## Halogen Oxidation Reactions of $(C_5Ph_5)Cr(CO)_3$ and Lewis Base Addition to $[(C_5Ph_5)Cr(\mu-X)X]_2$ : Electrochemical, Magnetic, and Raman Spectroscopic Characterization of $[(C_5Ph_5)CrX_2]_2$ and $(C_5Ph_5)CrX_2(THF)$ (X = Cl, Br, I) and X-ray Crystal Structure of $[(C_5Ph_5)Cr(\mu-Cl)Cl]_2$

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## Abstract

The 17-electron complex  $(C_5Ph_5)Cr(CO)_3$  reacts with halogens  $(C_6H_5I \bullet Cl_2, Br_2, and I_2)$  in  $C_6H_6$  to yield the dimeric oxidation products  $[(C_5Ph_5)Cr(\mu-X)X]_2$  as thermally stable solids. Reactions with other chlorinating agents similarly yield  $[(C_5Ph_5)CrCl_2]_2$ . An X-ray crystal structure of  $[(C_5Ph_5)Cr(\mu-Cl)Cl]_2$  was obtained. The magnetic properties of the  $Cl_2$ -bridged dimer have been determined and modeled using the usual isotropic Hamiltonian  $H = -2J\hat{S}_1 \bullet \hat{S}_2$ , which yields J/k) - 30 K. Low-temperature (77 K) Raman spectra of solid  $[(C_5Ph_5)CrX_2]_2$  (X) Cl, I) allow assignments to be made for the metal-ring and metal halogen stretching modes in the low-frequency region (<600 cm<sup>-1</sup>). Tetrahydrofuran (THF) cleaves these dimers to yield complexes of the form ( $C_5Ph_5$ )CrX<sub>2</sub>(THF).



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