

## Quick start-up for DAMQT\_3.2.0 (by R. López)

1. Once the package is installed, run it just writing DAMQT320.exe in any suitable directory (beware that the executable is accessible by PATH or alike).
2. Choose a language and start DAMQT320 (see fig 1).
3. When the GUI is open, press the  key placed at Project->Create Project->Import data from in the left-side menu. Navigate to any of the samples directories included in the package (\$DAMQT320)/samples/Molpro/C2H4/, for instance; see fig 2) and double click on file C2H4.out to launch Molpro's interface to DAMQT320.
4. Press the  key. The interface output will appear in the Results pannel (see fig 3).
5. Press on tab **Atomic densities** on the left side menu and click on the  key. The partition of the density will be carried out and the output including the multipolar moments of the atomic fragments will be printed in the viewer (see fig 4). Now, the .damqt file containing the fit of the radial factors of the fragments has been created and all the options will be accessible. (If your system has not mpi installed, the **Atomic densities** menu will look a bit different than in figure; in particular box labeled **Parallel computing** will be absent).
6. Press on tab **Density** on the left side menu, scroll down the menu with the right vertical rule, and click on the  key to compute the grid for the molecular density. It will take a few seconds to get the grid computed. Some output will be displayed in the **Results** panel (see fig 5).
7. To compute the molecular density deformations, instead of full density, check the **Density deformations** button and press the  key (see fig 6).
8. To compute full molecular density in a 2D grid, check radio buttons **Full electron density** and **2D grid**, select the plane YZ which is the molecular plane, and press the  key (see fig 7). Notice that box following grid type has suitably changed for the 2D grid specification.
9. Press on tab **Electrostatic potential** on the left side menu and click on the  key to compute the grid for the molecular electrostatic potential (see fig 8).
10. Check radio button **2D grid**, select YZ plane, and press the  key to generate a 2D grid tabulation (see fig 9).
11. Press on tab **Molecular orbitals** on the left side menu. In the **Input data from:**, press the  key to select a file with MO an select file C2H4.GAorba (see fig 10)). Select indices of MO orbitals to be displayed. Indices can be separated by commas. Ranges of indices separated by hyphens can be also specified (see fig 11). Once selected, press the  key to generate a grid.
12. Press on tab **Molecular topography** on the left side menu. Check the boxes labeled as **Construct molecular graph** and **Construct 3D atomic basin**, and click on the  key to compute the Topography of molecular density (see fig 12).
13. Check radio button **Molecular potential** and press the  key to compute the Topography of molecular electrostatic potential (see fig 13).
14. Press on tab **Mesp sigma hole** on the left side menu. In the **Import density from:**, press the  key to select a file with a 3D density grid. This grid will be used to generate a density isosurface with the contour chosen in the box labeled as **Density value**. Once selected, press the  key to compute the electrostatic potential on the isosurface (see fig 14).
15. Press on tab **Electric field** on the left side menu and click on the  key to compute electric field lines (see fig 15).

16. Press on tab **Density gradient** on the left side menu and click on the  key to compute 3D density gradient lines (see fig 16).
17. Check **2D grid** button and in **2D planes** check **YZ** plane to generate density gradient lines on the molecular plane (see fig 17).
18. Press on tab **H-F Forces on nuclei** on the left side menu and click on the  key to compute the Hellmann-Feynman forces on nuclei (see fig 18).
19. Press on tab **Radial factors** on the left side menu. Change **Step** to 0.02, and choose  $l$  and  $m$  values. Select the centers whose radial factors are to be displayed, check boxes for derivatives and press the  key (see fig 19).
20. Press on tab **Oriented multipoles** on the left side menu. Select the set of oriented multipoles to be computed with the **lmin** and **lmax** spinboxes, the centers defining the plane, and those whose oriented multipoles are to be computed. Press the  key to compute (see fig 20).
21. Press on tab **Zernike-Jacobi density expansion** on the left side menu. Press the  key to compute Canterakis-Zernike expansion of density (see fig 21).
22. Press on tab **Zernike-Jacobi density tabulation** on the left side menu. In the **Import data from:**, press the  key to select a file with a Canterakis Zernike expansion (see fig 22). Press the  key to compute Canterakis-Zernike expansion of density.

Many of the previous actions, besides the output data printed in the viewer and stored in **.out** files, have created files to be visualized with the 2D plotter or the 3D viewer. For 2D plotting do the following:

1. Press button **New 2D Plotter** on the right menu. A window for 2D plotting will be opened (see fig 23).
2. To visualize a 2D contour plot, select tab **Contour plots** and press the  key to select a file with grid data (see fig 24). Open the file and the contour plot will be displayed. Contour values can be displayed by double clicking on the lines (see fig 25).
3. To visualize 2D electric field lines (or density gradient lines), open a new 2D plotter and select tab **Field lines** and press the  key to select a file with grid data (see fig 26). Open the file and field lines will be displayed. Check **Show arrows** box to display arrows on the lines (see fig 27). Alternatively, lines can be displayed over the contour plot. To do this, in the plotter with 2D contour lines, select tab **Field lines** and proceed as before. You will be asked to superimpose image (see fig 28). Answering **yes** will cause the field lines to be superimposed on the contour lines (see fig 29).
4. To display the MESP sigma hole histogram, open a new 2D plotter and select the pertaining tab. Import a file with the histogram and carry out smoothing if desired (see fig 30). Several histograms can be displayed together. Each curve and its label can be edited by double clicking on the label (see fig 31).
5. To display radial factors, open a new 2D plotter and select the pertaining tab. Import a file with the radial factors or their derivatives (see fig 32). Several files can be imported in the same plot. Everytime you import a file, you will be prompted for superimposing (see fig 33). Curves and their labels can be edited by double clicking on their labels (see fig 34).
6. Critical points can be superimposed to contour lines and field lines or displayed alone. Go to the first plotter, which now contains the contour MESP and electric field lines and select tab **Critical points**. Import the **C2H4-cps-v.xyz** file containing MESP critical points. Increase the balls radii to make the CPs more visible (see fig 35).

7. Basins frontiers on the plane can be also superimposed in this 2D plot. To do this, select tab **Basins** and import *C2H4-v.basin2D* file. Increase pen thickness to make the MESP basins frontiers more visible (see fig 36).
8. Tab **Options** contains general options.
9. Tab **Image capture** allows to save plot to a file. Several formats are available and resolution can be scaled or user-defined.
10. Tab **Save/retrieve settings** allows to save current settings to a file to be retrieved when required.

For 3D visualizations do the following:

1. Press button **New 3D viewer** on the right menu. A window for 3D display will be opened (see fig 37).
2. In the right menu of the window, press button **Add molecule** and choose a file with molecular geometry. Choose file *C2H4.xyz* in this case (see fig 38) and open it. Use the left mouse button to rotate the molecule so that the molecular plane coincides with the screen (see fig 39).
3. Press button **Geometry measures**, choose **Distances** and check **Show/hide distances in a window** and **Show/hide distances** in the viewer. Next, while keeping **shift** key pressed, double click on pairs of atoms and the distances will be displayed on viewer and in a new window (see fig 40). You can repeat the operation selecting **Angles**, in which case three atoms must be selected, or **Dihedral angles**, which requires four atoms.
4. Press **Edit** button to edit molecule. A new window will be opened with editing options. Press **3D lines** button and import a file with lines. Choose file *C2H4.cam* (see fig 41). Increase arrows length and width to make them visible (see fig 42). Whenever the molecule editor is hidden by the viewer, it can be brought to forefront by pressing the **Edit** button.
5. Press **Critical points** button and import a file with MESP CPs, choose file *C2H4-cps-v.xyz*. Increase balls radii and slightly rotate the molecule to better visualize the CPs (see fig 43).
6. Uncheck **Show lines** box and press **Hide 3D lines manager**, and uncheck **(?,?)** CP boxes and press **Hide critical points manager** to hide lines and CPs.
7. Press **Add surface** button and import a file with a surface. Choose file *C2H4-d\_0.10E-02.sgh* which contains the MESP values on the density isosurface of contour 0.001. A spectrogram of MESP will be displayed on the isosurface (see fig 44).
8. In **Loaded surfaces** press the **Edit** button placed on the right of the surface file name. A menu for editing the surface will be displayed. In the menu, check the **Local maxima** and **Local minima** boxes. New options will appear in the men. Check **Show MESP values** box. Local extrema will be displayed with their MESP values (see fig 45).
9. In the surface editor, change the **Surface type** to **Wire frame**, check the box **Translucence correction** and move the slider **Opacity** to a value slightly lower than 100 to change surface look (see fig 46).
10. Check box **Only selected extrema**. CPs indices, symbols and MESP values will disappear. To make them visible in a given CP, double click on it (see fig 47).
11. Press button **Close** to close the surface editor and **Hide** button to hide surface. Then, press button **Add grid for isosurfaces** and choose a file with a 3D grid tabulation. Choose file *C2H4-v.plt* which contains a tabulation of MESP on a 3D grid. A menu for adding isosurfaces will be displayed. Press button **Add surface** and next **Edit**. An editor will be displayed for the isosurface. Choose a value in the box and press **Enter** key or, alternatively, move the slider. The isosurface will be displayed. Check **wire frame** option if desired (see fig 48).

For cluster optimization

1. Remove or hide displayed surfaces.
2. Add one more C<sub>2</sub>H<sub>4</sub> molecule in the canvas (see fig 49).
3. Deactivate the first C<sub>2</sub>H<sub>4</sub> molecule (host) and move the second one (guest) to a suitable position. Display some distances to check the relative positions of molecules and press the **Optimize cluster** button (see fig 50).
4. In the new menu, choose a name for the cluster files and, selecting the option **Choose guests from canvas** (see fig 51).
5. Select the charge model for the atoms in guests. If Open Babel is installed and working, charges can be obtained with any of the models built in that Open Babel. The available models depend on the Open Babel version, and are displayed in a ComboBox that is displayed when the button **Open Babel** is checked. Alternatively, charges can be supplied by the user checking the **User supplied** button and pressing the **Import** button. A navigation window is opened for loading a suitable file with charges (see fig 52). By default, a files with extension *mltmod* will appear in the window. Charges generated by DAMQT can be imported from these files. Alternatively, charges can be loaded from any suitable file containing *atom symbols* and *charges* (one pair per line).
6. Press the **Edit** button to check that the charges have been correctly loaded. A window will appear with the charges currently chosen (see fig 52). Charge values can be edited in the boxes if desired.
7. In the new menu, choose a name for the cluster files and, selecting the option **Choose guests from canvas**, press the **Exec** button (see fig 53).
8. Wait until the message of cluster optimization finished appears (see fig 54).
9. Display some distances to check the relative positions of molecules, select the file with the cluster optimization frames, move the system to change the point of view if desired, and press the **Replay** button to animate the optimization process (see fig 55). During animation, the point of view can be changed by interactively rotating or translating the cluster.
10. Remove the cluster from the viewer (see fig 56) and restore the guest molecule to its initial position (see fig 57).
11. Edit the host molecule and load its MESP critical points (CP), keep only (3, +3) CP selected and display CP symbols (see fig 58).
12. Check the option **Only selected CPs**, deactivate the guest molecule and activate the host. Rotate the host to see the CP and double click on one of them to select (see fig 59).
13. In the cluster optimization menu, change the name of the cluster files, check the options **Use template for guests** and **Only selected CPs**, and press the **Exec** button to carry out optimization using CP for starting guest positions (see fig 60).
14. Wait until optimization finishes. Load the file with frames, change the point of view if desired, display some distances and press **Replay button** to animate the optimization process (see fig 61).
15. Check the **Record optimization** option. Verify that the command for creating movie is correct (**fframe** must be installed and accessible in your system if this is the program chosen for this purpose). Select a name for the movie file and the option **Remove frame files at end** unless you want to keep the PNG files corresponding to the single frames (see fig 62). Repeat animation by pressing **Replay** and wait until recording ends. An *\*.mp4* file will be generated that can be reproduced with VLC, for instance. (Some multimedia programs, such as MSWindows multimedia, are unable to reproduce this file issuing format incompatibility).

You can test the different options at your will using this sample deck or any other included in the package.

Figure 1<sup>fig:1</sup>

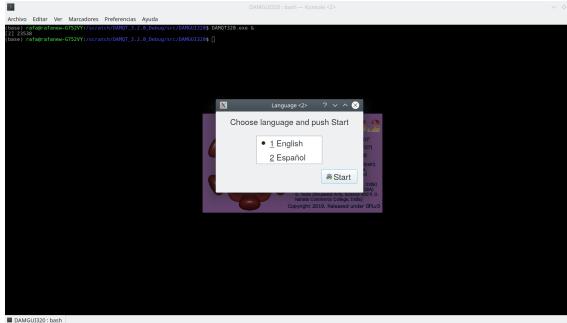


Figure 3<sup>fig:3</sup>

Figure 2<sup>fig:2</sup>

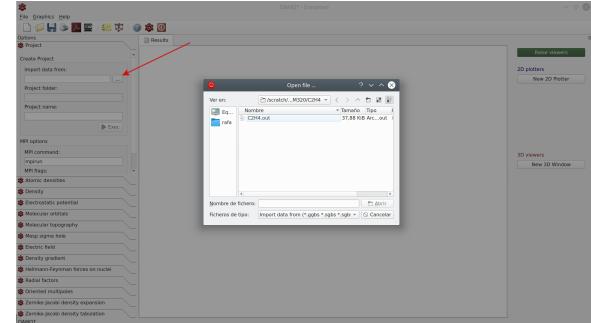


Figure 4<sup>fig:4</sup>

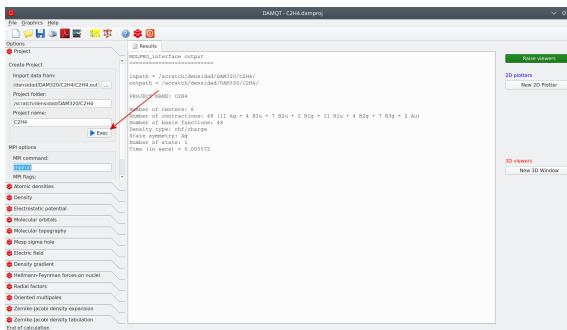


Figure 5<sup>fig:5</sup>

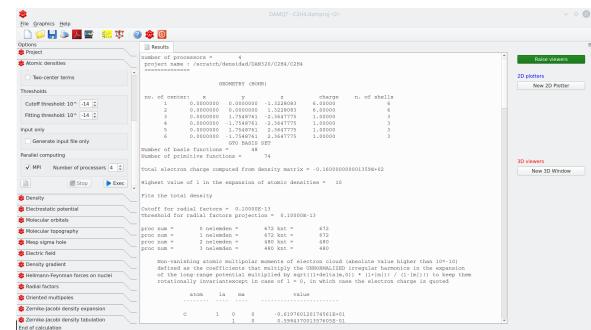


Figure 6<sup>fig:6</sup>

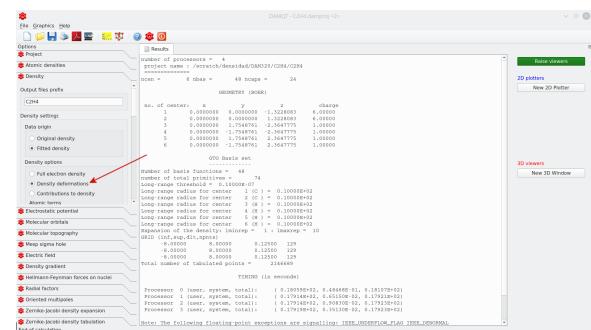
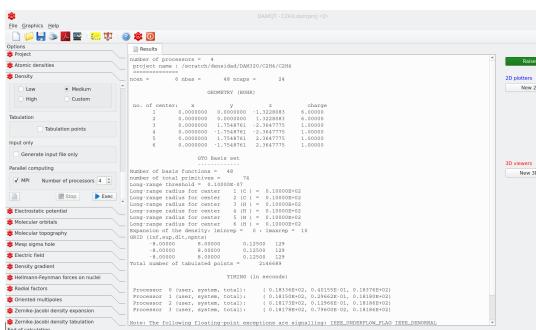


Figure 7<sup>fig:7</sup>

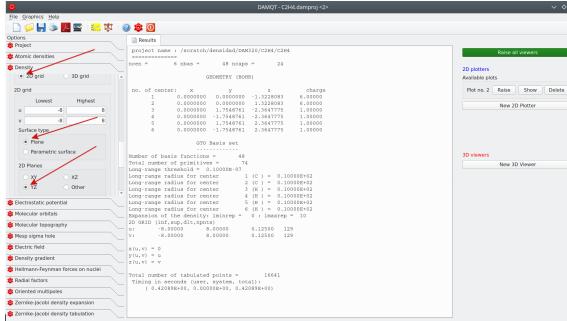


Figure 8<sup>fig:8</sup>

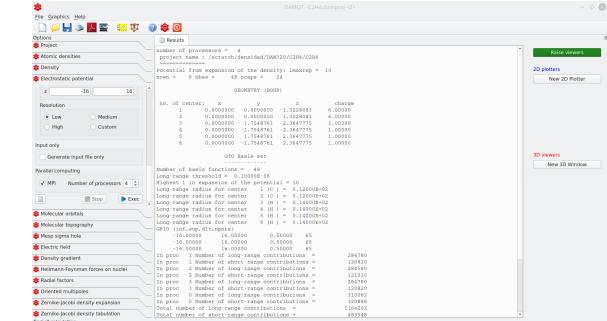


Figure 9<sup>fig:9</sup>

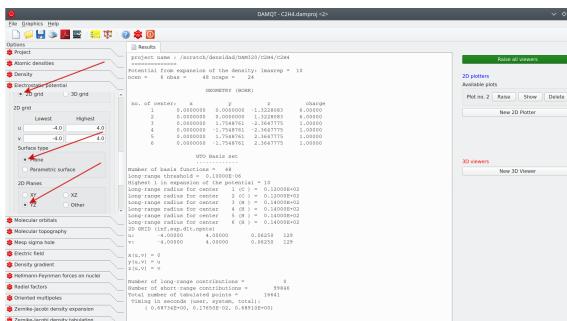


Figure 10<sup>fig:10</sup>

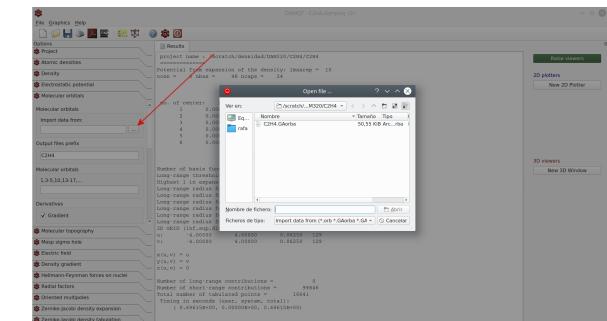


Figure 11<sup>fig:11</sup>

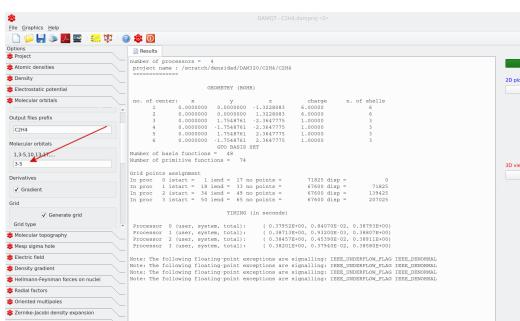


Figure 12<sup>fig:12</sup>

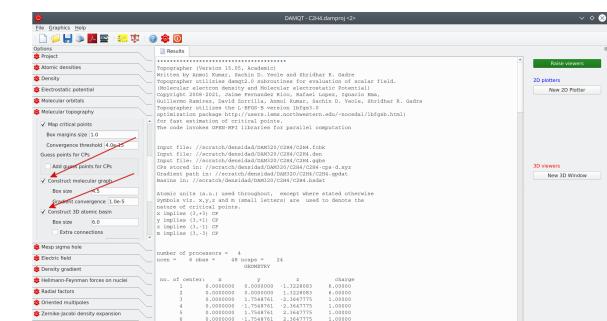


Figure 13<sup>fig:13</sup>

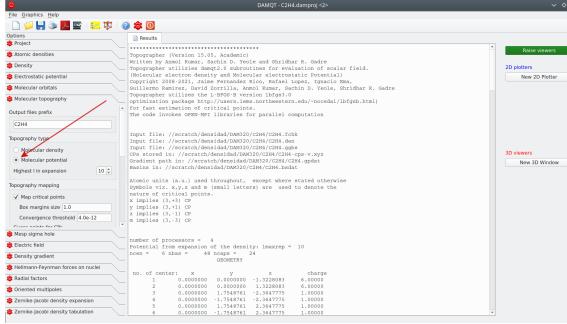


Figure 15<sup>fig:15</sup>

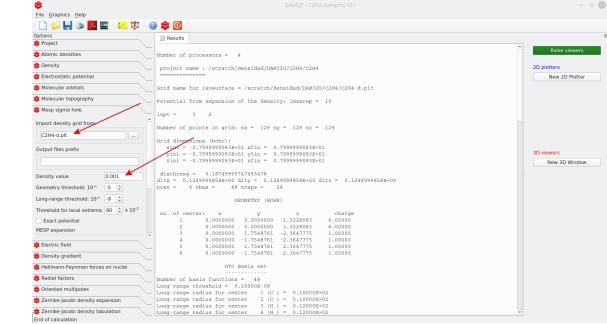


Figure 14<sup>fig:14</sup>

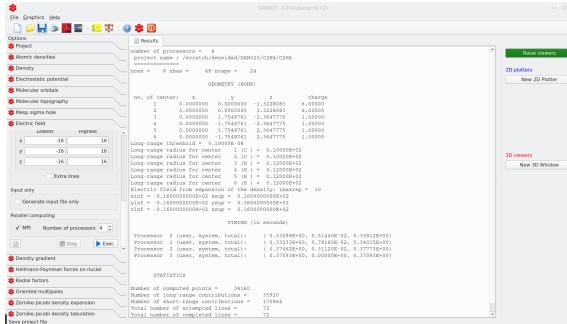


Figure 17<sup>fig:17</sup>

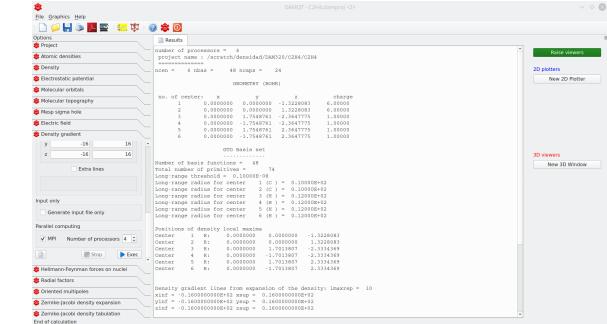


Figure 16<sup>fig:16</sup>

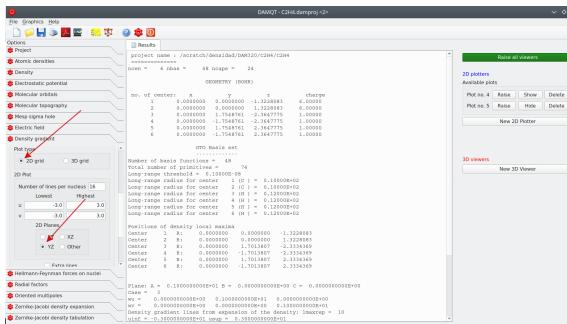


Figure 17<sup>fig:17</sup>

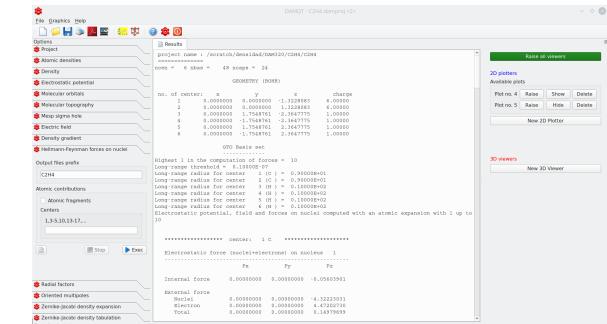


Figure 19<sup>fig:19</sup>

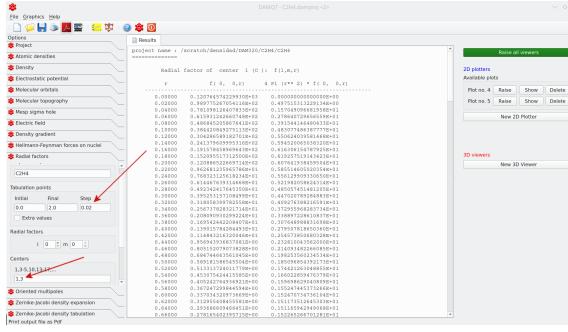


Figure 21<sup>fig:21</sup>

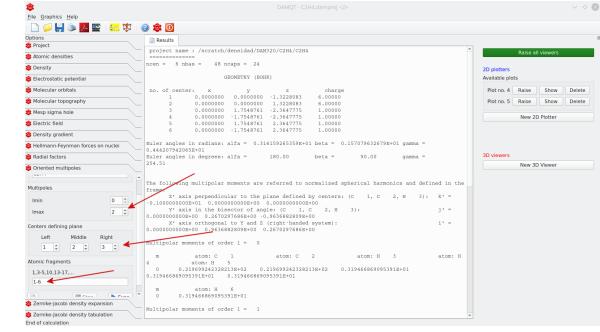


Figure 20<sup>fig:20</sup>

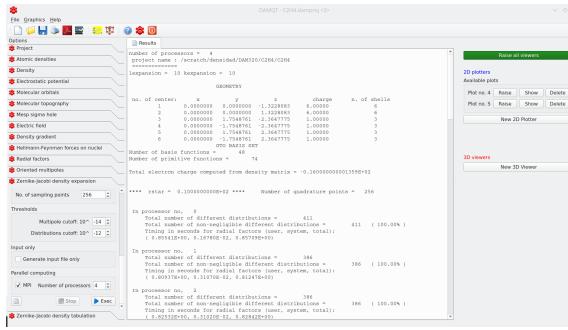


Figure 23<sup>fig:23</sup>

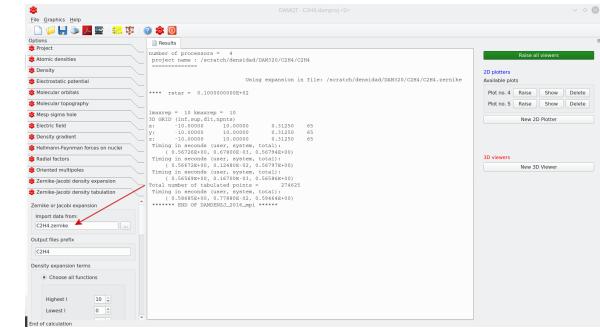


Figure 22<sup>fig:22</sup>

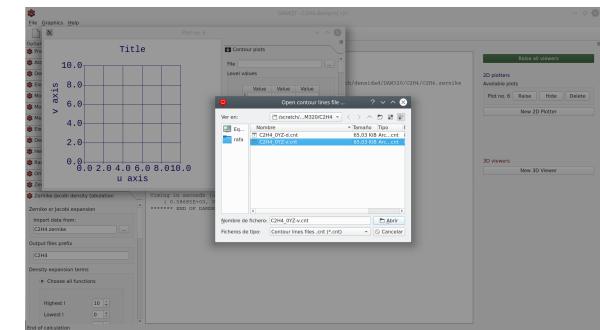
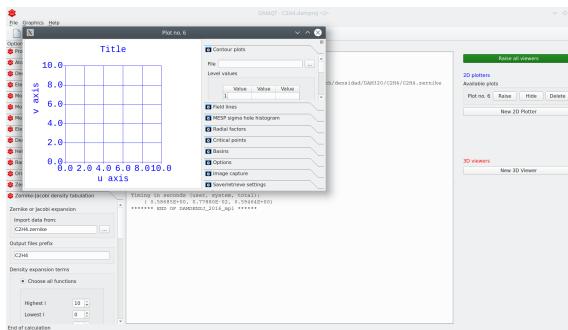


Figure 25<sup>fig:25</sup>

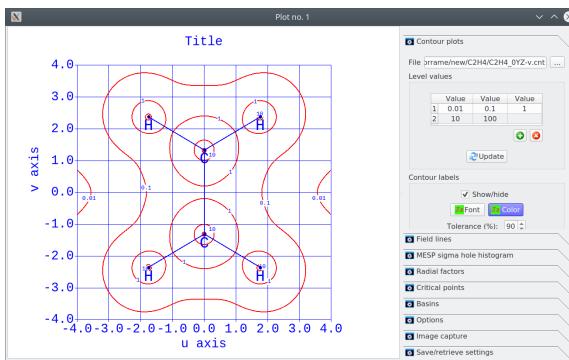


Figure 27<sup>fig:27</sup>

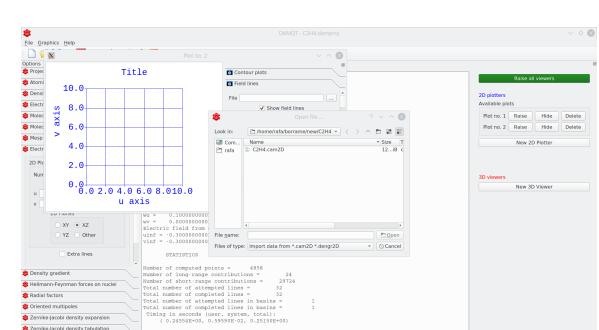


Figure 28<sup>fig:28</sup>

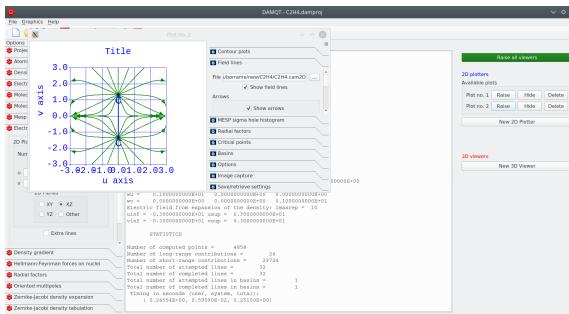


Figure 29<sup>fig:29</sup>

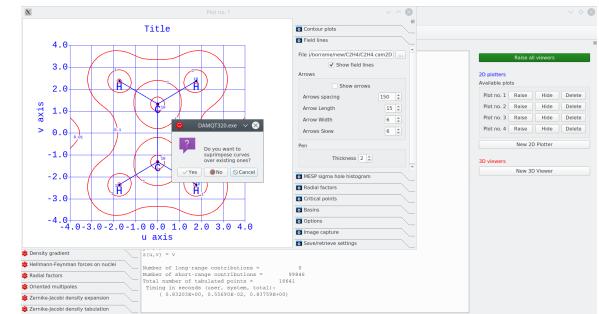


Figure 30<sup>fig:30</sup>

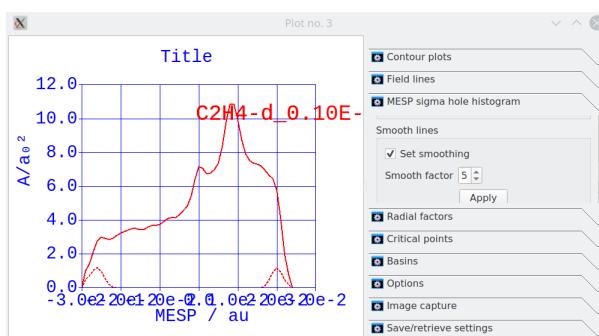
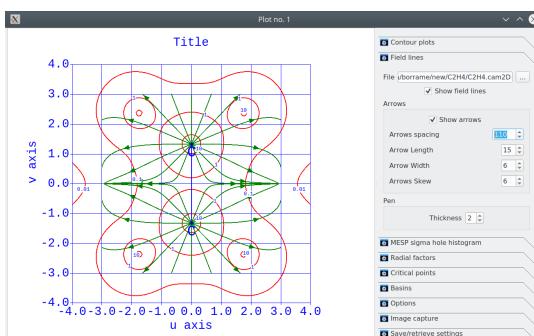


Figure 31<sup>fig:31</sup>

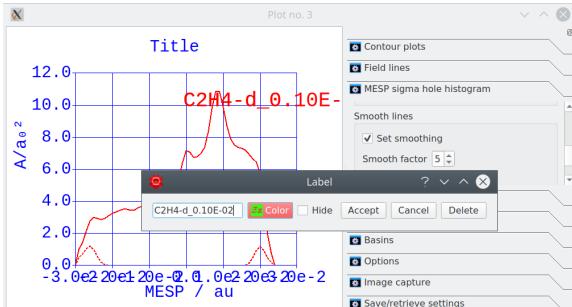


Figure 33<sup>fig:33</sup>

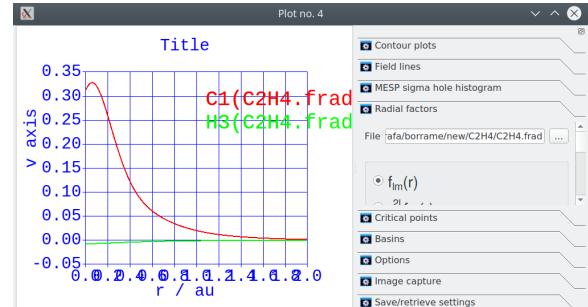


Figure 34<sup>fig:34</sup>

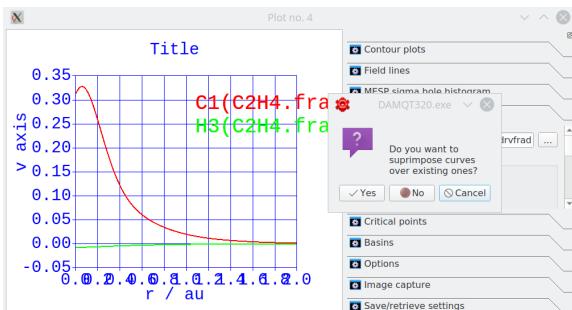


Figure 35<sup>fig:35</sup>

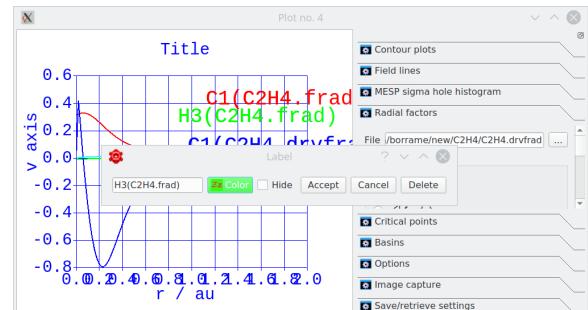


Figure 36<sup>fig:36</sup>

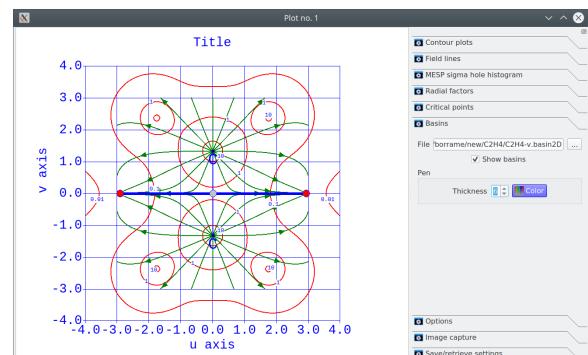
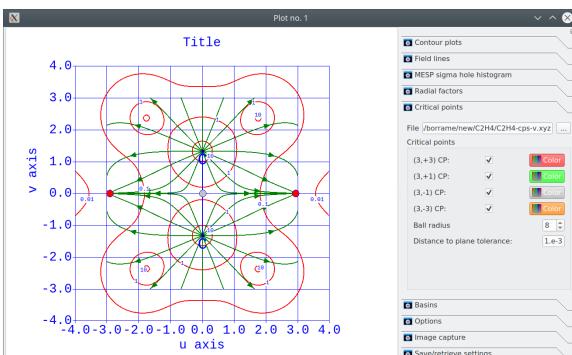


Figure 37 *fig:37*

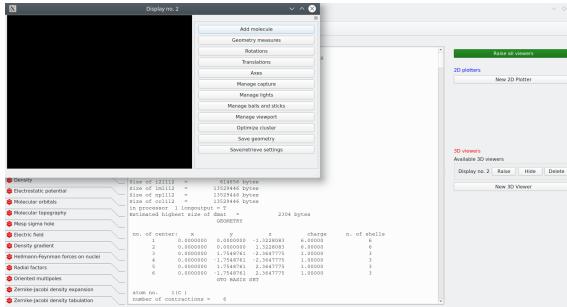


Figure 38 *fig:38*

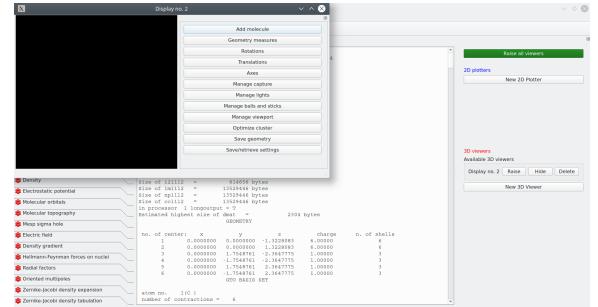


Figure 39 *fig:39*

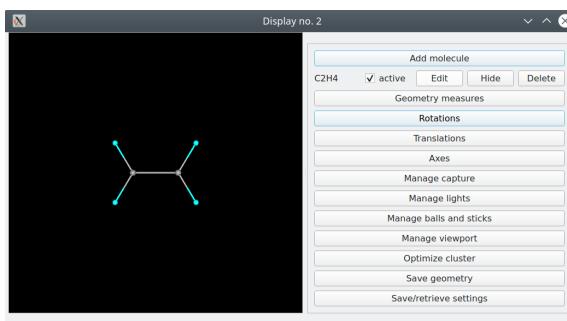


Figure 40 *fig:40*

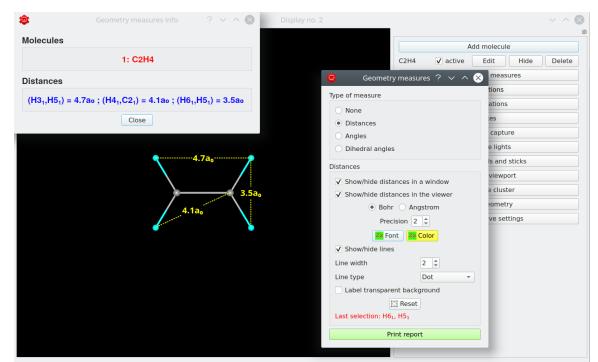


Figure 41 *fig:41*

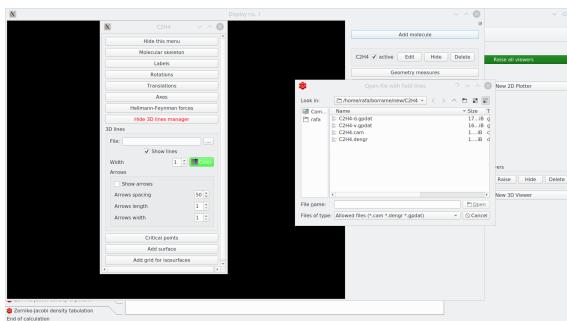


Figure 42 *fig:42*

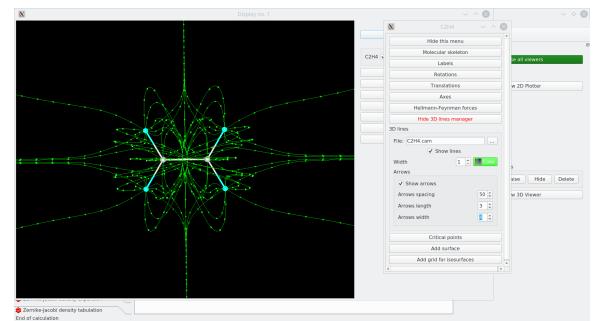


Figure 43<sup>fig:43</sup>

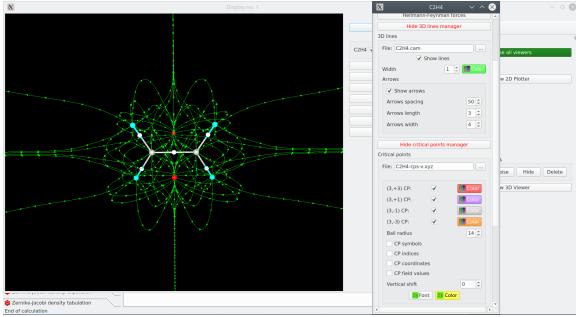


Figure 44<sup>fig:44</sup>

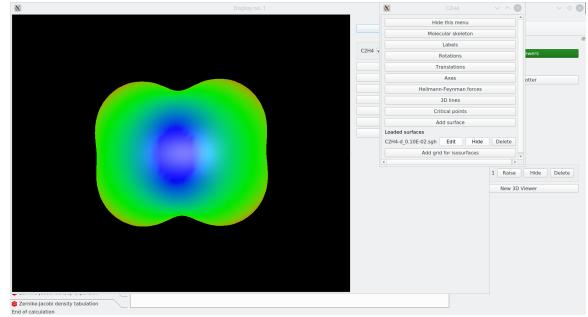


Figure 45<sup>fig:45</sup>

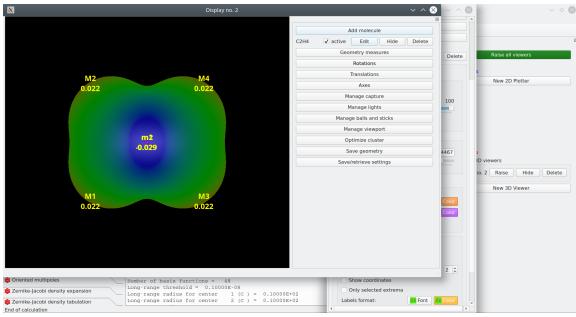


Figure 46<sup>fig:46</sup>

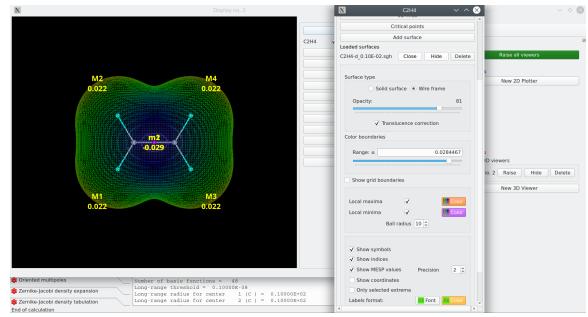


Figure 47<sup>fig:47</sup>

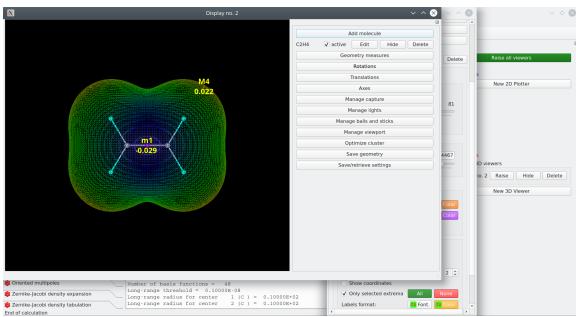


Figure 48<sup>fig:48</sup>

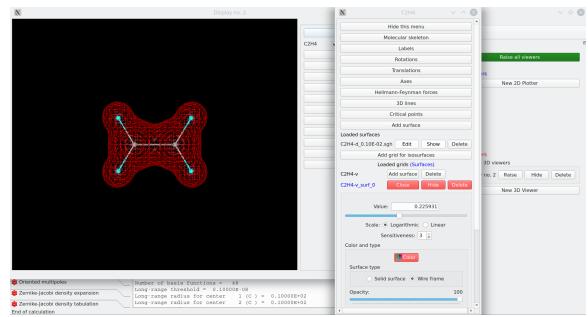


Figure 49<sup>fig:49</sup>

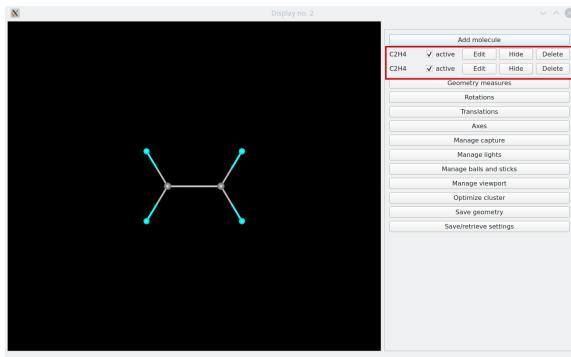


Figure 50<sup>fig:50</sup>

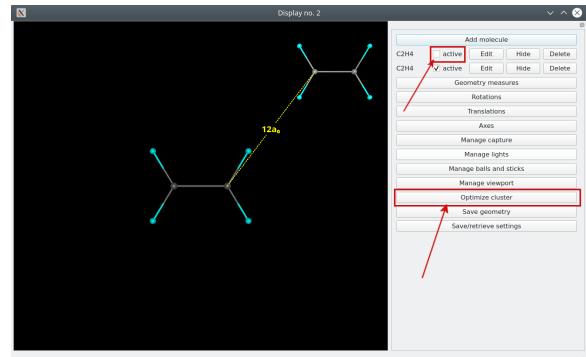


Figure 51<sup>fig:51</sup>

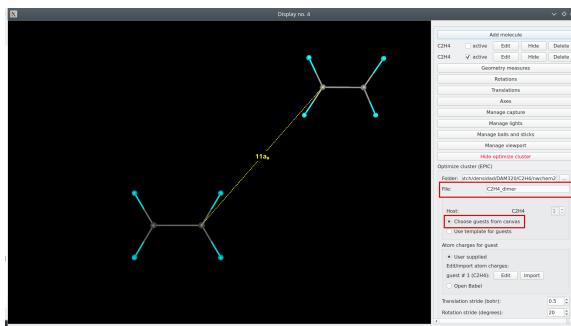


Figure 52<sup>fig:52</sup>

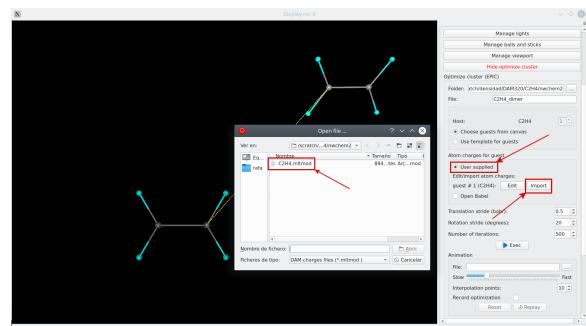


Figure 53<sup>fig:53</sup>

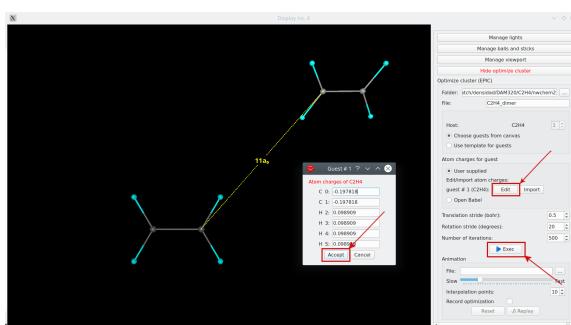


Figure 54<sup>fig:54</sup>

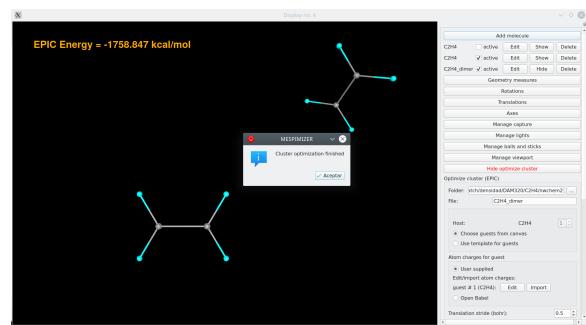


Figure 55<sup>fig:55</sup>

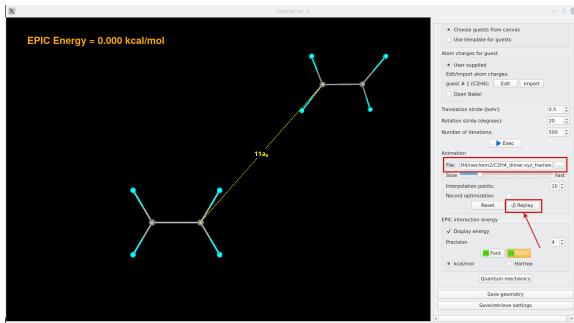


Figure 56<sup>fig:56</sup>

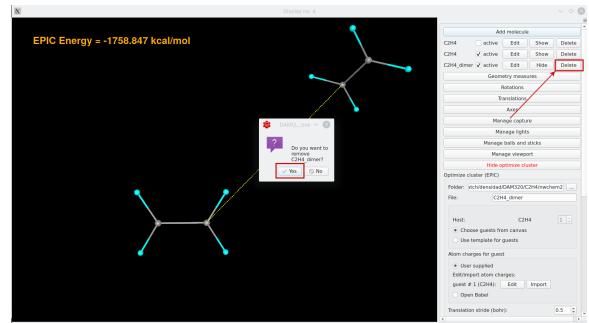


Figure 57<sup>fig:57</sup>

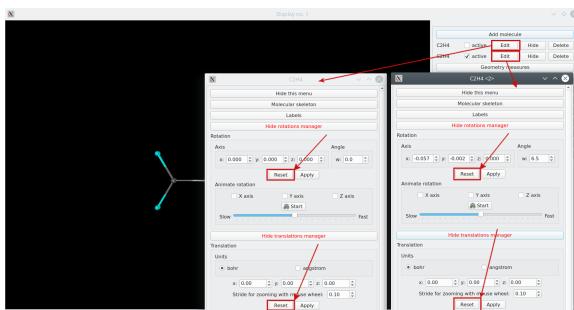


Figure 58<sup>fig:58</sup>

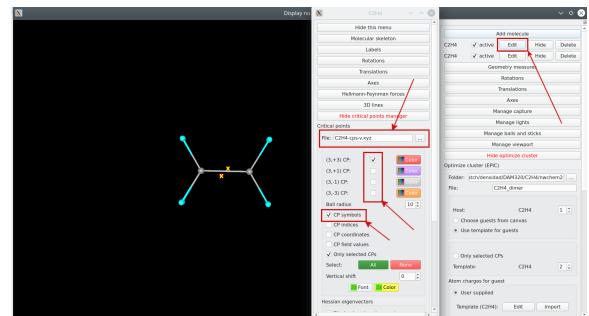


Figure 59<sup>fig:59</sup>

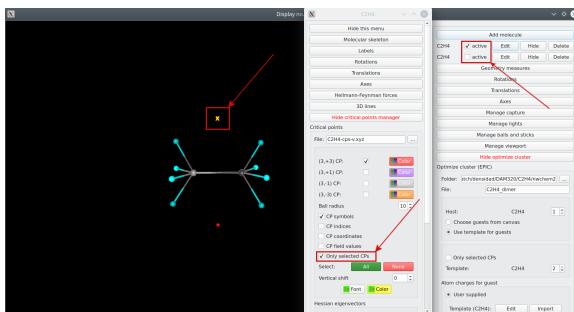


Figure 60<sup>fig:60</sup>

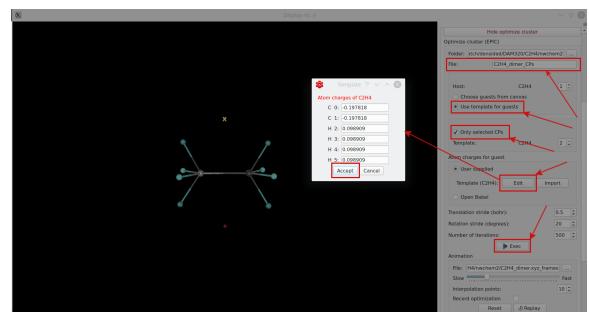


Figure 61<sup>fig:61</sup>

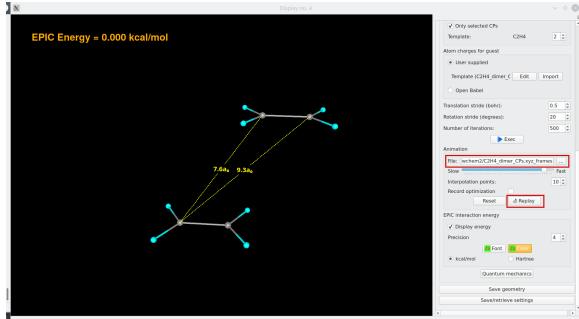


Figure 62<sup>fig:62</sup>

