1. a. Look up the 2010 crystal structure of bacterial nitric oxide reductase. What is the journal reference for its publication?

b. “The Protein Data Bank (PDB) archive is the single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids” (<http://www.rcsb.org/pdb/static.do?p=general_information/about_pdb/index.html>).

What is the pdb id# for the bacterial NOr in the 2010 paper?

c. From what bacterium was it isolated?

1. What ligands coordinate the non-heme iron center (FeB) in the crystal structure?
2. Write the balanced half-reaction for the reduction of NO to N2O in acidic conditions.
3. Discuss the HSAB nature of the ligands bound to the non-heme iron center, and their appropriateness to the function of the enzyme.
4. Use HSAB arguments to explain why the BMPA-Pr ligand complex would have a lower redox potential (i.e., why is it easier to make the ferric form) than the TPA complex on which it was based.
5. On page 16714, the authors state that “the isolated iron complexes are EPR silent in accordance with their Fe(II) oxidation states.” Explain why these Fe(II) complexes would be EPR silent.
6. Construct an MO diagram for nitric oxide. Identify the HOMO and the LUMO. How will NO- differ from NO?
7. On page 16716, the authors discuss the direct correlation between the Fe-NO and N-O stretching frequencies shown in Figure 3. They are careful to note that the “correlation between (Fe-NO) and (N-O) is *not* inverse, as would be expected for a change in Fe-NO back-bonding along this series.” Explain why one would expect to see an inverse relationship between the Fe-NO and N-O stretching frequencies if back-bonding were occurring between the Fe and NO ligand. That is, why would back bonding cause the N-O frequency to decrease as the Fe-NO frequency becomes larger.
8. List the techniques that were used in this communication.