Supplementary Materials: Chimera Diimine Ligands in Emissive [Cu(P^P)(N^N)][PF$_6$] Complexes

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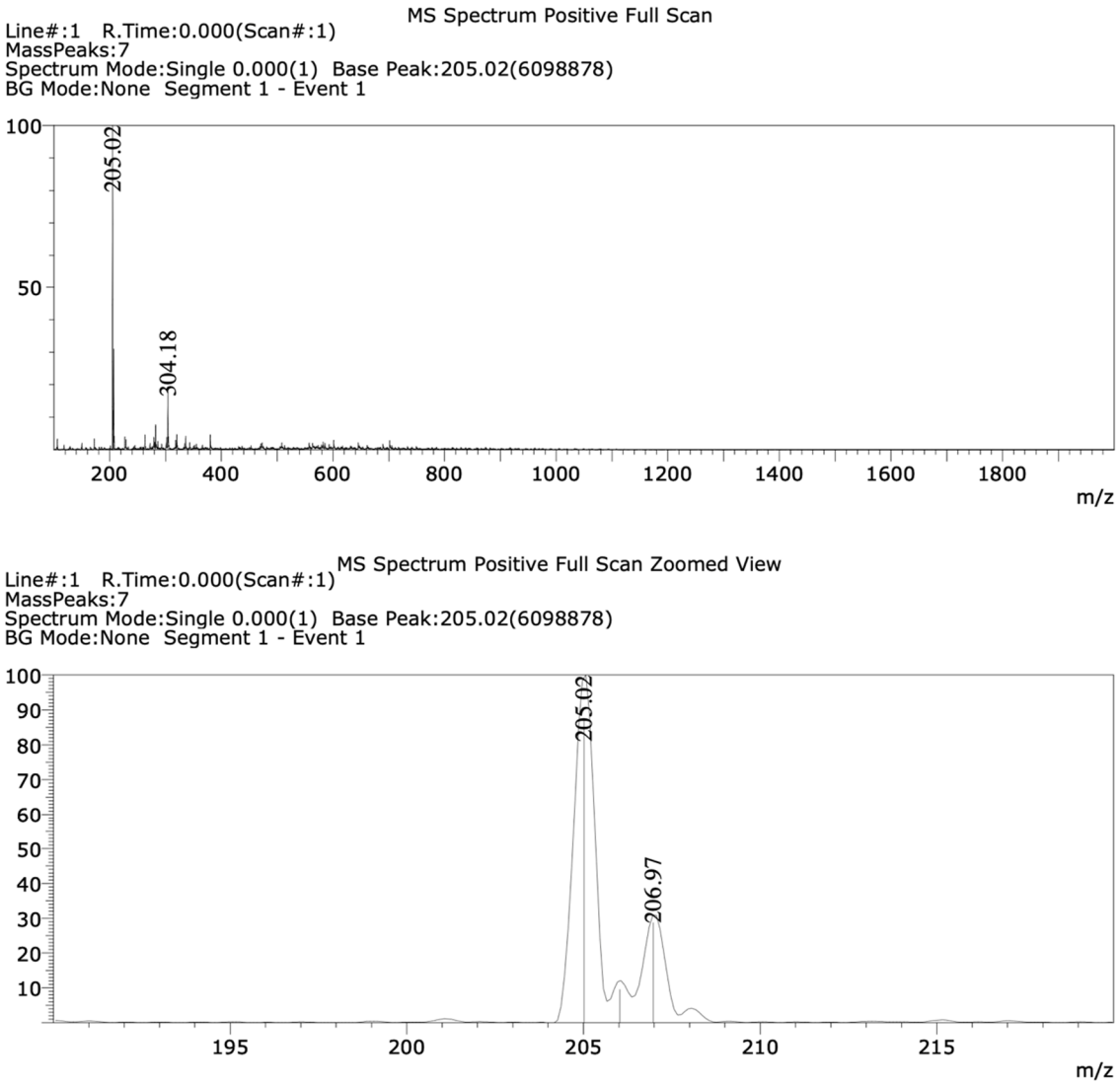

Figure S1. The ESI MS of 6-Cl-6'-Mebpy.

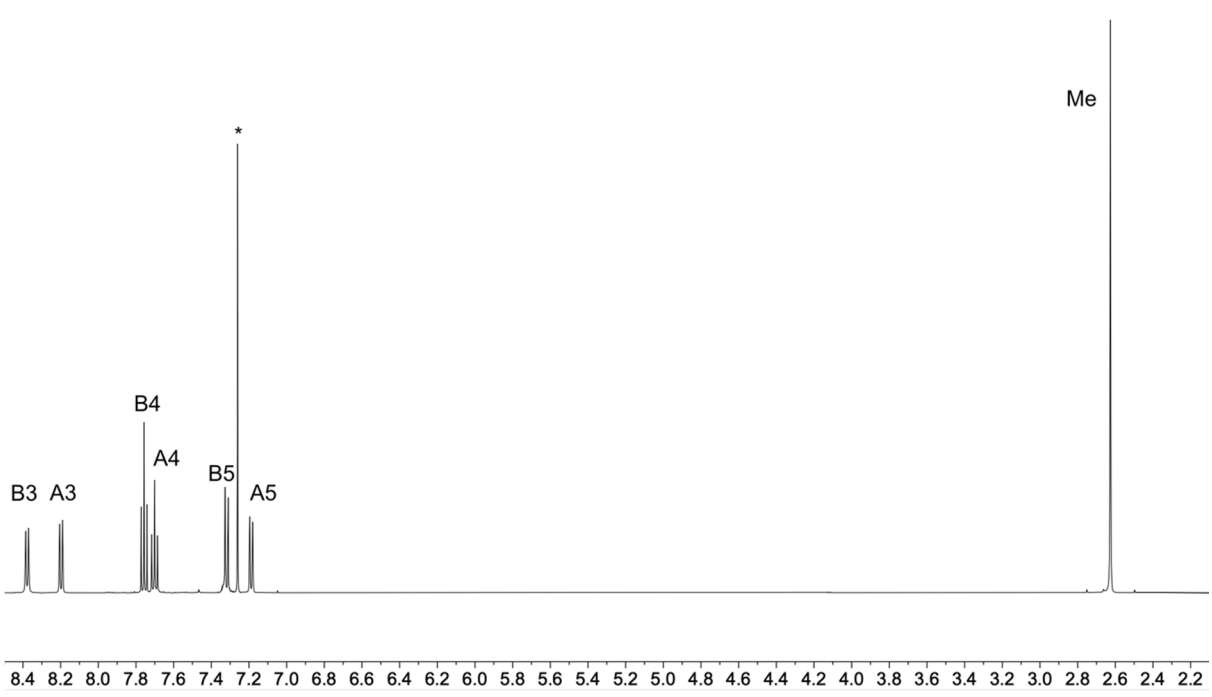

Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of 6-Cl-6'-Mebpy. Scale: δ / ppm. * = residual $CHCl_3$.

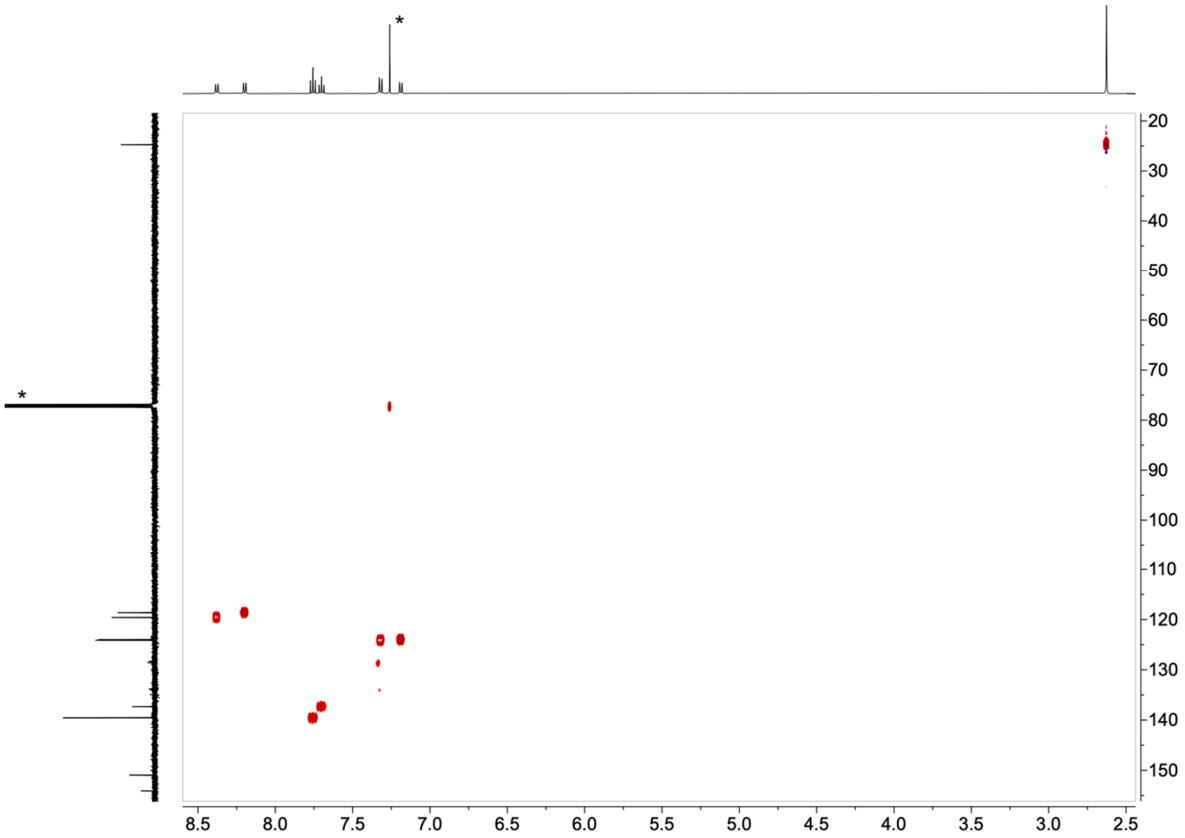

Figure S3. HMQC spectrum (500 MHz ^{1}H, 126 MHz $^{13}C\{^{1}H\}$, $CDCl_3$, 298 K) of 6-Cl-6'-Mebpy. Scale: δ / ppm. * = residual $CHCl_3$ (in ^{1}H) or $CDCl_3$ (in $^{13}C\{^{1}H\}$).

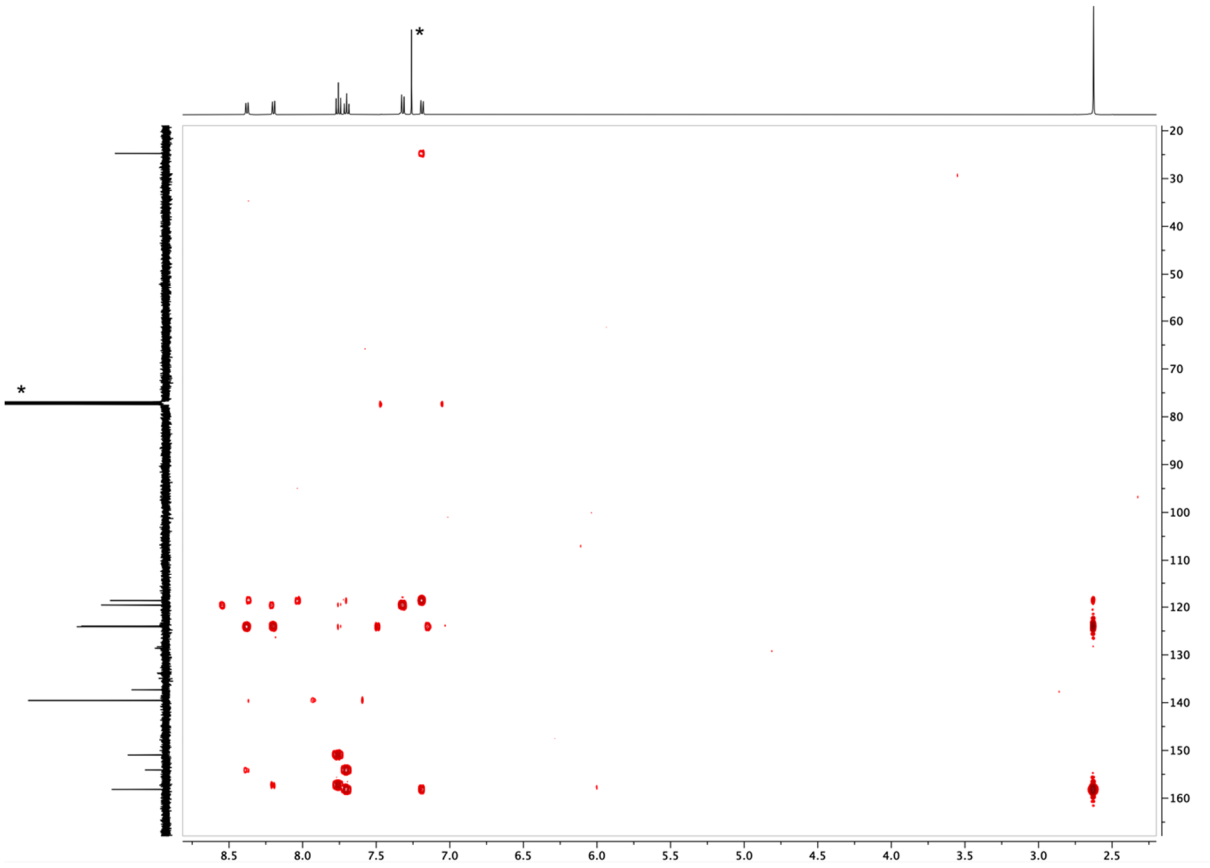

Figure S4. HMBC spectrum (500 MHz ^{1}H, 126 MHz ^{13}C{^{1}H}, $CDCl_3$, 298 K) of 6-Cl-6'-Mebpy. Scale: δ / ppm. * = residual $CHCl_3$ (in ^{1}H) or $CDCl_3$ (in ^{13}C{^{1}H}).

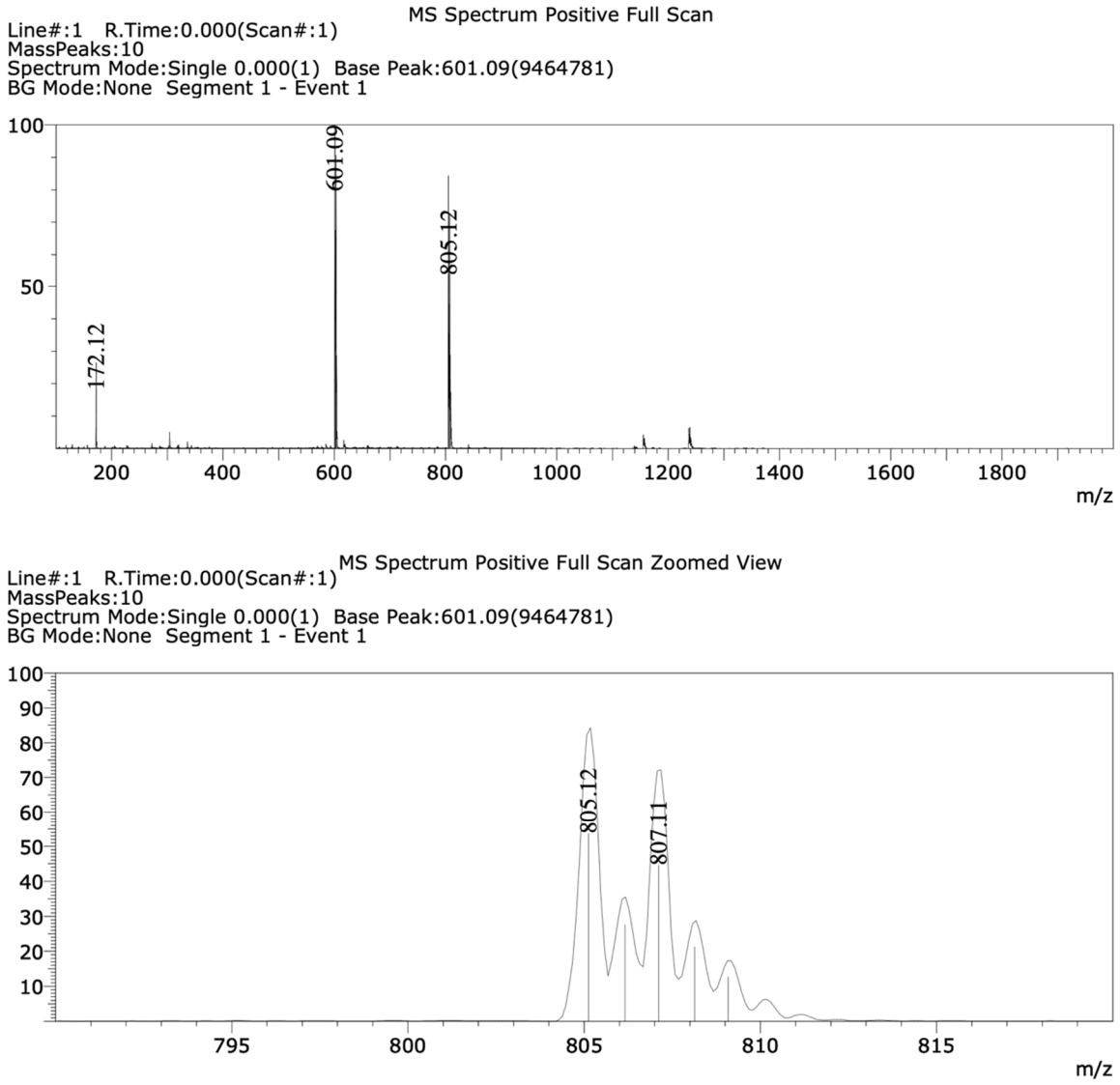

Figure S5. The ESI mass spectrum of [Cu(POP)(6-Cl-6'-Mebpy)][PF_6].

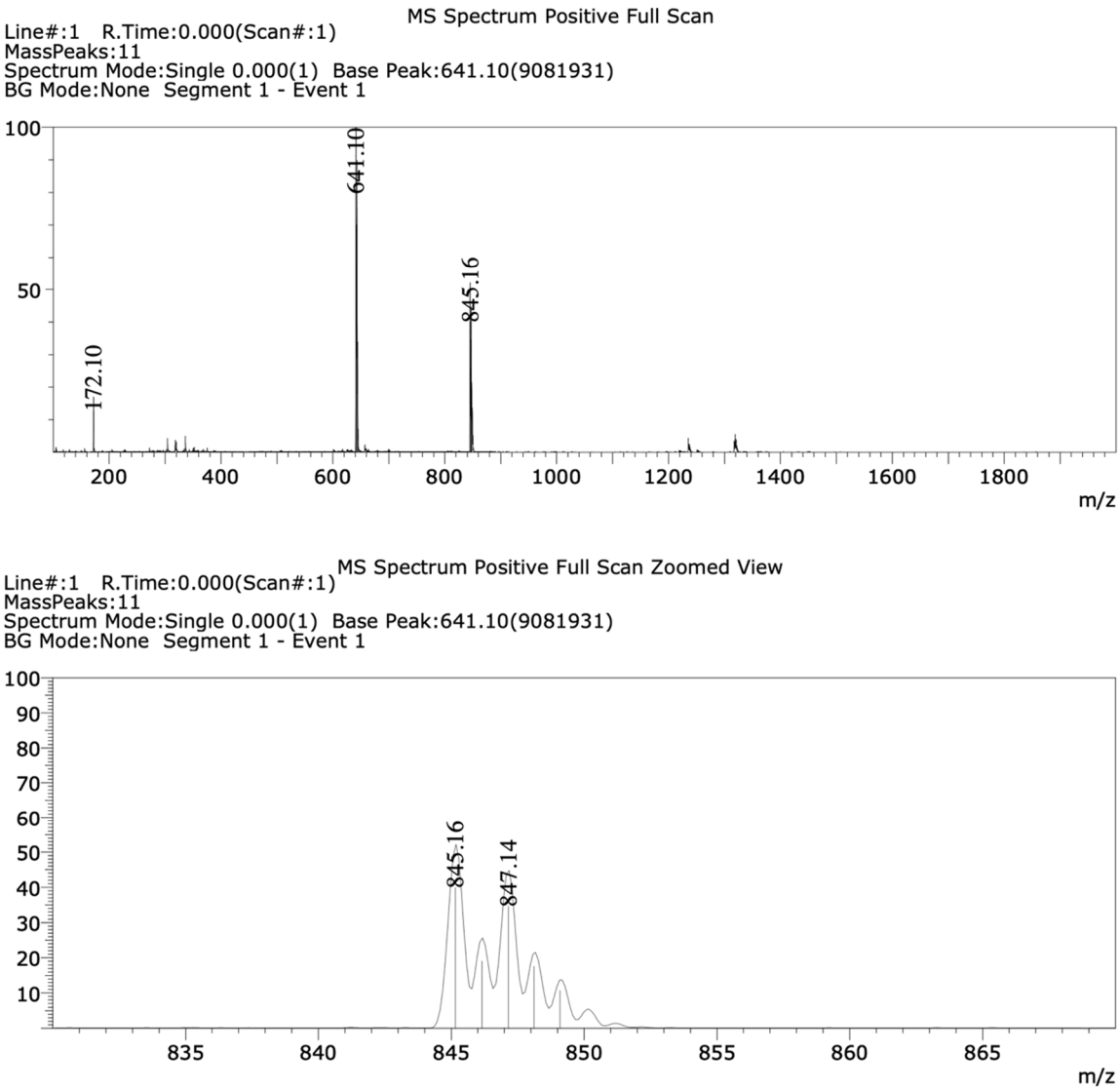

Figure S6. The ESI mass spectrum of [Cu(xantphos)(6-Cl-6'-Mebpy)][PF_6].

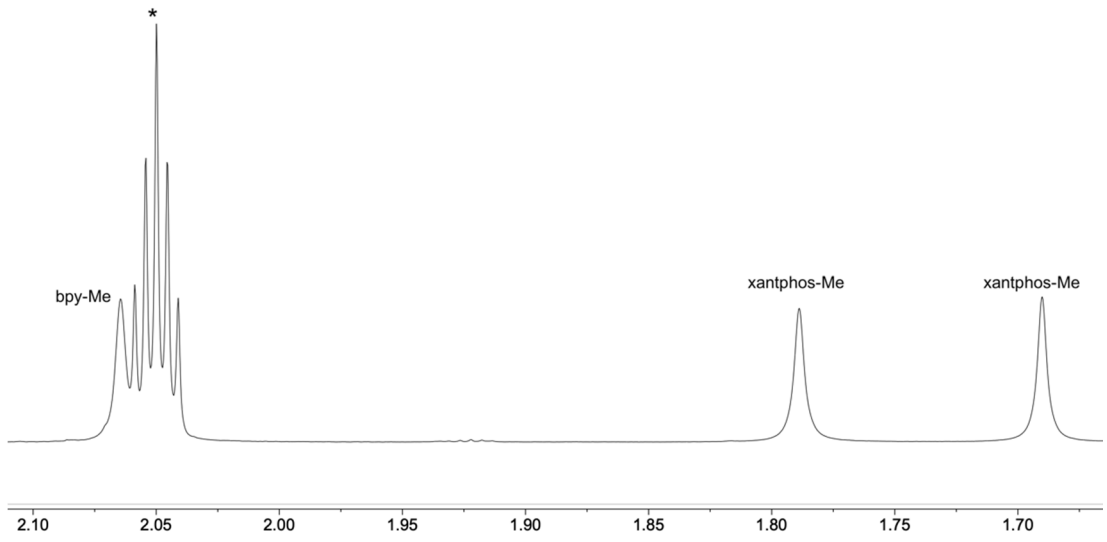

Figure S7. Methyl region of the ^{1}H NMR spectrum of [Cu(xantphos)(6-Cl-6'-Mebpy)][PF_6] (500 MHz, 298 K, acetone-d_6). * = residual acetone-d_5.

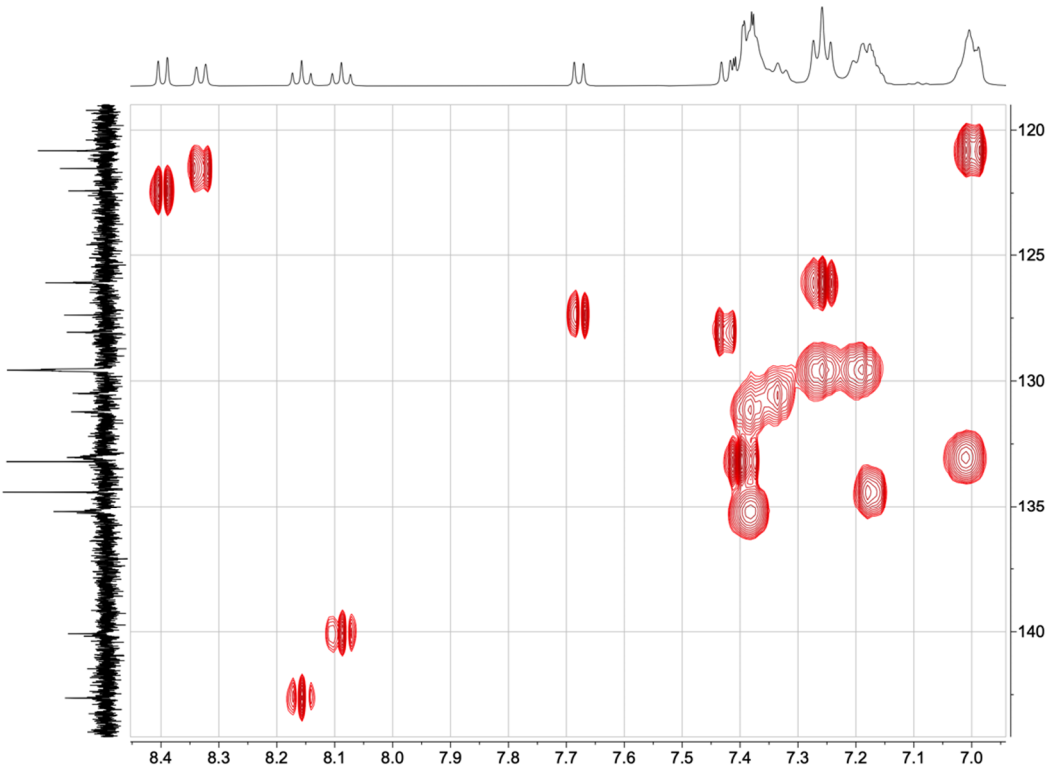

Figure S8. The aromatic region of the HMQC spectrum (500 MHz ^{1}H, 126 MHz ^{13}C{^{1}H}, acetone-d_6, 298 K) of [Cu(POP)(6-Cl-6'-Mebpy)][PF$_6$]. Scale: δ / ppm.

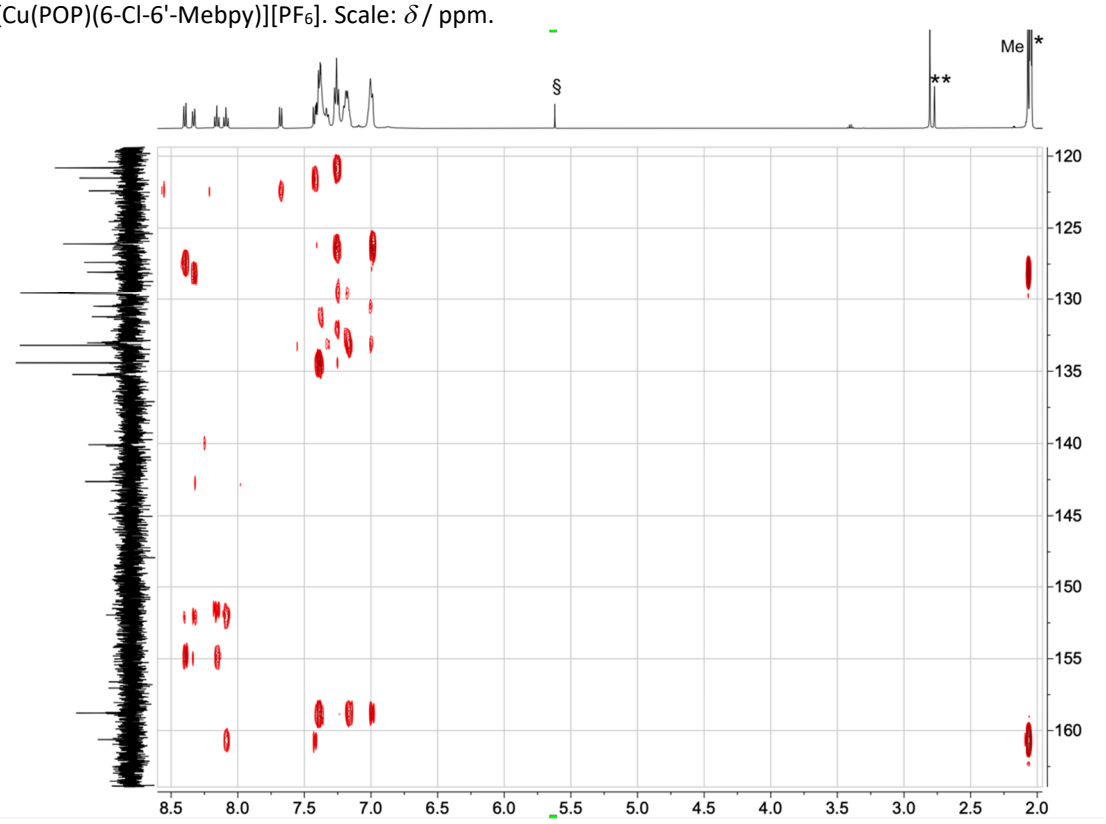

Figure S9. Part of the HMBC spectrum (500 MHz ^{1}H, 126 MHz ^{13}C{^{1}H}, acetone-d_6, 298 K) of [Cu(POP)(6-Cl-6'-Mebpy)][PF$_6$]. Scale: δ / ppm. * = residual acetone-d_5; ** = H_2O and HOD; § = CH_2Cl_2.

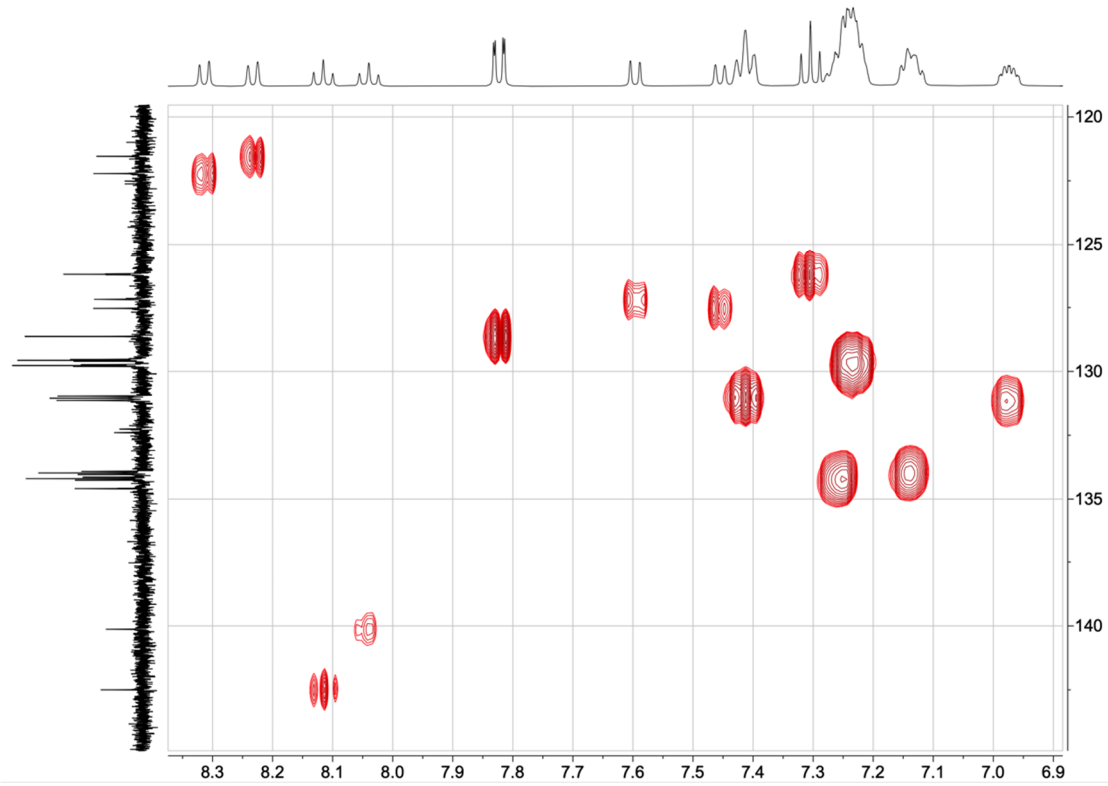

Figure S10. The aromatic region of the HMQC spectrum (500 MHz ^{1}H, 126 MHz ^{13}C{^{1}H}, acetone-d_6, 298 K) of [Cu(xantphos)(6-Cl-6'-Mebpy)][PF$_6$]. Scale: δ / ppm.

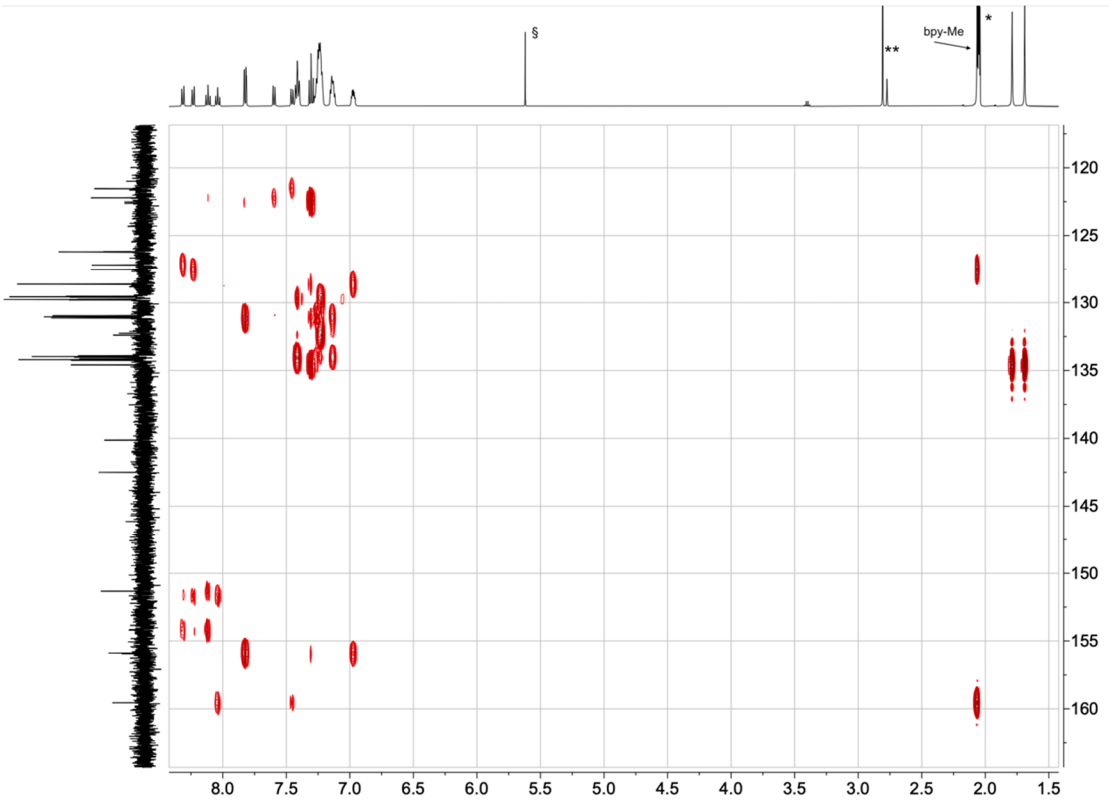

Figure S11. Part of the HMBC spectrum (500 MHz ^{1}H, 126 MHz ^{13}C{^{1}H}, acetone-d_6, 298 K) of [Cu(xantphos)(6-Cl-6'-Mebpy)][PF$_6$]. Scale: δ / ppm. * = residual acetone-d_5; ** = H_2O and HOD; § = CH_2Cl_2.

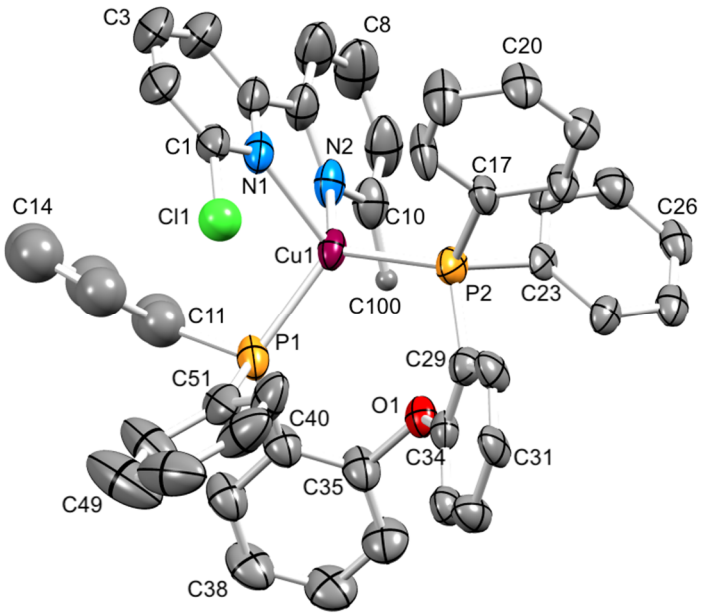

Figure S12. ORTEP representation of the structure of the $[Cu(POP)(6\text{-Cl-}6'\text{-Mebpy})]^+$ cation in $[Cu(POP)(6\text{-Cl-}6'\text{-Mebpy})][PF_6]$. One set of partical occupancy sites is shown (see Figure S13). Ellipsoids are plotted at a 40% probability level and H atoms are omitted. The phenyl ring with C11 was refined isotropically as it was not possible to identify two distinct orientations; atom C100 of the methyl group was also refined isotropically.

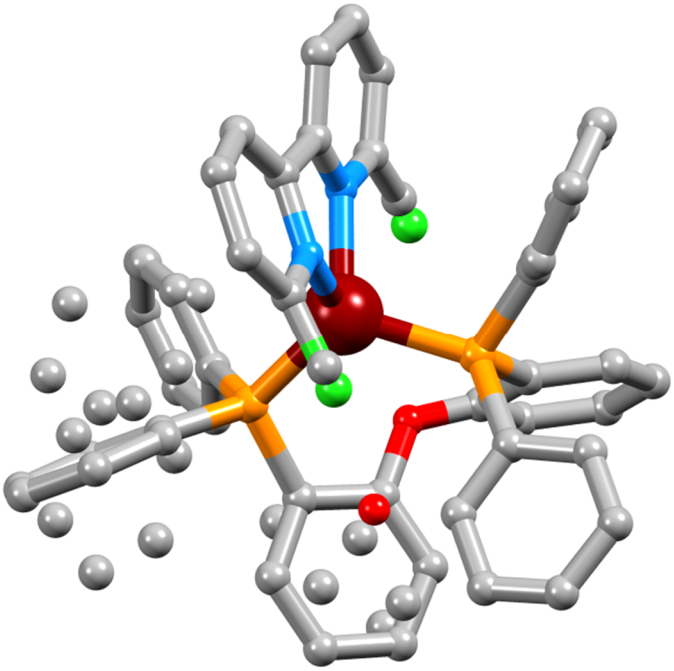

Figure S13. The disordered structure of the $[Cu(POP)(6\text{-Cl-}6'\text{-Mebpy})]^+$ cation in $[Cu(POP)(6\text{-Cl-}6'\text{-Mebpy})][PF_6]$. Each partial occupancy site was modelled with a 50% occupancy.

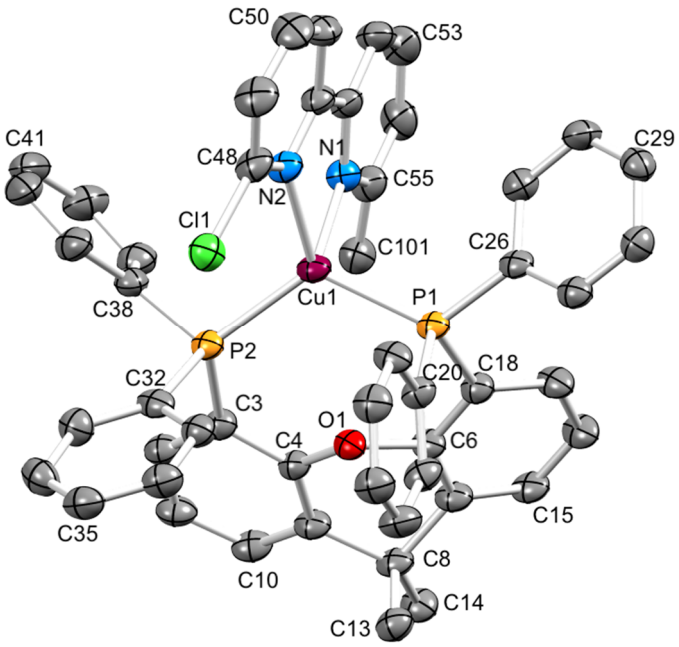

Figure S14. ORTEP representation of the structure of the $[Cu(xantphos)(6\text{-Cl-}6'\text{-Mebpy})]^+$ cation in $[Cu(xantphos)(6\text{-Cl-}6'\text{-Mebpy})][PF_6]$. Ellipsoids are plotted at a 40% probability level and H atoms are omitted. The Cl/Me positions are disordered (modelled with 50% occupancies) and one site for the 6-Cl-6'-Mebpy is shown.

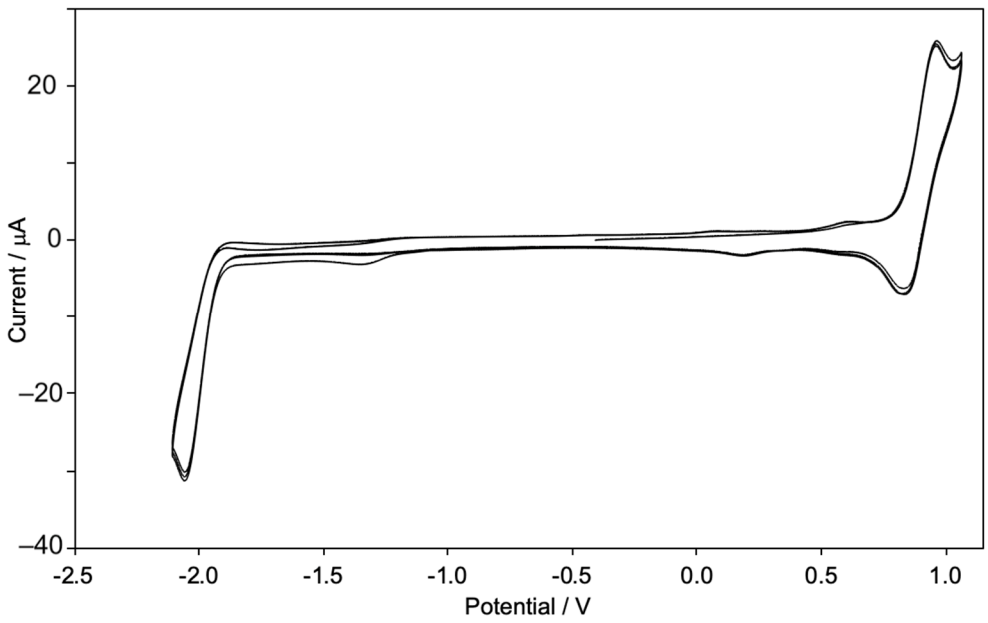

Figure S15. Three consecutive scans in the cyclic voltammogram of $[Cu(xantphos)(6\text{-Cl-}6'\text{-Mebpy})][PF_6]$ in CH_2Cl_2 solution (ca. 10^{-4} mol dm^{-3}) with $[^nBu_4N][PF_6]$ as supporting electrolyte and a scan rate of 0.1 V s^{-1} (referenced to internal Fc/Fc^+ = 0.0 V).

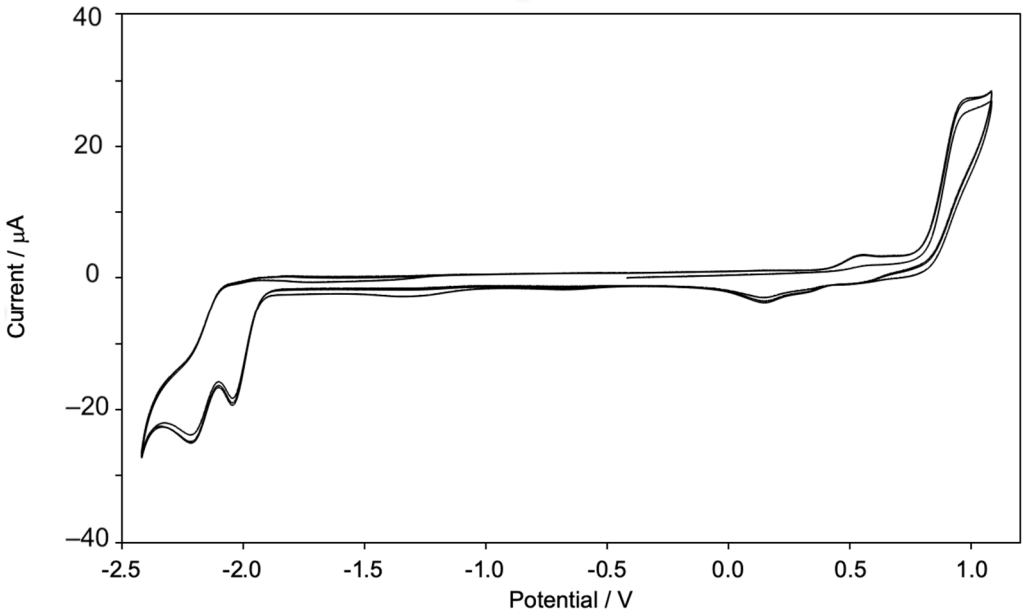

Figure S16. Three consecutive scans in the cyclic voltammogram of [Cu(POP)(6-Cl-6'-Mebpy)][PF_6] in CH_2Cl_2 solution (ca. 10^{-4} mol dm^{-3}) with [^{n}Bu$_4$N][PF_6] as supporting electrolyte and a scan rate of 0.1 V s^{-1} (referenced to internal Fc/Fc^+ = 0.0 V).