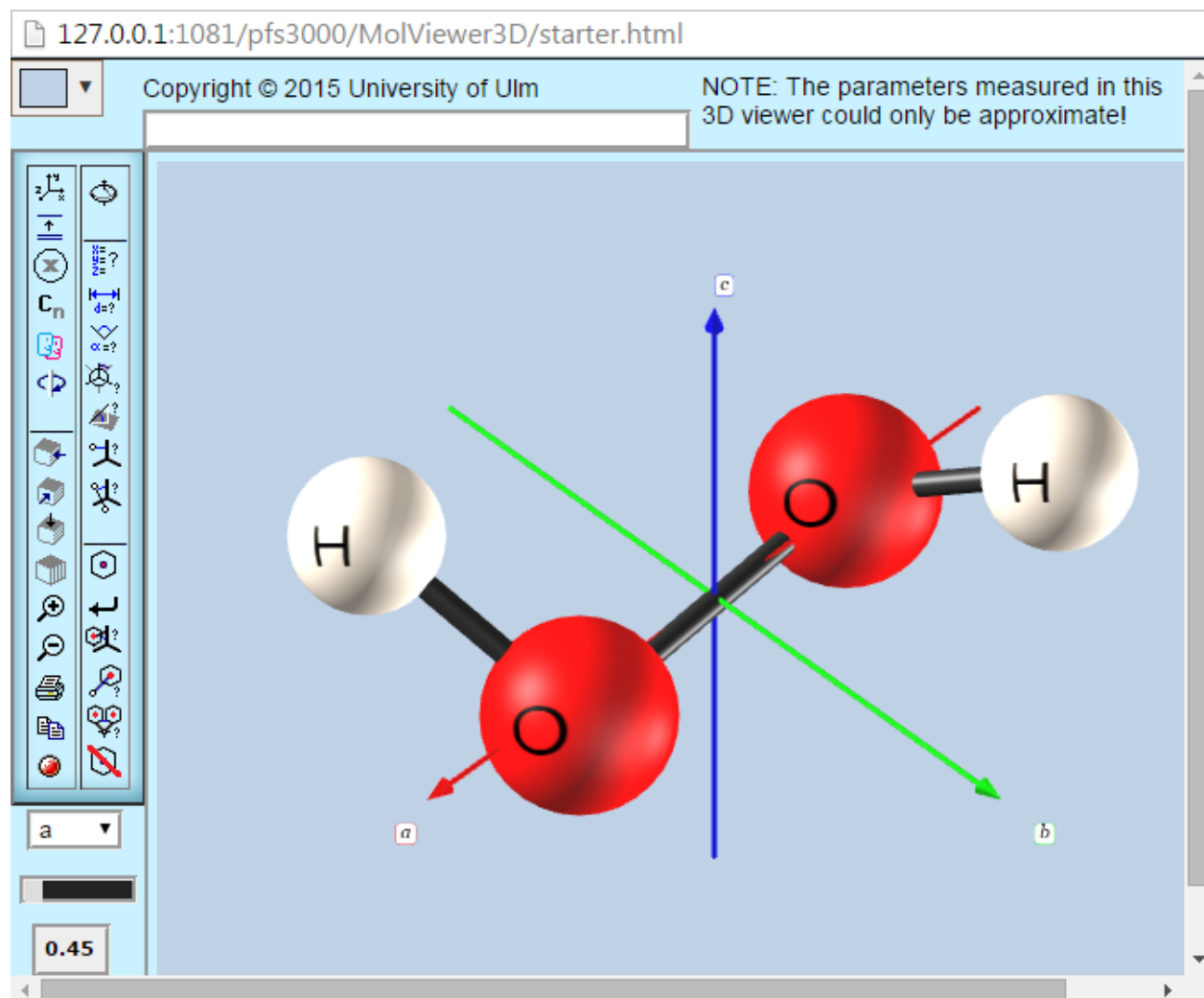# 3D Molecule Viewer of MOGADOC (JavaScript)

127.0.0.1:1081/pfs3000/MolViewer3D/starter.html

NOTE: The parameters measured in this 3D viewer could only be approximate!

a

0.45
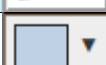
Movement of the Molecule

Rotation of the molecule: Use left mouse button to drag.

Translation of the molecule: Use right mouse button to drag.

Resize the molecule: a) Turn the mouse wheel, or b) press the wheel (central mouse button) while moving the mouse pointer up or down, or c) click on ⊕ or ⊖.

Tools (there are further explanations below this table)

	Options
	Show/hide coordinate axes in principal inertial axes system
	Show/hide bond orders
	Show/hide dummy atoms
	Show/hide atom labels
	Toggle between normal and anaglyph 3D view
	Turn on/off continuous rotation of the molecule
	Others
	View molecule along the *a*-axis
	View molecule along the *b*-axis
	View molecule along the *c*-axis
	Isometric view of the molecule
	Enlarge the view of the molecule
	Reduce the view of the molecule
	Print the image of the molecule
	Copy the image of the molecule to the clipboard or to a png file
	Reset last measurement (equivalent to Escape key press)
	Measurements
	Show the rotational constants of the molecule
	Show the cartesian coordinates of a selected atom/centroid a an arbitrary axis system
	Show the distance between two selected atoms/centroids
	Show the angle between the connecting lines through three selected atoms/centroids
	Show the dihedral angle between two planes through four selected atoms/centroids
	Show the angle between a plane through three atoms and a line through two atoms of four selected atoms/centroids
	Show the distance between a selected coordinate axis and a selected atom/centroid
	Show the angle between a selected coordinate axis and the line through two selected atoms/centroids
	Define the centroid of and the least-squares plane through selected atoms
	Finish the definition of a centroid/least-squares plane (equivalent to Enter key press)
	Show the angle between a selected coordinate axis and a selected least-squares plane
	Show the distance between a selected least-squares plane and a selected atom/centroid
	Show the angle between two selected least-squares planes
	Remove a selected centroid/least-squares plane
	Others
a ▼	Select a principal inertial axis
▼	Select a background color

Detailed description of selected functions

1. Coordinate Axes

MOGADOC uses a principal inertial axes system with an *a*-axis (shown in red), a *b*-axis (green) and a *c*-axis (blue). You can select an axis using [a ▼] and calculate distances or angles of selected parts of the molecule with this axis (see below). If you don't want to see the axes you can hide them by clicking [icon].

2. Bond Order

MOGADOC distinguishes between single, double and triple bonds, shown as one, two, or three parallel sticks. If you hide the bond order by clicking [icon], all bonds are shown as one stick. Note: Dotted lines can not be turned into a stick.

3. Anaglyph View

The anaglyph view shows two color-codes images, one for each eye. With red-cyan glasses this view produces a stereoscopic 3D effect. Note: This does not work with red-blue or red-green glasses.

4. Dummy Atoms

MOGADOC uses dummy atoms (small, magenta-colored, transparent balls) to mark certain points within the molecule (e.g. centers of mass or centers of bonds). When calculating geometric properties you can treat dummy atoms as normal atoms. You can hide all dummy atoms by clicking [icon].

5. Atom Labels

In the structural part of MOGADOC most documents contain tables with geometric properties of a molecule. As a reference to the structural formula or to the 3D-model of this molecule some atoms may have labels (normally a number). You can hide all labels of a molecule (if there is any) by clicking C_n . Note: It is not possible to hide the element symbol.

6. Print the image of the molecule

This opens a dialog window in which you can select a printer. By clicking on **Print** your image is printed. The kind of dialog window depends on your web browser.

7. Copy the image of the molecule

Some web browsers will open a new browser window or a new tab with the current molecule image. You can copy this image to the clipboard by right-click and selection of "Copy image" or by Ctrl/C. Other web browsers will ask you, if you want to save the image to a file or to open the image by a picture viewer. The default file format is "PNG".

8. Change Background Color

Click on [image]. In the following dialog you can select the lightness and saturation of the color in the left, and the hue in the right field.
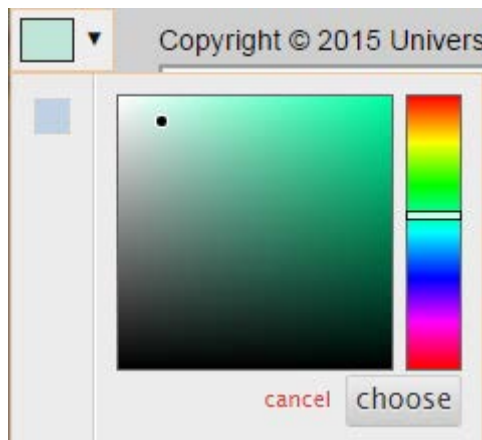
Confirm your selection by clicking on "choose".

9. Calculate Distances between Atoms

The distance between atoms or atoms and centroids can be calculated by clicking on [image] and then selecting two atoms/centroids. The value of the distance will appear in the image and at the top of the window. The atoms must not necessarily be connected by bonds.

10. Calculate Distances between Atoms and Planes

The distance between an atom and a least-squares plane can be calculated by defining the plane according to 18, clicking on [image] and then selecting the atom and the centroid representing the plane. The value of the distance will appear in the image and at the top of the window.

11. Calculate Distances between Atoms and Axes of Inertia

The distance between an atom and a principal axis of inertia can be calculated by clicking on [image] and then selecting an atom. A list field will appear which lets the user select the a-, b-, or c-axis of inertia. The value of the distance will appear in the image and at the top of the window.

12. Calculate Bond Angles

A bond angle between three atoms can be calculated by clicking on [image] and selecting three atoms. The value of the angle will appear in the image and at the top of the window.

13. Calculate Angles between Bonds and Axes of Inertia

The angle between a bond and an inertial axis can be calculated by clicking on [image] and then selecting the two atoms of the bond. A list field will appear which lets the user select the a-, b-, or c-axis of inertia. The value of the angle will appear in the image and at the top of the window.

14. Calculate Dihedral Angles

The dihedral angle through four atoms (= the angle between the plane through the first three atoms and the plane through the last three atoms) can be calculated by clicking on ⌖ and then selecting the four atoms of the dihedral angle. The value of the angle will appear in the image and at the top of the window.
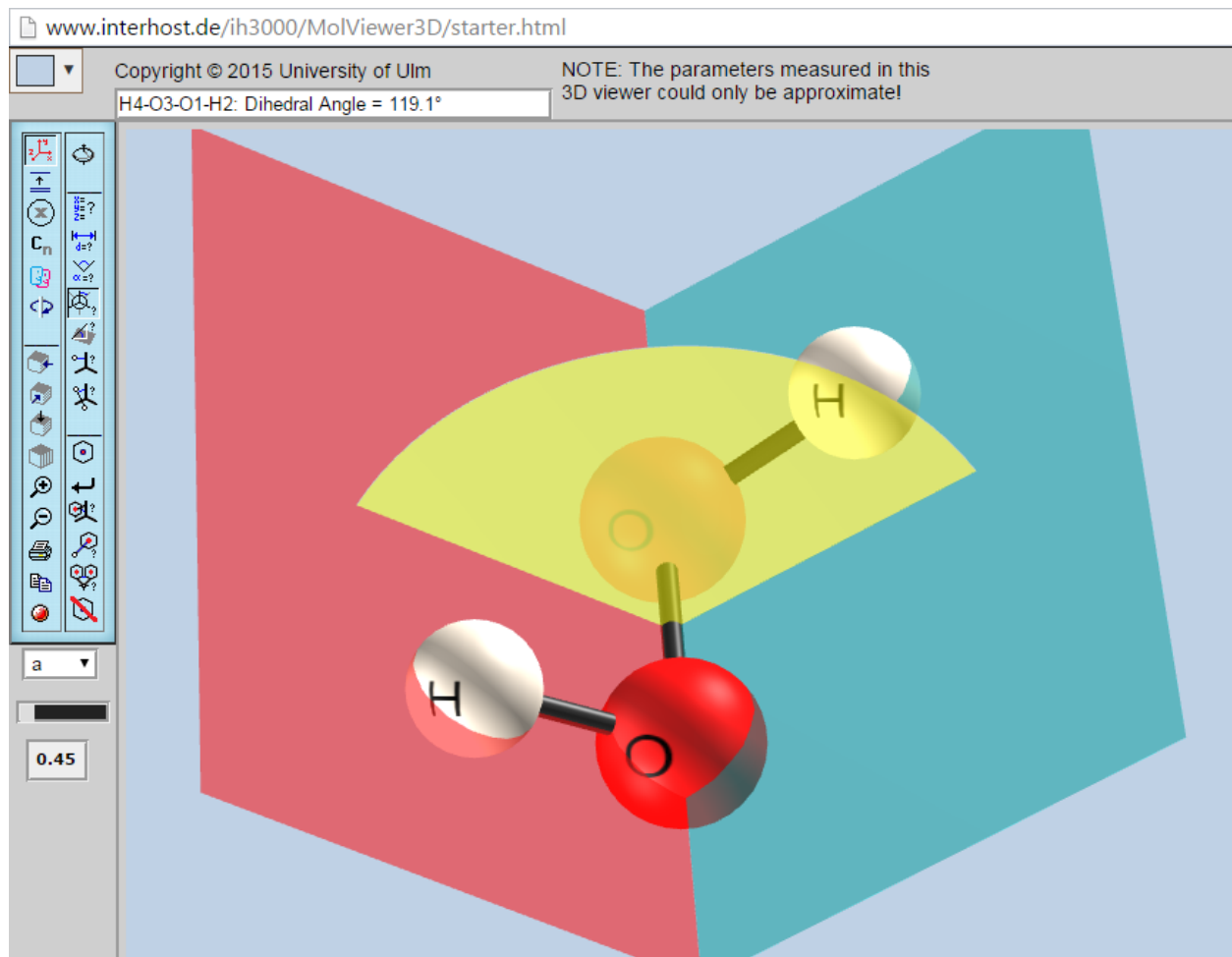

Dihedral angle

15. Calculate Elevation Angles

An elevation angle between a plane and a bond can be calculated by clicking and then selecting four atoms. The first three atoms define the plane and the angle between the bond from one of these atoms to the fourth atom will be calculated. If there is no bond between the fourth atom and one of the first three atoms, the line between the third and the fourth atom will be used instead. The value of the angle will appear in the image and at the top of the window.

Elevation angle

16. Calculate Angles between Planes and Axes of Inertia

An angle between a least-squares plane and an inertial axis can be calculated by defining the plane according to 18, clicking on and then selecting the cyan-colored sphere representing the plane. A list field will appear which lets the user select the *a*-, *b*-, or *c*-axis. The value of the angle will appear in the image and at the top of the window.

17. Calculate Angles between two Planes
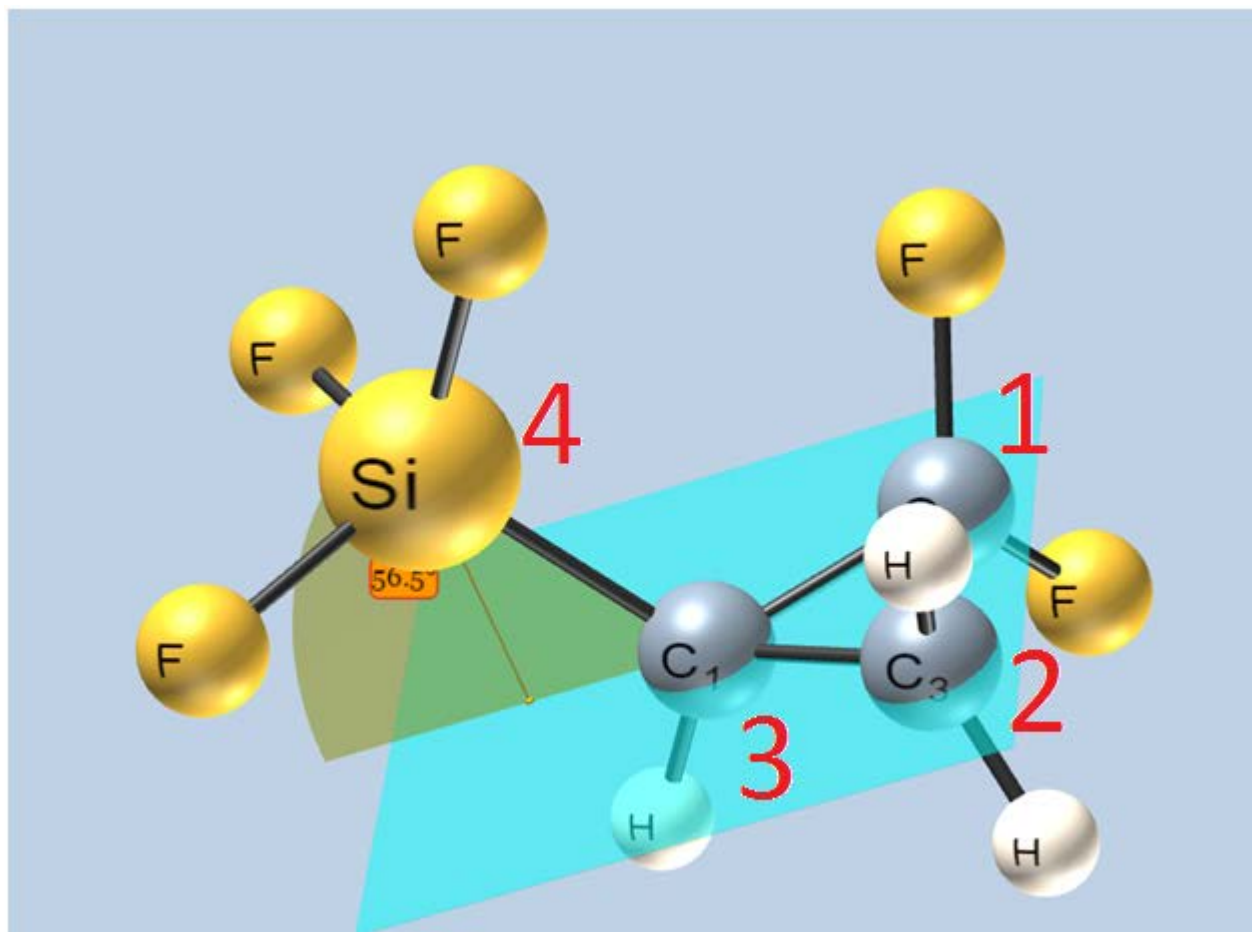
An angle between two least-squares planes can be calculated by defining the planes according to 18, clicking on and then selecting the two cyan-colored spheres representing the planes. The value of the angle will appear in the image and at the top of the window.

18. Define Centroids and Leastsquares Planes

A centroid is the unweighted average value of selected 3D coordinates (not to be confused with the center of mass!). First you have to click on ⬡ , then click on all atoms, dummy atoms and centroids you want to average. Finish the definition by pressing the RETURN key or clicking on ↵ . The centroid will appear as a cyan-colored small sphere. At the same time a least-squares plane of these atom positions will be calculated, which is also symbolized by the small magenta colored small sphere. When you use this sphere for your calculations it will be treated as a centroid or a plane, depending on the kind of calculation. If you accidentally click on the wrong atom, you can click on 🔴 or press the Esc key and start from the beginning.

19. Delete Centroids

You can delete a centroid and the corresponding plane by clicking on ⬡ and then on the cyan-colored sphere symbolizing this centroid/plane.

ATTENTION

The calculated values are sometimes a little bit different from the corresponding values in the document tables. The reason may be the method of measurement, which results in inconsistent angles and distances.

Web Browser Requirement

The 3D Molecule Viewer uses *WebGL*. *WebGL* is supported by *Mozilla Firefox* since version 4.0, by *Google Chrome* since version 9, *Safari* since version 6.0, *Microsoft Internet Explorer* since version 11 and *Opera* since version 11. In *Safari* and *Opera* you have to enable *WebGL* manually. In most cases you need a graphics card that is not too old.