**Theoretical Analysis of Fe K-Edge XANES on Iron Pentacarbonyl**

*Literature Discussion Activity*

“Theoretical Analysis of Fe K-edge XANES on Iron Pentacarbonyl”

by Wei-Ting Chen, Che-Wei Hsu, Jyh-Fu Lee, Chih-Wen Pao, and I-Jui Hsu\*

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**Discussion Questions:**

1. What was the research problem that these scientists were attempting to solve?
2. What are the two geometries (and respective point groups) of iron pentacarbonyl investigated in this work and what are the differences between the two structures?
3. What does the Walsh diagram indicate about the occupied MOs of Fe(CO)5?
4. What is K-edge XANES? What is EXAFS? What can these characterization techniques elucidate about a chemical structure?
5. Consider the data presented in Figures 5 and 6. What did the authors measure computationally to obtain these figures and how did they analyze the data to produce these plots? What conclusions did they draw from these results?
6. Comparing Figures 7-8, what are the main differences in the convolution profiles between the two geometries. Why does this change occur?
7. Explain how this paper combines group theory, symmetry, MO theory, ligand field theory, and spectroscopy.