

Oxo-Bridged Dinuclear Chromium(III) Complexes: Correlation Between the Optical and Magnetic Properties and the Basicity of the Oxo Bridge

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Supplementary Material

Table S1. Crystallographic data for **8**(ClO₄)₂·2H₂O and **11**(PF₆)₄·2CH₃CN.

Figure S1. Optical absorption spectrum of [Cr(CNCH₃)₆]²⁺ in CH₃CN:CH₃NC (*V/V* = 2:1).

Figure S2. Contour plot of p*K*_a from -8 to 8 in intervals of 2 vs. (*r*, *E*_{CT}). Calculated from eqs 4–7 and 12 with *a* = 1.04×10⁵ cm⁻¹, *b* = -1.24 Å⁻¹, *U* = 90000 cm⁻¹, and *E*₀ = 235.8 kJ mol⁻¹.

Table S1 Crystallographic data for **8**(ClO₄)₂·2H₂O and **11**(PF₆)₄·2CH₃CN.

Compound	8 (ClO ₄) ₂ ·2H ₂ O	11 (PF ₆) ₄ ·2CH ₃ CN
Formula	C ₄₂ H ₃₆ Cl ₂ Cr ₂ N ₁₀ O ₁₁ S ₂	C ₂₄ H ₃₆ OCr ₂ F ₂₄ N ₁₂ P ₄
<i>M</i> (g mol ⁻¹)	1095.92	1192.53
Crystal size (mm ³)	0.400 x 0.282 x 0.074	0.358 x 0.220 x 0.169
Crystal system	Monoclinic	Monoclinic
Space group	P 2 ₁ /c	P 2 ₁ /c
<i>a</i> (Å)	17.854(9)	10.3130(12)
<i>b</i> (Å)	16.428(8)	22.2650(19)
<i>c</i> (Å)	15.648(8)	12.431(1)
α (°)	90	90
β (°)	96.55(4)	122.232(8)
γ (°)	90	90
<i>U</i> (Å ³)	4560 (4)	2414.5(4)
<i>Z</i>	4	2
<i>D_x</i> (g cm ⁻³)	1.588	1.640
<i>T</i> (K)	123(2)	123(2)
μ	0.757	0.713
No. measured/observed reflections	164881 / 8659	28297 / 5847
Parameters refined	641	347
Final <i>R</i> 1	0.0555	0.0702
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.1243	0.1967
<i>R</i> 1, <i>wR</i> ₂ (all data)	0.0822, 0.1591	0.0881, 0.2206
<i>S</i> (GoF)	1.140	1.116

Figure S1. Optical absorption spectrum of $[\text{Cr}(\text{CNCH}_3)_6]^{2+}$ in $\text{CH}_3\text{CN}:\text{CH}_3\text{NC}$ ($V/V = 2:1$)

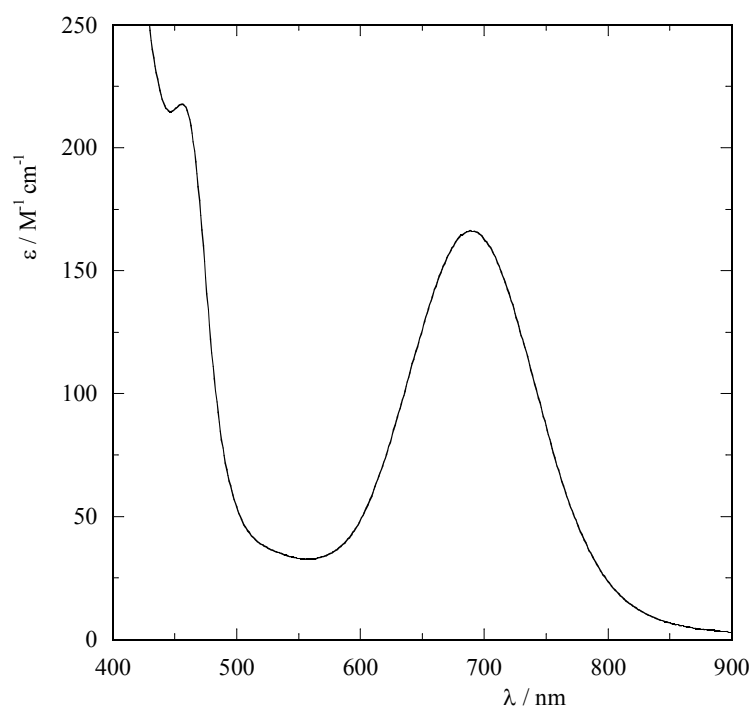


Figure S2. Contour plot of pK_a from -8 to 8 in intervals of 2 vs. (r, E_{CT}) with the data for **1**, **10**, and **11** included ($\square$). Calculated from eqs 4–7 and 12 with $a = 1.04 \times 10^5 \text{ cm}^{-1}$, $b = -1.24 \text{ \AA}^{-1}$, $U = 90000 \text{ cm}^{-1}$, and $E_0 = 235.8 \text{ kJ mol}^{-1}$.

