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MOLECULAR EDITOR DEMO

public-domain demonstration version of a software-based molecular model kit developed at Drexel University

With Molecular Editor, you can construct and view molecules or crystal structures of over 100 atoms in a three-dimensional representation (this demo version permits molecules of up to 15 atoms only). Atoms or ions are drawn as patterned circles with radii proportional to the element's radius. Bonds are drawn as either simply patterned rectangles for single, double, triple, or other bond types, or as lines (a wireframe representation). You can draw molecules in a number of ways: all atoms and all bonds, atoms only, or bonds only.

You can rotate a molecule through any angle about any of three orthogonal axes, either by single steps or continuously. You can also rotate only a portion of a molecule with respect to another portion, thus producing conformational changes about a single bond. You can place any atom at the origin of the screen coordinate system (the center of the drawing window), and you can orient any bond attached to that atom along the x-axis. You can invert the coordinates of any or all atoms through the origin. You can also reflect any or all atoms through the XY, XZ, or YZ planes. You can rescale the molecular display, or independently rescale the whole set of atomic radii while leaving bond lengths unchanged. This latter feature permits continuous variation from a touching-hard-sphere model to a bonds-only model.

You can edit any molecular structure from the screen. You can change covalent bond types, make atomic substitutions from a palette of 10 atom types, and delete atoms or bonds using the backspace key. The default palette contains the elements C, H, O, S, N, P, F, Cl, Br, and I, but on a 512 k Mac these may be easily changed to any element of the periodic table, each with its own editable pattern.

You can measure the distance between any two atoms, the angle between any two bonds attached to the same atom, and the torsional angle about a bond. You can change the perspective, or viewing angle, from which the molecule is seen.

The standard Macintosh commands Cut, Copy, and Paste are implemented in three dimensions in Molecular Editor. This feature allows you to build virtually any molecule from an initial collection of basic structures and functional groups.

In the full release of Molecular Editor (not in this demo version), you can store structures on disk and retrieve them as Molecular Editor files. If you rotate a molecule, you can see either the transformed cartesian coordinates or the original coordinates in the coordinate table. You can choose the rotated form as the identity, or at any time revert to the original coordinates stored in the Molecular Editor file for that molecule.

You can open up to 20 files at one time and flip the display manually between them. If you are running Molecular Editor on a 512 k Mac with at least 256 k bytes of memory

allocated to the program, you can also run through a sequence of open files rapidly (about five frames per second) using an animation feature.

On a 512 k Mac in the full release of Molecular Editor, you can print the molecule in the active window to a printer (Imagewriter or Laserwriter) directly from Molecular Editor. On a 128 k Mac, a print file is spooled to the disk, and can be printed from the Finder using the Print command. You can also print out the coordinate table as well as the connectivity table (a table indicating which atoms are connected to other atoms by what types of bonds). All printing is disabled in this demo version. There is an extensive Help Menu which explains the features of Molecular Editor in more detail.

With this demo disk, we have included a few files of structures we have built and use in undergraduate chemistry and materials engineering courses at Drexel: an organic molecule, a crystal structure, and several basic shapes. [I haven't found those files - TwZ] Try the Copy and Paste procedures to modify the organic molecule by adding functional groups. Try drawing the crystal structure with atoms only, bonds only, and both; then try changing the points to some atom type and redisplaying. Open all four shapes (they will look identical at first) and identify the shape by rotating about various axes. Then use atomic substitution to make an actual molecule which has that structure.

As of February 26, 1986, final arrangements are being made for the sale of the full version of Molecular Editor. If you are interested in the full version, write Special Projects Coordinator, Microcomputer Program

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for the current status of the availability of Molecular Editor.