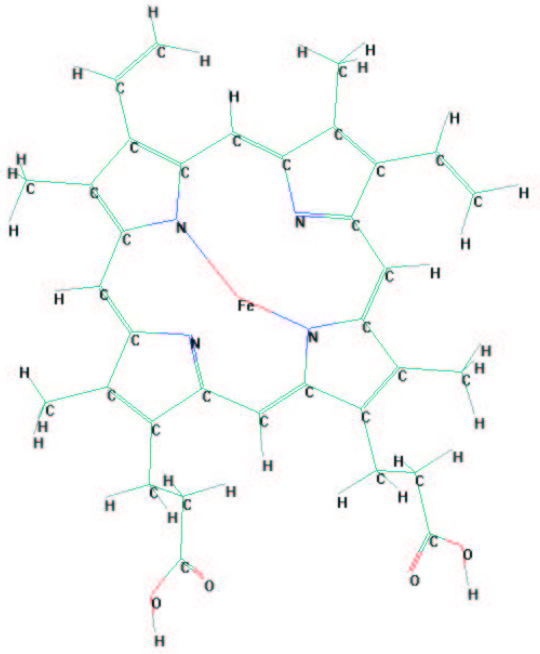
Laboratory 3
HyperChem, Hem B

Lesson	Information covered	Time to complete
Creating Hem B	Creating molecule and using model builder.	10 minutes
Geometry Optimization of Hem B	Geometry optimization and vibrational analysis.	45 minutes
Building and optimizing geometry parameters	Build and optimize geometry for isolated O_2, CO_2 and CN^-. Use PM3 and ZINDO method.	15 minutes
Building and optimizing geometry parameters	Build and optimize geometry for complexes $HemB + O_2$, $HemB + CO_2$ and $HemB + CN^-$. Use PM3 and ZINDO method.	65 minutes

Creating Hem B



L-click on Explicit Hydrogens of the Build menu until it is not selected. Select Default Element of the Build menu to bring up the periodic table dialog box...create molecule shown above... Select Add H & Model Build of the Build menu to create Hem B at the standard model builder geometry.

Geometry Optimization of Hem B

In this lesson you will use a semi-empirical method PM3. To perform calculation select Setup, semi-empirical, PM3. Then Compute, Geometry optimization. Write down energy you have obtain. One again select Setup, semi-empirical, ZINDO(1). Now select Compute, Single point calculation. Write down the energy from ZINDO. To perform a vibrational analysis: select Setup, semi-empirical, PM3, OK. Compute, Geometry optimization. Select Vibrations from the Compute menu to perform a vibrational analysis at the optimized geometry. It takes a while. Select Vibrational Spectrum from the Compute menu to display the vibrational spectrum.

Save the structure as hem.hin!!!!!

Geometry Optimization of O_2, CO_2 and CN^-

Build O_2 molecule. Optimize geometry using PM3 method. Write down the energy. Do single point calculations for ZINDO(1) method. Perform a vibrational analysis. Save structure!!!!! Do the similar things for CO_2 and CN^- molecules.

Geometry optimizations for complexes $HemB+O_2$, $HemB+CO_2$ and $HemB+CN^-$

Reopen hem.hin. Create complex $HemB + O_2$ (put O_2 molecule above Fe). Optimize geometry PM3(geometry optimization, then ZIND(1) single point). Perform a vibrational analysis. Write down the energy. Save structure!!! Do the similar things for complexes $HemB + CO_2$ and $HemB + CN^-$.

Analysis

Calculate:

$$\Delta E_1^{PM3} = E^{PM3}(ComplexHem + O_2) - E^{PM3}(Hem) - E^{PM3}(O_2) \quad (1)$$

$$\Delta E_1^{ZINDO} = E^{ZINDO}(ComplexHem + O_2) - E^{ZINDO}(Hem) - E^{ZINDO}(O_2) \quad (2)$$

$$\Delta E_1^{PM3} = E^{PM3}(ComplexHem + CO_2) - E^{PM3}(Hem) - E^{PM3}(CO_2) \quad (3)$$

$$\Delta E_1^{ZINDO} = E^{ZINDO}(ComplexHem + CO_2) - E^{ZINDO}(Hem) - E^{ZINDO}(CO_2) \quad (4)$$

$$\Delta E_1^{PM3} = E^{PM3}(ComplexHem + CN^-) - E^{PM3}(Hem) - E^{PM3}(CN^-) \quad (5)$$

$$\Delta E_1^{ZINDO} = E^{ZINDO}(ComplexHem + CN^-) - E^{ZINDO}(Hem) - E^{ZINDO}(CN^-) \quad (6)$$

Write down conclusions.