Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for

Synthesis and Characterization of Phosphorescent Platinum and Iridium Complexes with Cyclometalated Corannulene

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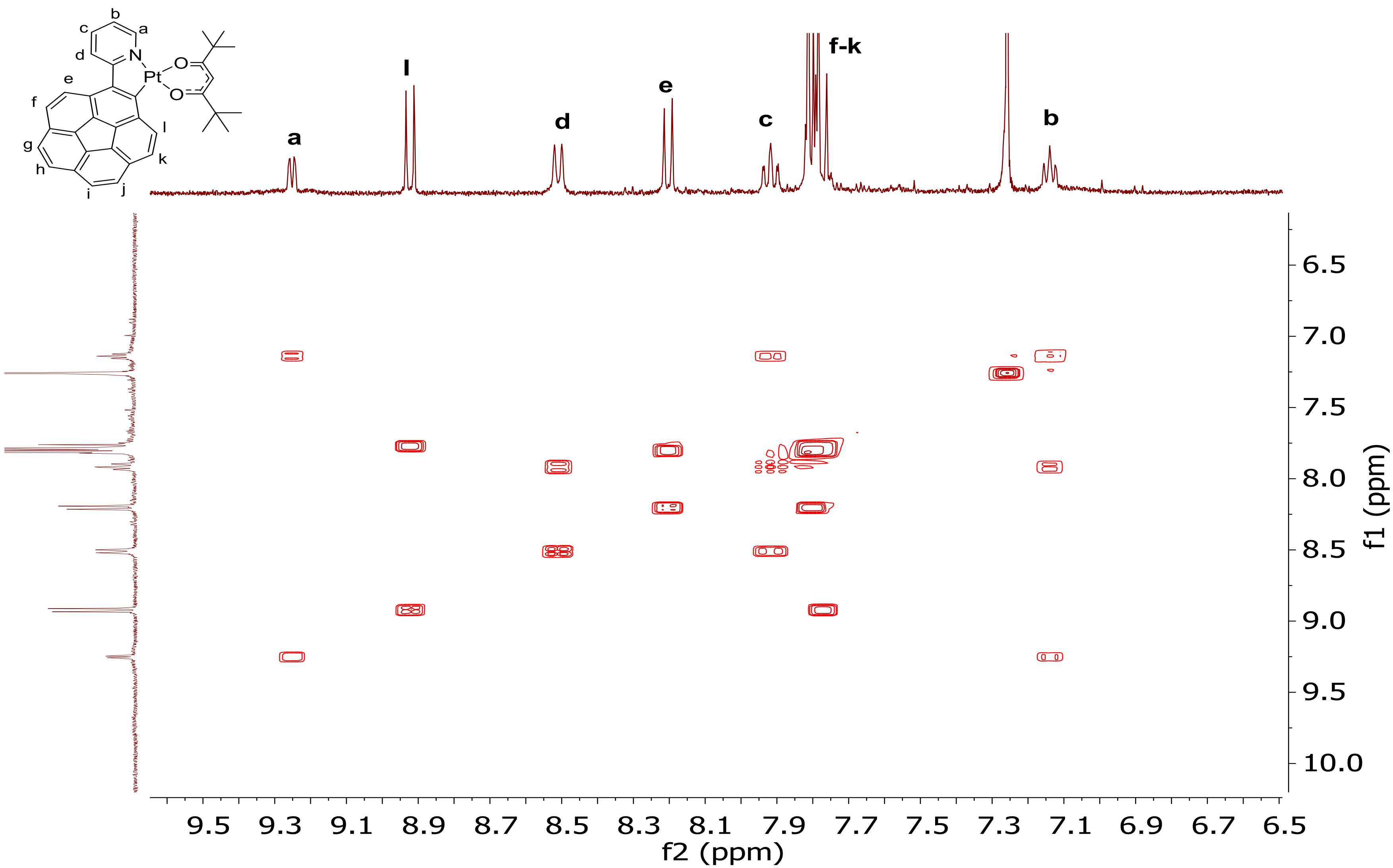
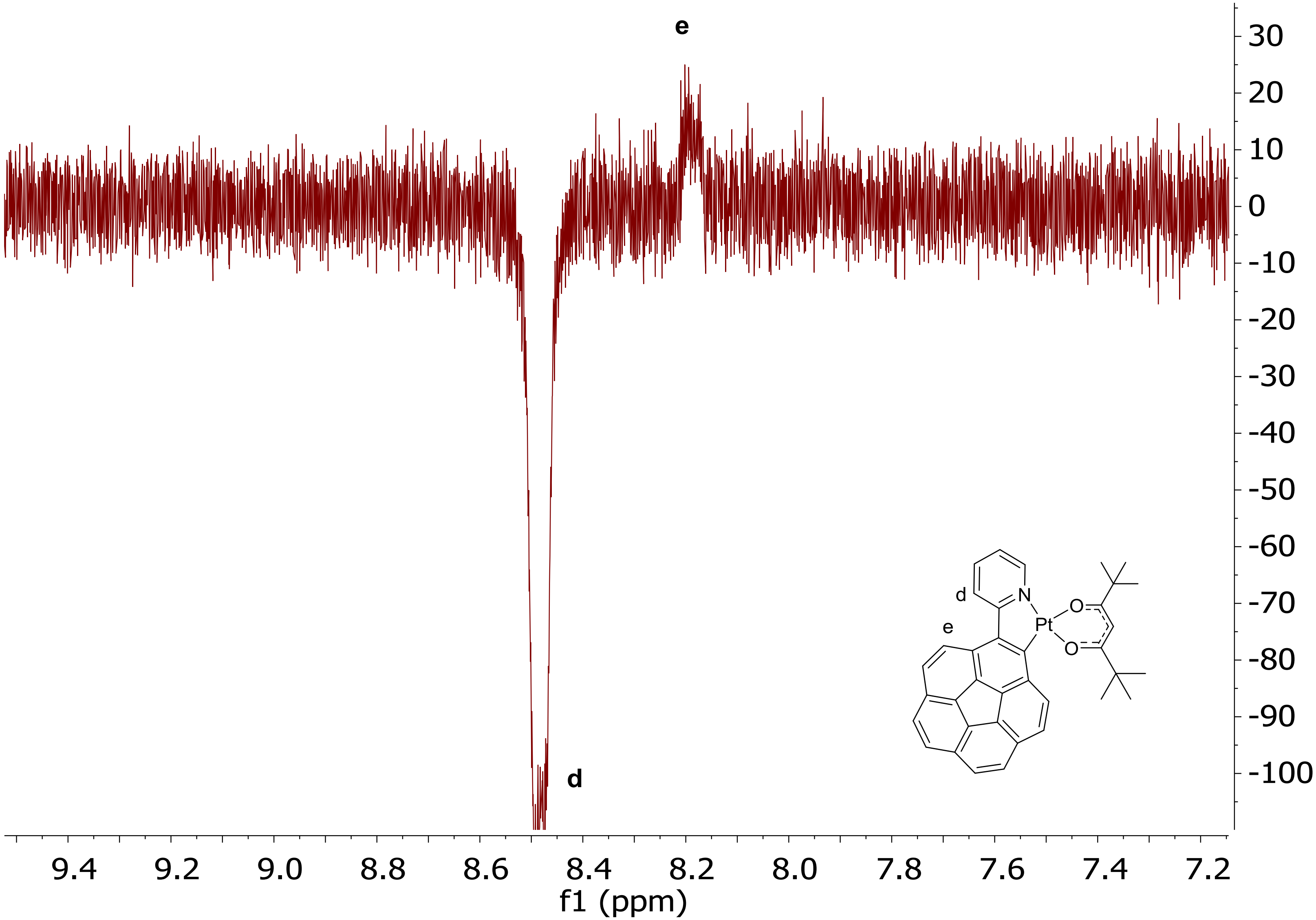


S-2. 1D NOESY of (corpy)Pt(dpm) irradiation at 8.5 ppm in $CDCl_3$.



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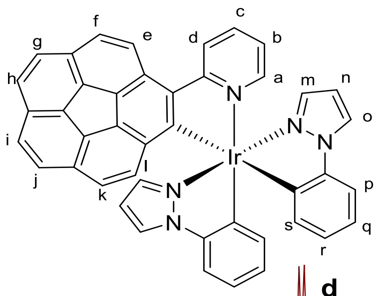
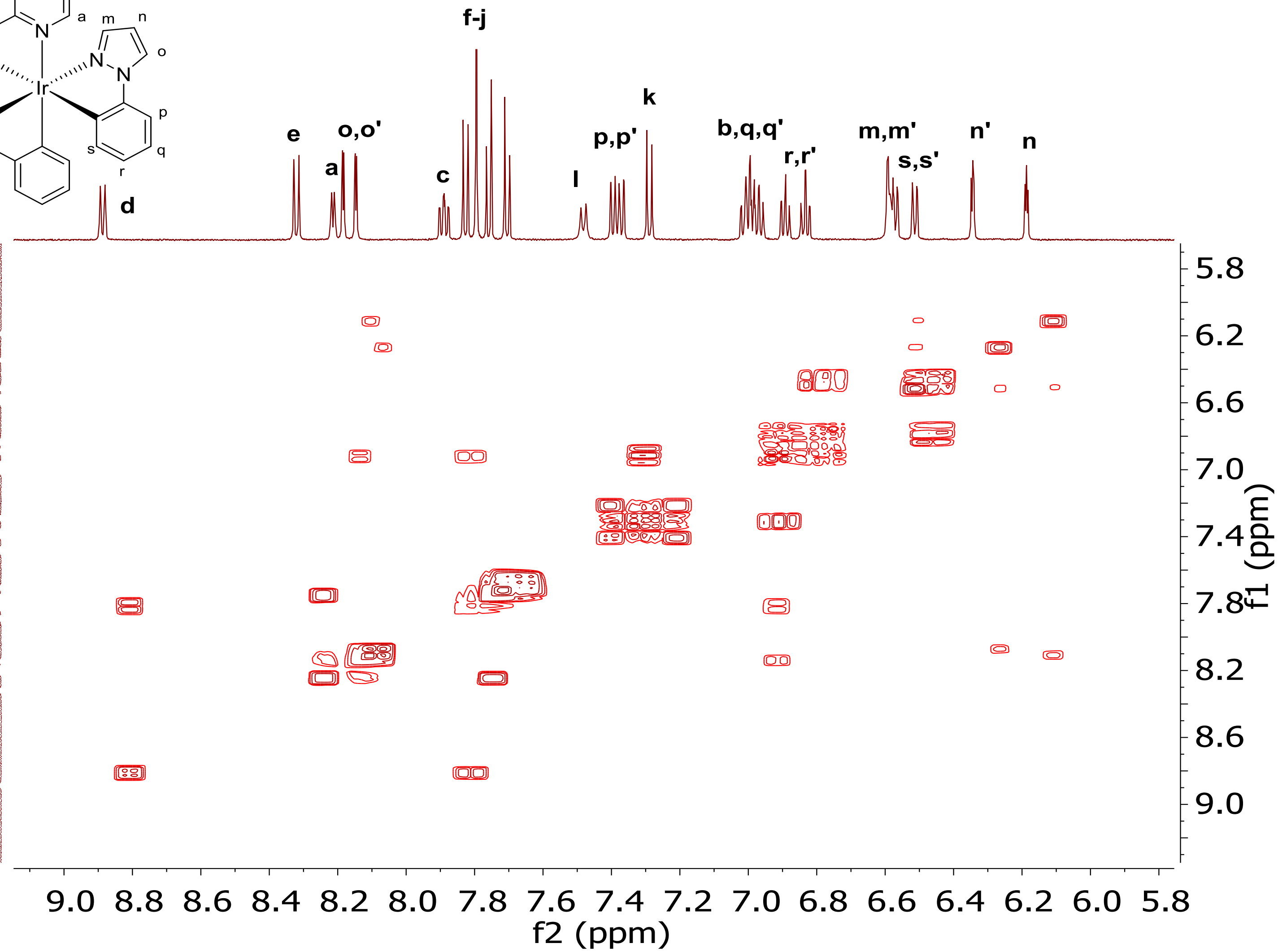
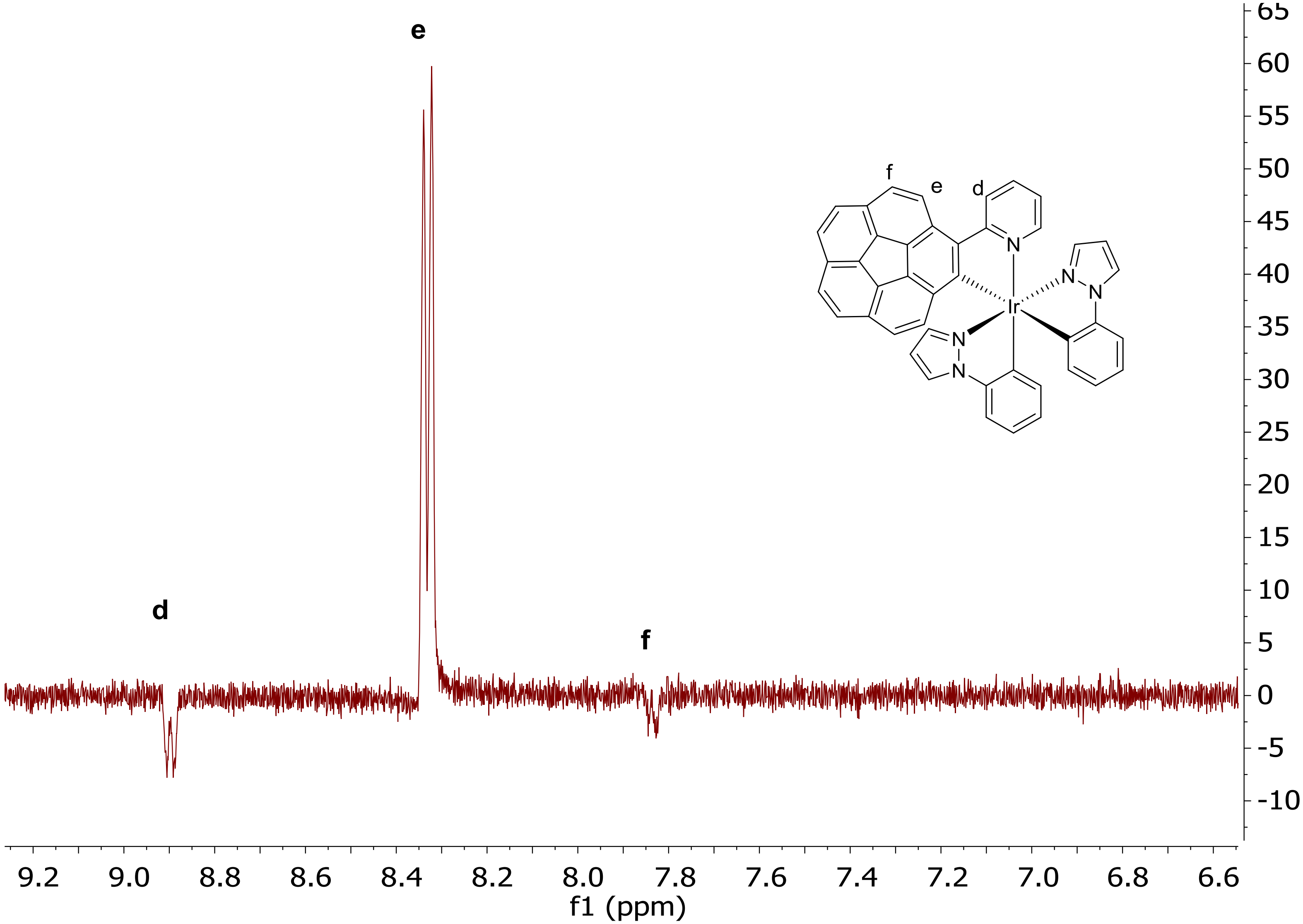




S-4. 1D

S-4. 1D NOESY of (corpy)Ir(ppz)$_2$ irradiation at 8.33 ppm in 2:1 CD_2Cl_2: acetone.



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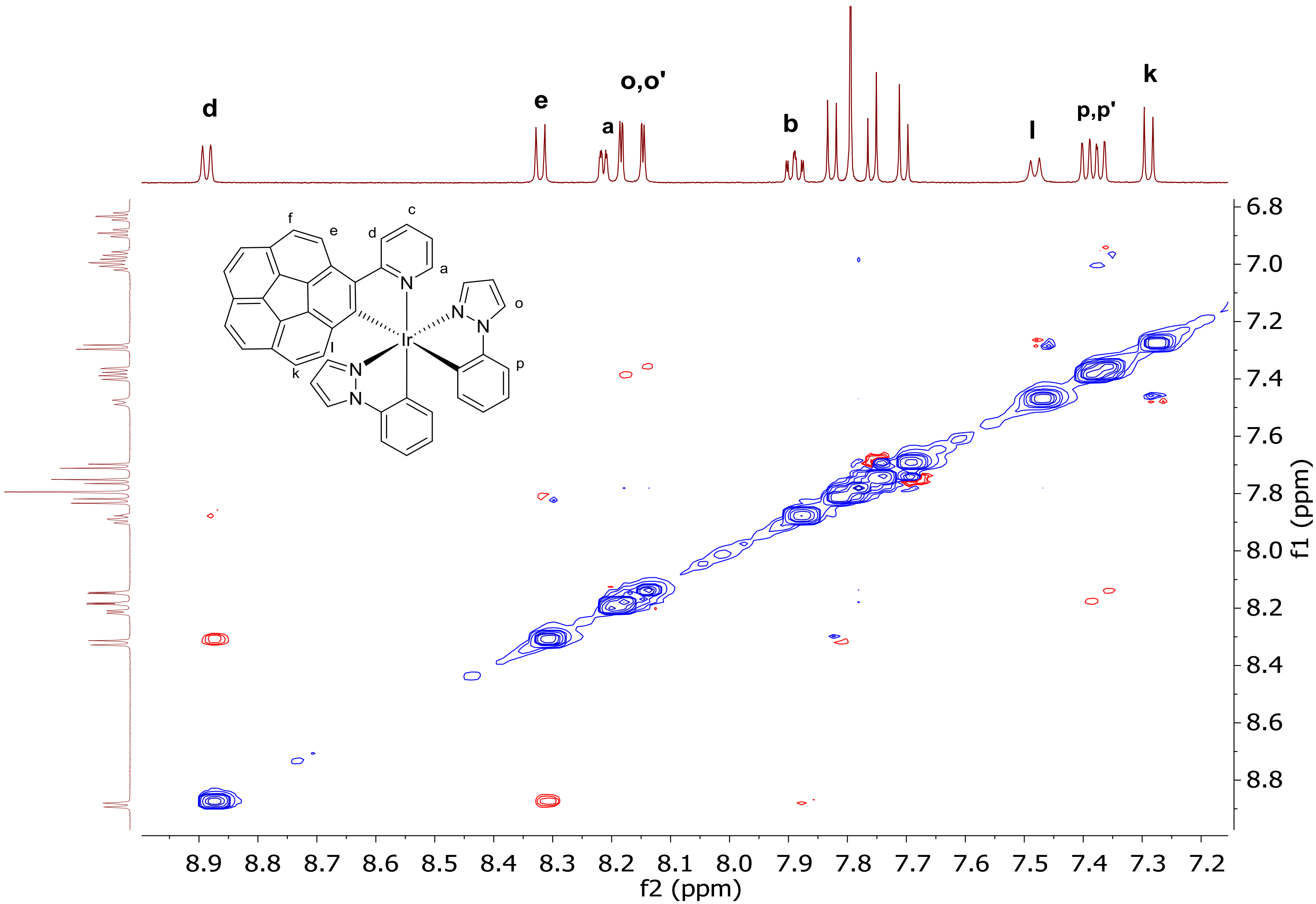

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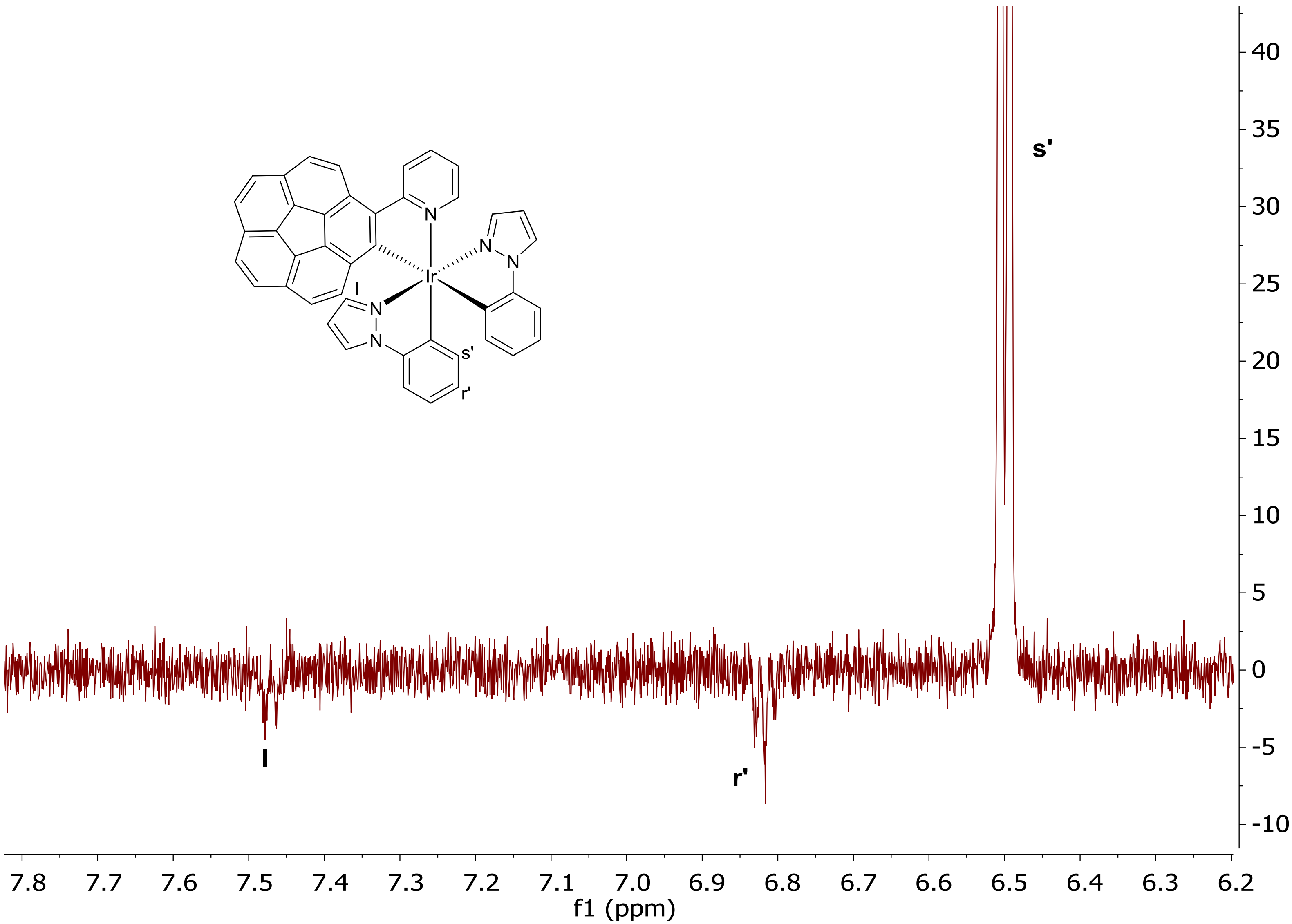
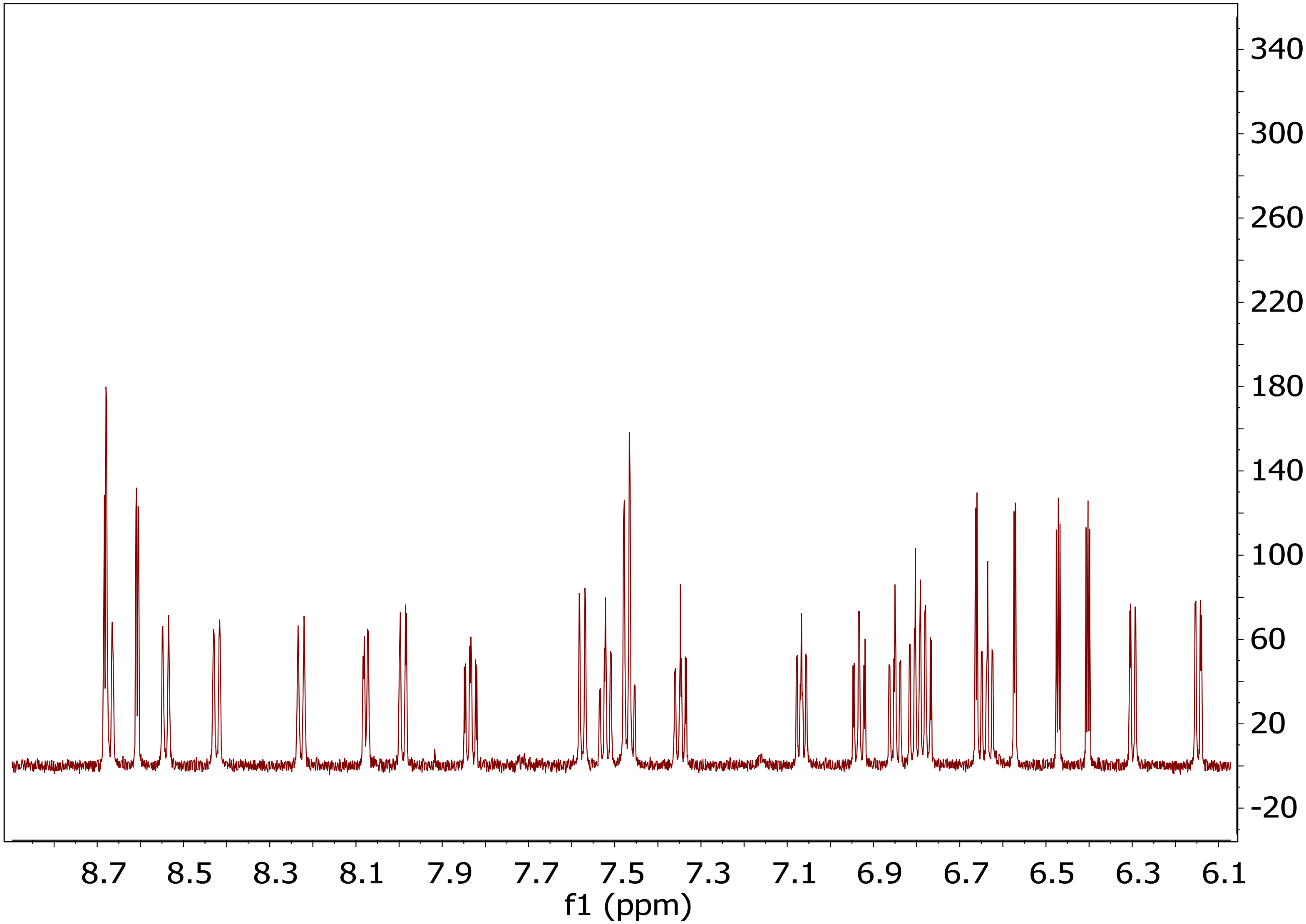
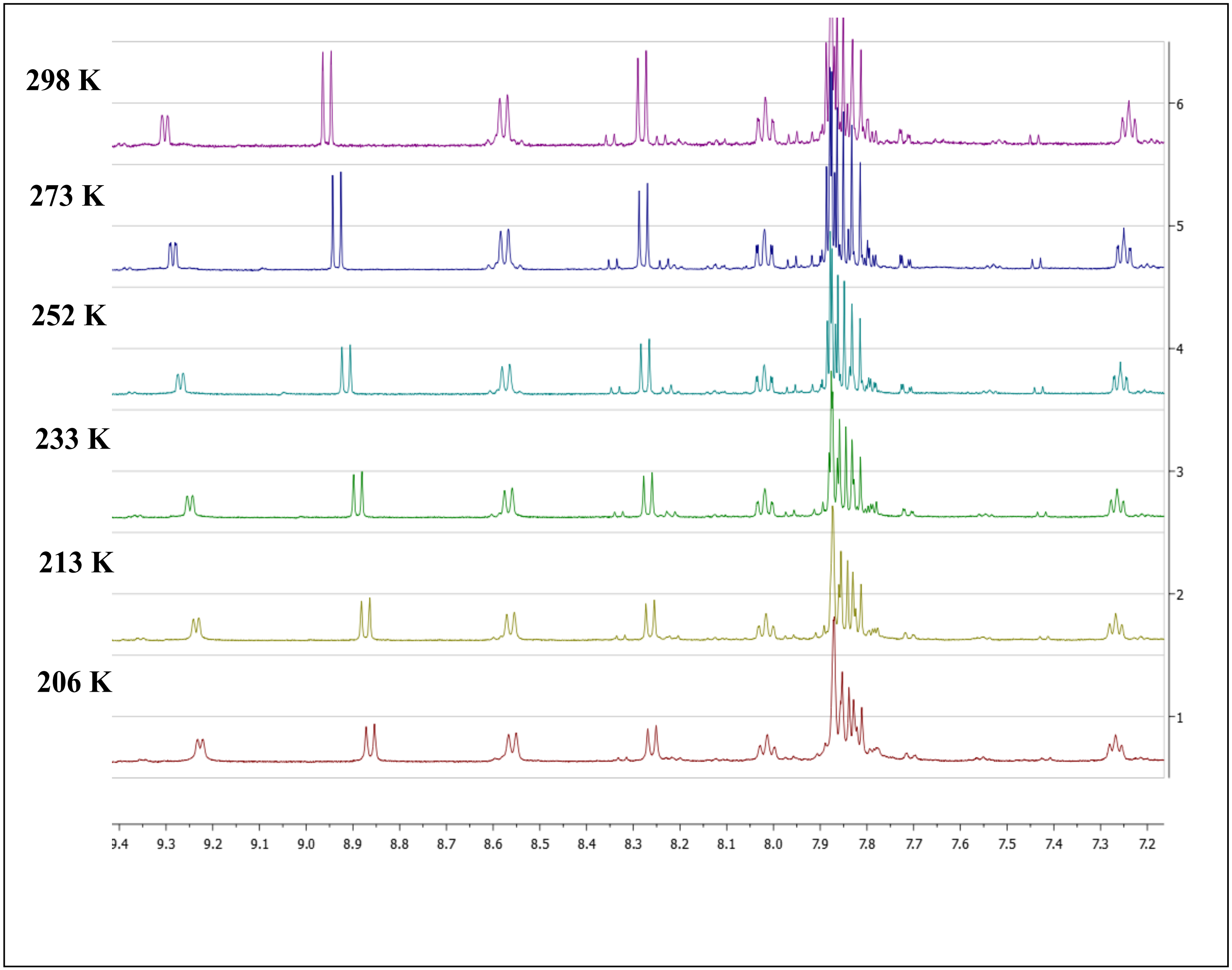


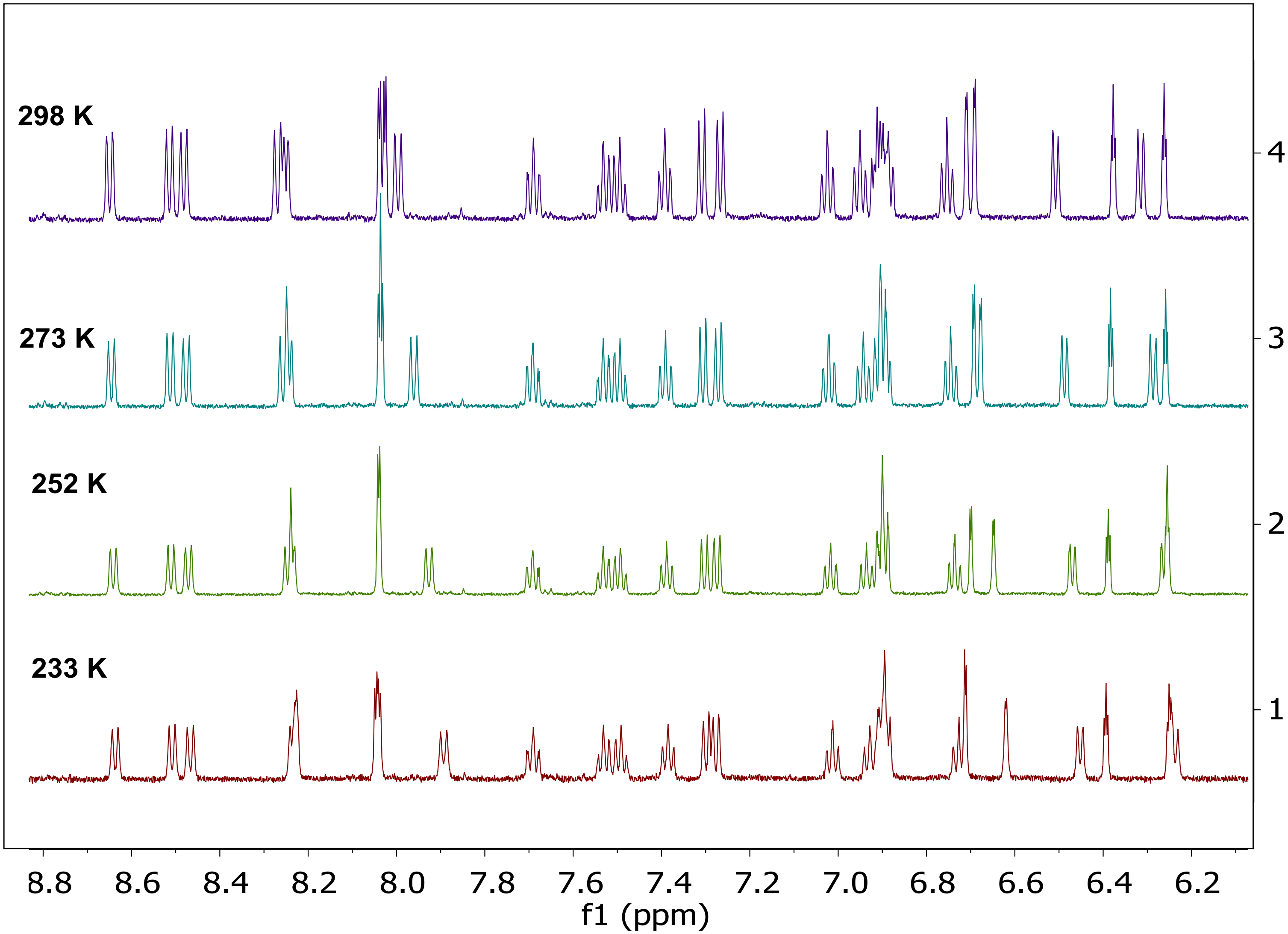
S-7. NMR of (phenpy)Ir(ppz)$_2$ in $(CD_3)_2SO$.



S-8. VT NMR of (corpy)Pt(dpm) in CD_2Cl_2.



S-9. VT NMR of (phenpy)Ir(ppz)$_2$ in CD_2Cl_2.



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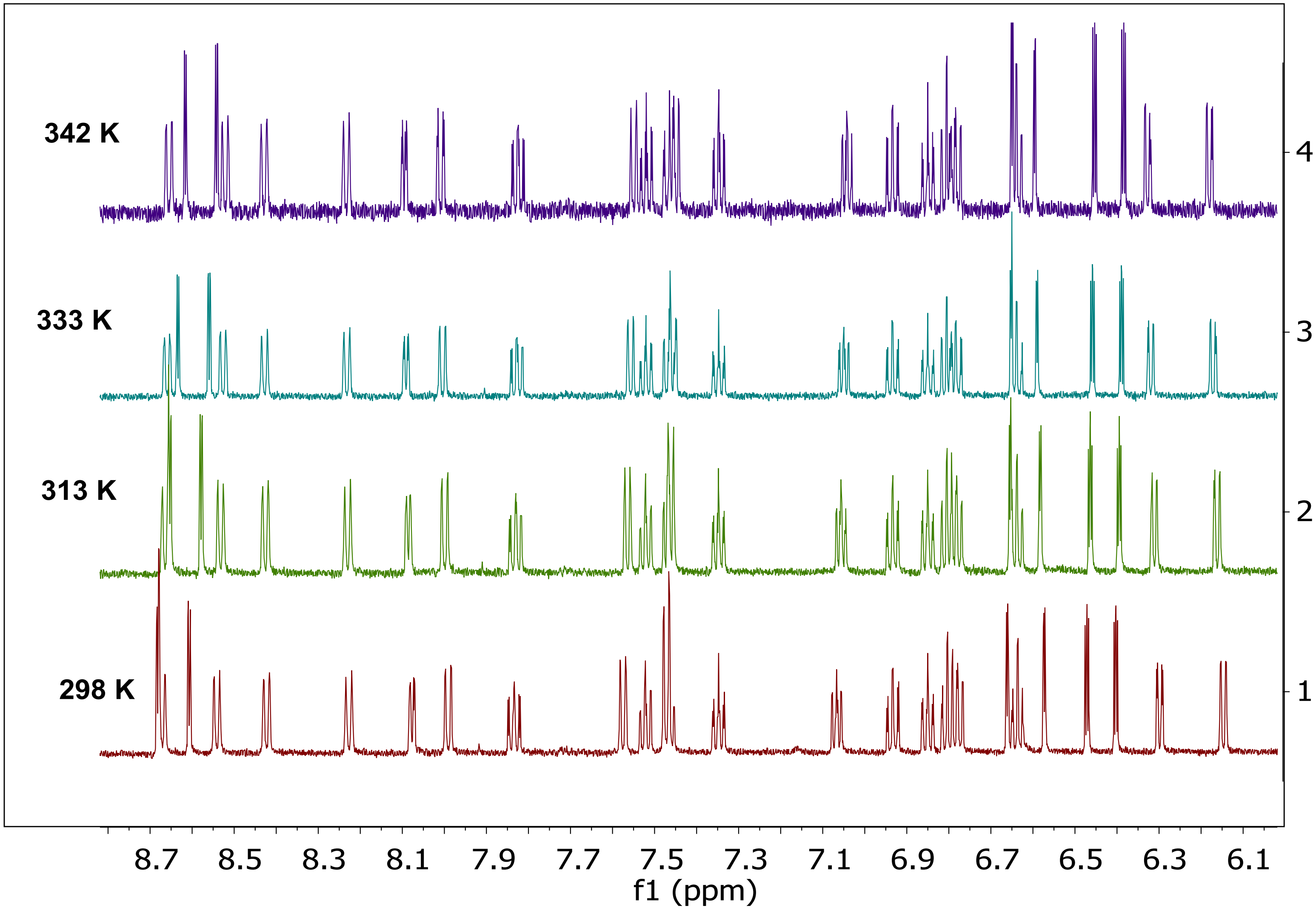
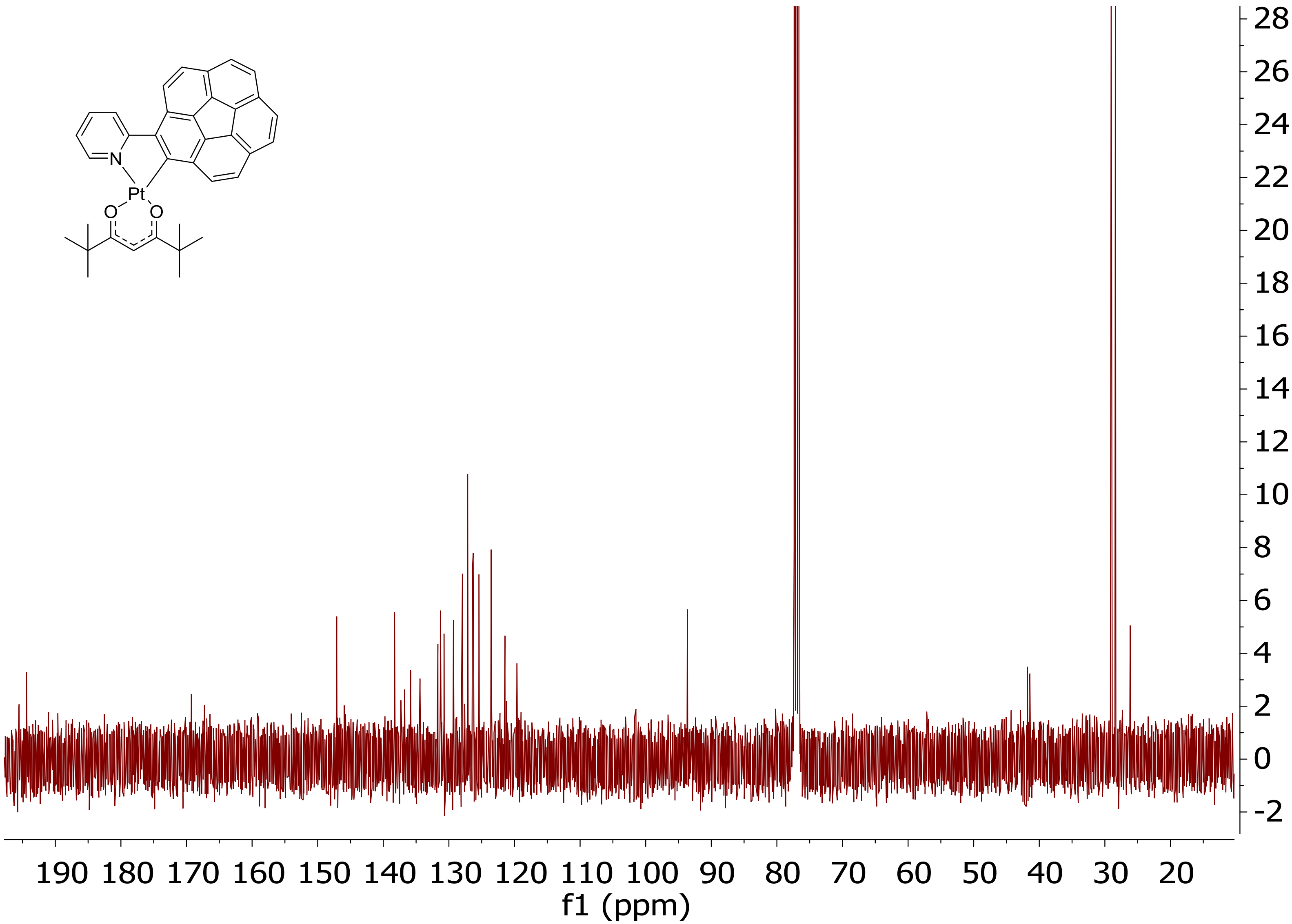


S-11. ^{13}C NMR of (corpy)Pt(dpm) in $CDCl_3$.



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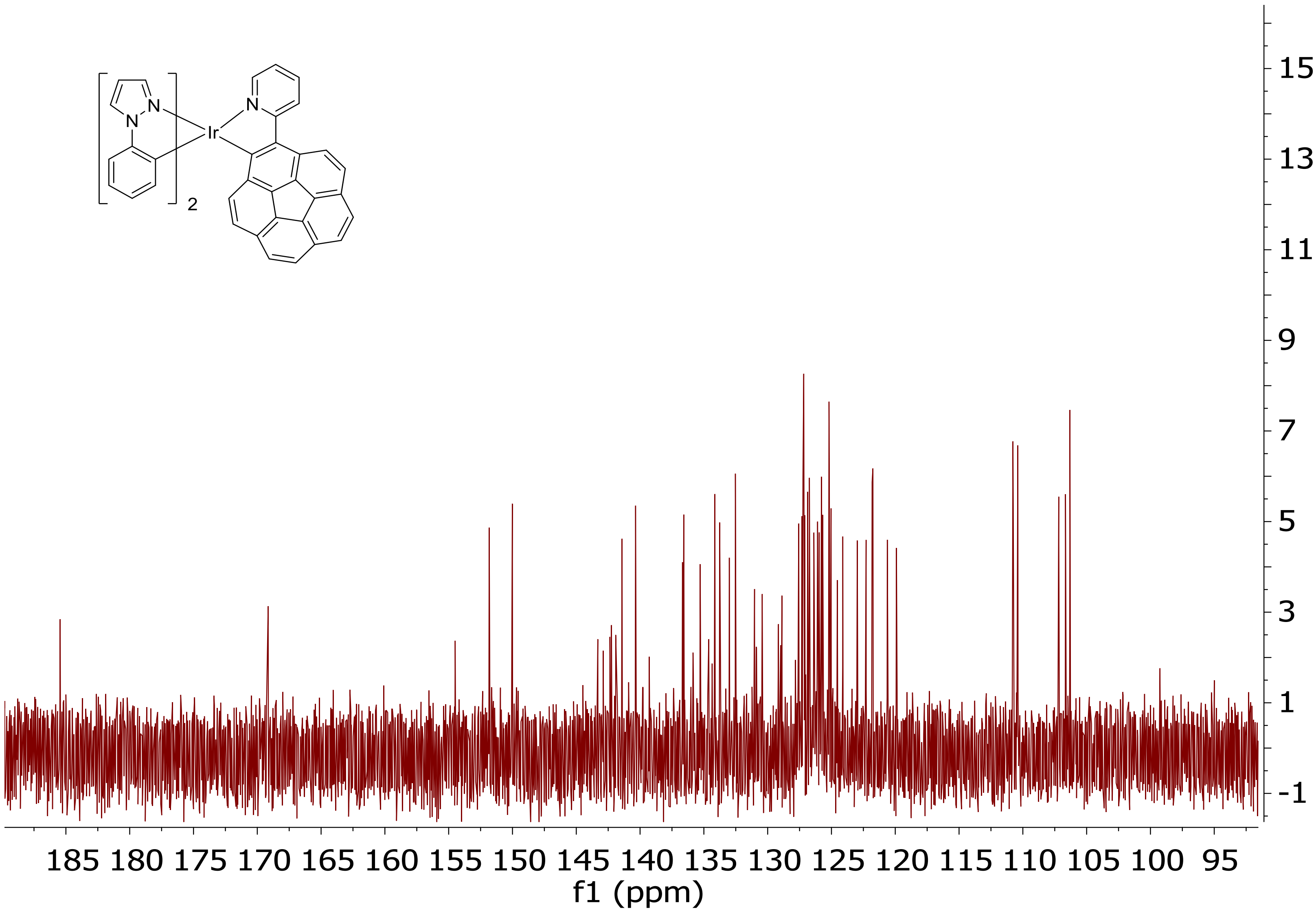

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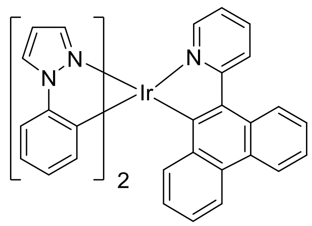
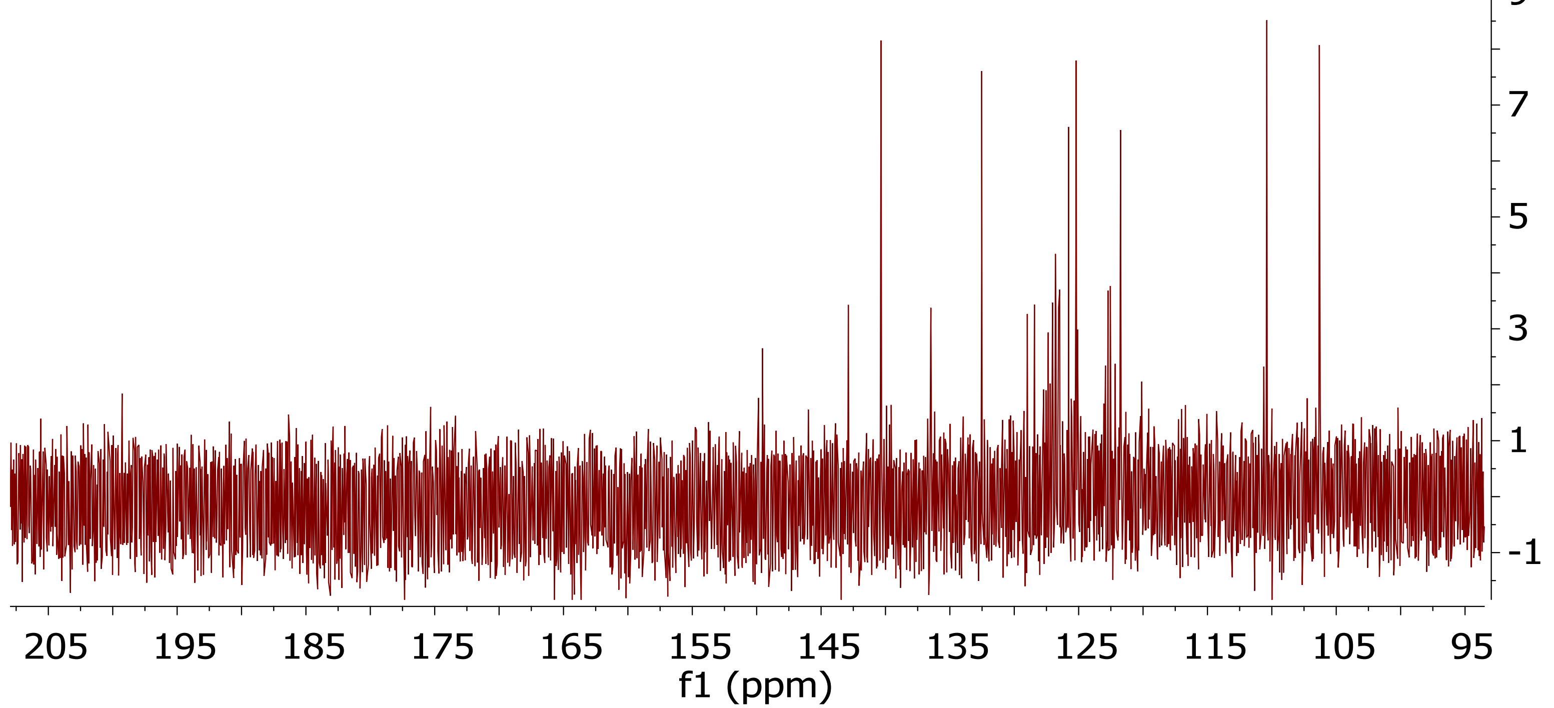
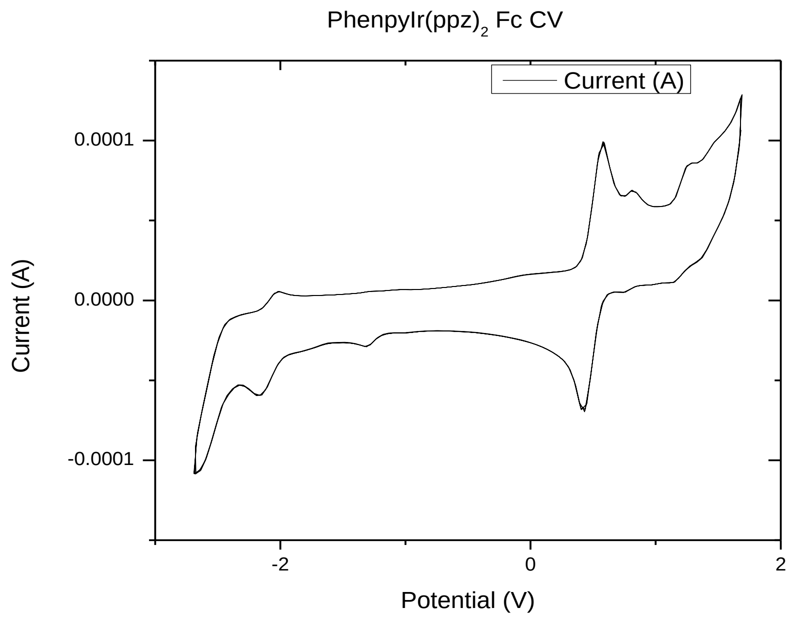




S-14. Cyclic Voltammetry of (phenpy)Ir(ppz)$_2$ vs Fc/Fc$^+$



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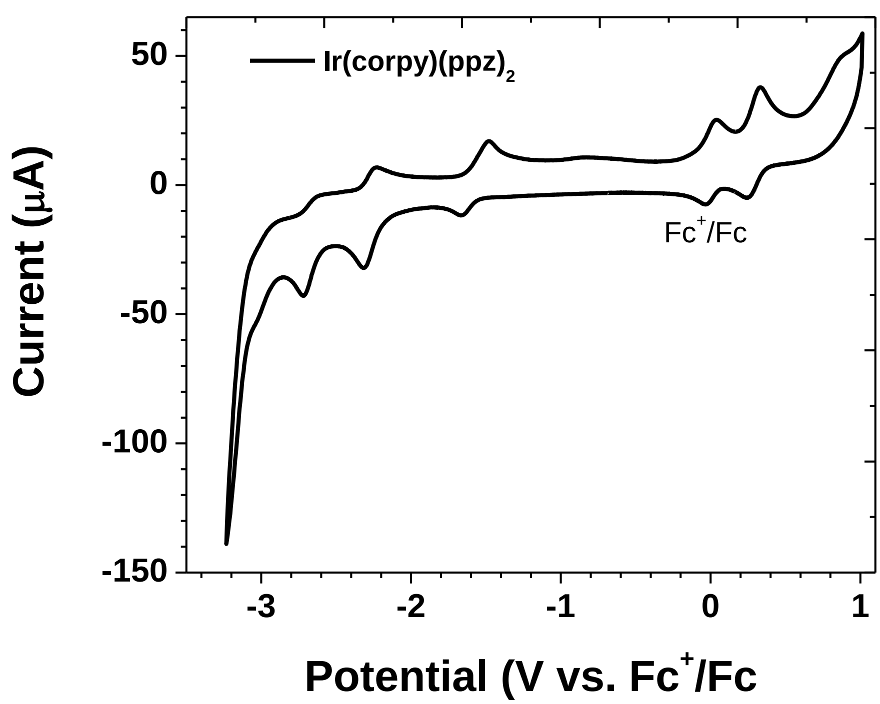

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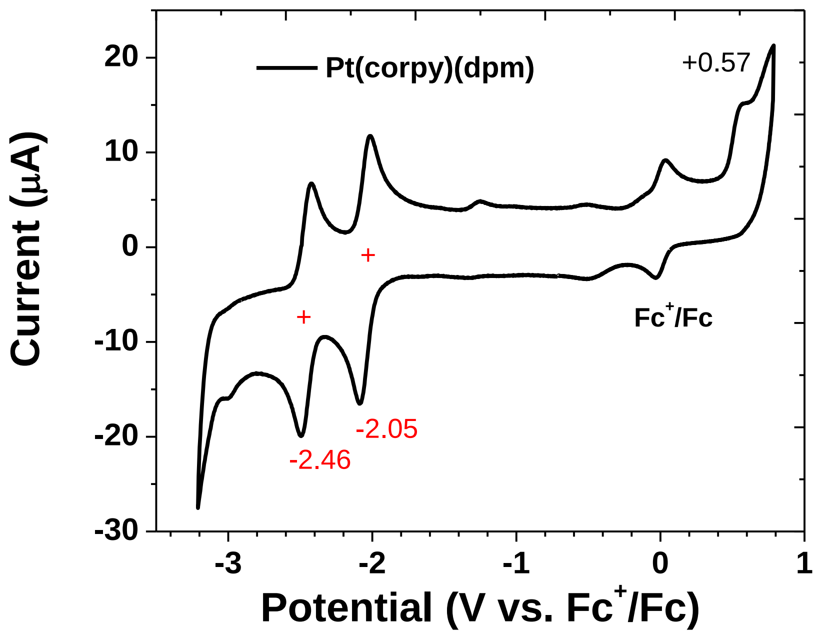

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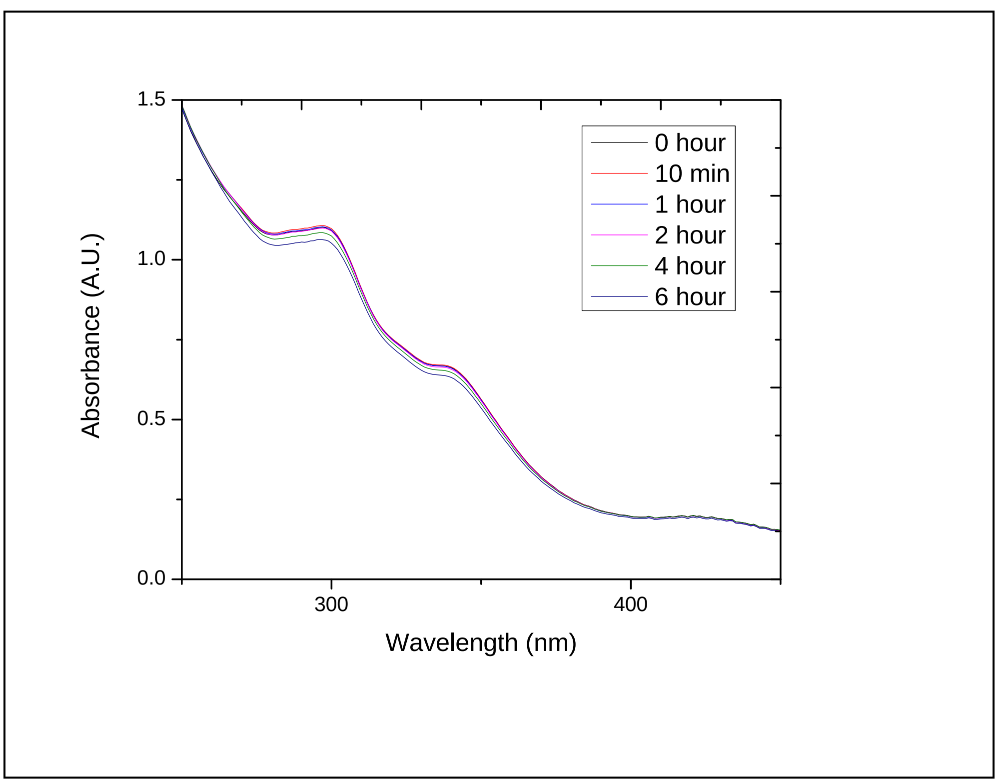

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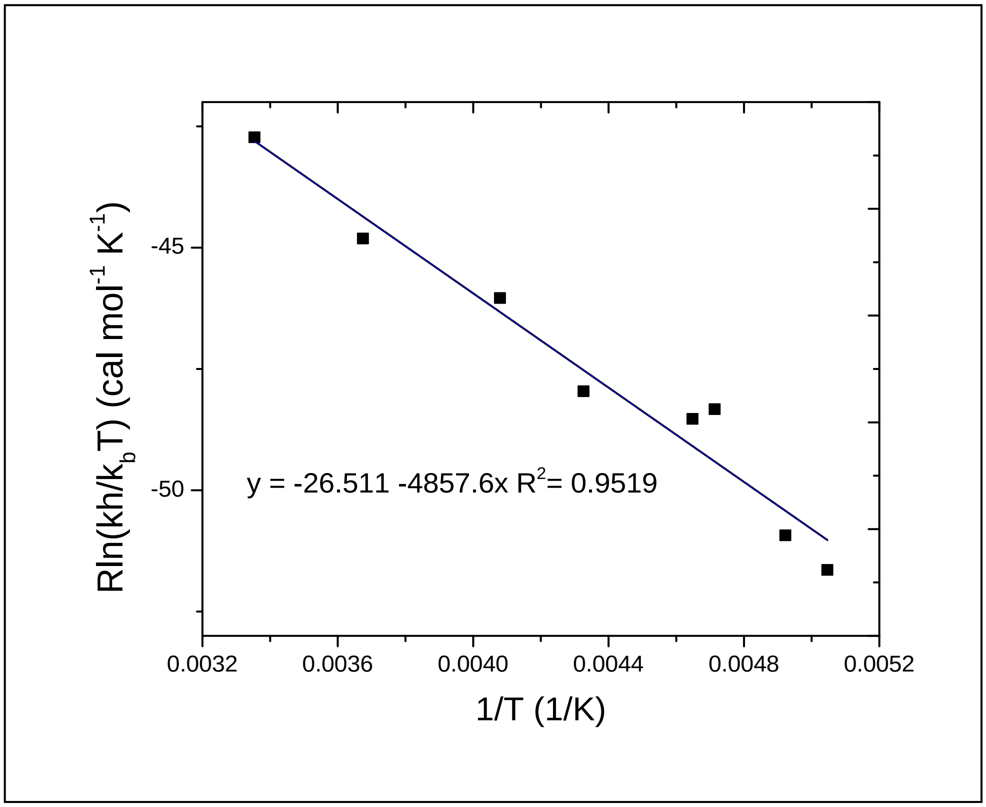

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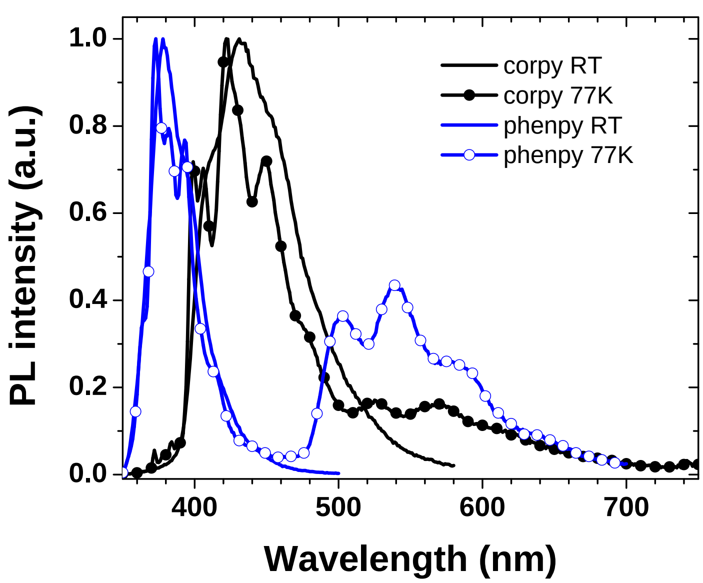

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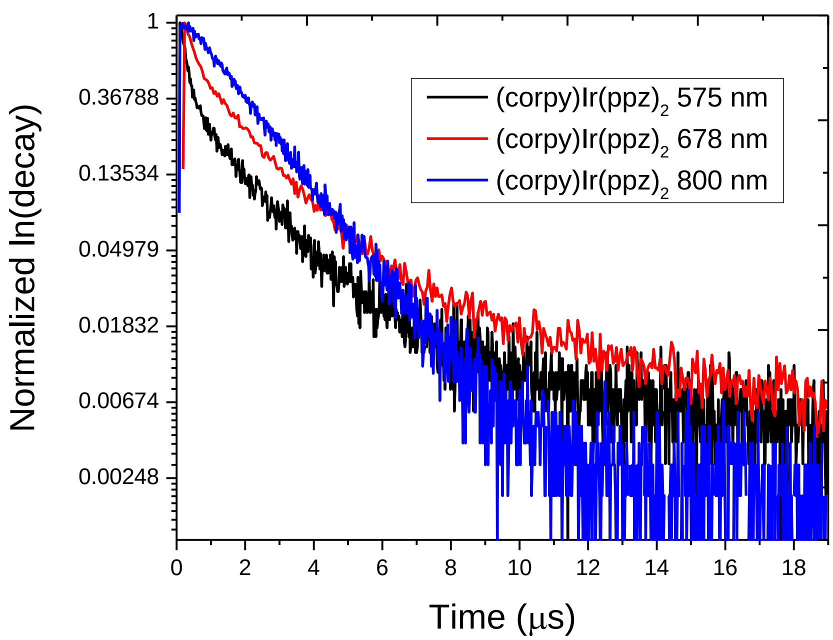
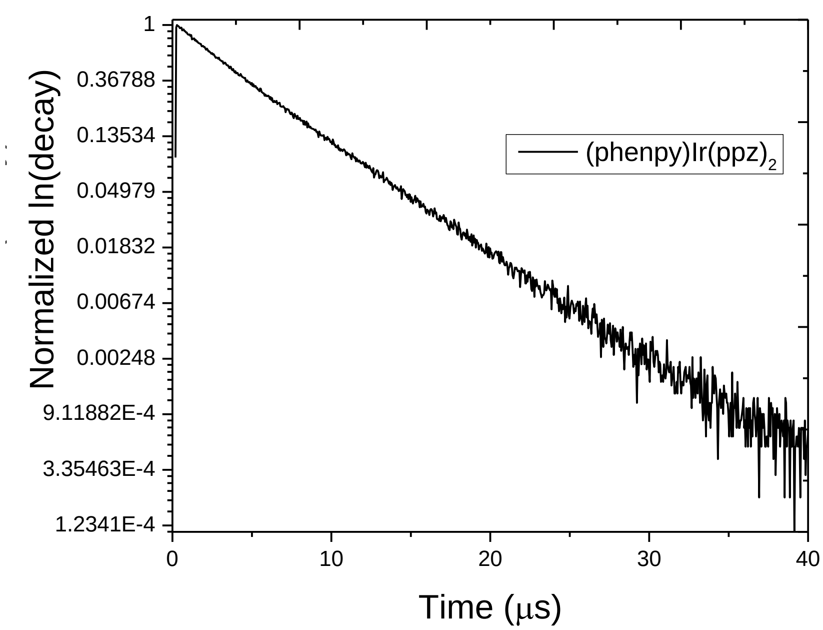


S-21. Emission Decay Spectra of (phenpy)Ir(ppz)$_2$



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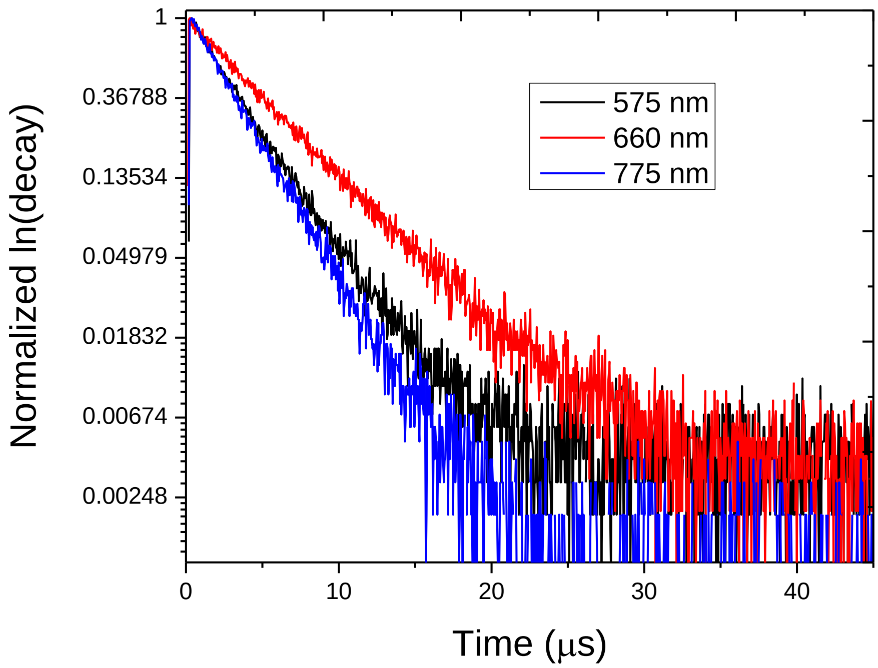


Table S1. Orbital contributions calculated for $S_0 \rightarrow T_1$ transition of (corpy)Pt(dpm).

(λ = 581 nm)				
transition			%	assignment
120	=>	121	88.9	MLCT
120	=>	122	2.8	MLCT
119	=>	121	3.0	LC
119	=>	122	1.9	LC
118	=>	121	3.4	ML'LCT

91.7% MLCT, 4.9% LC, 3.4% ML'LCT

Figure S23. Molecular orbitals for $S_0 \rightarrow T_1$ transition of (corpy)Pt(dpm).

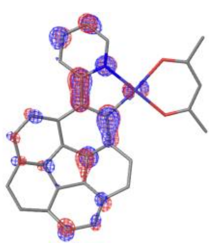
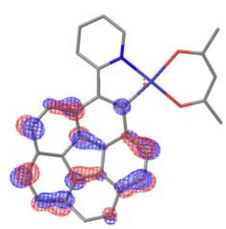
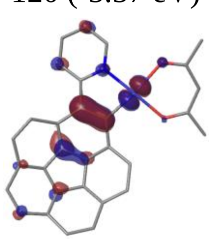
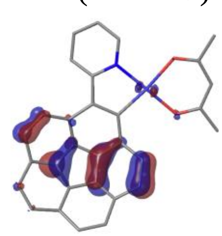
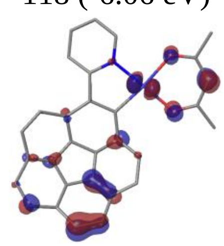
121 (-2.14 eV)	122 (-1.68 eV)	
		
120 (-5.57 eV)	119 (-5.99 eV)	118 (-6.06 eV)
		

Table S2. Orbital contributions calculated for $S_0 \rightarrow T_1$ transition of (corpy)Ir(ppz)$_2$.

(corpy)Ir(ppz)$_2$ Λ-P (λ = 558 nm)					(corpy)Ir(ppz)$_2$ Λ-M (λ = 565 nm)				
transition			%	assignment	transition			%	assignment
168	=>	169	11.4	L'LCT	168	=>	169	4.5	L'LCT
168	=>	170	1.2	L'LCT	167	=>	169	77.7	MLCT
167	=>	169	67.4	MLCT	167	=>	170	7.4	MLCT
167	=>	170	6.6	MLCT	166	=>	169	3.4	L'LCT
166	=>	169	7.4	L'LCT	165	=>	169	2.1	MLCT + LC
165	=>	170	1.3	MLCT + LC	165	=>	170	1.3	MLCT + LC
164	=>	169	4.7	MLCT +LC	163	=>	169	3.5	MLCT + LC
80.0% MLCT, 20.0% L'LCT					91.1% MLCT, 8.9% LLCT				

Figure S24. Molecular orbitals for $S_0 \rightarrow T_1$ transition of (corpy)Ir(ppz)$_2$ Λ-P.

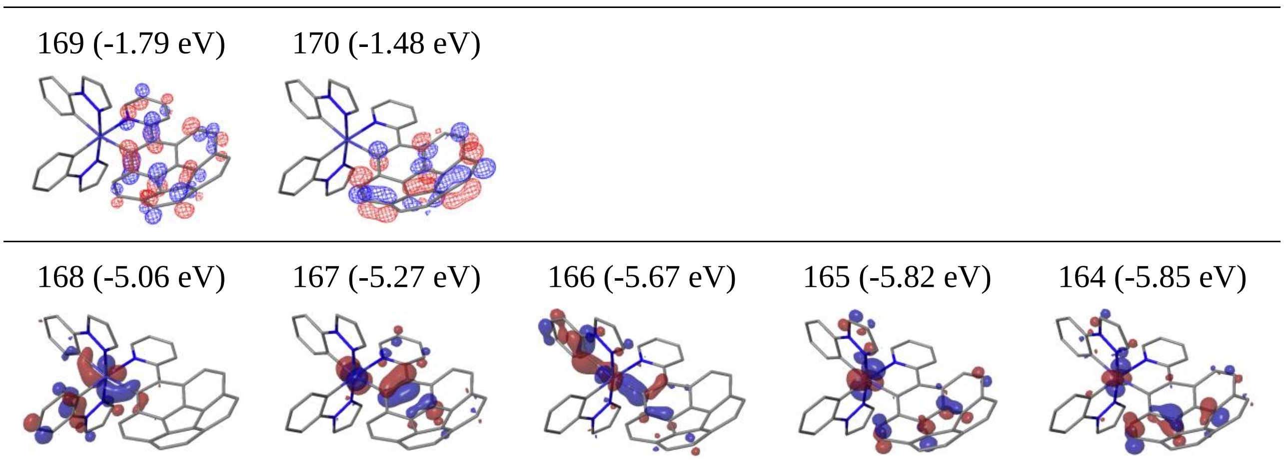


Figure S25. Molecular orbitals for $S_0 \rightarrow T_1$ transition of (corpy)Ir(ppz)$_2$ Λ-M.

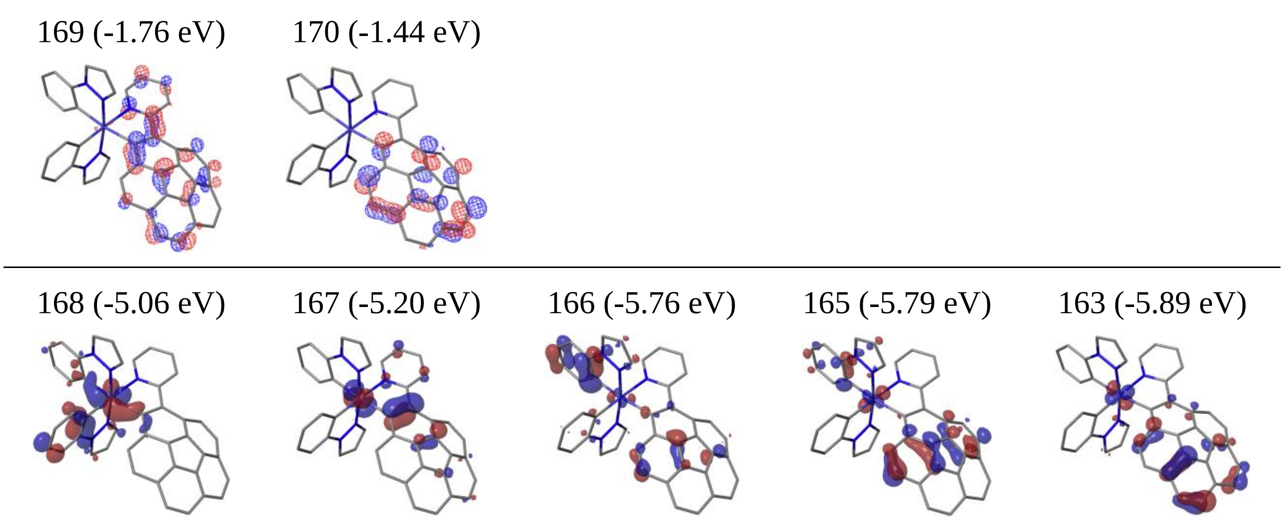


Table S3. Orbital contributions calculated for $S_0 \rightarrow T_1$ transition of (phenpy)Ir(ppz)$_2$.

(phenpy)Ir(ppz)$_2$ Λ-P (λ = 546 nm)					(phenpy)Ir(ppz)$_2$ Λ-M (λ = 565 nm)				
transition			%	assignment	transition			%	assignment
150	=>	151	25.0	L'LCT	150	=>	151	76.5	MLCT
149	=>	151	69.2	MLCT	150	=>	154	2.1	MLCT
149	=>	154	1.7	MLCT	149	=>	151	18.8	L'LCT
148	=>	151	1.9	L'LCT	148	=>	151	2.5	L'LCT
146	=>	151	2.1	L'LCT					
70.9% MLCT, 29.1% L'LCT					78.6% MLCT, 21.4% L'LCT				

Figure S26. Molecular orbitals for $S_0 \rightarrow T_1$ transition of (phenpy)Ir(ppz)$_2$ Λ-P.

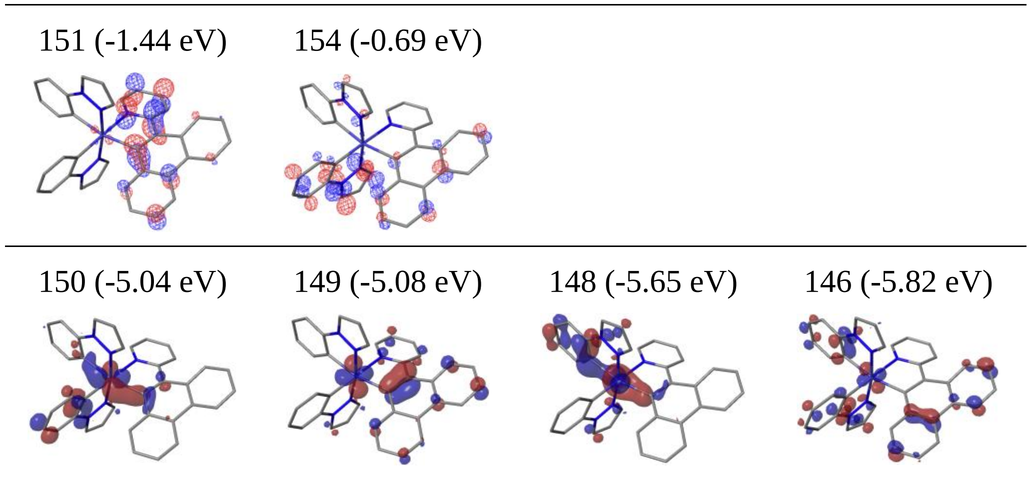


Figure S27. Molecular orbitals for $S_0 \rightarrow T_1$ transition of (phenpy)Ir(ppz)$_2$ Λ-M.