

Perturbation of the Charge Density between two Bridged Mo₂ Centers: the Remote Substituent Effects

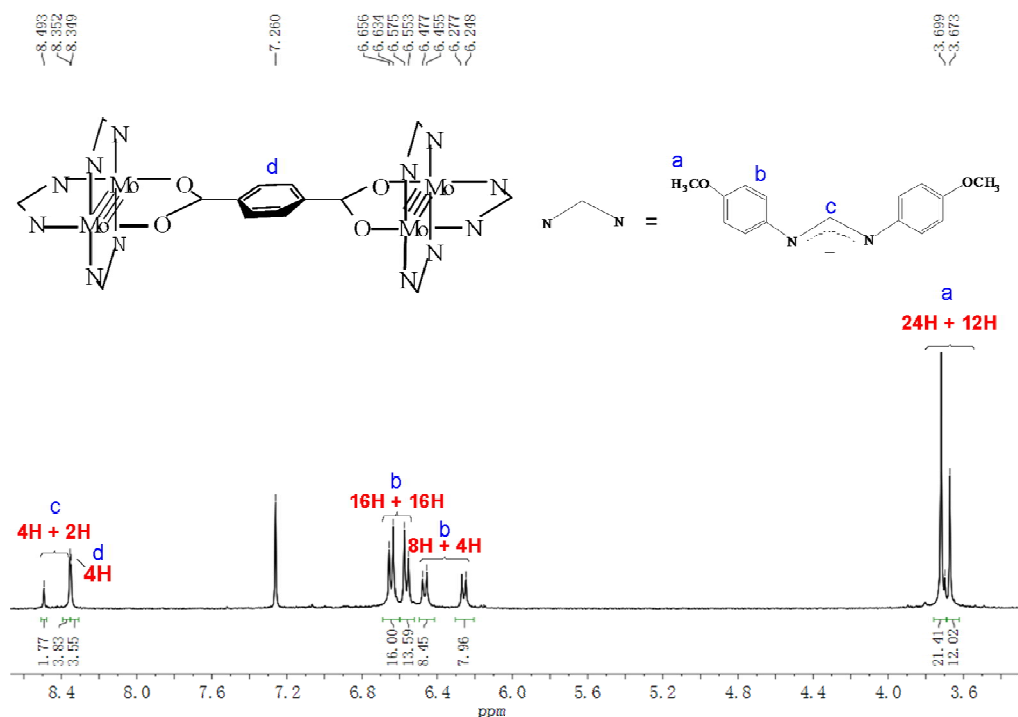
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Supporting Information Contents

¹H NMR spectra



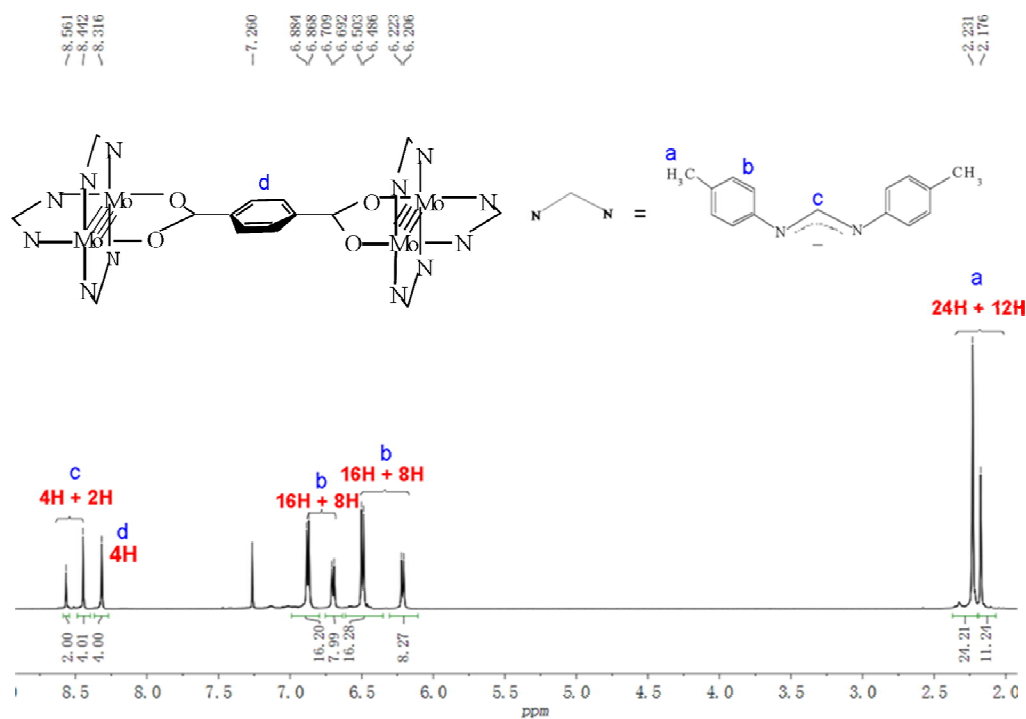


Figure S2. ¹H NMR spectrum for **2**.

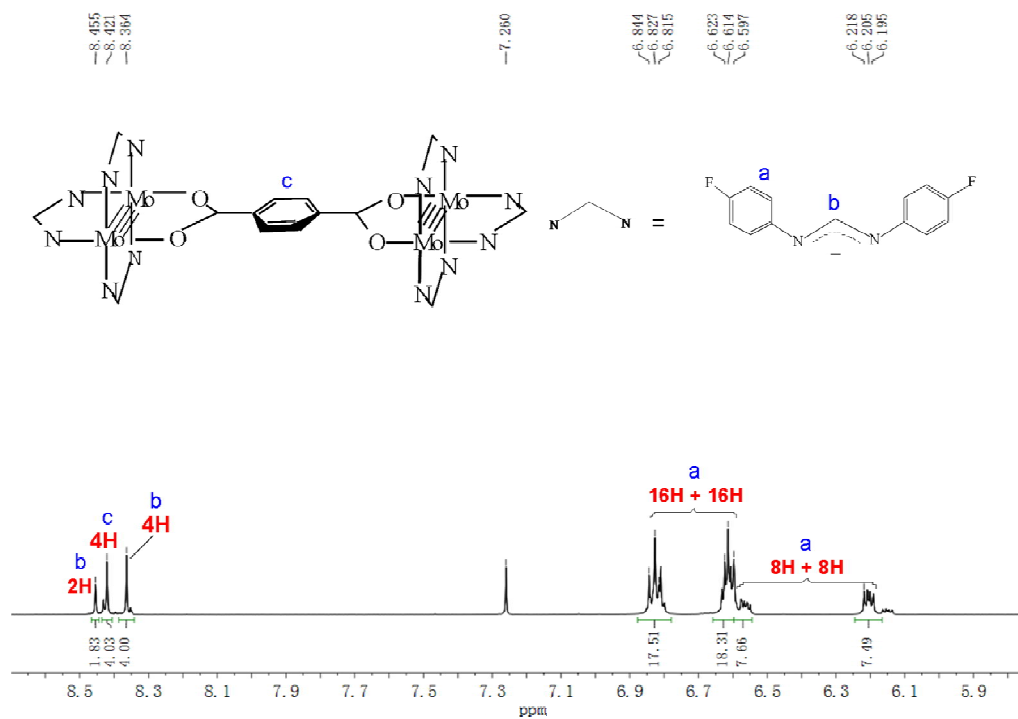


Figure S3. ¹H NMR spectrum for **3**.

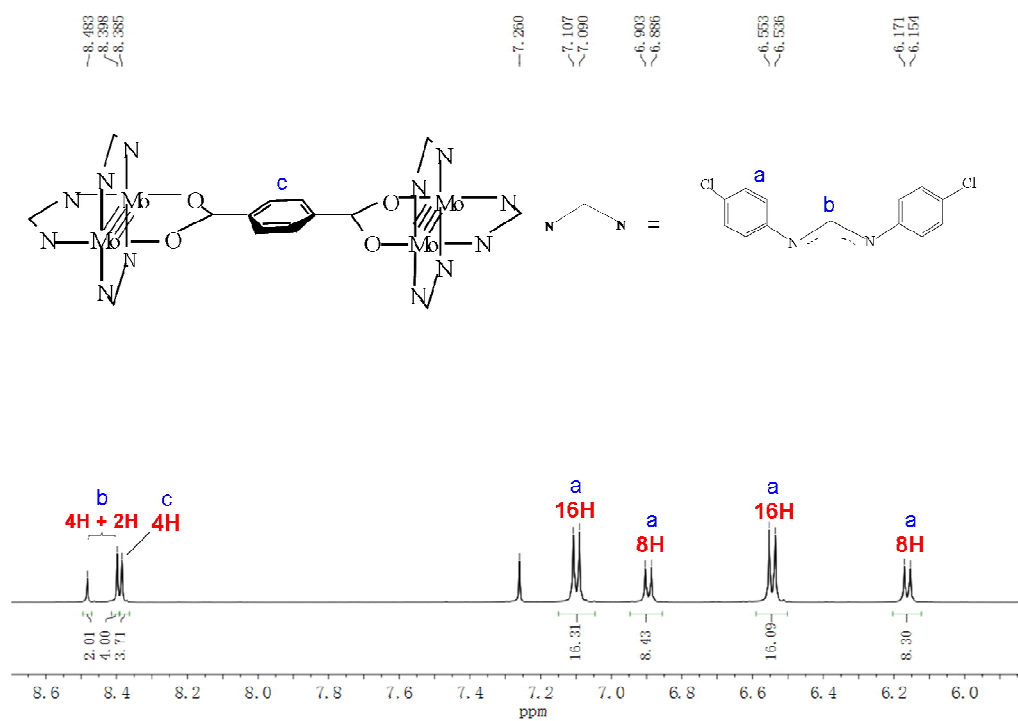


Figure S4. ¹H NMR spectrum for **4**.

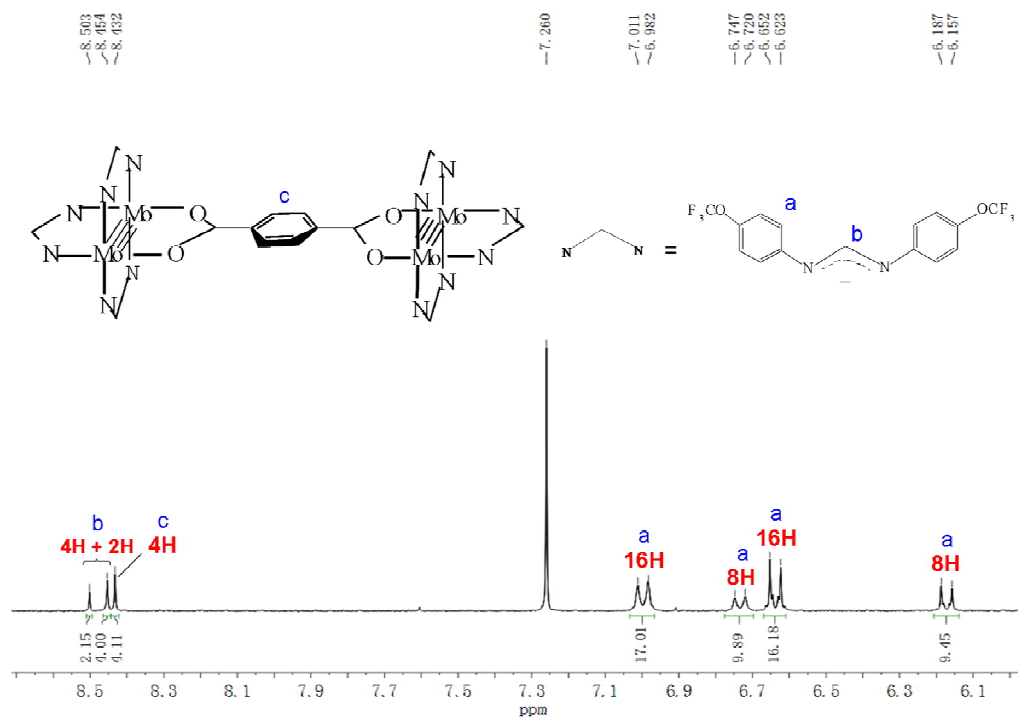


Figure S5. ¹H NMR spectrum for **5**.

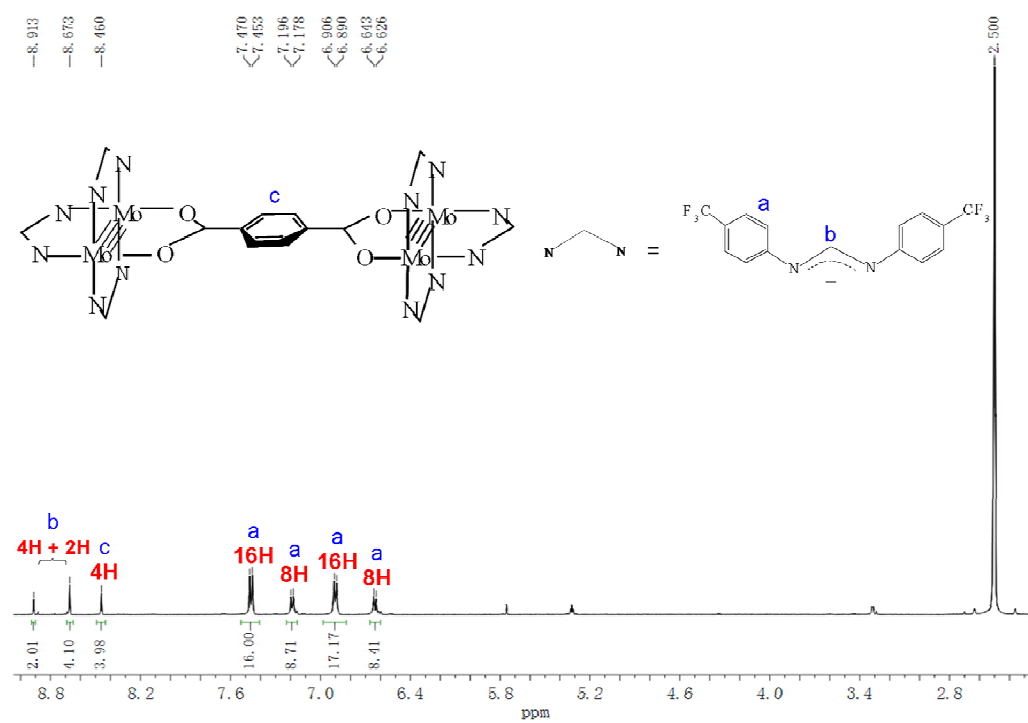


Figure S6. ^1H NMR spectrum for **6**.

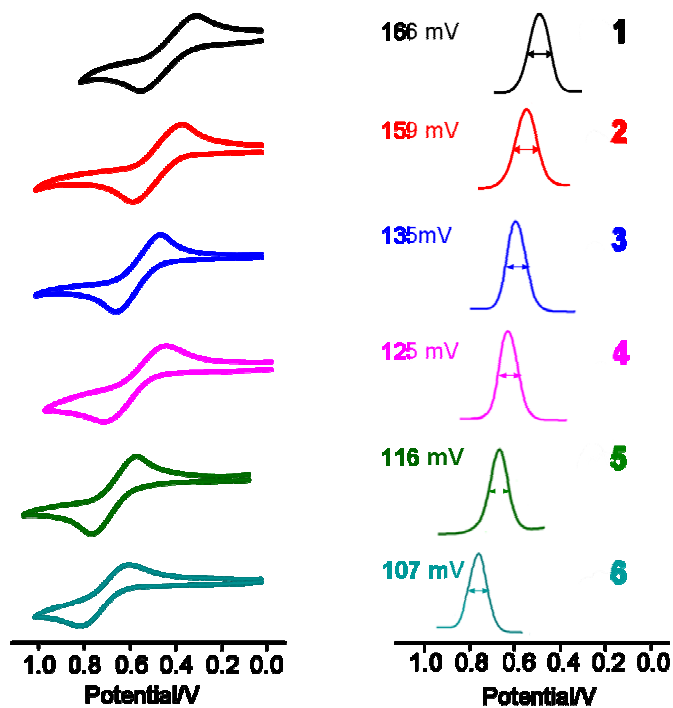


Figure S7. Electrochemical cyclic voltammograms (CVs, left) and differential pulse voltammograms (DPVs, right) for complexes **1-6** as labeled in different colors. The half-height widths ($i_{\max}/2$) are measured from the DPV plots.

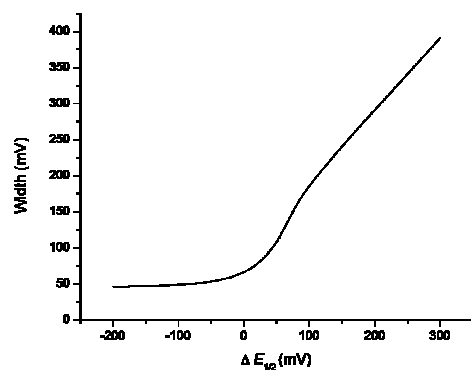


Figure S8. Working curve, generated from the data in ref 22 (Richardson, D. E.; Taube, H. *Inorg. Chem.* **1981**, 20, 1278–1285), for electrochemical data analyses.

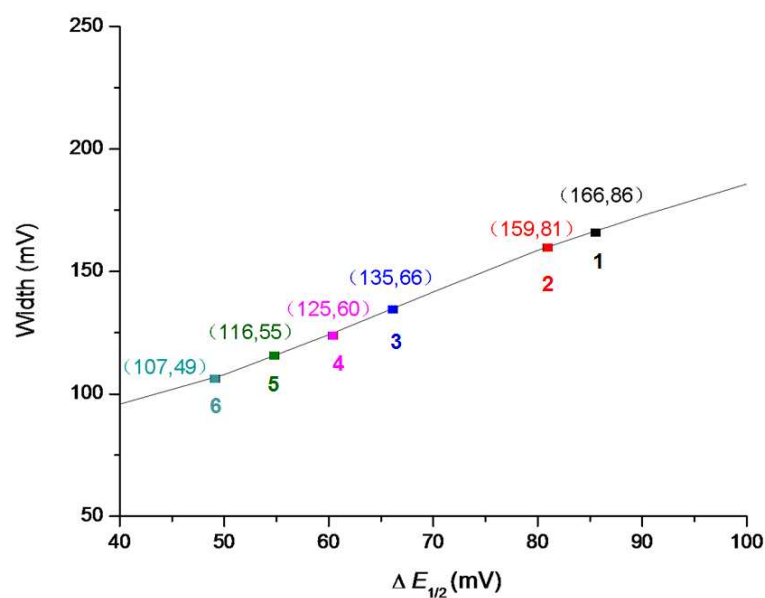


Figure S9. $\Delta E_{1/2}$ data derived for complexes **1-6** from the working curve (**Figure S8**).

Table S1. The values of width and $\Delta E_{1/2}$ for complexes **1-6**.

parameter	1 (OCH ₃)	2 (CH ₃)	3 (F)	4 (Cl)	5 (OCF ₃)	6 (CF ₃)
Width (mV)	166	159	135	125	116	107
$\Delta E_{1/2}$ (mV)	86	81	66	60	55	49

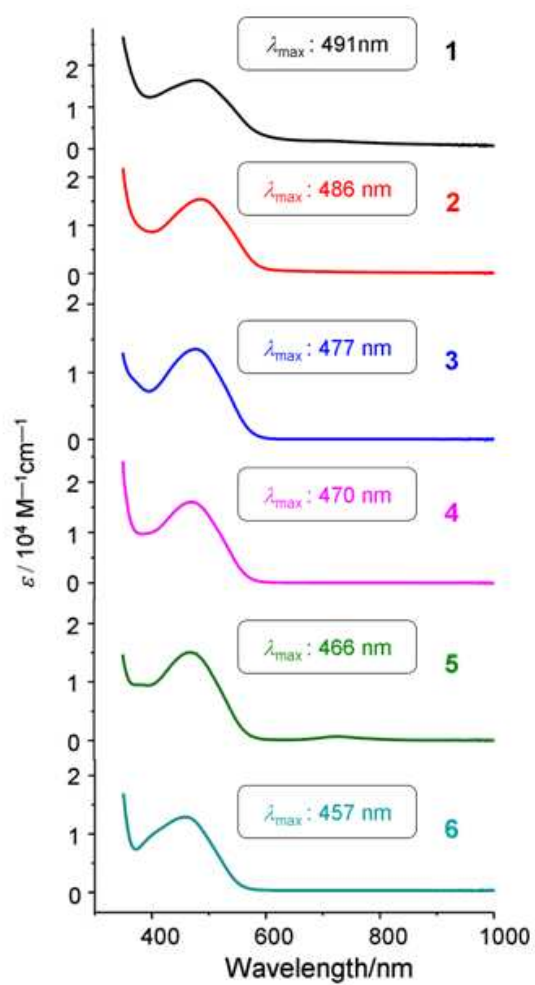


Figure S10. Electronic spectra showing the metal to ligand charge transfer (MLCT) absorption bands for complexes **1-6**.