CHEM 5620, Physical Methods in Chemistry; Spring 2003, Dr. Omary Department of Chemistry, University of North Texas Homework set #5 EPR. Due in class Wednesday, April 29.

<u>Part 1:</u> Do the following end-of-chapter problems from the handout you were given from Chapter 4 of the textbook by Wertz, J. E. and Bolton, J. R. "Electron Spin Resonance: Elementary Theory and Practical Applications":

Problems 4-2, 4-4, 4-5, 4-9, 4-10, 4-11, and 4-13.

Part 2: Answer the following questions from the work of Cotton et al. J. Am. Chem. Soc. 2003, 125, 2026-2027.

(a) Construct an MO diagram that shows the interaction of the metal d orbitals for each of compounds 1 and 2 in the paper to form dimers with metal-metal bonds. Explain how your MO diagrams account for the following:

(i) the M-M bond orders stated by the authors for the two compounds.

(ii) one of the two compounds should be EPR active.

(b) Explain the experimental evidence that the authors use to suggest that the M-M bond orders are different for the two compounds 1 and 2.

(c) Sketch a diagram that shows the interaction of the unpaired electron with the nuclear spins of the suitable atoms in compound 1 to give a EPR pattern that accounts for the one observed experimentally. If the number of lines predicted by your diagram is different from the 15-line pattern stated by the authors, explain any reasons that might have led to the difference.