Viewing Gaussian Difference Densities with Gabedit

Gabedit reads the cube file created from a Gaussian calculation. This example looks at several of the excited states of acrolein.

Generating Cube Files

- For a Ground State Density
    - CIS/6-31G(d) density(SCF) cube=density
    - At the end of input information
        - Blank line > filename_gs.cube > Blank line
- For an Excited State Density
    - Input information located directly below last blank line from Ground State Density input information
        - --link1--
        - %chk=filename.chk
        - # geom=allcheck guess(read, only) density(checkpoint,cis=n) cube=density
            - Where n represents the number for the excited state (example: n=2 for the second excited state)
        - Blank line > filename_ex.cube > Blank line

Note: There are numerous ways to generate cube files. The method instructed above is simply the way chosen for this particular demonstration.

Here is an input file :

%chk=acrolein_cube2.chk

CIS/6-31g(d) density(SCF) cube=density

Acrolein

0	1						
O							
C	1	B1					
C	2	B2	1	A1			
C	1	B3	2	A2	3	D1	
H	2	B4	1	A3	4	D2	
H	4	B5	1	A4	2	D3	
H	3	B6	2	A5	1	D4	
H	3	B7	2	A6	1	D5	

  B1   2.42760000

B2	1.35513230
B3	1.25839101
B4	1.06999778
B5	1.07000357
B6	1.07004978
B7	1.06999778
A1	146.67462980
A2	33.32258955
A3	93.32180987
A4	119.99543395
A5	120.00421600
A6	120.00356032
D1	0.00000000
D2	180.00000000
D3	180.00000000
D4	180.00000000
D5	0.00000000

acrolein1_gs.cube

--link1--
%chk=acrolein_cube2.chk
geom=allcheck guess(read,only) density(checkpoint,cis=2) cube=density

acrolein_ex2.cube

Visualizing Difference Densities in Gabedit

First Click to "Display Density/Orbitals/Vibration" icon(toolbar, top of window).

Right mouse click in the new window. Select **Cube/Load gaussian cube/Density only File**.

Find the **ground** state cube. Select OK.

Right mouse click. Select **Cube/Save**. Save your density in tmp.gcube

Right mouse click. Select **Cube/Load gaussian cube/Density only File**.

Find the **excited** state cube. Select OK.

Right mouse click. Select **Cube/Subtract.** Find the tmp.gcube. Select OK.

Adjust the iso value(Right mouse click **Set/IsoValue)** until you obtain a visualization of the difference densities that is ideal.

| File Name : acrolein_ex2.cube | File Type : Gaussian Cube | Geometry : Ok | Mol. Orb. : Nothing |
| At. Orb. : Nothing | Grid : Ok | IsoSurface : Ok | Right mouse button for popup menu. |

Cancel