SUPPLEMENTARY MATERIAL

B.T. Donovan-Merkert, P.H. Rieger, W. E. Geiger, "Reactions of Odd-Electron Cobaltacycles..."

The proton-NMR assignment for 2^{2} (Figure 4) is aided by an NOE difference experiment. The Cp singlet at $\delta=4.19$ was irradiated and a spectrum recorded. Then a second spectrum was obtained upon irradiation about 100 Hz away from the Cp resonance. Subtraction of the two spectra yielded the difference spectrum shown as Figure 1, Supplementary material. Note that the downfield signal is enhanced while the remaining cobaltacyclic peaks have negative difference intensities. Since we expect that proton 1 should be most highly affected by the Cp irradiation, we make the assignment: proton 1, $\delta=8.28$ (doublet) and the other assignments follow from the observed multiplicities: 2, $\delta=6.15$ (triplet); 3, $\delta=6.27$ (triplet); 4, $\delta=7.18$ (doublet).

FIGURE CAPTIONS

Figure 1, SM: NOE Difference spectrum of a solution of the dianion 2² in THF-d₈ irradiated on and off the cyclopentadienyl resonance.

Figure 2, SM: Simulation of frozen solution ESR spectrum of 2 with the parameters given in the text.

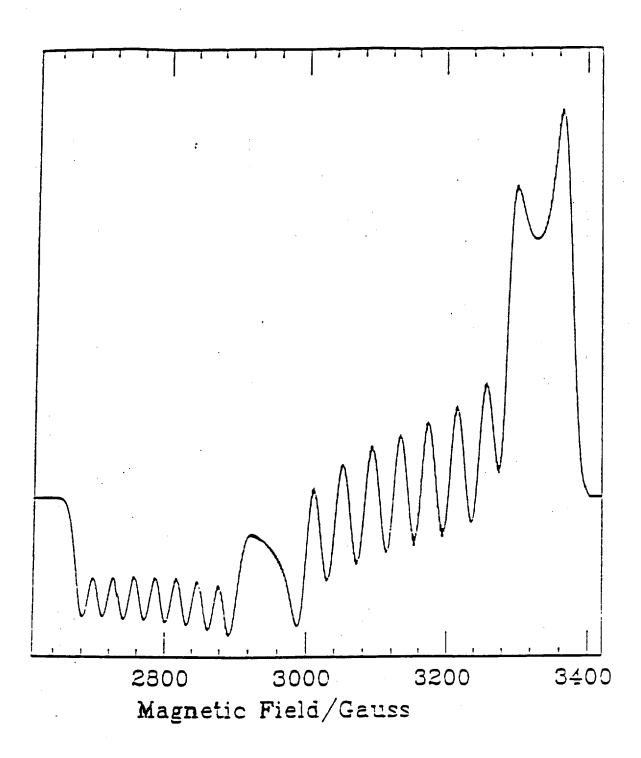


Figure 2, SM: Simulation of frozen solution ESR spectrum of 2 with the parameters given in the text.

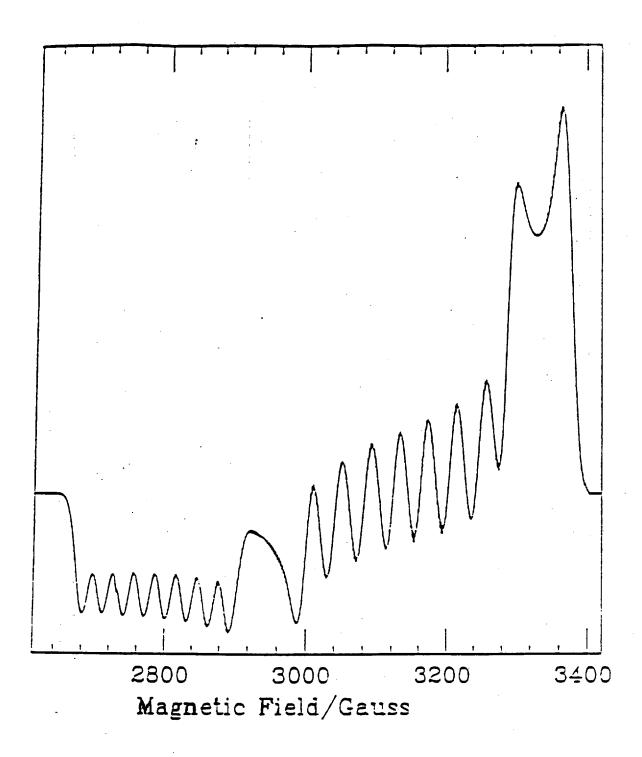


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