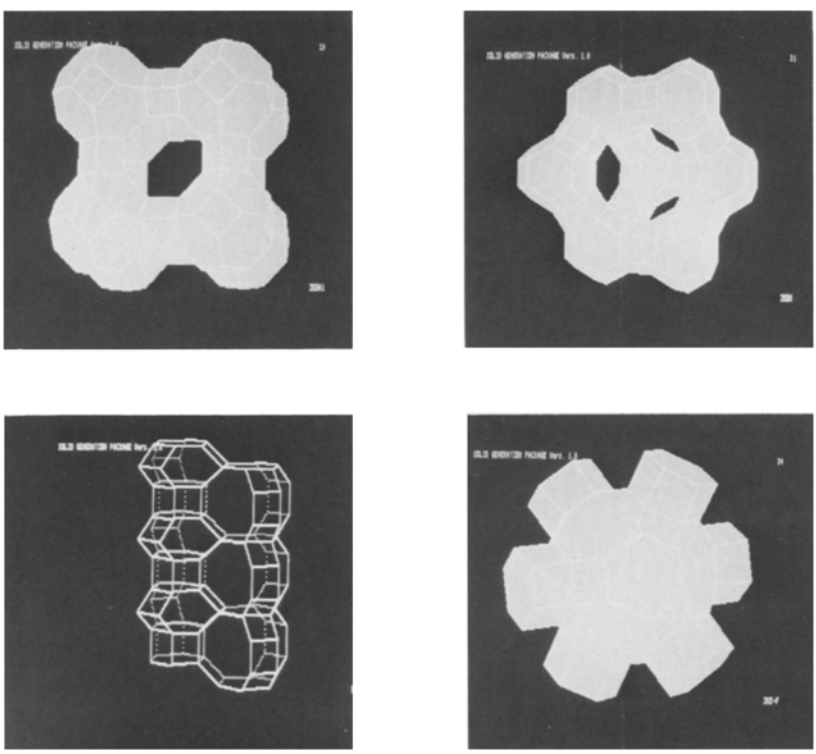

Figure 2. Examples of screen display of zeolite frameworks: a) Zeolite A; b) Zeolite X; c) Offretite; d) Zeolite ZK5