

University of Groningen

Complexed nitrogen heterosuperbenzene

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SUPPORTING INFORMATION

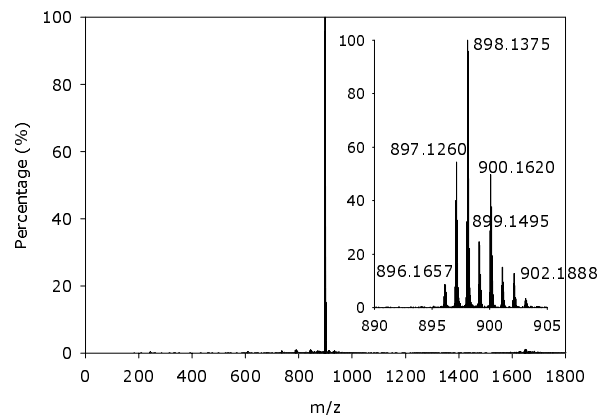


Figure 1. The ESI-mass spectrum of $[\text{Pd}(\eta^3\text{-C}_3\text{H}_5)(\mathbf{1})]^+$, **2** in methanol.

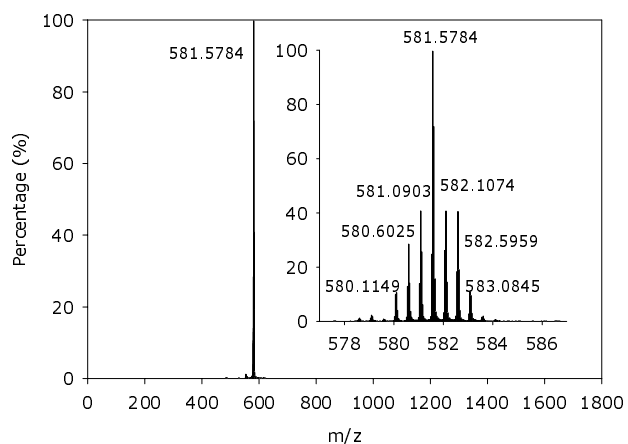


Figure 2. The ESI-mass spectrum of $[\text{Ru}(\text{bpy})_2(\mathbf{1})]^{2+}$, **3a** in acetonitrile.

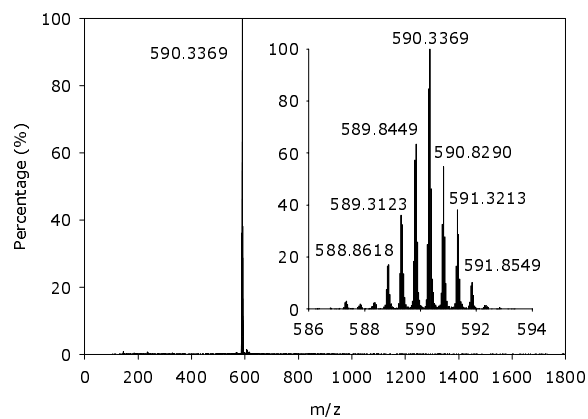


Figure 3. The ESI-mass spectrum of $[\text{Ru}(d_8\text{-bpy})_2(\mathbf{1})]^{2+}$, **3b** in acetonitrile.

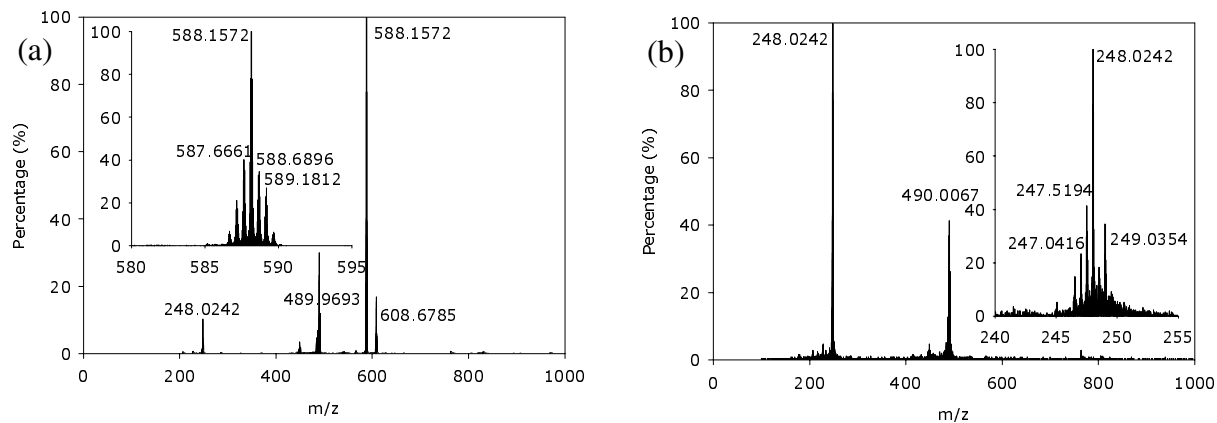


Figure 4. The ESI-mass spectrum of $[\text{Ru}(\text{bpy})_2(\mathbf{4})]^{2+}$, **5** in acetonitrile after (a) 0 and (b) 200 seconds of irradiation (125-W Mercury lamp). Peak assignments: 588.2 = **5**, $[\text{M}-2\text{PF}_6]^{2+}$; 608.7 = $[\text{Ru}(\text{bpy})_2(\mathbf{4})(\text{CH}_3\text{CN})]^{2+}$, $[\text{M}-2\text{PF}_6]^{2+}$; 248.0 = $[\text{Ru}(\text{bpy})_2(\text{CH}_3\text{CN})_2]^{2+}$, $[\text{M}-2\text{PF}_6]^{2+}$. (The envelope in both spectra at $m/z=490$ is assigned to the unreacted starting material $[\text{Ru}(\text{bpy})_2\text{Cl}_2]$)

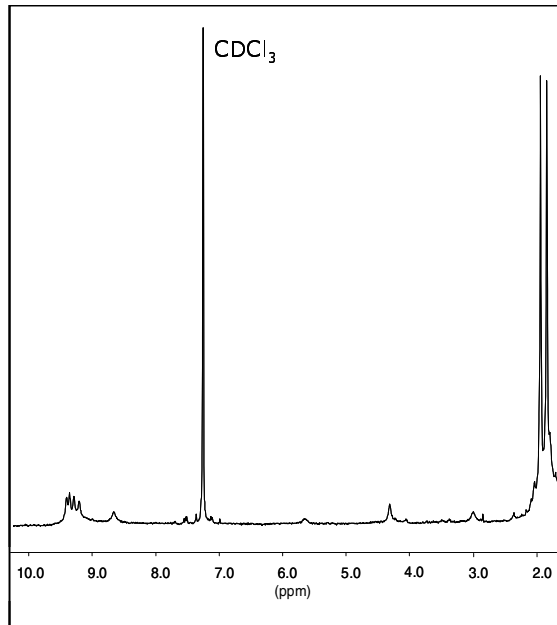


Figure 5. The ^1H NMR spectra of $[\text{Pd}(\eta^3\text{-C}_3\text{H}_5)(\mathbf{1})]\text{PF}_6$, **2** (CDCl_3 , 40°C, 400 MHz).

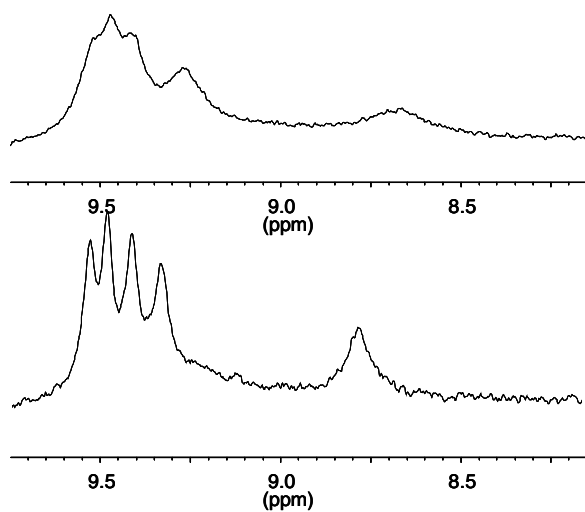


Figure 6. The aromatic region of the ^1H NMR spectrum of **2** at 21°C and 40°C (CDCl_3 , 400 MHz).

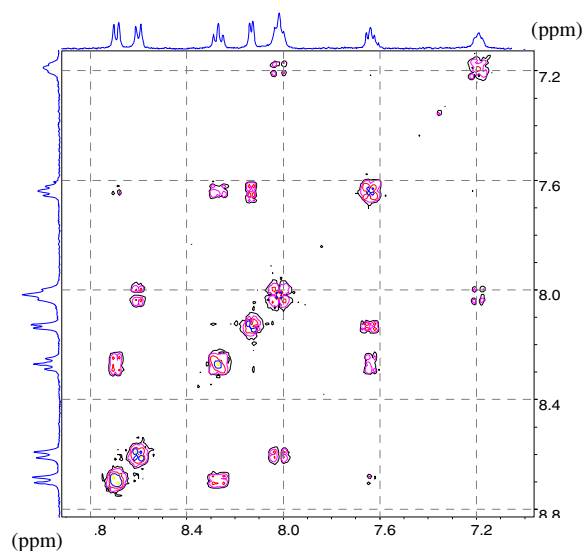


Figure 7. The aromatic region of the ^1H - ^1H TOCSY NMR spectra of $[\text{Ru}(\text{bpy})_2(\mathbf{1})]^{2+}$, **3a** (CD_3CN , 23 K, 400 MHz).

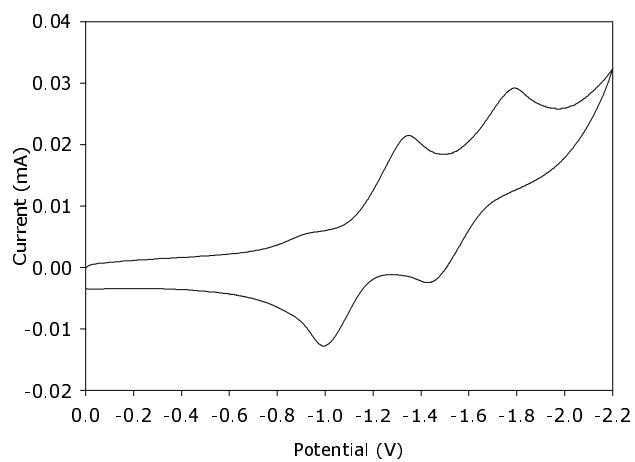


Figure 8. The Cyclic voltammogram of **1** in chloroform. Supporting electrolyte: Bu_4NPF_6 (0.1 M); glassy carbon working electrode, Pt wire auxiliary electrode, SCE reference electrode.