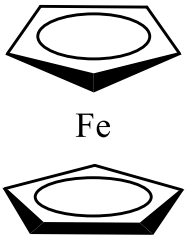
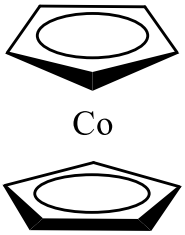
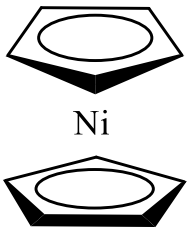
Ch112
In class problem
Oct 13, 2016

Consider $FeCp_2$, $CoCp_2$ and $NiCp_2$.

1. What is the d-electron count in each?
2. If paramagnetic, what is the number of unpaired electrons?
3. Order them from least to most reducing. Which is the most reducing? Why?

	 Fe	 Co	 Ni
d^n	6	7	8
Paramagnetic? / S = ?	No	Yes, S = 1/2	Yes, S = 1
Rank $E_{1/2}(MCp_2/MCp_2^+)$	Least reducing	Most reducing	In the middle

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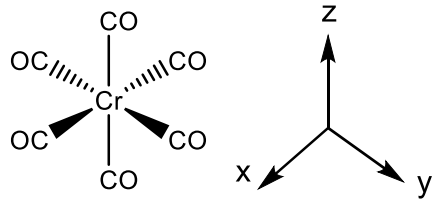
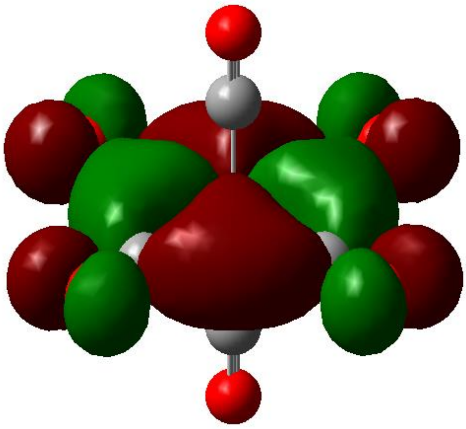
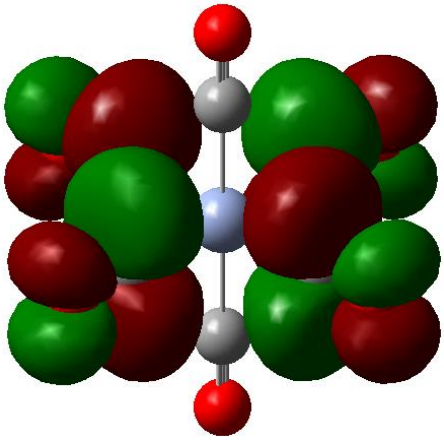
Problem 1

Consider $Cr(CO)_6$. Shown below are pictures of calculated molecular orbitals. Assign each orbital as σ/σ*, π/π*, or non-bonding with respect to the M-ligand interaction. Name the contributing metal based orbital.

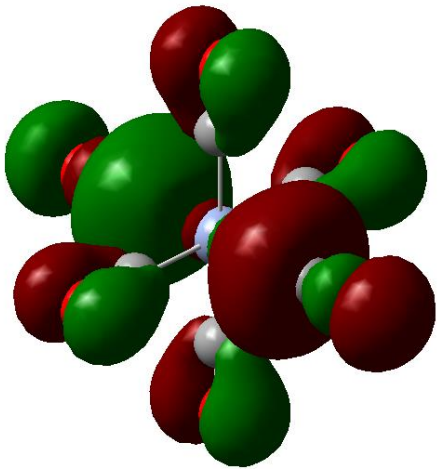




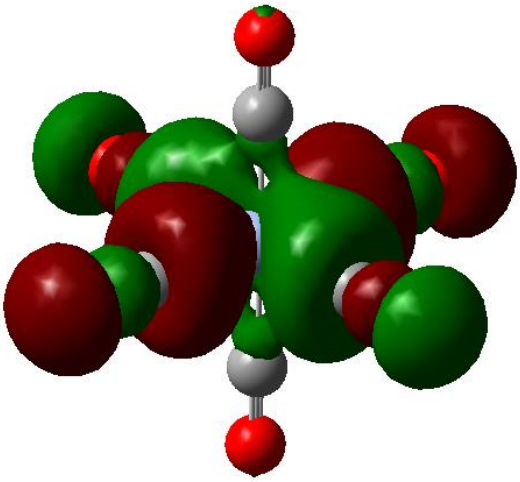
π, d_{xy}



nb



σ, p_y



σ, d_{x2-y2}

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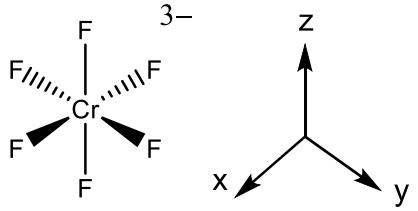
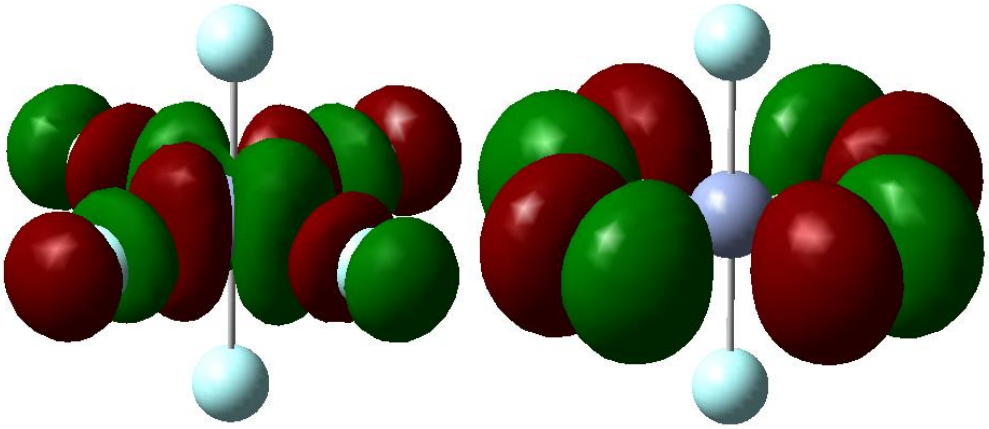
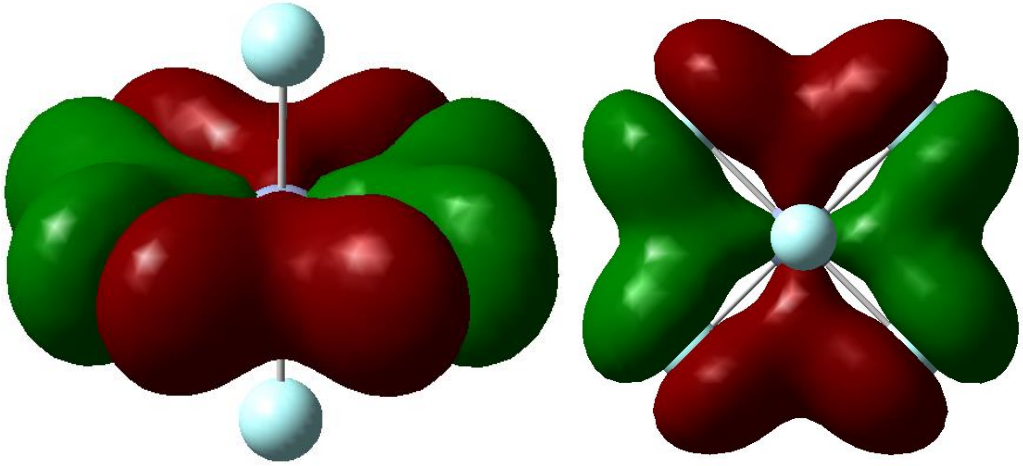
Problem 1

Consider $[CrF_6]^{3-}$. Shown below are pictures of calculated molecular orbitals. Assign each orbital as σ/σ*, π/π*, or non-bonding with respect to the M-ligand interaction. Name the contributing metal based orbital.





σ*, d_{x2-y2} **nb**



π, d_{xy} **(another view along Cr−F bond**