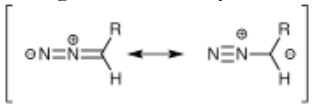
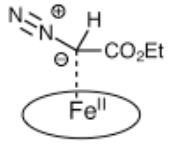
Problem Set #10 – Chemistry 391 Name_____
Due in class on 11/29/18

1. Suggest (a) why this paper might have excited the editors of science and (b) why the authors might even have thought to pursue this project.

2. To form an understanding of how cyclopropanation might work, suggest an arrow-pushing mechanism for the reaction in which an Fe(IV) oxo species reacts with an alkene to make an epoxide (oxene transfer, Figure 1).

3. What evidence is there that the active species of $P450_{BM3}$ is Fe^{II} rather than Fe^{III}? With that evidence in place, suggest an arrow pushing mechanism that starts as shown below with a second resonance form of the diazo compound. Be sure you can arrive at the Fe(IV) carbene intermediate and get all the way to the cyclopropane species that ends with Fe(II).





4. Hemin (heme in Fe^{III} state) is set up as the baseline in this study. Discuss its performance as a catalyst, and a regio- and stereo-selective catalyst compared to $P450_{BM3}$.

5. The productivity of catalysts are evaluated by several metrics. Define each of the ones show below.

TTN

Yield

Cis/trans

ee

6. Walk me through the development of BM3-CIS-T438S as a superior catalyst of the *cis* product. What are the individual steps? It will be easiest to set those steps up as bullet points.

7. Comparably, what turns out to be the best catalyst for the *trans* product. How was it developed?