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PROJECT II
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The Problem

Mixing $\text{Ag}(\text{CN})_2$ and $\text{Ni}(\text{CO})_4$ in chloroform under a CO atmosphere, you isolate a solid precipitate that micro-analysis and mass spectroscopy indicate to be $\text{NiC}_4\text{N}_2\text{O}_2$. A ^{13}C NMR spectrum of the precipitate in chloroform with $\text{Ni}(\text{CO})_4$ added as an internal standard shows a strong peak 6.6 ppm upfield from $\text{Ni}(\text{CO})_4$ and a much smaller peak 8.4 ppm upfield from $\text{Ni}(\text{CO})_4$. There is also a very strong peak 84 ppm upfield from $\text{Ni}(\text{CO})_4$.

An IR spectrum of the precipitate in a KBr pellet shows a strong absorption at 2154 cm^{-1} and very weak absorptions/shoulders at 2143, 2170, and 2188 cm^{-1} . After three recrystallizations from diisopropyl ether, your solid is composed of beautifully twinned light orange crystals. NMR and IR spectra of the recrystallized solid show only the strong peaks noted above, and none of the weak ones. An ultraviolet spectrum of the recrystallized solid in freon shows absorptions at 310 and 333 nm.

Questions

1. What is the structure of the molecules in the recrystallized solid?

In a narrative fashion, describe in some detail how you came to your conclusion.

2. To what electronic transitions do the two peaks in the UV spectrum correspond (Show pictures of the orbitals?) Based on the nature of these transitions, how might you expect the geometries of the first and second excited states to differ from the ground state. Infer from the orbitals but possibly perform an excited-state geometry optimization.