StrukEd—The Structural Chemistry Interface

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StrukEd is a PC program which draws chemical structures. It is mouse-driven and menu-oriented and can generate 2D or 3D structures which can be transferred *via* the clipboard to other Window applications.

INTRODUCTION

The program StrukEd is a molecule-editor, handling chemical structures in a very comfortable way, like drawing the valence formula on a sheet of paper. The program is menu-oriented and mouse driven. To speed up drawing, fragment and group libraries can be used, expanded, and changed by the user easily.

From the 2D drawing (internal representation as Connection Table, CT) the program automatically generates reliable 3D structures, which can be modified in all degrees of freedom. The different modes of visualization of structures give a good three-dimensional impression to the user.

Fast internal calculation routines can be used to generate atomic charges, Hueckel Molecular Orbitals, and polarizabilities. The calculated numerical values are visualized inside the structure.

Structural data can be read from commonly used data formats. The structure can be exported as input files for molecular mechanics and quantum mechanics calculations. The essential output from these calculations can be filtered by StrukEd for graphical representation.

Within the Windows environment the user can very easy transfer structural information via the clipboard or DDE (dynamic data exchange) to other Windows applications (text processing, spreadsheet calculation, or graphics).

Context-sensitive helps or the printed manual (about 100 pp) describes all the capabilities of StrukEd and gives references to the programmed methods and algorithms.

StrukEd has an universal, user-friendly, and easy to use graphical interface for structural chemistry. It can be successfully used to support structural thinking in chemical education by quantitative numbers and instructive pictures or to do first steps in molecular modeling.

SYSTEM REQUIREMENTS

The minimum system configuration for using StrukEd is a PC 386 with 4 MB RAM, 5 MB free space on hard disk, a VGA card with 16 colors and an operating system of Microsoft Windows 3.11 or higher.

The program and the examples are provided each on one floppy disk.

An optimal computer configuration is a Pentium processor based PC and with fast graphics card of at least 256 colors.

THE INTERNAL STRUCTURE OF STRUKED

Most of the features of the program can be seen from a survey of the pull-down menus.

In addition to the menu functionality listed in Table 1, the program has element symbols, types of chemical bonds, and fragment and group libraries available. Depending on the content of the window (2D or 3D structure) one can switch between both of these two representations. ZOOM, ROTATE, CENTER, and MOVE buttons change the visualization by moving the mouse. The display options (wire, stick, ball and stick, CPK-model, perspective, illumination and position of the light source) can be chosen after clicking the "OPTION" button.

STRUCTURE INPUT

The program helps to avoid errors at the structure entry, by exploring the drawn structure for chemical plausibility. By pushing the DRAW button, the structure will be redrawn by updating the free valences with hydrogens and scaling the valence formula to fit into the window. The brutto formula and the molecular weight fields are also updated. For each atom one can change the bonding number. One can also assign charges or radical character to atoms. 2D structure information can be stored in a compressed CT in sequential files.

GENERATION OF THREE-DIMENSIONAL STRUCTURES

From the connection table of the 2D structures StrukEd generates very fast realistic three-dimensional structures by heuristic rules.[1]

For cyclic conformers, the user can interactively choose from the generated structures (e.g., in the six-membered cyclohexane: chair, boat, or twist conformation). There are tools for changing the geometry of substructures (e.g., cis/trans isomers for double bounded substructures) and chiral centers by rotation, reflection or corner-flipping. The UNDO function can back up the last 100 steps of structure modification. The use of "dummy" atoms is very helpful in the construction of complex structures (e.g., for placing cyclopentadienyl ligands as templates to coordination compounds) and for the orientation of structures with respect to the coordinate system.

All degrees of geometrical freedom (bond length, bond angle, and torsional angle) can be changed interactively.

INTERFACES

Interfaces to molecular mechanics, semiempirical, and ab initio quantum mechanics programs are available from the menu for generating input jobs for external application programs (normally running on UNIX workstations). The

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Table 1. Menu Structure of the Program StrukEd

File	
New	Open a new empty document
Close	Close current document
Open...	Load a structure in a new document
Save	Save structure from current document
SaveAs...	Save the structure in new file
Import...	Import a structure in new document
Export...	Export the structure from current document
Print	
All In File	Print all structures of the database-file
Structure...	Print current document
Printer Setup...	Change printer settings
Exit	Exit the program
Edit	
Undo	Undo the changes in structures
Select...	Select atoms for other actions
Delete	Delete selected atoms
Cut	Copy selected atoms in clipboard and delete
Copy	Copy selected atoms in clipboard
Paste	Paste atoms from clipboard
Options	
Property...	Display molecular properties
Surface...	Change settings for surfaces
Atom Display...	Change settings for atom-display
System-Settings...	Change program-settings (e.g. Fonts, Units, ...)
Load-Settings...	Change load-settings (e.g. auto-orientation, auto-center, ...)
Edit-Settings...	Change settings for edit-operations (e.g. Updating of bondlength)
Clipboard-Settings...	Change settings for Clipboard-Export
Export-Settings...	Change options for structure export in file (for Gaussian, MOPAC, ...)
Save On Exit	Activate the save options on Exit Feature
Save Settings now	Save all settings
Structure	
Build-3D-Struc	Generate 3D-coordinates from 2D-structure
Stereoconformer	Change the stereo-chemistry of structure
Ring Conformer	
Change	Change the conformation of rings (chair, boat)
Flip Corner	Flip a corner in a ring
Numbering	
Define	Change the numbering of atoms interactively
AtomType...	Automatic numbering of atoms by type
Change Geometry	Change geometry (Distances, Angles, Torsion Angles)
Centre of Mol	Set center of molecule between all selected atoms
Mass weighted	in mass average
Coord weighted	in coordinate average
Dummy Atoms	Set a dummy atom between all selected atoms
Mass weighted	in mass average
Coord weighted	in coordinate average
View	
Geometry	Measure geometry (Distances, Angles, Torsion Angles)
Z-Matrix...	Generating and editing Z-Matrix
Fit-Structures...	Fit two structures and calculate RMS-value
Monitor...	Set monitor on geometry for measure
Orientation	
Settings...	Change settings for automatic orientation of molecule
Plane Orientation	Orient molecule in a plane
Axis Orientation	Orient molecule on coordinate axis
Optimal Show	Calculate a optimal show for molecule
New Image	Calculate a new image for 2D-structure
Calculate	
HMO	Start a Hueckel MO-calculation
Export	and export the results in external Text-Editor
Graph	or display the results in Window
Charges	Calculate charges
PEOE	with PEOE-method
Del Re	with method from Del Re
Cheleq	with Cheleq method
Mol.-Polari	Calculate molecular polarisability
Mom.of Inertia	Calculate Moment of Inertia
Surface	Calculate vdW-surface
Quality	Calculate electrostatic potential on VdW-surface
Tools	
Makro	
Define...	Define a sequence of commands
Start	and start it
DDE-Export	
Init...	Initiate the DDE-export
Export	and export the selected values
DrawMO...	Display MO-diagram
Vibration...	Display the modes of vibration
FileManager	Start the Windows File-Manager
Recorder	Start the Windows Recorder
Editor	Start an external Text-Editor
Window	Show and hide Windows in StrukEd
Rotate Axis	Window for rotation around several (coordinate-)axis
Output-Window	Window with Text-Output from measurements and calculations
Status-Window	bottom and top Status-Windows
Select-Window	the Window with settings for input and editing structures
Help	
Mouse-Help...	Display/hide a Window with on-line Help-Text for Mouse Commands
About	Display the About Information

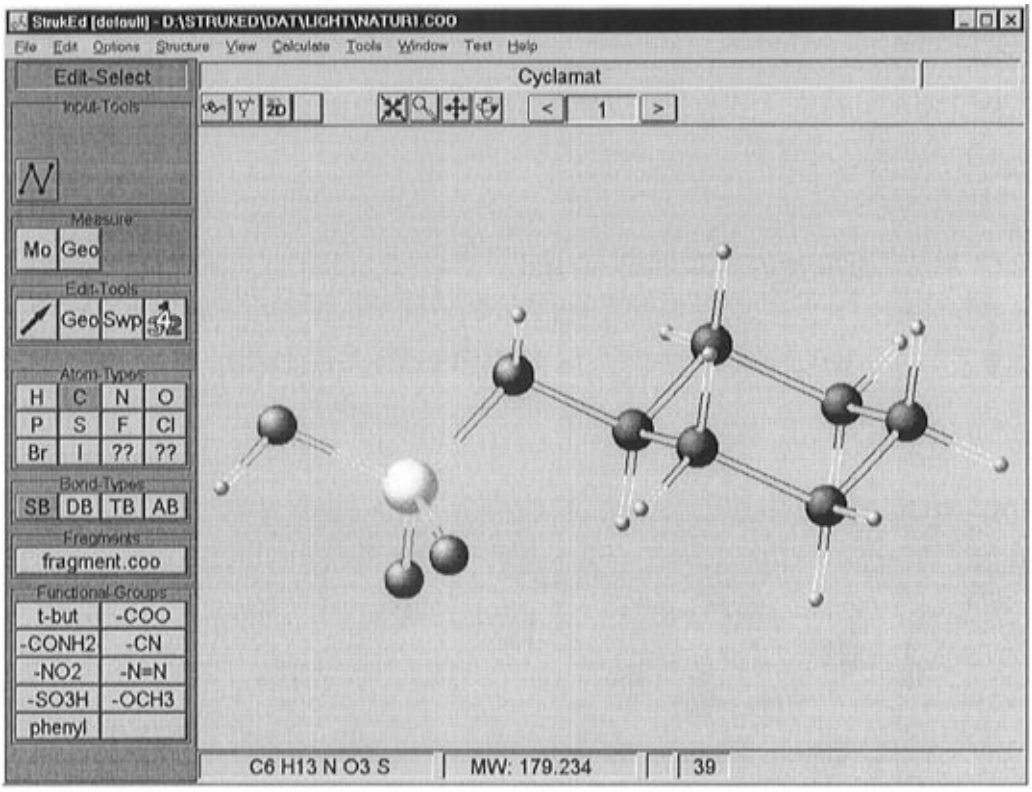

Figure 1. Shows the working area of the StrukEd (Cyclamat is the first of 39 datasets in the file).

essential data from these programs can be imported back to StrukEd for visualization of structures and calculated properties.[2] The following interfaces to application programs are available: MOPAC, PIMM, ZINDO, GAUSSIAN94, TURBOMOLE, and Z-matrix to other programs. For MOPAC nearly all interesting results, like charges, populations, molecular orbitals, and vibrations can be visualized or animated with the structure.

For comparison of similar structures, StrukEd can fit two substructures and calculating RMS values. Distances and angles can be selected for display in a window or for drawing to the picture of the structure. Up to 20 documents can be opened simultaneously in separate windows for comparison of structures and charge distributions.

The program can read the file formats of important structural databases: CSD, PDB, MOL, SMD, and others.

SOFTWARE DISTRIBUTION

The software package StrukEd is available within the pool of BRUKER spectroscopic programs and can be ordered from the Umschau-Verlag, POB 1247, D-58207 Schwerte (Germany); Tel. ++49-2304-81854; Fax ++49-2304-83271; e-mail: clb@ellmer.un.eunet.de. The price for the slightly reduced version of StrukEd LITE is 295.-DM (approx. $200) including the printed manual. This LITE version can handle only one document at the same time, and the interface is reduced to the semiempirical MOPAC program.

For further details please see our www homepage http://ibm530.chemie.uni-halle.de/usr/www/software.htm or contact boegel@chemie.uni-halle.de for any questions or remarks.

REFERENCES AND NOTES

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(2) Dettmann, J.; Bögel, H.; Thiele, H. StrukEd - ein universelles Grafikinterface für die Strukturchemie. *Software Developments in Chemistry*; Springer Verlag: Berlin, Heidelberg, 1995; pp 235−239.

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