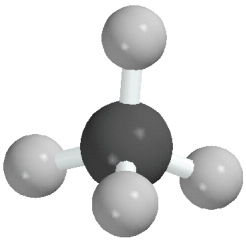
Electron Density Lab Exercise
Chemistry 221

You might find it helpful to work through the electron density tutorial at the website first: web.pdx.edu/~shusteg

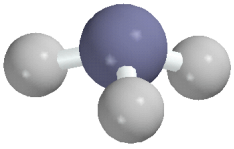
For the molecules listed below:

- Draw a Lewis dot structure model
- Use the ball and stick models below and electronegativities to predict if the molecules are polar

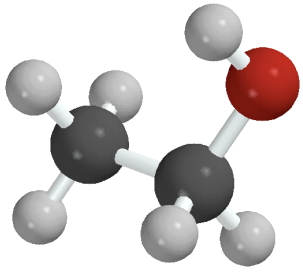
A) CH_4



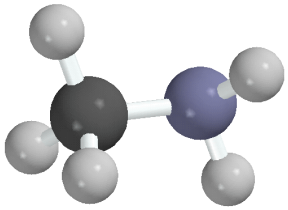
B) NH_3



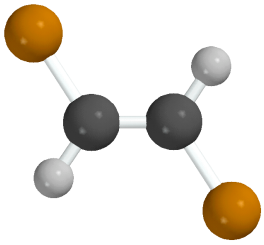
C) CH_3CH_2OH



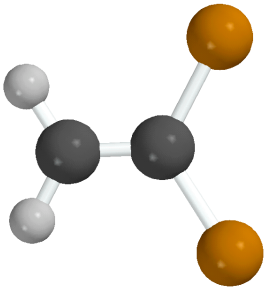
D) CH_3NH_2



E) $CHClCHCl$



F) CCl_2CH_2

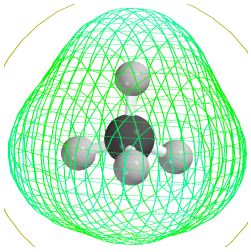


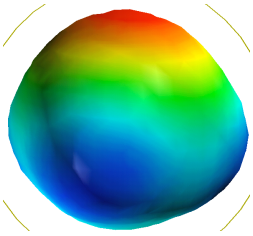
Below are electron density models of the molecules you drew Lewis structures for. These are surfaces where the value of the electron density

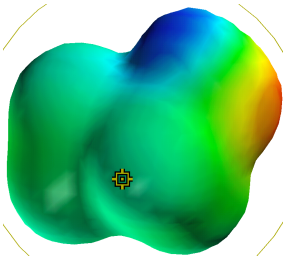
is the same everywhere. The value of the electron density chosen to generate these surfaces is that which can be interpreted as a "size" surface. This is how big the molecule is.

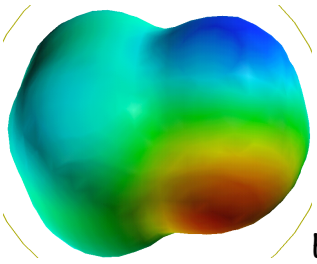
Additional information is included in these graphical images. Regions where the surface is most negative are colored red and regions where the surface is most positive are colored blue. The rainbow of colors between red and blue are used for intermediate charges. The charge on the surface is the result of the combination of nuclear charge and the electron charge distribution at that point. When the nuclear charge exceeds the electron charge the result is a positive region of the surface, and vice versa for negative.

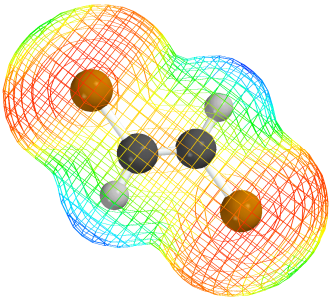
Evaluate the electron density surfaces below and compare the quantum mechanical predictions to your simpler Lewis model and electronegativities.

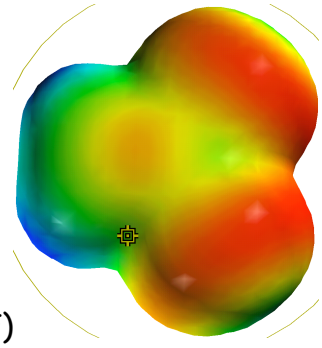
A) 

B) 

C) 

D) 

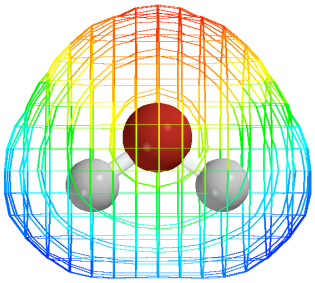
E) 

F) 

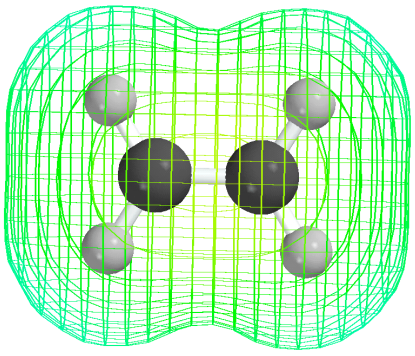
Now that you are more familiar with the electron density models, which molecules below you would expect to be most soluble in water?

In addition, indicate the relative attraction you would expect between these molecules and a surface or column that was coated with a very polar material. Can you use this as a separation scheme to separate these compounds?

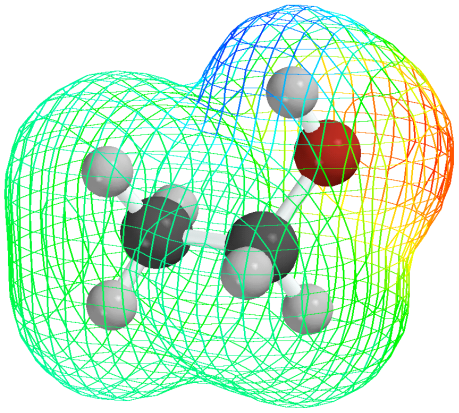
Water:



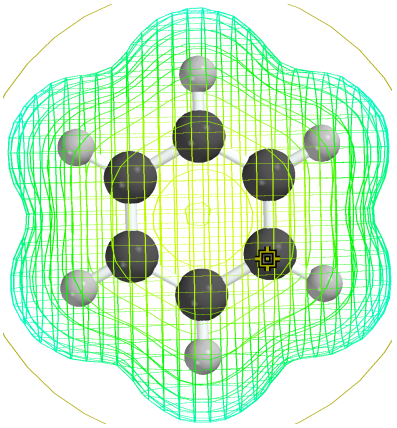
1)



2)



3)



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