Complexed nitrogen heterosuperbenzene

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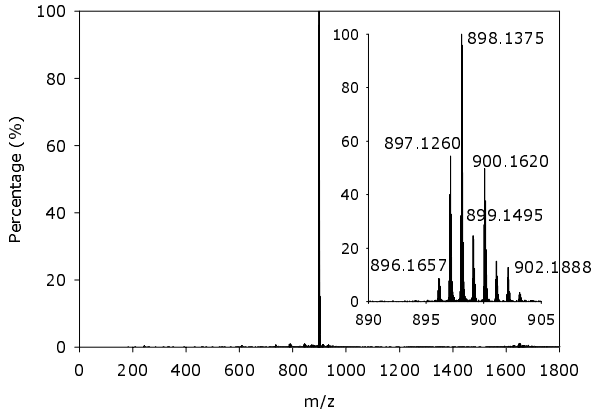

Figure 1. The ESI-mass spectrum of $[Pd(\eta^3\text{-}C_3H_5)(\mathbf{1})]^+$, **2** in methanol.

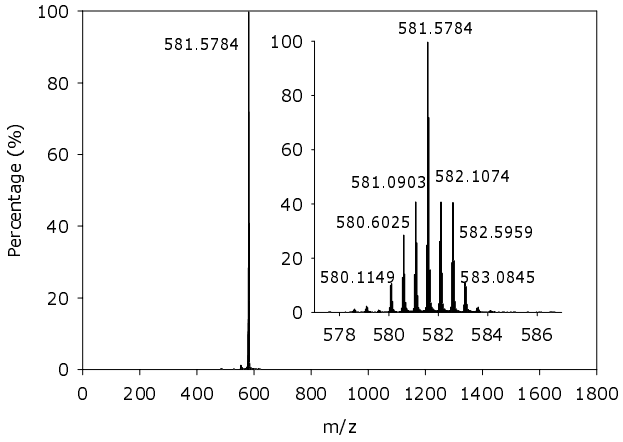

Figure 2. The ESI-mass spectrum of $[Ru(bpy)_2(\mathbf{1})]^{2+}$, **3a** in acetonitrile.

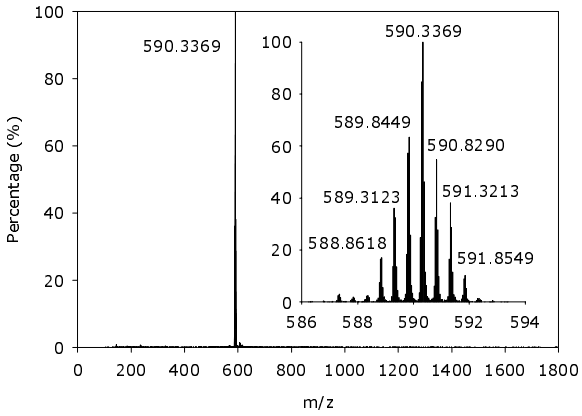

Figure 3. The ESI-mass spectrum of $[Ru(d_8\text{-bpy})_2(\mathbf{1})]^{2+}$, **3b** in acetonitrile.

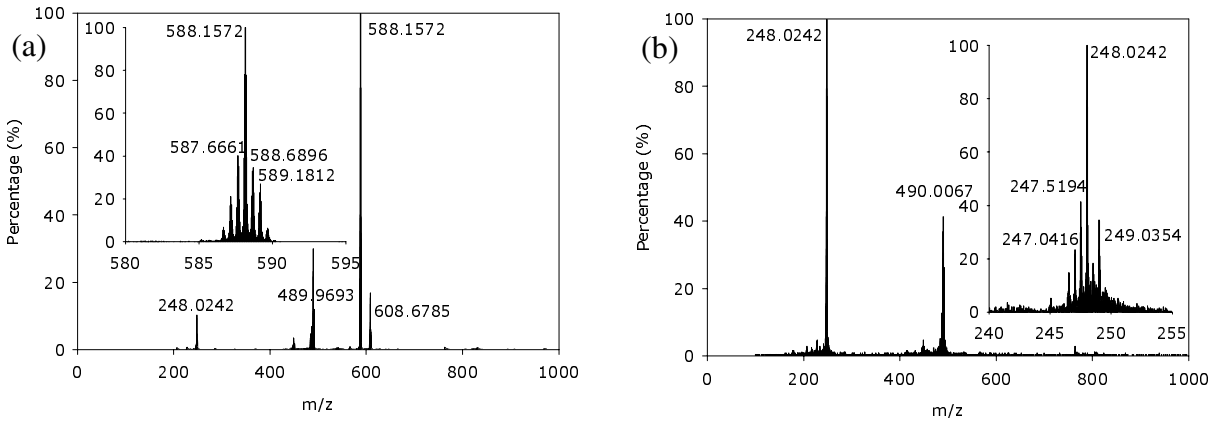

Figure 4. The ESI-mass spectrum of $[Ru(bpy)_2(\mathbf{4})]^{2+}$, **5** in acetonitrile after (a) 0 and (b) 200 seconds of irradiation (125-W Mercury lamp). Peak assignments: 588.2 = **5**, $[M\text{-}2PF_6]^{2+}$; 608.7 = $[Ru(bpy)_2(\mathbf{4})(CH_3CN)]^{2+}$, $[M\text{-}2PF_6]^{2+}$; 248.0 = $[Ru(bpy)_2(CH_3CN)_2]^{2+}$, $[M\text{-}2PF_6]^{2+}$. (The envelope in both spectra at *m/z*=490 is assigned to the unreacted starting material $[Ru(bpy)_2Cl_2]$)

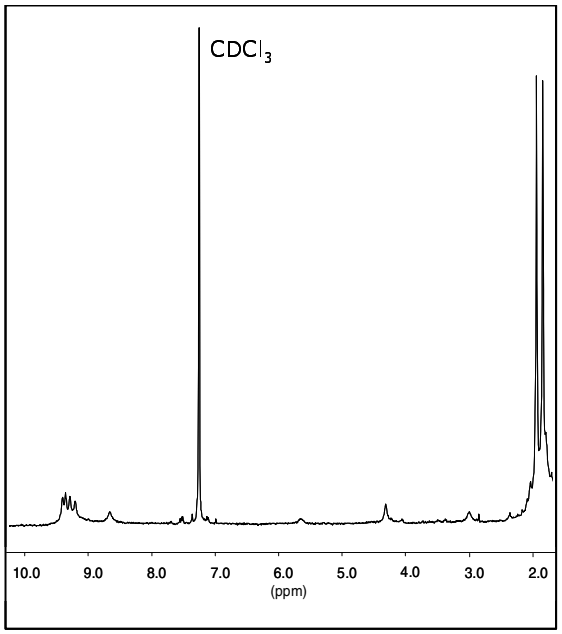

Figure 5. The ^{1}H NMR spectra of $[Pd(\eta^3\text{-}C_3H_5)(\mathbf{1})]PF_6$, **2** ($CDCl_3$, 40ºC, 400 MHz).

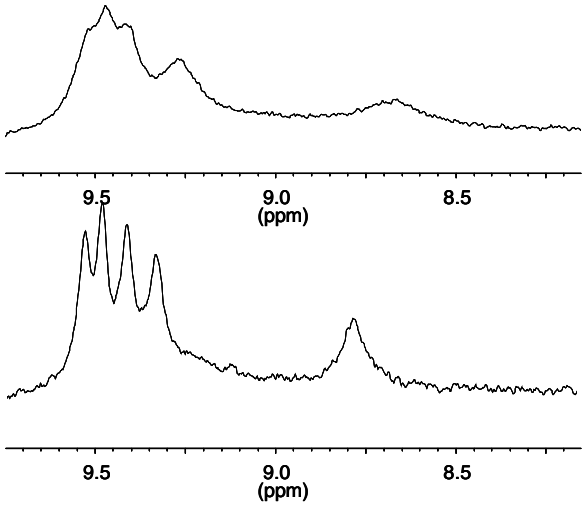

Figure 6. The aromatic region of the ^{1}H NMR spectrum of **2** at 21°C and 40°C ($CDCl_3$, 400 MHz).

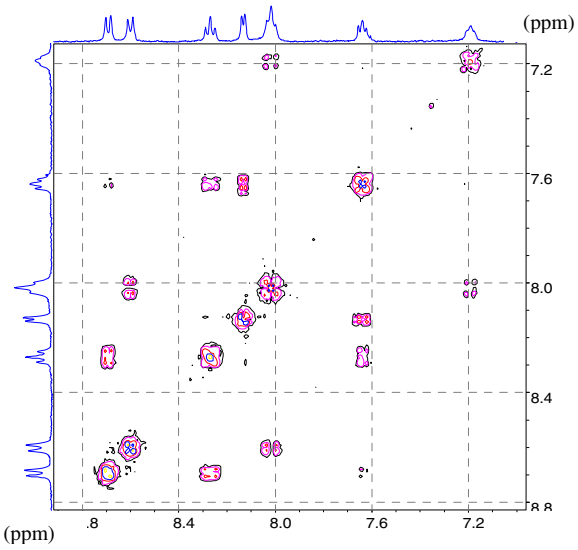

Figure 7. The aromatic region of the ^{1}H-^{1}H TOCSY NMR spectra of $[Ru(bpy)_2(\mathbf{1})]^{2+}$, **3a** ($CD_3CN$, 23 K, 400 MHz).

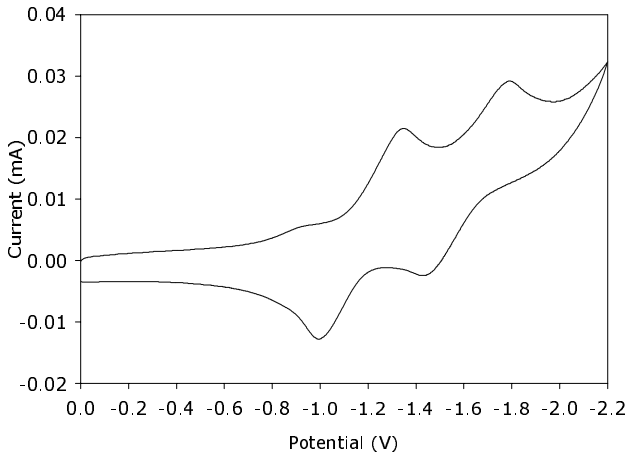

Figure 8. The Cyclic voltammogram of **1** in chloroform. Supporting electrolyte: Bu_4NPF_6 (0.1 M); glassy carbon working electrode, Pt wire auxiliary electrode, SCE reference electrode.