



















## Quick start-up for DAMQT\_2.1.2 (by R. López)






1. Once the package is installed, run it just writing DAMQT212.exe in any suitable directory (beware that the executable is accessible by PATH or alike).
2. Choose a language and start DAMQT212 (see fig ??).
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 (\$DAMQT212)/samples/Molpro/C2H4/, for instance; see fig ??) and double click on file C2H4.out to launch Molpro's interface to DAMQT212.
4. Press the  key. The interface output will appear in the *Results* pannel (see fig ??).
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 ??). 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 that 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 deformations. It will take a few seconds to get the grid computed. Some output will be displayed in the *Results* panel (see fig ??).
7. To compute the full molecular density instead of the deformations, change the file name in the **Density-> Output files prefix** box (if you wish to keep the files with the deformations, otherwise the files will be overwritten with the new information), change the value in the spinbox **Density->Density settings->Atomic terms->Lowest** 1 from 1 to 0 and press the  key (see fig ??).
8. To compute full molecular density in a 2D grid, check radio button *2D grid* and press the  key (see fig ??). 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 ??).
10. Check radio button *2D grid* and press the  key to generate a 2D grid tabulation (see fig ??).
11. Press on tab **Molecular topography** on the left side menu. Check the boxes labeled as *Construct molecular graph* and *Construct atomic basin*, and click on the  key to compute the Topography of molecular density (see fig ??).
12. Check radio button *Molecular potential* and press the  key to compute the Topography of molecular electrostatic potential (see fig ??).
13. 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 ??).
14. Press on tab **Electric field** on the left side menu and click on the  key to compute the electric field lines. Increase **Higher number of points** and **Higher number of lines** by a factor of ten and click on the  key (see fig ??).
15. 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, and press the  key (see fig ??).




16. 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 ??).
17. Press on tab **Molecular orbitals** on the left side menu. Press the  key to select a file with MO (.GAOrba)). Select indices of MO orbitals to be displayed. Indices will be separated by commas. Ranges of indices separated by hyphens can be also specified (see fig ??). Once selected, press the  key to generate a grid.

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. To plot 2D grids do the following:

1. Press on tab **2D Plots** in the main panel to access the 2D plotter (see fig ??).
2. Press on tab **Import data** and select a file in the **File** box. The  key allows to navigate through the directories tree to choose a file (see fig ??).
3. Selecting a *.frad*, *.drvfrad* or *.drv2frad* file, radial factors (or their derivatives) will be plotted (see fig ??). Tab **Radial factors** on the right menu contains specific options for this type of plots.
4. Selecting a *.cnt* file, a contour plot will be displayed (see fig ??). Tab **Contour plots** on the right menu contains specific options for this type of plots.
5. Tab **Options** contains general options.

To visualize 3D grids do the following:

1. Press on tab **3D Pictures** in the main panel to access the viewer (see fig ??).
2. Press the tab **Geometry** in the right side menu and click on the  key. A window will be opened with the available *.gghs* and *.xyz* files of the project containing the geometry (see fig ??). **Do not choose -cps-d.xyz or -cps-v.xyz files**, since they correspond to critical points coordinates, not to atoms coordinates. Open the file by double clicking on the name or clicking once and pressing the  key. A figure with the molecule will be visualized. You can choose among four schemes for visualizing the molecular skeleton. Fine tuning of the display is also possible. Use the mouse buttons for reorienting or displacing the molecule (this can be done also in the **Options** tab; see fig ??).
3. Press the tab **Geometry measurements** in the right side menu and check the **Distances** radio button. Check also the boxes labeled as *Show/hide distances in a window* and *Show/hide distances in the viewer*. Next, hold the shift key and double click on a pair of centers. Distance between the selected centers will be displayed both in the viewer and in a pop window (see fig ??). You can repeat with angles (choosing three centers) and dihedral angles (four centers). Angles can be displayed only in a pop window (see fig ??).
4. Press the tab **Surfaces** in the right side menu and click on the  key for selecting a 3D grid to be visualized (files *.plt*). A window with the *.plt* files available will be opened (see fig ??). Choose one by double clicking on it. Use the ruler or the box to choose a contour value. To change sign of contour, press on the  or  keys. The contour surface will be dynamically rendered (see fig ??). Each contour to be displayed must be selected in a different tab. Up to 8 contours can be visualized at the same time. Single contours can be shown or hidden by checking (unchecking) the **Show/hide contour surface** checkbox.
5. Hide surfaces by unchecking the boxes labeled **Show/hide contour surface** (see fig ??).

6. Press the tab **Molecular topography** in the right side menu(see fig ??). Click on the  keys for selecting a *-cps-d.xyz* or *-cps-v.xyz* file with the critical points (CP) of density (the former) or electrostatic potential (the latter) to be visualized. (See fig ??). CP symbols, indices and field value at CP can be also displayed for all CPs (see fig ??), or only for selected ones (see fig ??). Hessian eigenvectors at CPs can be displayed as well (see fig ??). Choose a file *-d.gpdatt* or *-v.gpdatt* with a gradient path to display gradient lines of density or electrostatic potential (see fig ??). Choose a file *-d.bswir*, *-d.bssol*, *-v.bswir* or *-v.bssol* in the **Atomic basins** section to display atomic basins (see fig ??). Hide CPs, atomic basins, gradient lines and hessian eigenvectors by unchecking the pertaining boxes.
7. Press the tab **Forces** in the right side menu and click on the  keys for selecting a *.forces* file with the Hellmann-Feynman forces to be visualized. Increase vectors lengths if required (See fig ??). Hide vectors by unchecking the boxes.
8. Press the tab **Field lines** in the right side menu and click on the  keys for selecting the file with the electric field lines to be visualized. (See fig ??).

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

Figure 1:



Figure 2:



Figure 3:

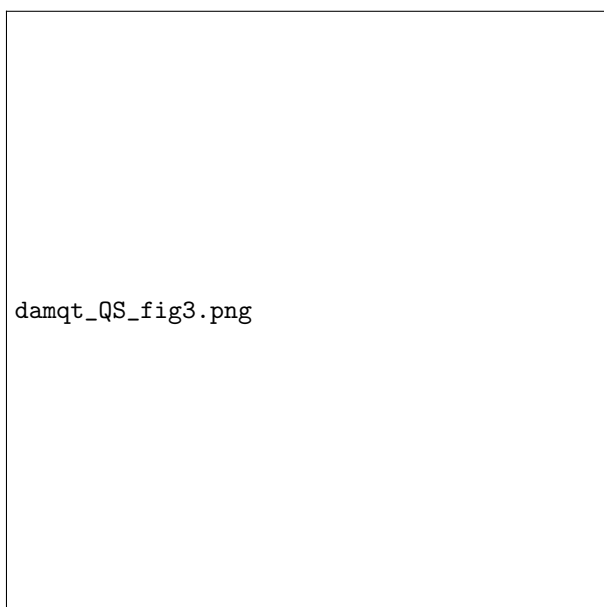


Figure 4:

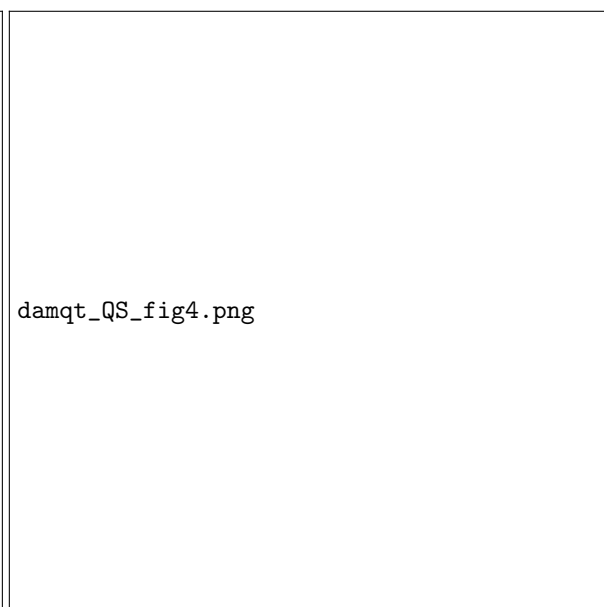


Figure 5:

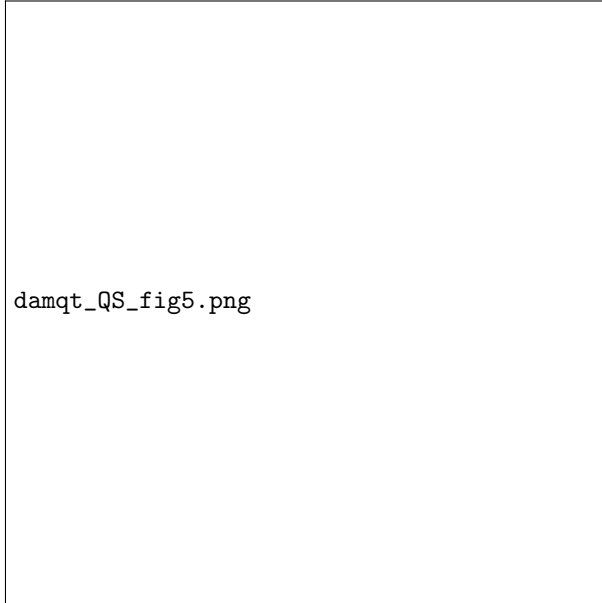


Figure 6:

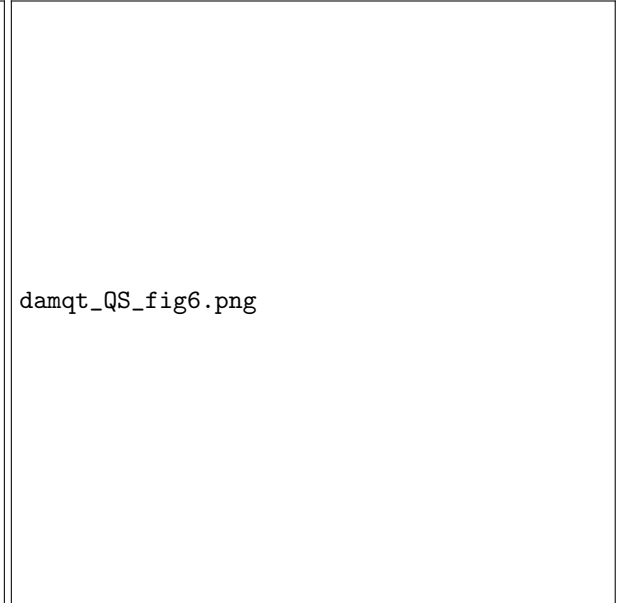


Figure 7:



Figure 8:

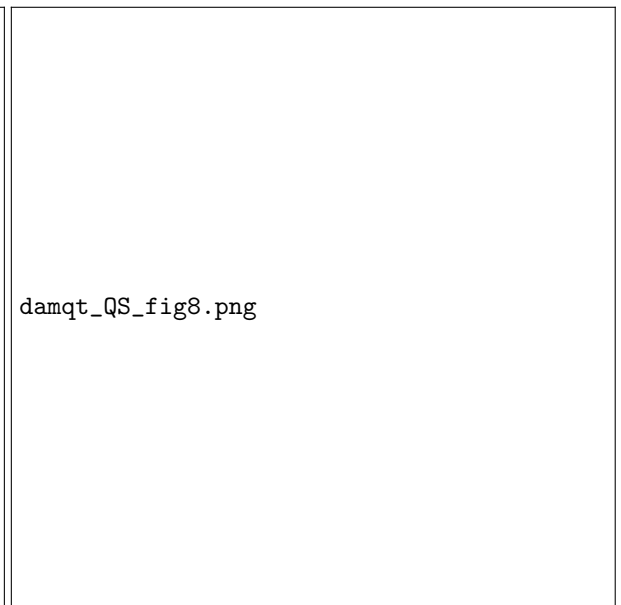


Figure 9:

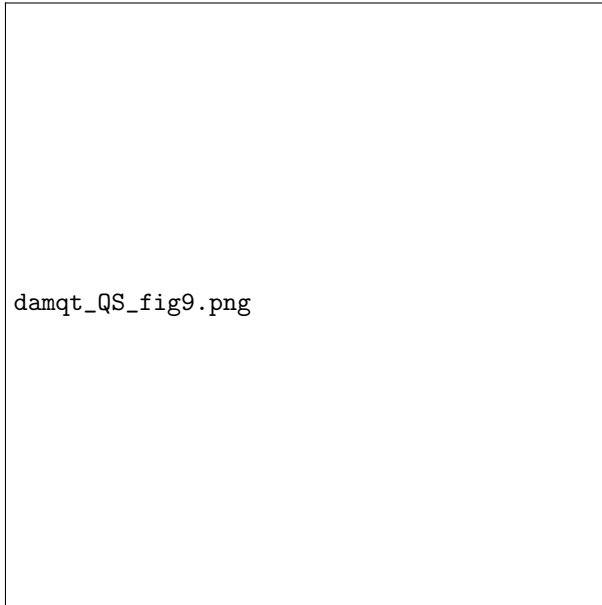


Figure 10:



Figure 11:



Figure 12:



Figure 13:



Figure 14:

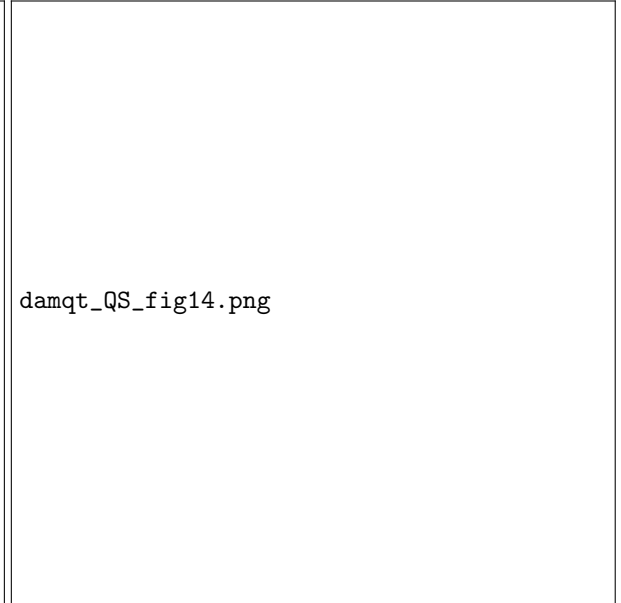


Figure 15:



Figure 16:

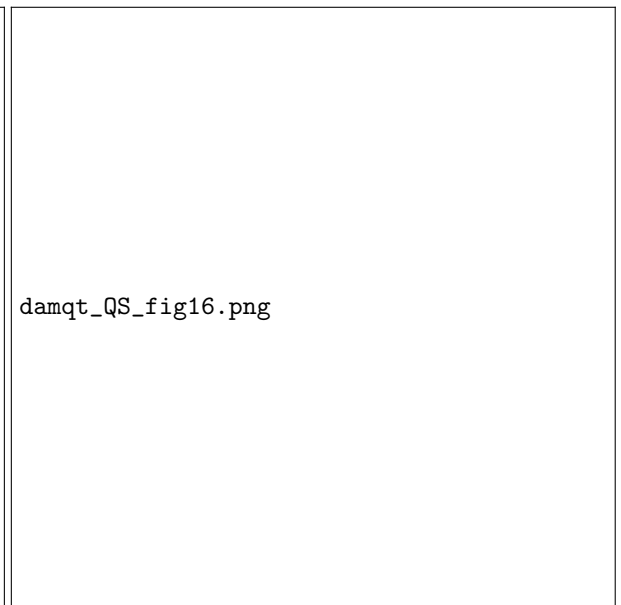


Figure 17:



Figure 18:

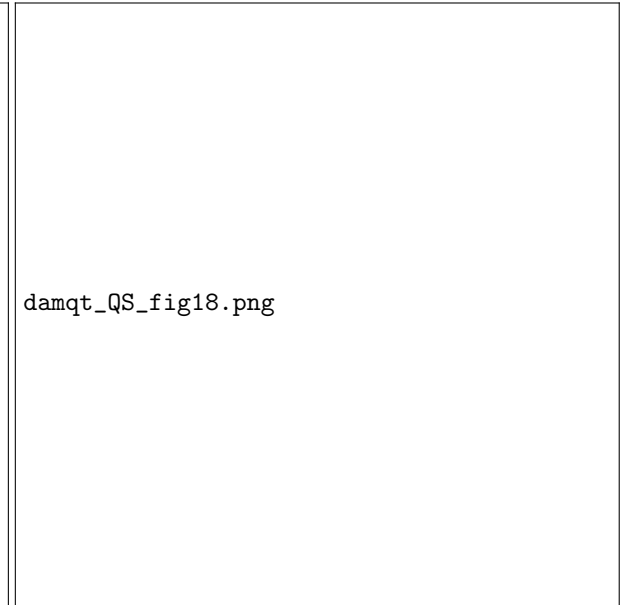


Figure 19:

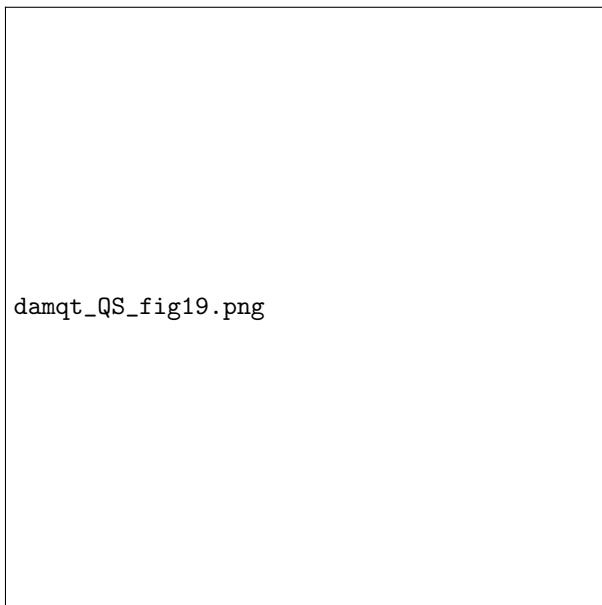


Figure 20:

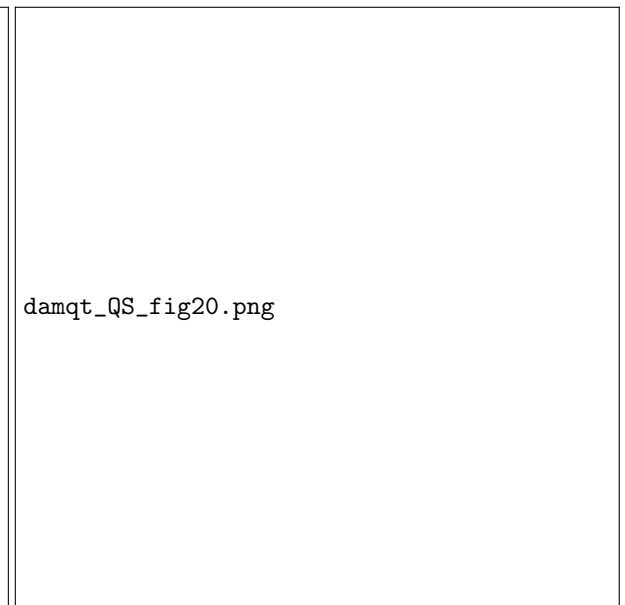




Figure 21:



Figure 22:



Figure 23:



Figure 24:

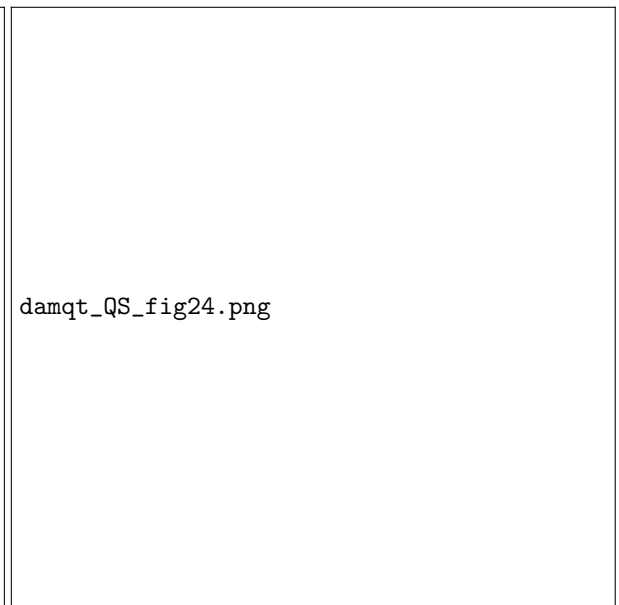


Figure 25:



Figure 26:



Figure 27:



Figure 28:



Figure 29:



Figure 30:

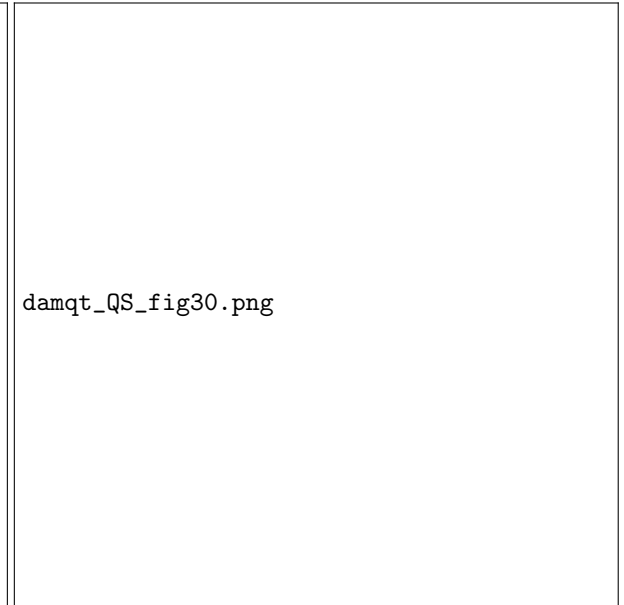


Figure 31:



Figure 32:



Figure 33:



Figure 34:



Figure 35:



Figure 36:

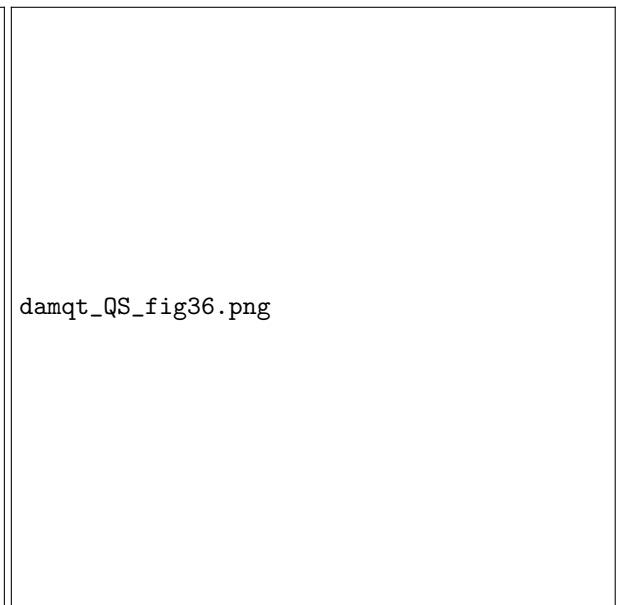


Figure 37:

