

Pointers on using CAChe

1. open the workspace (located under CAChe on the program menu)
2. To build water select O and sp³ hybridization and click in the workspace
3. You can add the H's by selecting valence under the beautify menu
4. to measure or change the angle select the select tool on the workspace (topmost tool). Click one H, and holding down the shift key click the other two atoms. A box will pop up giving you the angle which you can modify.
5. Now choose Experiment, new
6. In the menu that pops up select homo-5 to lumo+4 under properties
7. click start on the popup menu
8. When the calculation finishes, you can display the orbitals using show surfaces under the analyze menu
9. to get the orbital energies choose chemical properties under analyze. On the properties popup sheet select molecular.