MIT Inorganic Chemistry 5.04 Homework

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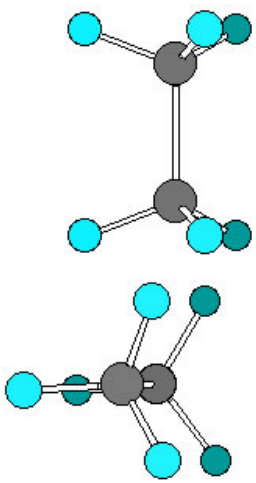
March 18, 2019

Part 1: Finding Symmetry Elements

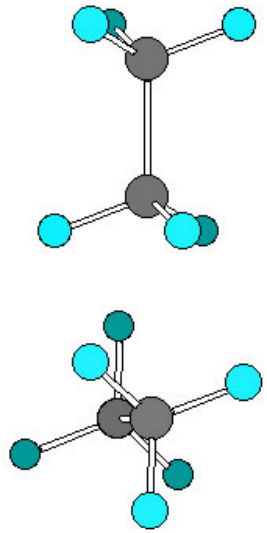
First, a refresher: Symmetry elements are the axes, planes, and points that one can apply our discovered symmetries about to achieve a symmetry. The first half of this assignment is listing the symmetry elements of molecules, and that I shall do.

Symmetry of Ethane: Eclipsed & Staggered

Ethane has two different forms, Eclipsed and staggered, as we can visualize using the following image:



Eclipsed

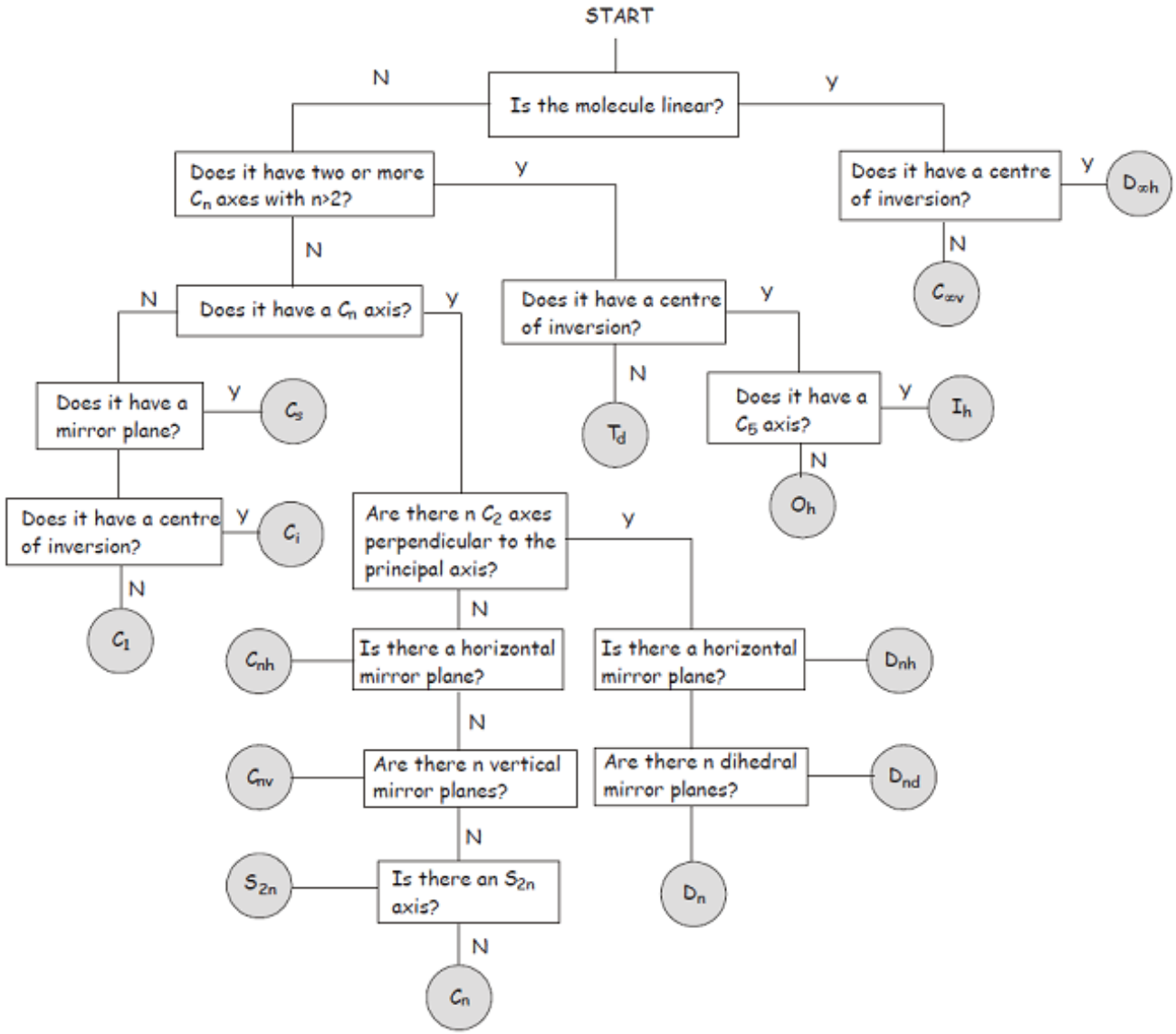


Staggered

Ethane Continued

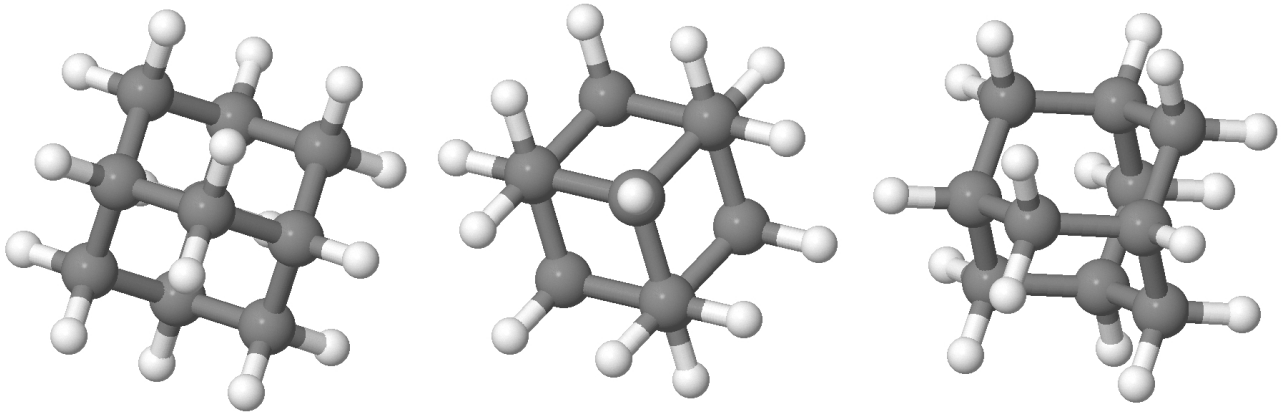
Both of these forms exhibit 3 planes of symmetry through the $\mathrm{C}-\!\!-\mathrm{C}$ bond and one of the hydrogen atoms offset; However, the eclipsed ethane also exhibits a mirror plane perpendicular to the ones previously mentioned. We also see that the staggered ethane exhibits an S_6 improper rotation axis, while the eclipsed merely has an S_3 improper rotation axis. The flowchart seen on the next page enables us to assign point groups quickly, and allows us to see that staggered ethane has a D_{3d} point group, while eclipsed has a D_{3h} point group.

Assigning Point Groups: The Flowchart



Adamantane

Rather than do all of the solutions, I have presented the easiest to get the concepts out of the way, and now shall do what appears to be the hardest and is coincidentally organic, adamantane. After a short bit of exploration, I notice something unimaginable beautiful (and useful) about adamantane, its cross-section when viewed at certain angles (or in the case of the third, when it is not):



Adamantane Continued

These "hexagonal" and "square/grid" cross sections give us some very interesting information to work with; we note that if we imagine the viewpoint being an axis going through the molecule at that angle, then there exist some symmetries as follow: In the case of an axis as seen from any of the the "square" positions, there exist C_2 (180°) symmetries and S_4 improper axis symmetries. In the case of the "hexagonal" axes, these exhibit C_3 (120°) symmetries. We also see that there exist *many* mirror planes. Overall, adamantane exhibits a T_d point group.

Part 2: Working from point groups

We are given a peculiar point group to work from, C_{2h}. This means that the molecule we are looking for is:

1. Not linear
2. Does not have more than one C_n axes with $n > 2$.
3. Has a C_n axis
4. Has no axes perpendicular to the principal axis
5. Has a horizontal mirror plane

Finding a suitable molecule

So it would seem that we have a planar molecule that exhibits rotational symmetry about an axis perpendicular to the plane. My first thought was to think of C_2H_2 this is both acetylene and unfortunately linear, so we want something to inspire the element "hanging off" to bend, and an easy way to do that without Lewis structures, is find some other atom that forces it away.