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TECHNICAL NOTE

UNIVIS-2000: An indigenously developed comprehensive visualization package

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This paper describes features of UNIVIS-2000, an indigenously developed MS-WINDOWS-based package for physicists, chemists and molecular biologists interested in modelling medium-sized molecules and visualization of molecular scalar functions defined over a regular grid or on a variety of molecular surfaces. The code is written in C^{++} using freely available public domain graphics library, COSMO3D. The package provides essentially all the traditional features of molecular viewing softwares as well as visualization of scalar fields using planar pixel plots, contours and isosurfaces. A novel feature of UNIVIS-2000 is its ability to create composites of the functions, allowing scientists to quickly view an overall effect of one function over the other. For chemists, such a feature presents an opportunity to view the effect of one molecule on another with a change in their relative positions, providing valuable guidelines for exploration of molecular interactions without doing expensive calculations.

THE complexity of molecular systems engenders huge amounts of data generated by a variety of experiments or simulations. In view of this, visualization has become an invaluable tool for the modern chemist. There are several freely available packages[1–8] for chemists that allow viewing of molecules and a variety of molecular surfaces. Connolly[9] has recently presented an excellent and comprehensive review of the computation and visualization of molecular surfaces.

UNIVIS-2000 is a visualization package for computational physicists, chemists and biologists who are not only interested in carrying out molecular modelling, but

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also need a tool for the examination of scalar functions defined over a regular grid. It may be noted[10,11] that the modern chemist is interested in the visualization as well as topography mapping of a variety of molecular scalar fields in order to obtain condensed information regarding their significant features. Molecular electron density (MED), the Laplacian of MED, molecular electron momentum density, molecular electrostatic potential (MESP) as well as the electron localization function (ELF) are some of the scalar functions that have been subjected to such detailed probing[10,11].

The present version of UNIVIS-2000 has been written for MS-WINDOWS using the COSMO3D library. COSMO3D is a scene graph API developed upon OpenGL (www.opengl.org) and made freely available by Silicon Graphics (SGI). A scene graph is a tree structure used for organizing and controlling the rendition of its constituent objects. COSMO3D comes as a C^{++} graphics library and it allows applications to use a higher-level interface than the lower-level OpenGL language that it is based on. Further details can be found on SGI's website (www.sgi.com).

Molecular visualization tools

UNIVIS-2000 provides a set of tools that a modeller may find very handy. These include display of ball-and-stick, tube, line, space-fill and van der Waals models. Weak hydrogen bonding, whenever present, is displayed. The package also allows interrogation of various attributes such as bond lengths, bond angles and dihedral angles. For generation and manipulation (changing lengths and angles) of existing molecular geometries, the package provides a *Z*-matrix editor. UNIVIS-2000 allows manipulation of molecules in place, unlike most of the molecular modelling packages, which place the first atom at (0, 0, 0), the second atom on one of the standard axes, and so on. UNIVIS-2000 can handle multiple systems at a time. Geometry of an individual molecule being viewed can be manipulated and transformed (rotation/translation) independent of the geometries of the other molecules and it can also be duplicated many times to form a cluster of molecules. In order to facilitate modelling, UNIVIS-2000 is provided a facility to track the distance between the selected pairs of atoms. The tracker displays the distances in Angstrom or a.u. as requested and these are updated whenever there is relative movement. The user can also change the colour of the weak bonds, tracker, atoms and the atom labels and also vary the background colour.

With UNIVIS-2000, one can animate various vibrational frequency modes and geometry optimization steps, whenever corresponding data are provided. Chemists can also view the IR spectral graph on screen and can view the animation of the selected frequency mode. Figure 1 displays the IR spectrum of anthracene molecule computed at the HF/6-31G** level along with its optimized structure, while Figure 2 depicts the HF/6-31G** optimized structure of formamide...$(H_2O)_{12}$ along with the tracker to probe the desired bond lengths. For geometry optimizations the user has an option of looking at any intermediate geometry during the course of optimization or get an animation of the progress of geometry optimization. With UNIVIS-2000, the user can also build a new molecule by entering the data in the form of a *Z*-matrix.

Visualization of molecular scalar fields

Scientists dealing with scalar fields[10] will also find UNIVIS-2000 useful. Some of the popularly used scalar functions such as MED, molecular electrostatic potential (MESP), the highest occupied molecular orbital (HOMO), as well as the lowest unoccupied molecular orbital (LUMO) are of interest to the molecular scientists' community at large. These functions are normally evaluated over a regular grid for further visualization and analysis. In UNIVIS-2000, the user is provided with a standard set of visualization tools such as:

- Standard and oblique textured cuts through the data set.
- Contours in 2D and 3D and on oblique cuts.
- Constant-valued (Iso) surfaces.

With textured cuts, the user can view the function variations across the desired area, whereas contours and iso-surfaces help in tracking the desired function value over an area or volume. These variations in the function can be quickly viewed over a specified range of function values using the 'Quick View' option. The package provides with a facility to colour iso-surfaces with a different front and back colour – such a tool is useful in unambiguously identifying the inner and outer parts of the surface. The transparency of the iso-surfaces and the textured planes can also be adjusted to visualize the unseen regions of the molecule. UNIVIS-2000 also provides for visualization of a continuous range of function values through what are called as fuzzy volumes. Fuzzy volumes are shown as a set of dots over the region defined by two bounding function values – these are thus a generalization of iso-surfaces, where both function values are the same. The dots can be coloured depending on the function value they represent, thus generating a colour-graded fuzzy volume. The colour range is displayed on the bottom right hand side of the screen when the property data set is loaded.

As with molecular geometries, UNIVIS-2000 can handle multiple data sets (functions) at the same time. Since UNIVIS-2000 can juggle between multiple mole-

cules and data sets at the same time, the user can (especially for large systems) split the evaluation of the property into smaller sections in different files. Moreover, the iso-surfaces or molecular surfaces can be textured with any of the available data sets. For instance, a chemist can texture MESP onto a constant electron density surface[11] by supplying MESP and MED for the required system. The user can also interrogate the coordinates and function value at any point on such a surface. If there are more than one data sets, then the information is given for all the data sets. Figures 3–11 illustrate the various features of visualization of molecular scalar fields (discussed above) provided in this package for a variety of molecules. The features illustrated in these figures include iso-surfaces, contours, textured planes, planar cuts, etc.

In order to avoid cluttering the display screen, UNIVIS-2000 provides a utility for hiding the molecules and data sets whenever they are not immediately needed. Once the required image has been created the user can add captions using a caption editor provided in the package.

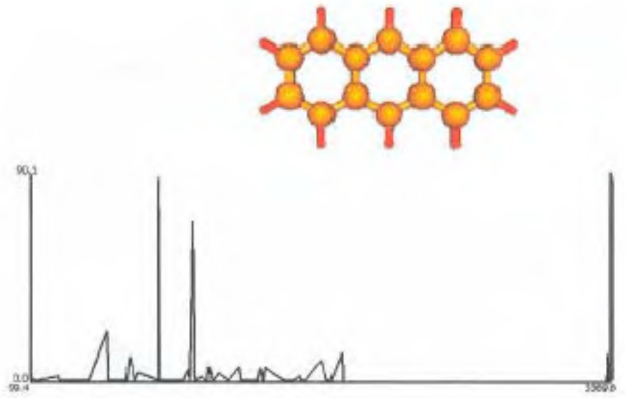

Figure 1. IR spectrum of anthracene along with its HF/6-31G** optimized structure.

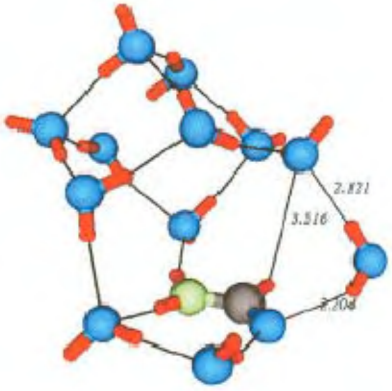

Figure 2. HF/6-31G** optimized structure of formamide...$(H_2O)_{12}$ displaying the distances between the weakly bonded atoms using the tracking facility.

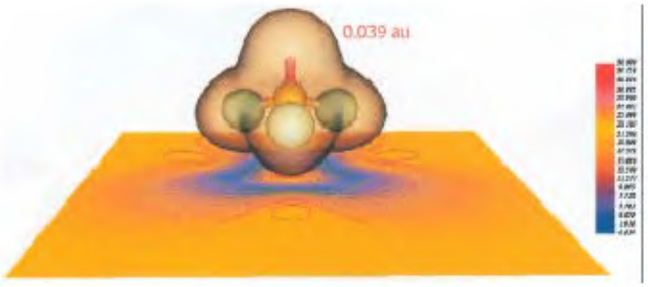

Figure 3. Chloroform molecule enveloped by its constant-valued MESP (0.039 a.u.) (iso) surface. Also shown is the MESP-textured plane with 2D contours. Green dots represent MESP minima.

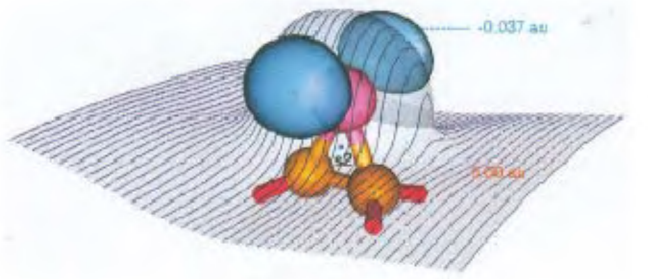

Figure 4. Thiirane molecule viewed with its zero MESP iso-surface (made transparent in order to visualize the atoms) along with zero-valued contours. The negative MESP (–0.037 a.u.) iso-surface is also shown with the corresponding minima inside.

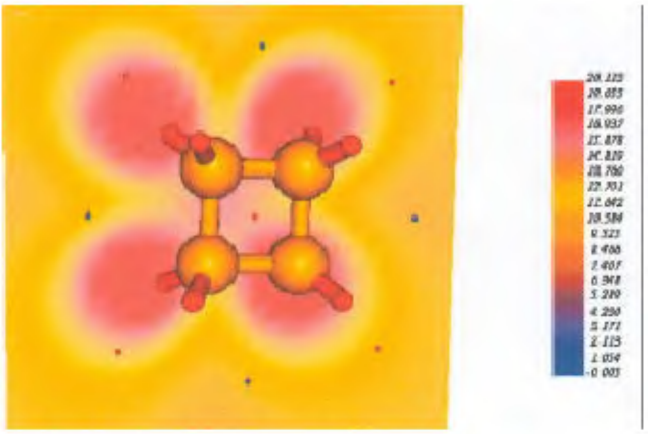

Figure 5. Cyclobutane molecule shown with its MESP-textured plane. The texturing is done according to the given colour range. Red and the blue spots indicate the minima and saddle points, respectively.

The package can read input from GAUSSIAN 94/98 input/output files, GAMESS input/output files and UNIVIS-2000 formatted files. With UNIVIS-2000 formatted files, the user can feed in the data generated from a program other than those mentioned above, e.g. using UNIVIS-2000 to view simulated annealing data. UNIVIS-2000 can also read in surfaces created by the

user and these can be manipulated exactly like any other surface generated in UNIVIS-2000. The package can also read the molecular property files generated using 'Cube=' keyword from GAUSSIAN 94/98 program.

The package can export the molecular geometries in GAUSSIAN, GAMESS and UNIVIS-2000 format. The geometries can be saved in angstrom or a.u. and in Cartesian or *Z*-matrix format. The images can be exported

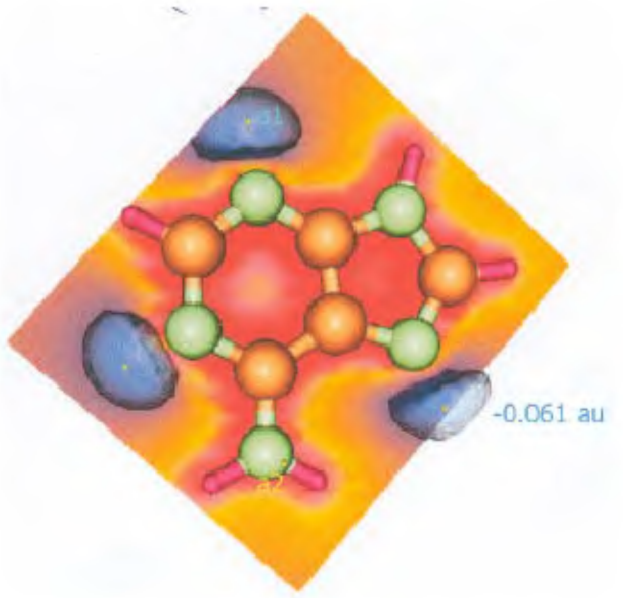

Figure 6. MESP-textured plane of the adenine molecule, with the negative MESP (– 0.061 a.u.) iso-surfaces. Yellow dots represent minima.

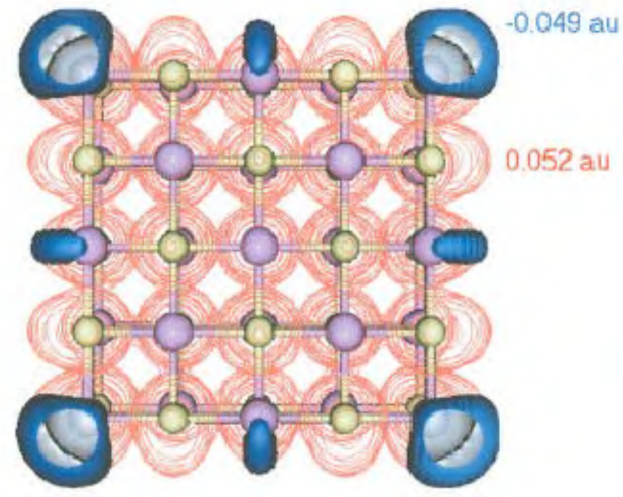

Figure 7. Sodium chloride (100) surface shown with its positive-valued MESP contours and negative MESP iso-surfaces. The iso-surfaces with different front and back colours are also illustrated to identify their inner and outer parts.

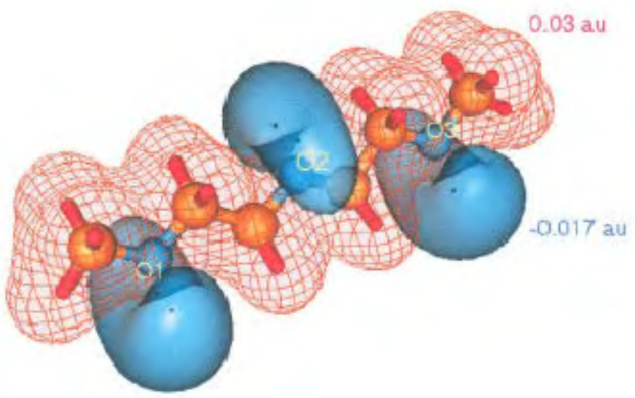

Figure 8. Diethylene glycol dimethyl ether (Diglyme) shown with different MESP regions, with the blue-coloured iso-surfaces (value – 0.017 a.u.), enclosing the minima. Red-coloured contours covering the molecule represent positive (0.03 a.u.) MESP.

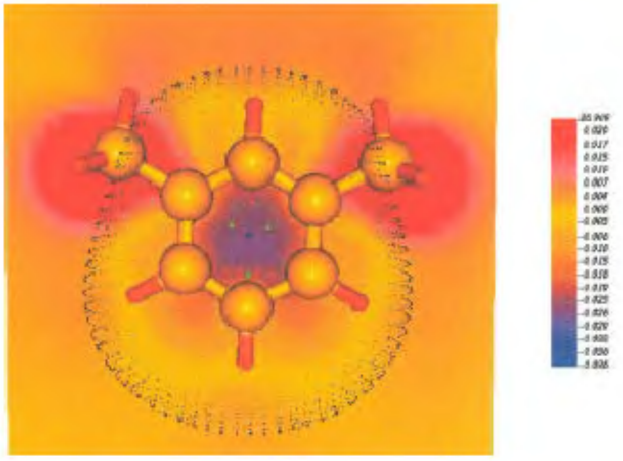

Figure 9. The MESP-textured plane of *m*-xylene viewed with a distribution of constant valued (–0.0066 a.u.) MESP points around it.

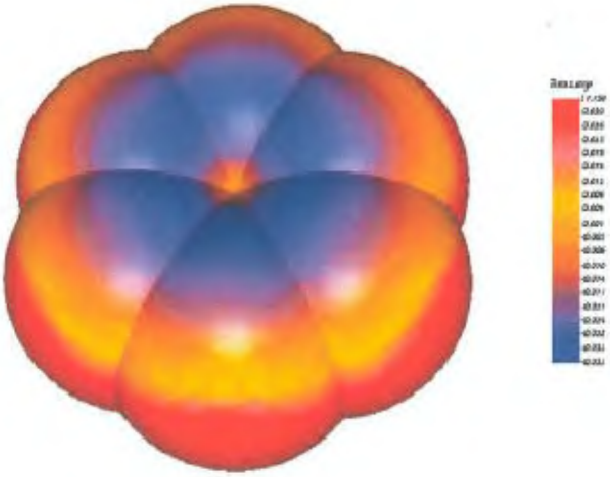

Figure 10. MESP-textured van der Waals surface for benzene. MESP colour coding is as indicated.

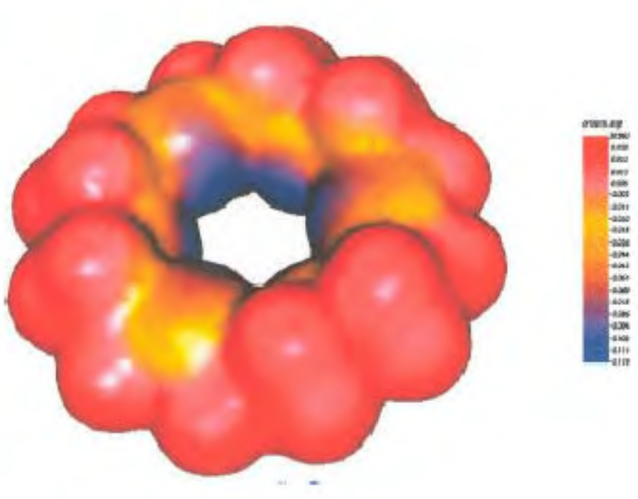

Figure 11. MESP-textured electron density ($\rho = 0.003$ a.u.) isosurface for crown ether (18C6). MESP colour coding is as indicated.

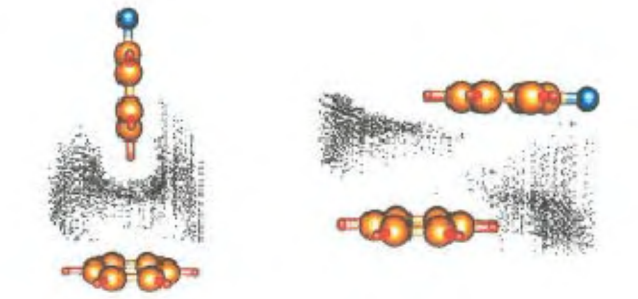

Figure 12. Composite (lock-and-key) MESP property generated over –0.003 to 0.003 a.u. for two benzene... fluorobenzene complex geometries.

as a VRML 97 file (www.web3d.org). Molecular geometries and surfaces that are visible at the time of export are saved in VRML 97 format.

Composite functions

Apart from the above-mentioned traditional tools, UNIVIS-2000 provides a novel method for looking at multiple functions. It provides a way to visualize composites of functions. Two or more data sets may be combined together in various ways to form a composite data set. A composite data set is defined only in the region where the data sets (points) involved in its creation overlap. This facility is provided for quick handling of interacting data sets. There are four possible composite data sets (of the sets A and B) provided in the package:

- Plus: (A + B)
- Minus: (A – B)
- Product: (A * B)
- Lock-and-key: (A & B)

Composite data set value at a point will be the combination of values of the corresponding parent data sets at the reference point, combined in one of the four possible ways listed above. For example, if at a point in the overlapping region we have the value due to data set A as 0.5 and the value at the same point due to B as 2.0, then UNIVIS-2000 defines values at that point for the first three composite data sets as

- Plus: $A + B = 2.5$
- Minus: $A - B = -1.5$
- Product: $A * B = 1.0$

Lock-and-key is different from the above three composite data sets, in the sense that it has additional criteria that need to be satisfied before a point in the overlapping region can assume some value. Lock-and-key is very similar to Plus. It has been implemented primarily to serve as a visual aid for the computational chemists/biologists with a view to help them identify a complementary long-range interaction between the molecules. In the case of lock-and-key composite, the interacting data sets are combined as follows. Add the data set values in the overlapping region provided they satisfy two conditions:

1. The two data sets have opposite signs, viz. sign (A) = –sign (B).
2. They lie numerically close to each other, viz. $|A + B| <$ a pre-specified small threshold value.

The first condition ensures that the interacting data sets have opposite signs – a necessary condition for interacting species to come close enough for interaction. The second condition says that the two data sets tend to cancel each other. The user specifies the threshold value, thus controlling the numerical closeness. Lock-and-key composite data set gives visual clues regarding the interacting species when created from two MESP data sets. Figure 12 illustrates these features for the benzene... fluorobenzene interactions in T-shaped and shifted parallel geometry, respectively. The dark blue dots represent the composite property generated over the range –0.003 to 0.003 a.u. of MESP. Thickly populated dots may be considered as an indication of relatively strong interaction for these T-shaped and shifted parallel goemetries. Scientists interested in exploring complementary intermolecular interactions may find this an extraordinarily useful utility in dealing with appropriate problems. Composite data sets thus provide computational scientists with a novel way of looking at interacting molecular systems.

An earlier (albeit primitive) attempt to indigenously develop a DOS-based molecular visualization package was made[12] at the authors' group several years ago. However, most of the facilities available in UNIVIS-2000 (such as visualization of modes of vibration, vibrational spectra, *Z*-matrix utilities, geometry tracking, multiple and composite surfaces, versatility of cut iso-surfaces as well as fuzzy surfaces) were conspicuous by their absence in that package[12]. Several object-oriented features of C^{++} and COSMO3D have also been exploited in UNIVIS-2000. All these have resulted into a far more sophisticated and portable MS-WINDOWS-based package of wide utility in scientific computing.

Concluding remarks

In summary, UNIVIS-2000 provides the chemists, molecular physicists, biologists as well as material designers with a set of useful and comprehensive visualization tools. The package indeed has almost all the traditionally available facilities for manipulation of molecules. However, the visualization of scalar fields, in general, and the composite utilities in particular, are the special features of this indigenously-developed package. A smaller version of the package UNIVIS-2000 is available[13] from the authors to academic users. It can be downloaded from the site http://chem.unipune.ernet.in/univis2000.exe.

1. MSV: Developed at the molecular graphics laboratory of the Scripps Research Institute. See Sanner, M. F., *J. Mol. Graphics Modelling,* 1999, **17**, 57–61. [http://www.scripps.edu/pub/olson-web/people/sanner/home.html].
2. PMV: Also developed at the molecular graphics laboratory of the Scripps Research Institute. [http://www.scripps.edu/pub/olson-web/share/python/pmv/webpmv.html].
3. Visual Molecular Dynamics (VMD) package allowing visualization and analysis of proteins, amino acids, lipid bilayer assemblies, etc., developed by the Theoretical Biophysics Group at the University of Illinois. For details, see Humphrey, W., Dalke, A. and Chulten, K., *J. Mol. Graphics*, 1996, **14**, 33–38. [http://www.ks.uiuc.edu/Research/vmd/].
4. Raster3D Photorealistic Molecular Graphics: Generates high-quality raster images of proteins or other molecules. It also renders spheres, triangles, cylinders and quadric surfaces with specular highlighting. Developed by the Biomolecular Structure Center at the University of Washington. See Merritt, E. A. and Bacon, D. J., *Methods Enzymol.*, 1997, **277**, 505–524. [http://www.bmsc.washington.edu/raster3d/raster3d.html].
5. PYMOL developed by DeLano, W. L., at the DeLano Scientific, generates molecular images and movies. cf. [http://pymol.sourceforge.net].
6. CyberMol developed by Yoshida, H., at the University of Hiroshima, enables the visualization of molecular models on www by the use of VRML viewer. [http://vbl01.chem.sci.hiroshima-u.ac.jp/CyberMol].
7. Protein Explorer developed by Martz, E., at the University of Massachusetts. [http://www.umass.edu/microbio/rasmol].
8. MOLDA is a molecular-model building program that provides views in VRML format. Developed by Yoshida, H., at the University of Hiroshima. [http://cssj.chem.sci.hiroshima-u.ac.jp/molda/molda.htm].
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10. Gadre, S. R., in *Computational Chemistry: Reviews of Current Trends* (ed. Leszczynski, J.), World Scientific, Singapore, 1999, vol. 4, pp. 1–53.
11. Bader, R. F. W., *Atoms in Molecules: A Quantum Theory*, Oxford University Press, Oxford, 1990.
12. See Limaye, A. C., Inamdar, P. V., Dattawadkar, S. M., Gadre, S. R., *J. Mol. Graphics*, 1996, **14**, 19–22.
13. The smaller version of UNIVIS-2000 is available free of cost to academic users. Please contact S.R.G. for further information.

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