New Features in the 3D-Applet of the Forthcoming MOGADOC Update

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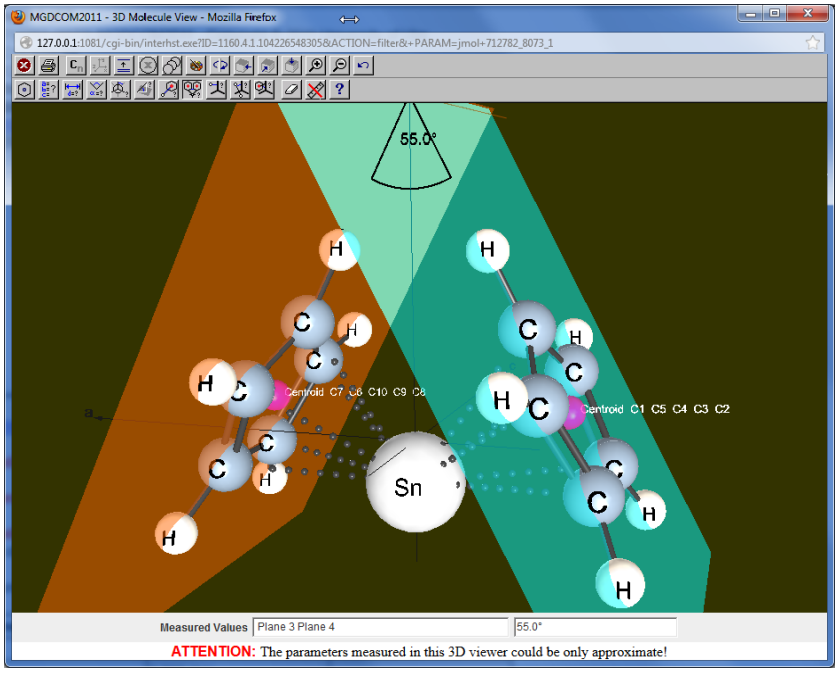
The MOGADOC database (MOlecular GAs-phase DOCumentation) was presented on various conferences of this series. In the meantime the database has grown up to 11,500 inorganic, organic, and organometallic compounds, which were studied in the gas-phase by microwave spectroscopy, radioastronomy, and electron diffraction. The database also contains about 9,000 numerical datasets with internuclear distances, bond angles, and dihedral angles. Most of the corresponding molecular structures are also given as a 3D presentation (ball-stick-models).

The retrieval features of the HTML-based database have been described elsewhere in details [1,2]. Some years ago a Java-based applet has been developed, which enables the 3D-visualization of the molecular structures. The user can interactively rotate, shift, and scale the 3D-models; moreover one can "measure" atomic distances as well as bond, dihedral and elevation angles [3].



Recently new "measurement" features have been supplemented (such as distances between centroids, angles between ring planes, etc.).

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[1] J. Vogt, N. Vogt, and R. Kramer, *J. Chem. Inform. Comput. Sci.* **2003**, *43*, 357.
[2] J. Vogt and N. Vogt, *J. Mol. Struct.* **2004**, *695*, 237.
[3] N. Vogt, E. Popov, R. Rudert, and J. Vogt, *J. Mol. Struct.* **2010**, *978*, 201.