Created by Chip Nataro, Lafayette College (nataroc@lafayette.edu); Barbara A. Reisner, James Madison University (reisneba@jmu.edu); Sheila R. Smith, University of Michigan Dearborn (sheilars@umich.edu) and Joanne Stewart, Hope College (stewart@hope.edu) and posted on VIPEr (www.ionicviper.org) on March 12, 2024.

Read this paper before class.

Jiang, J.; Koch, S. A. New Members of the Class of $[Fe(CN)_x(CO)_y]$ Compounds. *Inorg. Chem*. **2002**, *41(2)*, 158-160. DOI: 10.1021/ic015604y.

To prepare for our discussion, write out the answers to these questions and bring them to class.

1. $[Fe(CN)_3(CO)_3]^-$ symmetry and structure
   a. Sketch and label the two possible geometric isomers of $[Fe(CN)_3(CO)_3]^-$. Which isomer do the authors observe?
   b. Provide sketches that show the symmetry elements of $[Fe(CN)_3(CO)_3]^-$. (Do not include the counterion.)
   c. Assign the point group of $[Fe(CN)_3(CO)_3]^-$.
2. $[Fe(CN)_4(CO)_2]^{2-}$ symmetry and structure.
   a. Sketch and label the two possible geometric isomers of $[Fe(CN)_4(CO)_2]^{2-}$. Which isomer do the authors observe?
   b. Provide sketches that show the symmetry elements of $[Fe(CN)_4(CO)_2]^{2-}$. (Do not include the counterion.)
   c. Assign the point group of $[Fe(CN)_4(CO)_2]^{2-}$.
3. Using group theory, predict how many IR and Raman bands should be observed for the *fac*-isomer and *mer*-isomer of $[Fe(CN)_3(CO)_3]^-$.
4. Using group theory, predict how many IR and Raman bands should be observed for the *cis*-isomer and *trans*-isomer of $[Fe(CN)_4(CO)_2]^{2-}$.
5. Use the CBC method of electron counting to classify each compound. Determine the electron number, ligand bond number, metal valence, and d^n count for *fac*-$[Fe(CN)_3(CO)_3]^-$ and *cis*-$[Fe(CN)_4(CO)_2]^{2-}$.
6. How do the authors confirm the structure? Does the vibrational spectral data make sense? Why or why not? What are potential reason(s) you can use to rationalize your answer?
7. How would you rationalize this statement by the authors "In the $[Fe^{II}(CN)_{(6-x)}(CO)_x]^{(x-4)}$ series, both the CO and CN stretching frequencies are shifted to higher energy with increasing CN^- by CO substitution."?
8. The authors state "Aqueous solutions of **2** decay on the order of minutes into a mixture of products including **1** and $[Fe^{II}(CN)_5(CO)]^{3-}$. As monitored by IR spectroscopy, added NaCN inhibits this reaction." What insight does the second sentence provide in terms of a potential mechanism for this decay?
9. Professor Koch and his colleagues suggest that the compounds characterized in this paper may be of special interest due to their similarity to metal centers found in two hydrogenase enzymes. This area of chemistry, ***biomimetic*** chemistry, has been a driving force for the synthesis of a wide range of complexes, many of which were deemed unlikely until found in nature.
   a. What is the function of a hydrogenase enzyme? Write the balanced chemical equation carried out by a hydrogenase.

b. Locate the primary article referenced in 1a in the current paper. Attach a screenshot of the title and abstract.

c. Compare and contrast the iron center in Figure 1A of the current paper and the iron center in Figure 1B of the JACS paper.