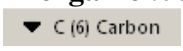
Chem 201, 2009
HW #4, due Th, Oct 8, 12 PM

Loudon problems from chapter 5: 28AGHO 30ABG, 32H, 42, 45AB, 48DF, 50

- I've assigned lots of problems because there are many ways to approach chemical reactions and I want to make sure you see several *types* of problems.
- #28, 30, 45 have short answers. Just draw a structural formula for each.
- #32 has a short answer. Just draw a synthetic step (or series of synthetic steps).
- #48 requires mechanism drawings. Include curved arrows or fishhooks as needed (see book for guidance). Do not draw energy diagrams.
- #42 requires some arithmetic. Show your work.
- #50 should lead you down to the computer lab to use *SPARTAN* to build and compare models of the boranes that are actually observed (Figure 5.50) with models of the expected *tri*alkylboranes.

SPARTAN instructions for #50:

1. **File: New** or 
2. Select **Inorganic** toolkit
3. Click 

in toolkit and change to 

4. Click  and click in work area to install a trigonal B
5. Select **Organic** toolkit
6. Select sp^3 C and add as needed to make desired borane (*see building tip*)
7. **Build: Minimize** or  (this "cleans up" the most egregiously distorted bond distances, bond angles, and van der Waals repulsions, but the "cleaned up" model is not terribly reliable; proceed to step #8)
8. **Submit: Calculations** and calculate **Equilibrium Geometry** using **Semi-Empirical AM1** (click Submit)
9. What hits you? (see *analysis tip*)

Building tip – You may need to rotate alkyl groups (or parts of alkyl groups) into unencumbered locations to generate a plausible model. To do this:

- If necessary, select 
- Select bond that needs to be rotated. A red band will be wrapped around the bond.
- Press **Alt** and work the mouse while pressing the *left* mouse button

Analysis tips – This is really an energy problem, but I don't want you to calculate energies. Instead, I want you to simply look at the models and use what you have learned about structure-energy relationships. To put it another way, you are supposed to *see* something that looks destabilizing in each *tri*alkylborane. Possibly useful tools:

- **Model: Space-filling** will give you an idea how much space each atom fills
-  will let you find out the distances between pairs of atoms
-  will let you find out angles between three atoms*
-  will let you find out dihedral angles between four atoms*

* with these tools, the order in which you select atoms is important