Electronic Supplementary Information (ESI)

Templating an N-Heterocyclic Carbene (NHC)-Cyclometalated Cp*Ir[III]-Based Oxidation Precatalyst on a Pendant Coordination Platform: Assessment of the Oxidative Behavior via Electrochemical, Spectroscopic and Catalytic Probes

Suraj K. Gupta, and Joyanta Choudhury*

Organometallics & Smart Materials Laboratory, Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhauri, Indore By-pass Road, Bhopal 462 066, INDIA.

E-mail: joyanta@iiserb.ac.in.
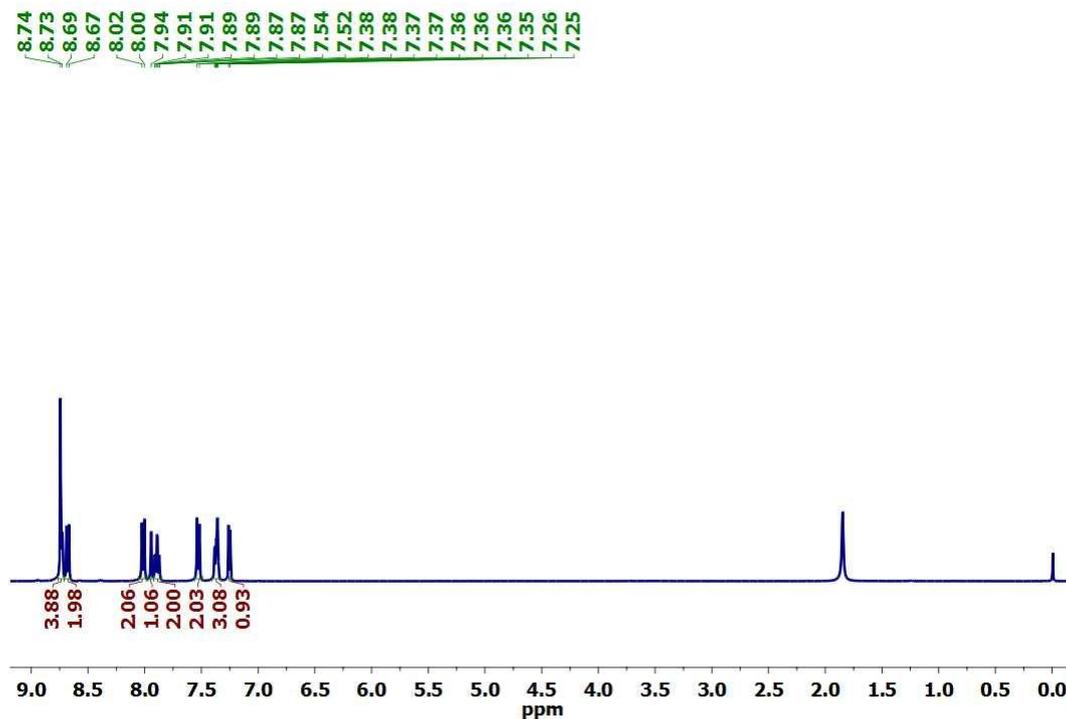
Figure S1 ^{1}H NMR spectrum of **4'-[4-(Imidazol-1-yl)phenyl]-2,2':6',2''-terpyridine** (400 MHz, CDCl$_3$, 300 K).
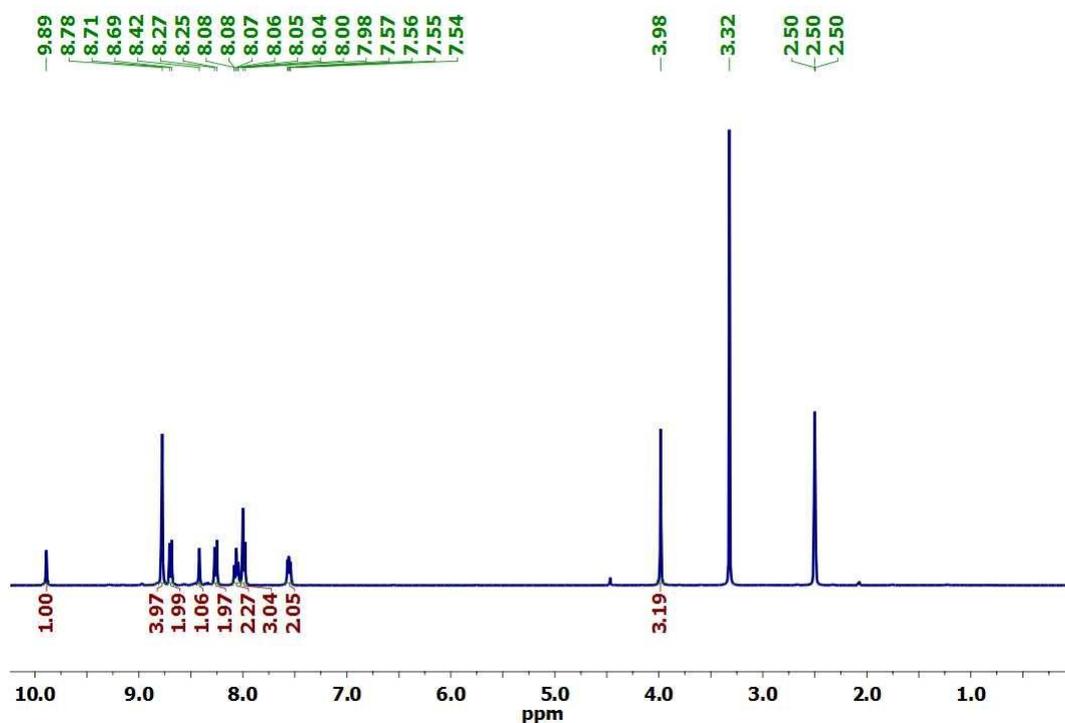
Figure S2 ^{1}H NMR spectrum of **[L^{1}H]$^+$I$^-$** (400 MHz, DMSO-d_6, 300 K).
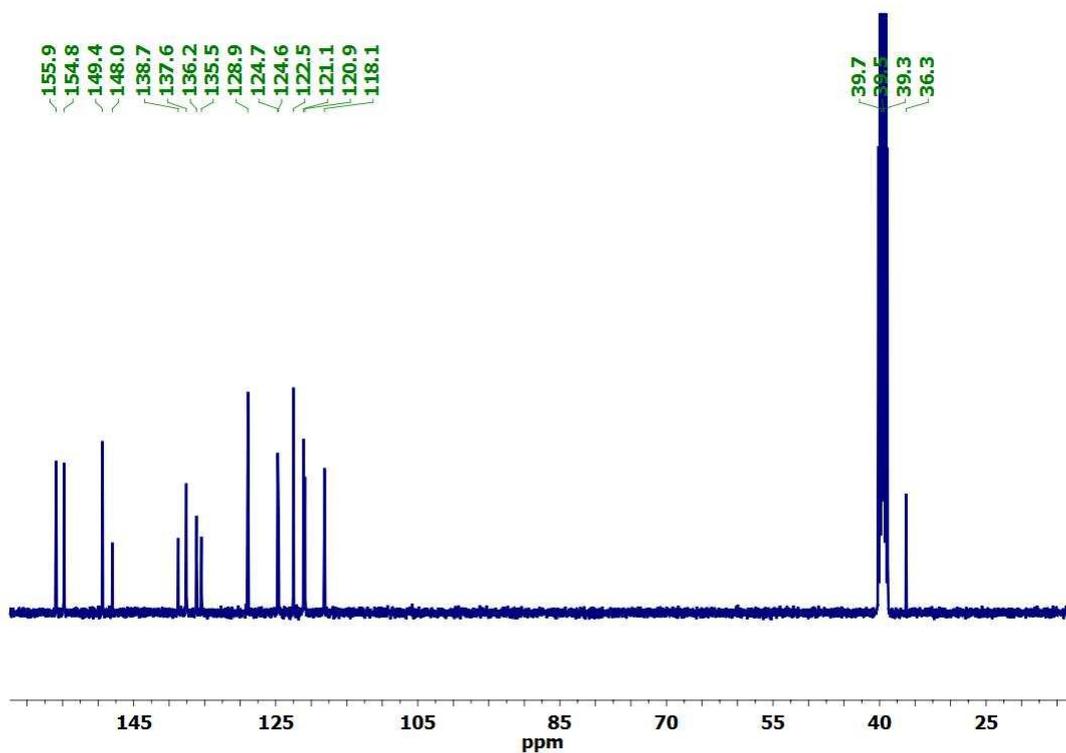
Figure S3 $^{13}C\{^1H\}$ NMR spectrum of $[\mathbf{L^1H}]^+\mathbf{I}^-$ (100 MHz, DMSO-d_6, 300 K).
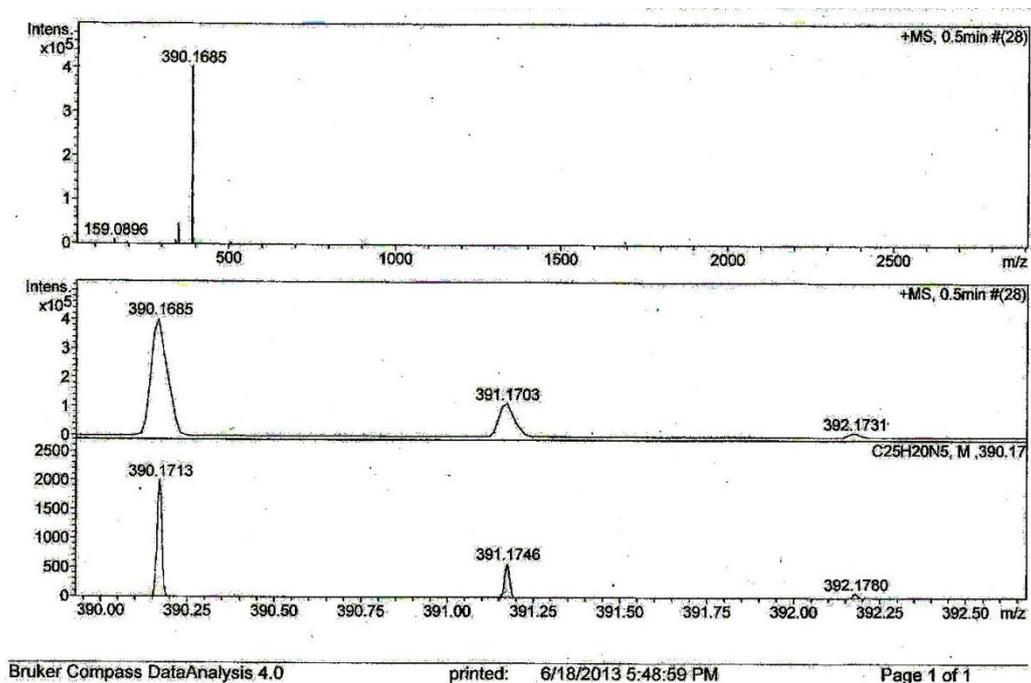
Figure S4 ESI-MS (positive ion mode) spectrum of $[\mathbf{L^1H}]^+\mathbf{I}^-$.
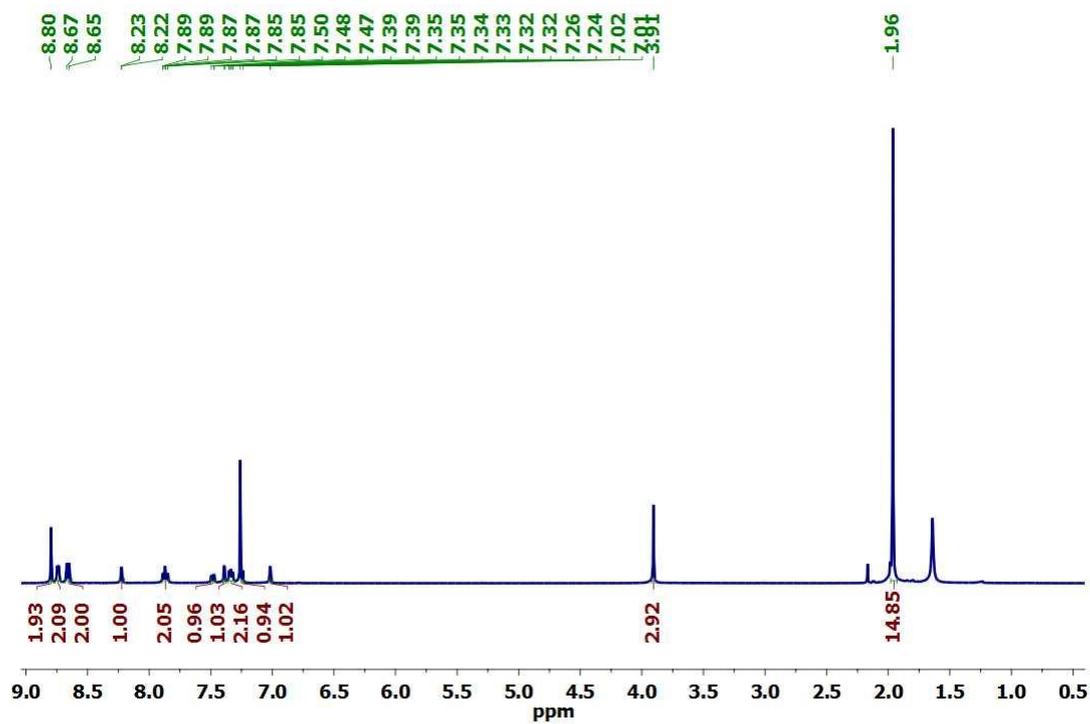
Figure S5 ^{1}H NMR spectrum of **1** (400 MHz, CDCl$_3$, 300 K).
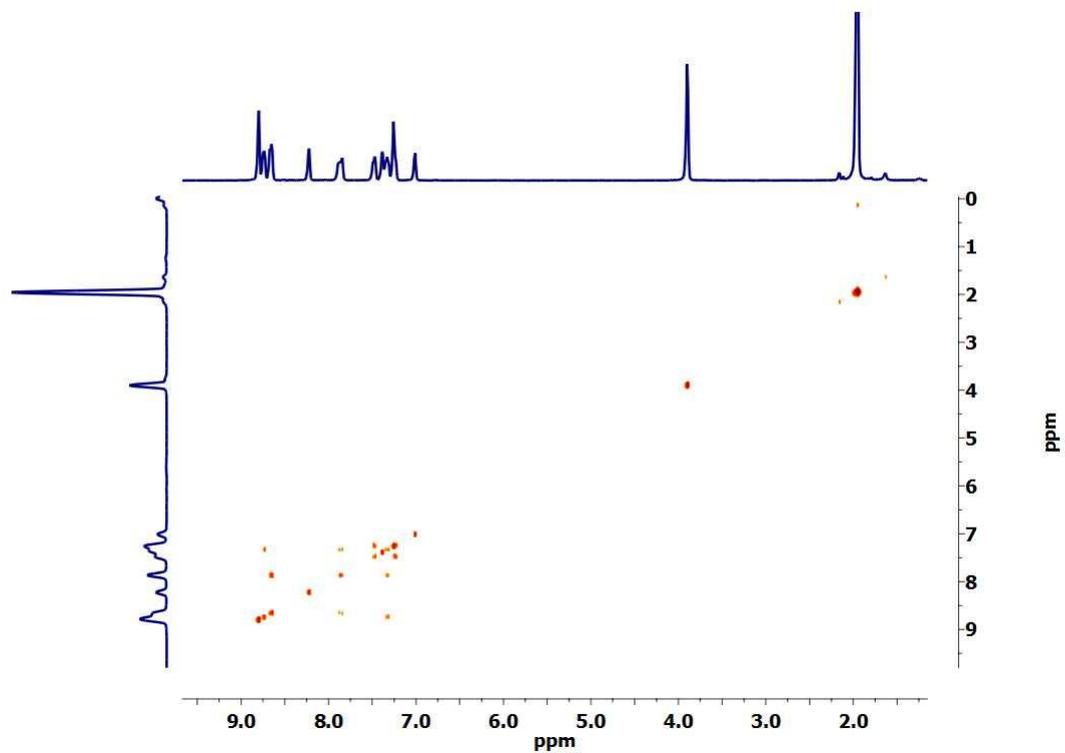
Figure S6 ^{1}H-^{1}H COSY NMR spectrum of **1**.
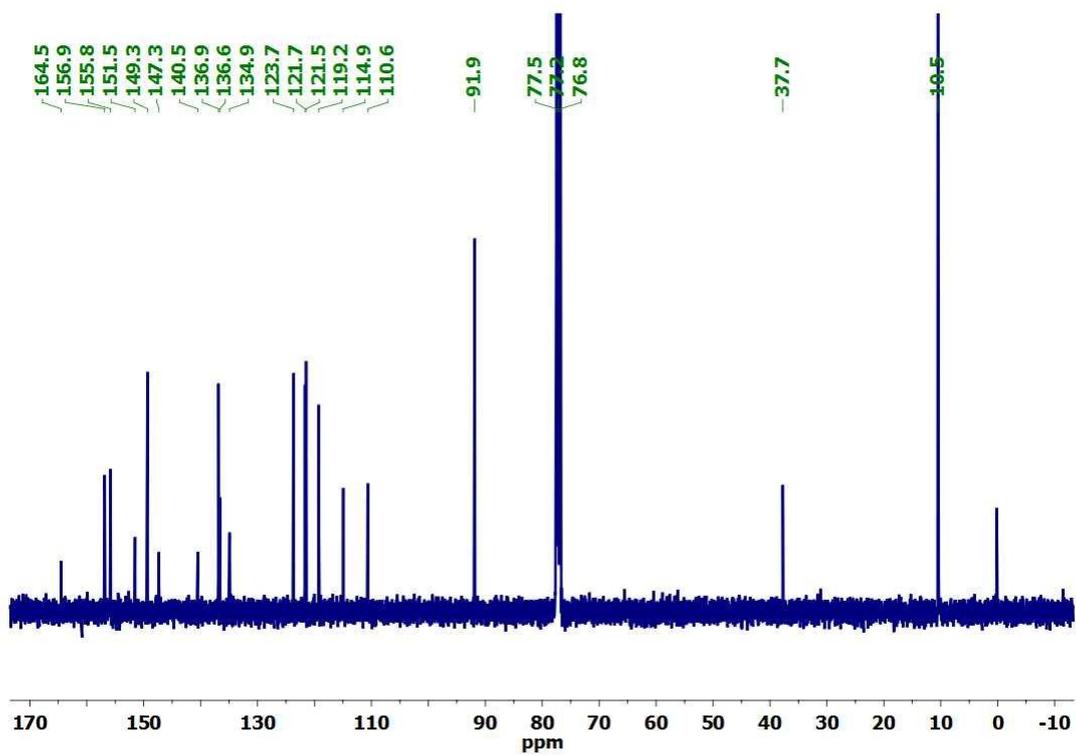
Figure S7 $^{13}C\{^1H\}$ NMR spectrum of **1** (100 MHz, CDCl$_3$, 300 K).
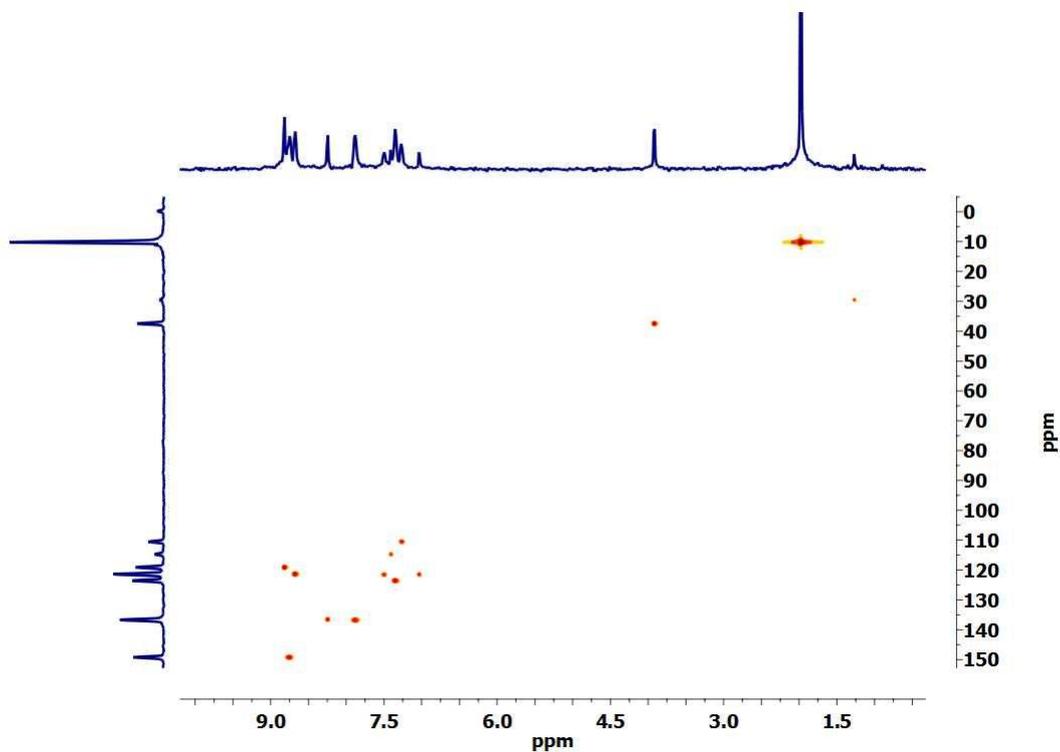
Figure S8 ^1H-^{13}C HSQC NMR spectrum of **1**.
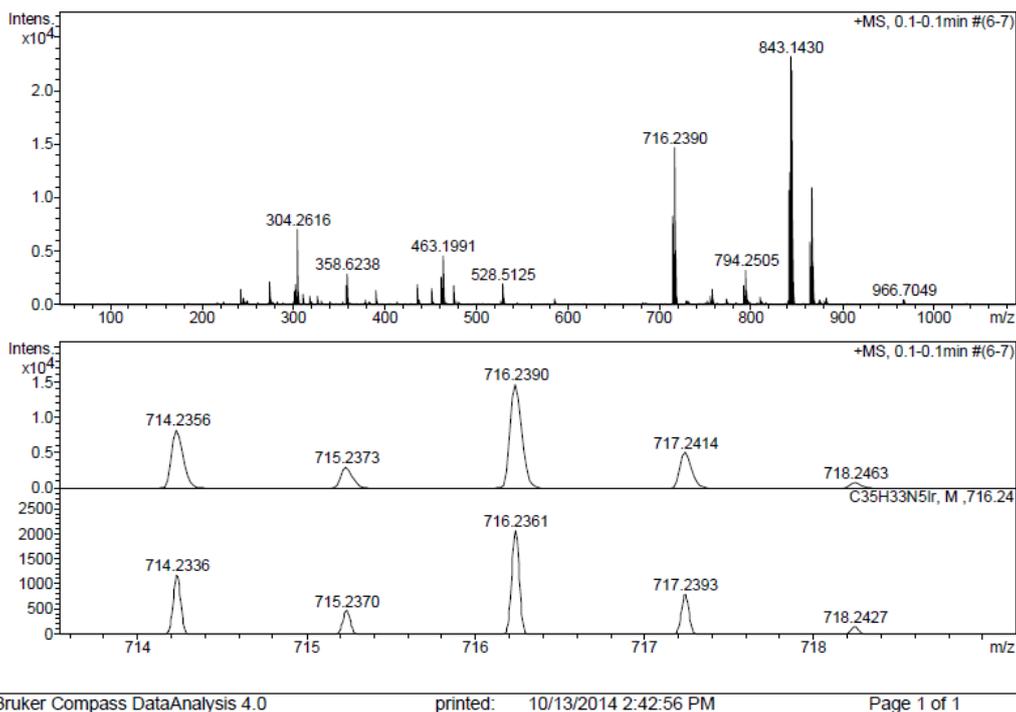
Figure S9a ESI-MS (positive ion mode) spectrum of **1**. The peak at 716.2390 is due to the [**1**−I]$^+$ cation.
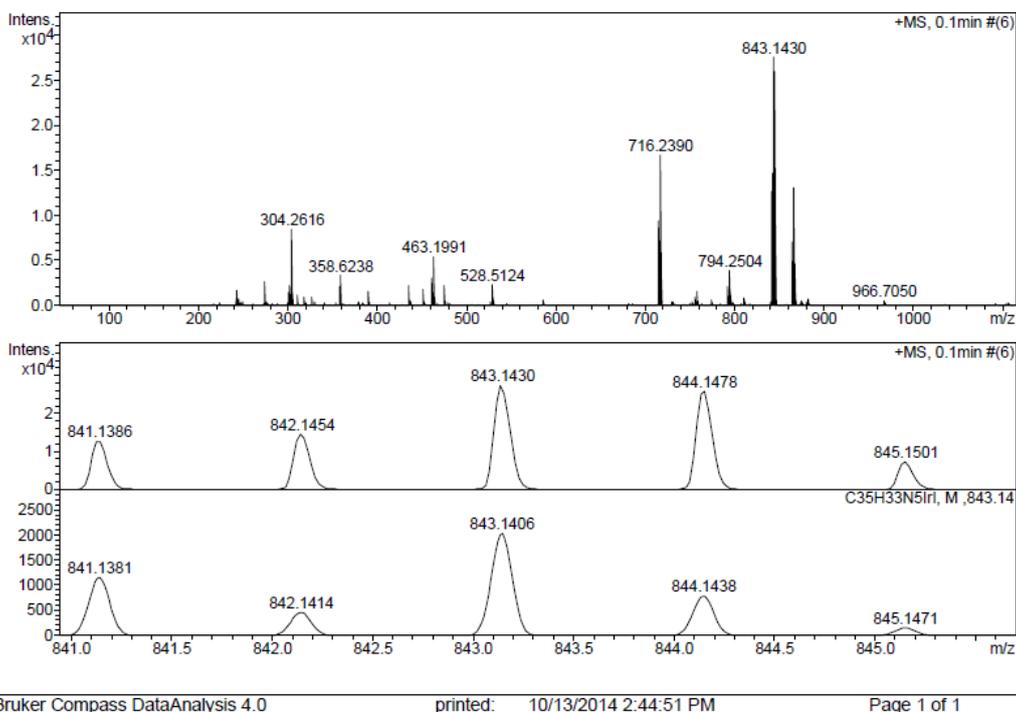
Figure S9b ESI-MS (positive ion mode) spectrum of **1**. The peak at 843.1430 corresponds to the complex **1** which might be due to oxidation under ESI-MS conditions.
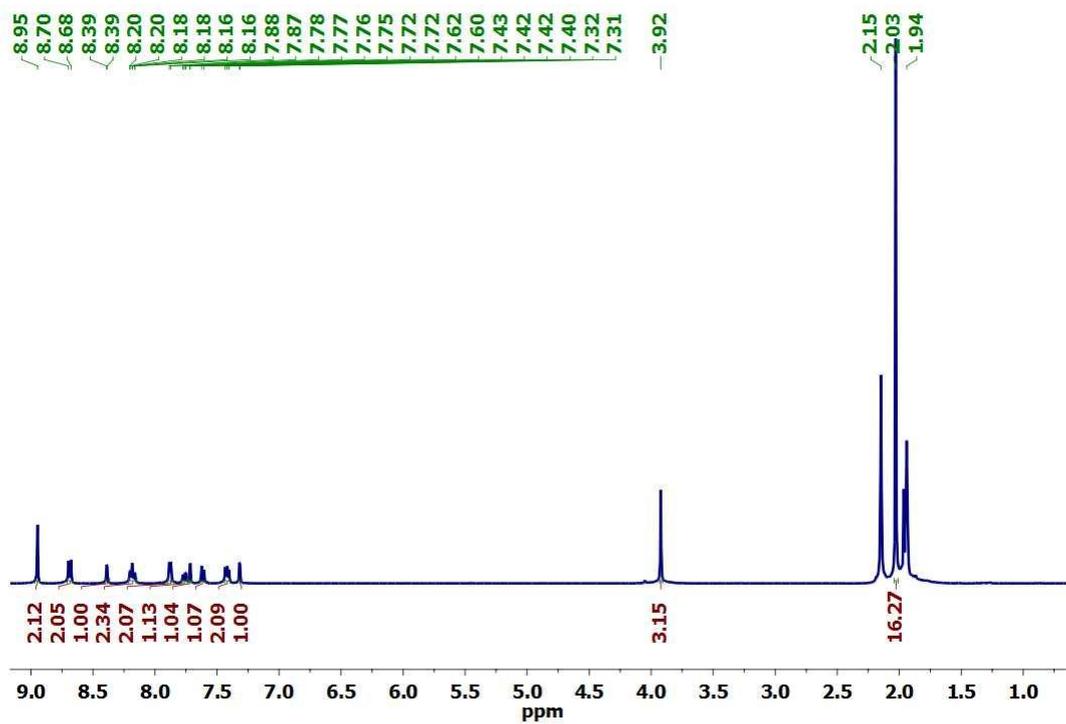
Figure S10 ^{1}H NMR spectrum of **2** (400 MHz, CD$_3$CN, 300 K).
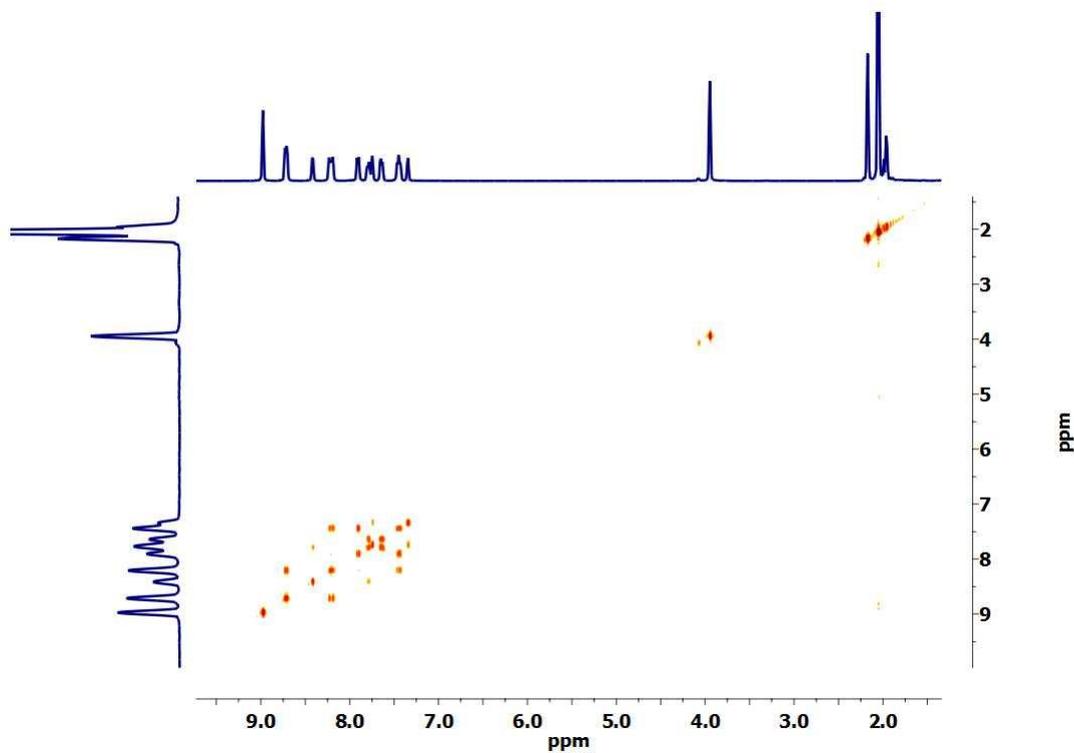
Figure S11 ^{1}H-^{1}H COSY NMR spectrum of **2**.
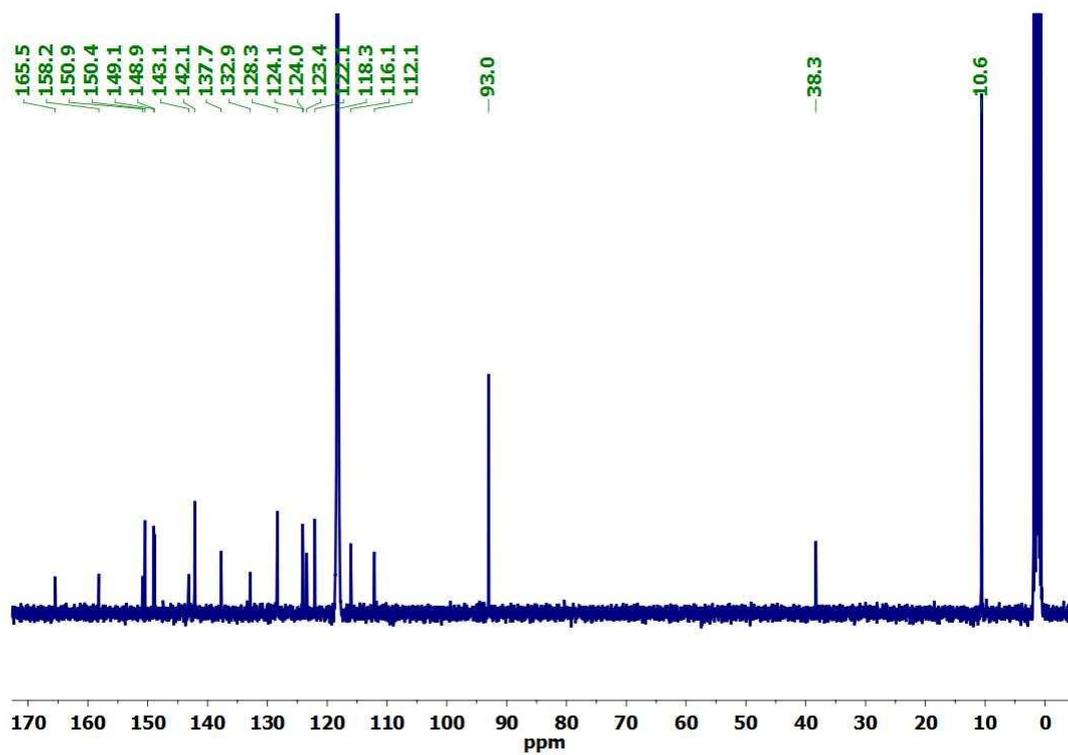
Figure S12 $^{13}C\{^1H\}$ NMR spectrum of **2** (100 MHz, CD$_3$CN, 300 K).
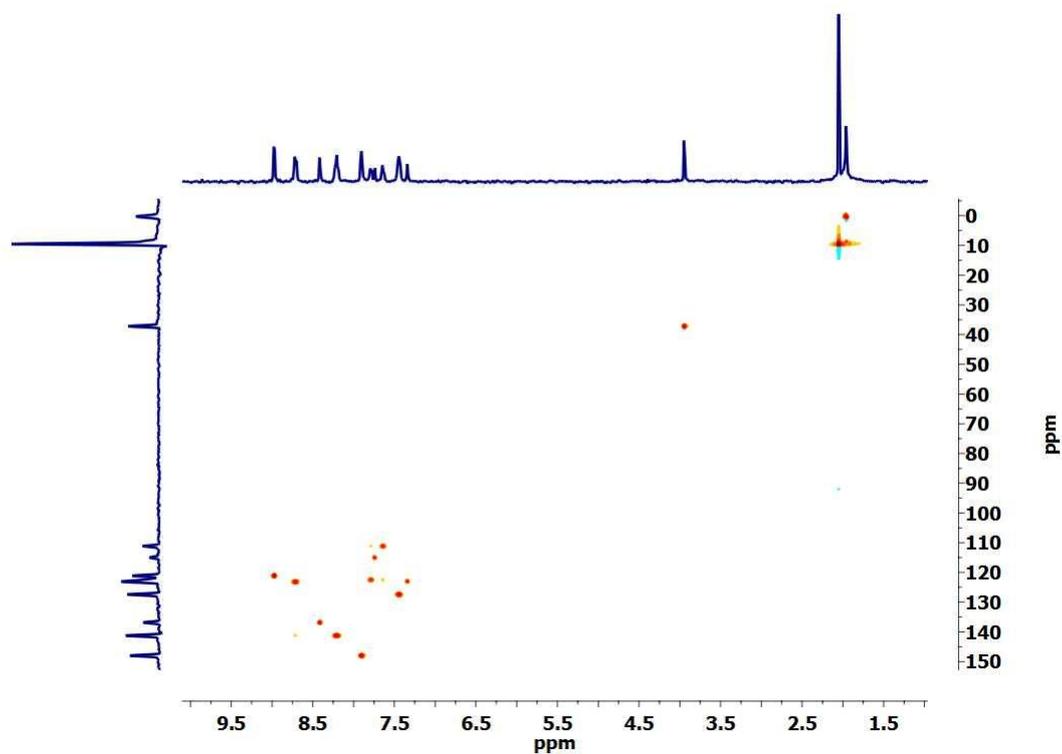
Figure S13 ^1H-^{13}C HSQC NMR spectrum of **2**.
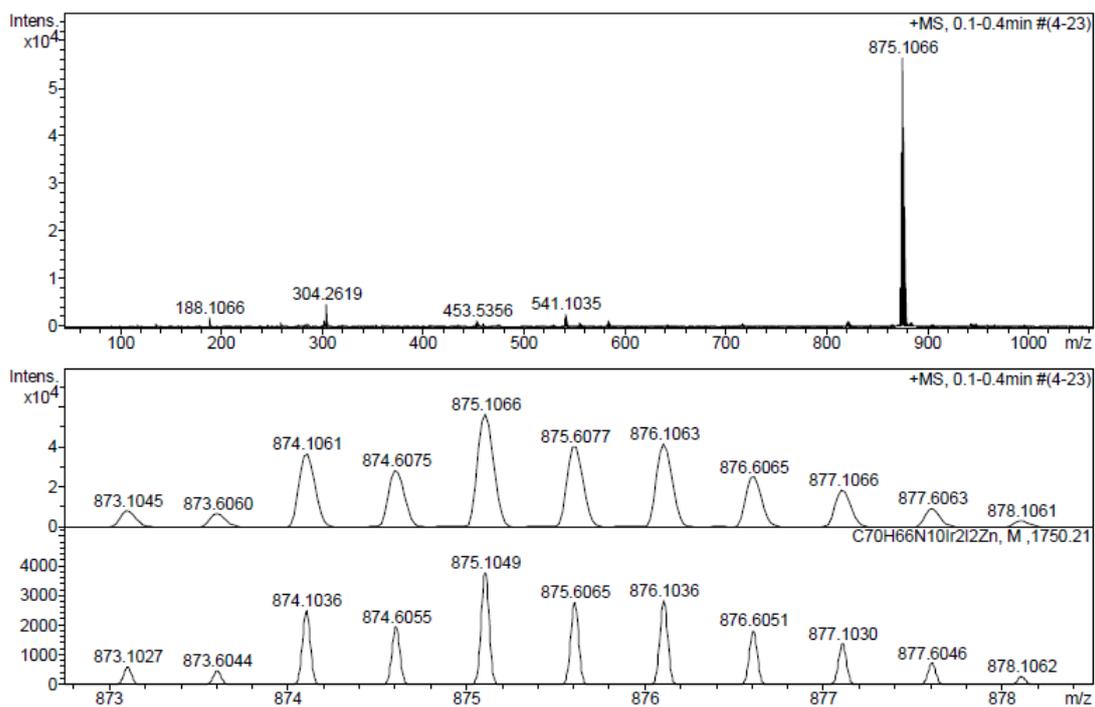
Figure S14 ESI-MS (positive ion mode) spectrum of **2**. The peak at 875.1066 corresponds to the $[Zn(\mathbf{1})_2]^{2+}$ cation.