ESP with ORCA

(E-Mail Vahideh 16/06/2021; files unter k15:Desktop/ORCA(R)ESP_charges/)

To calculate ESP with ORCA you first need a start structure as xyz-file "input.xyz". On this structure you perform a single point calculation, for example with input.inp and run.bash (attachment). If you want to optimize the structure in the step you may use the opt.inp as input.inp. With the attached run file "run.bash" you will have a folder named "opt_out0" which contains .gbw file, continue in the folder opt_out0.

Now the fun part for ESP starts (after the calculation is finished you use):
`/home/software/cluster/orca_4_0_1_linux_x86-64/orca_plot input.gbw -i`

In the upcoming dialogue you choose:
For (1) `Enter type of plot --> 2`-electron density
For (4) `Enter number of grid intervals -->Enter NGRID: 80`
For (5) `Select output file format --> 7-` gaussian cube
Then, you start the calculation with 10. This should run fast.

Use the script "mep.py" (attachment) in the corresponding folder like ./mep.py input 80
This may take a while...
You should have two cube files:
"input.eldens.cube" with the electron density
"input_mep.cube", with the electrostatic potential

Thus, now you need to visualize. To visualize it with VMD in the same style I chose, you first have to open the "input.eldens.cube" with VMD. Now you load the "input_mep.cube" into the same molecule (!!!). You can now choose the representations in a way, that you have
1. a CPK representation → "input_mep.cube"
2. an isosurface, with "Vol" chosen as "vol0:input.eldens.cube", the isovalue as 0.004 and the draw "Wireframe".
Now you choose the coloring method as "Volume" with "1:input_mep.cube" as parameter. In the "Trajectory" slide you change the color scale range to something like 0.00 and 0.20 or whatever is looking meaningful. Finally, you may try in the Graphics->Colors window the slide "Color Scale" and change it to RGB.

Additional info:

- make geometry optimization with ORCA and produce .gbw file
- get .molden file with:
  /home/software/cluster/orca_4_0_1_linux_x86-64/orca_2mlk orca -molden
- boot file with multiwfn
- for RESP: choose (7), then (18) and (1)
- restricting the calculations with regard to symmetry of the studied molecule is possible when calculating ESP charges