ELECTRONIC SUPPLEMENTARY INFORMATION

Selective synthesis, reactivity and luminescence of unsymmetrical bis-cyclometalated Pt(IV) complexes

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1. NMR spectra of new compounds

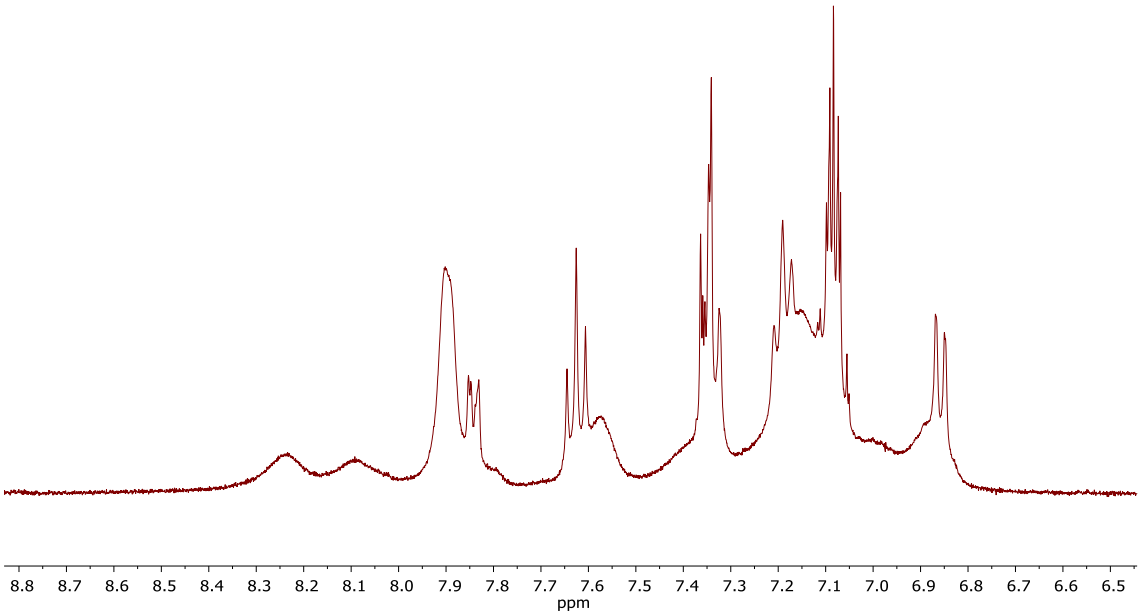


Figure S1. ^{1}H NMR spectrum of complex **2af** (aromatic region, CD_2Cl_2, 400 MHz).

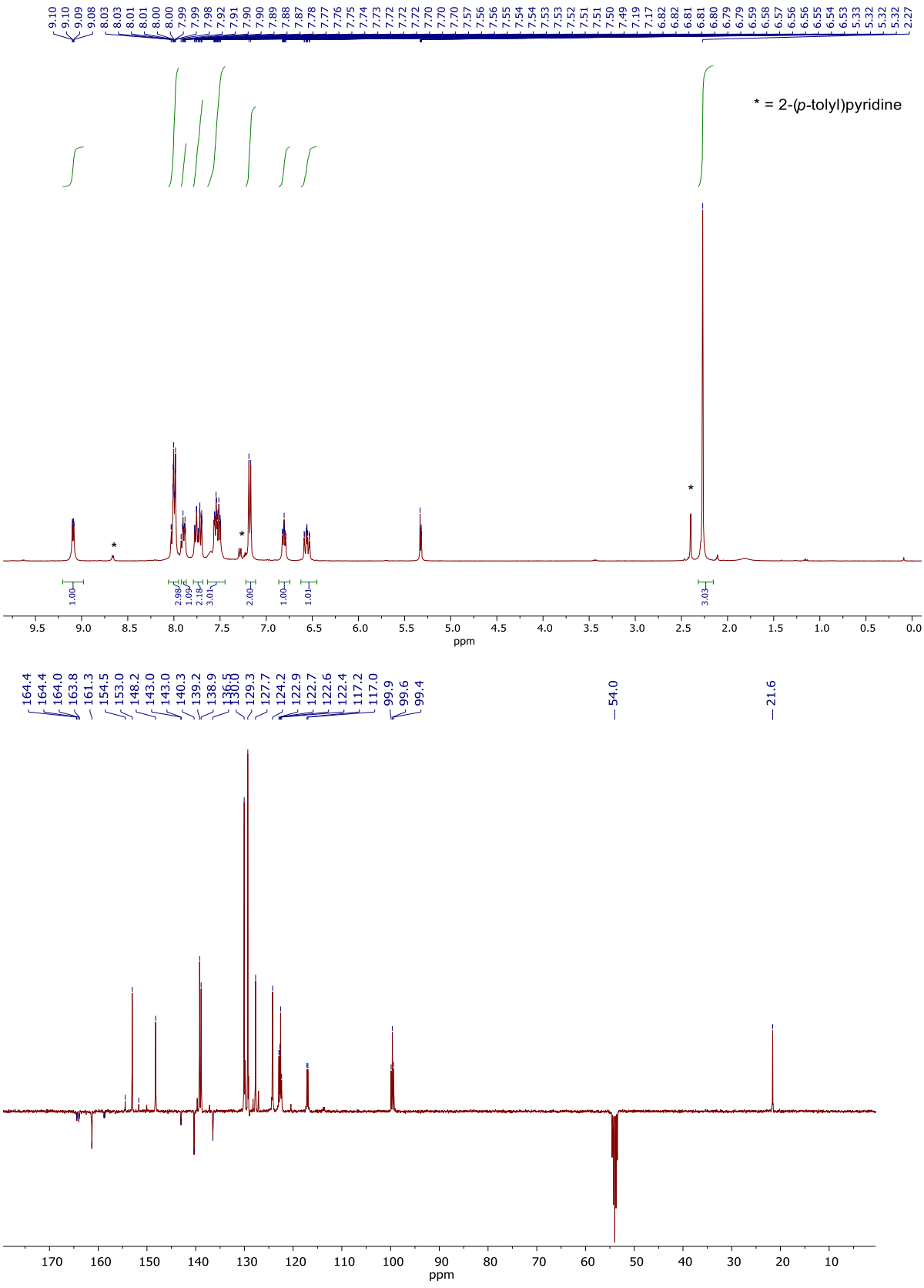


Figure S2. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2cd** (CD_2Cl_2, 400 and 100 MHz, respectively)

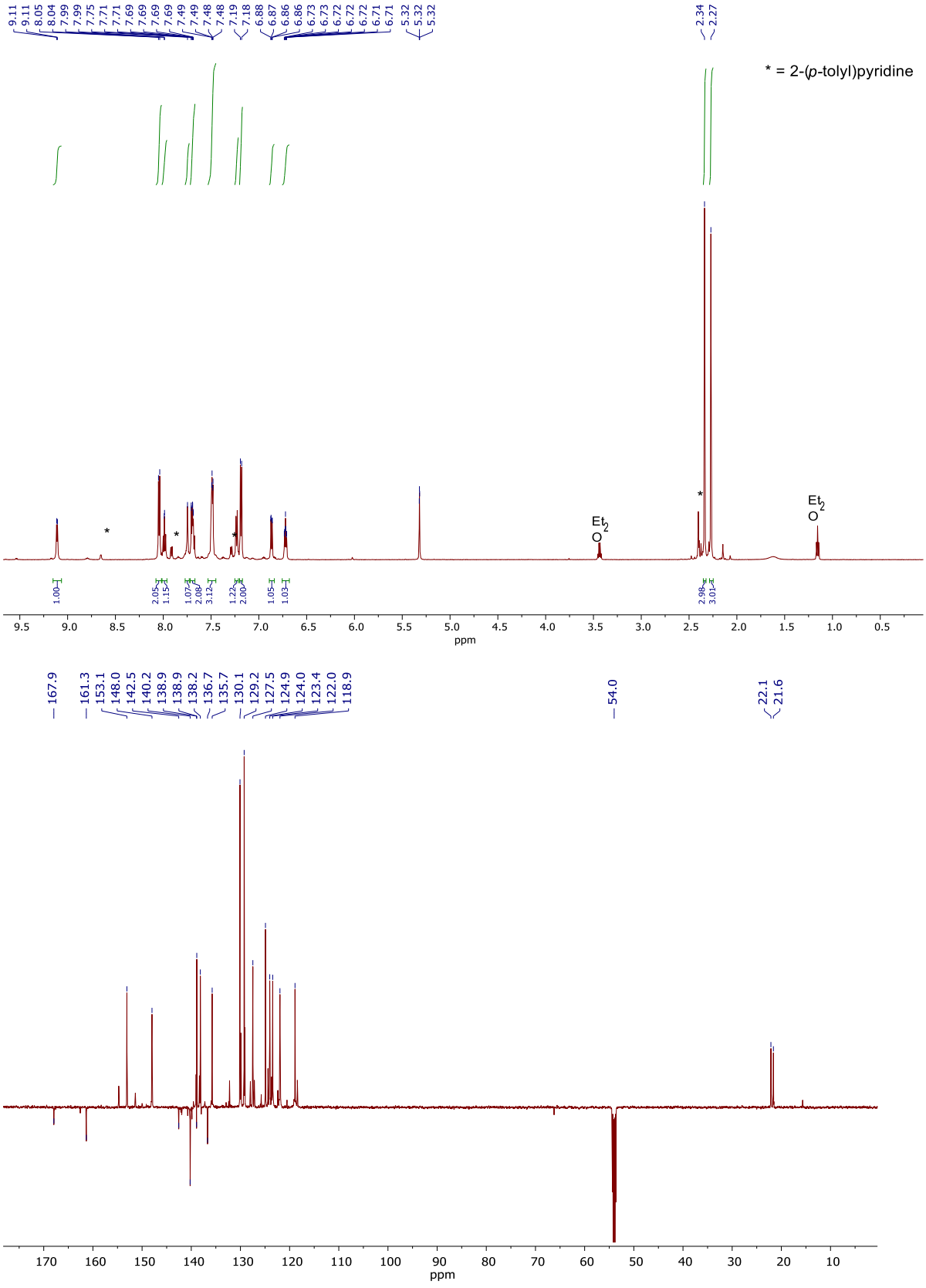


Figure S3. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2dd** (CD_2Cl_2, 600 and 151 MHz, respectively)

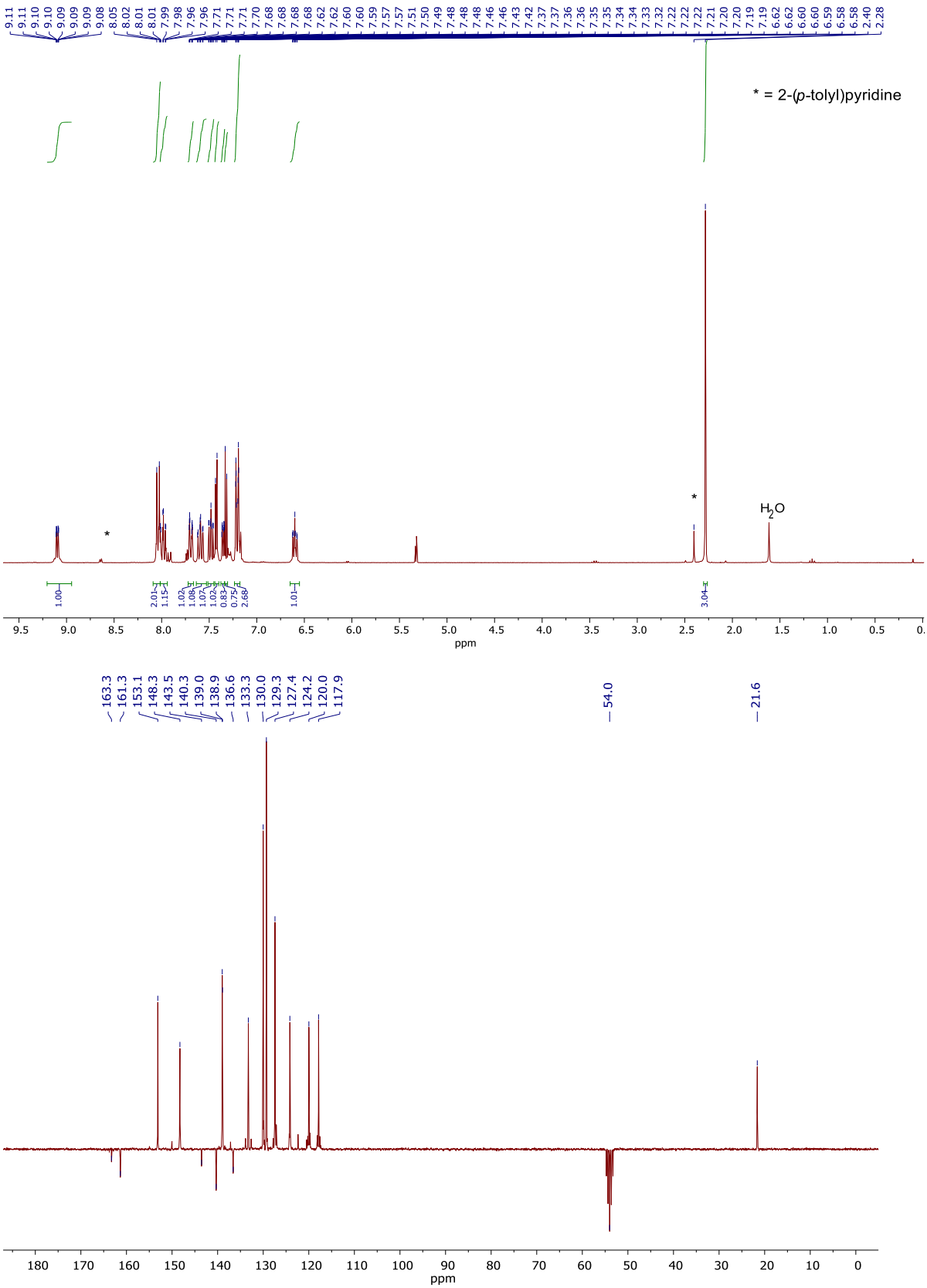


Figure S4. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2ed** (CD_2Cl_2, 300 and 75 MHz, respectively)

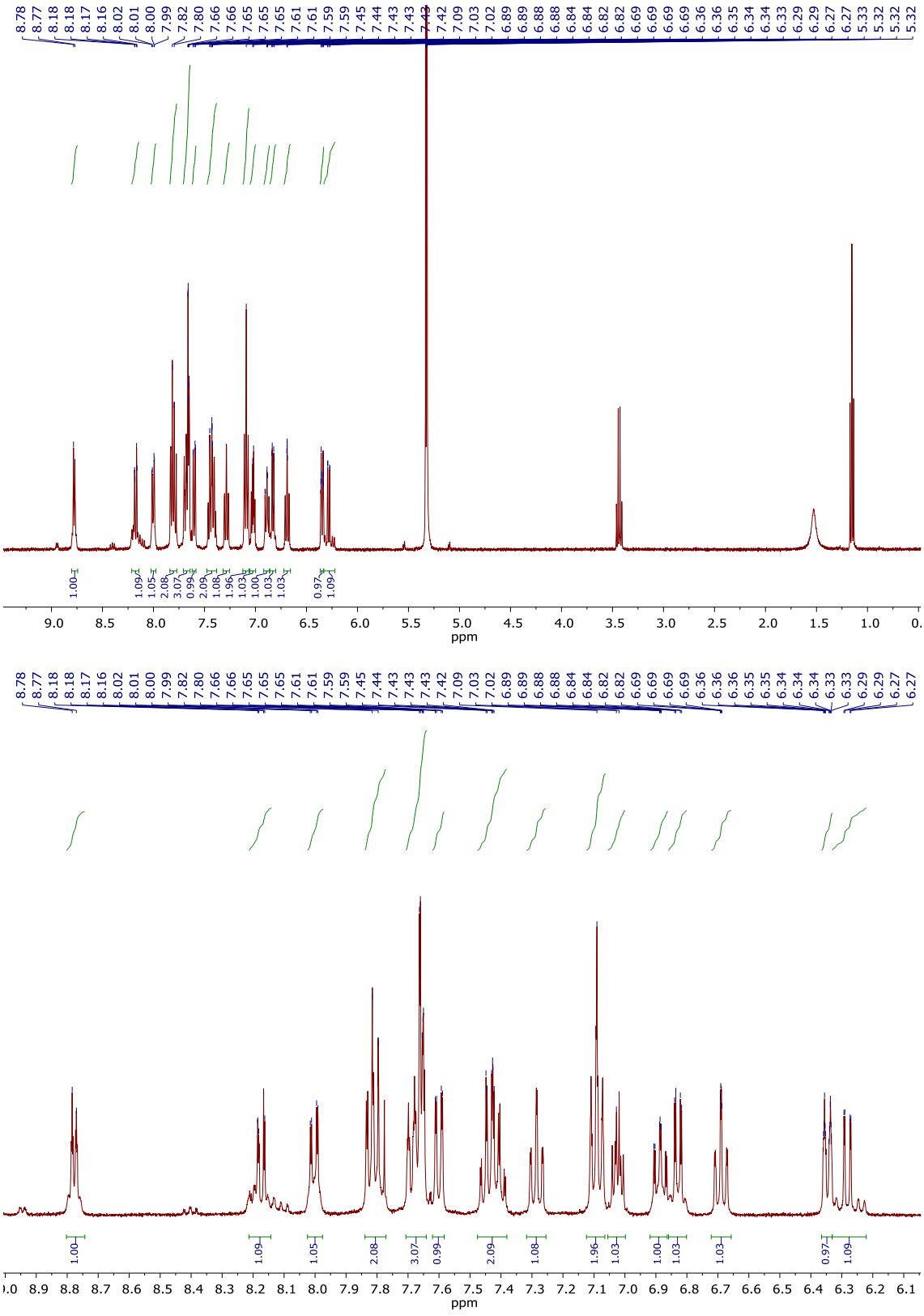


Figure S5. ^{1}H NMR spectrum of complex **3af** (CD_2Cl_2, 400 MHz). Top: complete spectrum. Bottom: aromatic region.

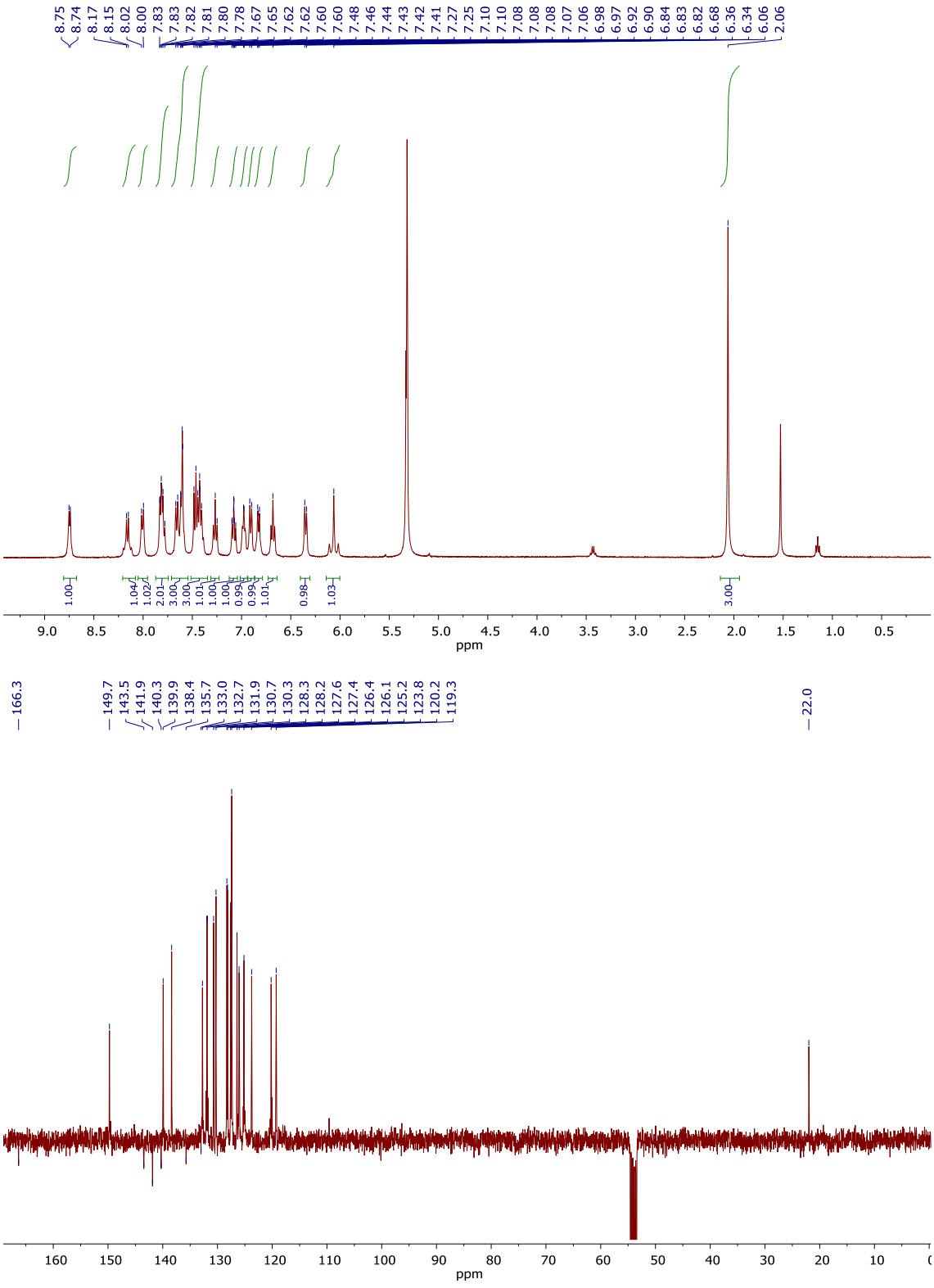


Figure S6. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3ad** (CD_2Cl_2, 400 and 100 MHz, respectively)

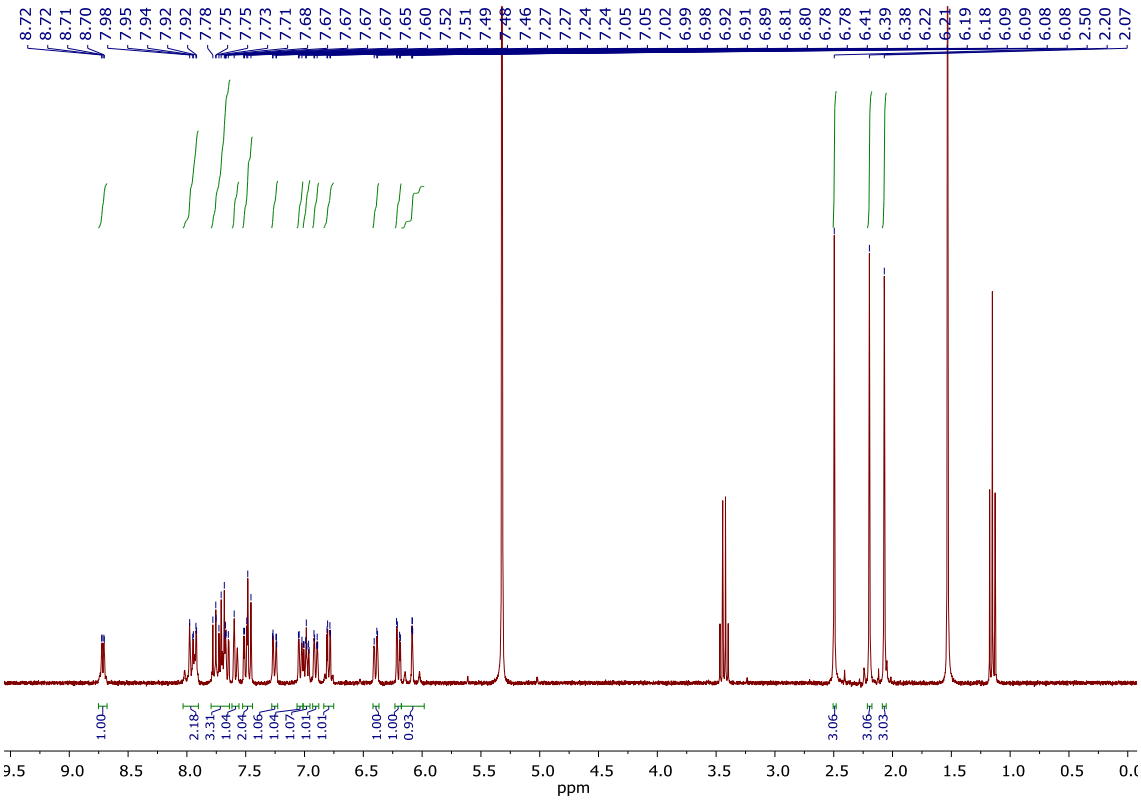


Figure S7. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3bd** (CD_2Cl_2, 300 MHz)

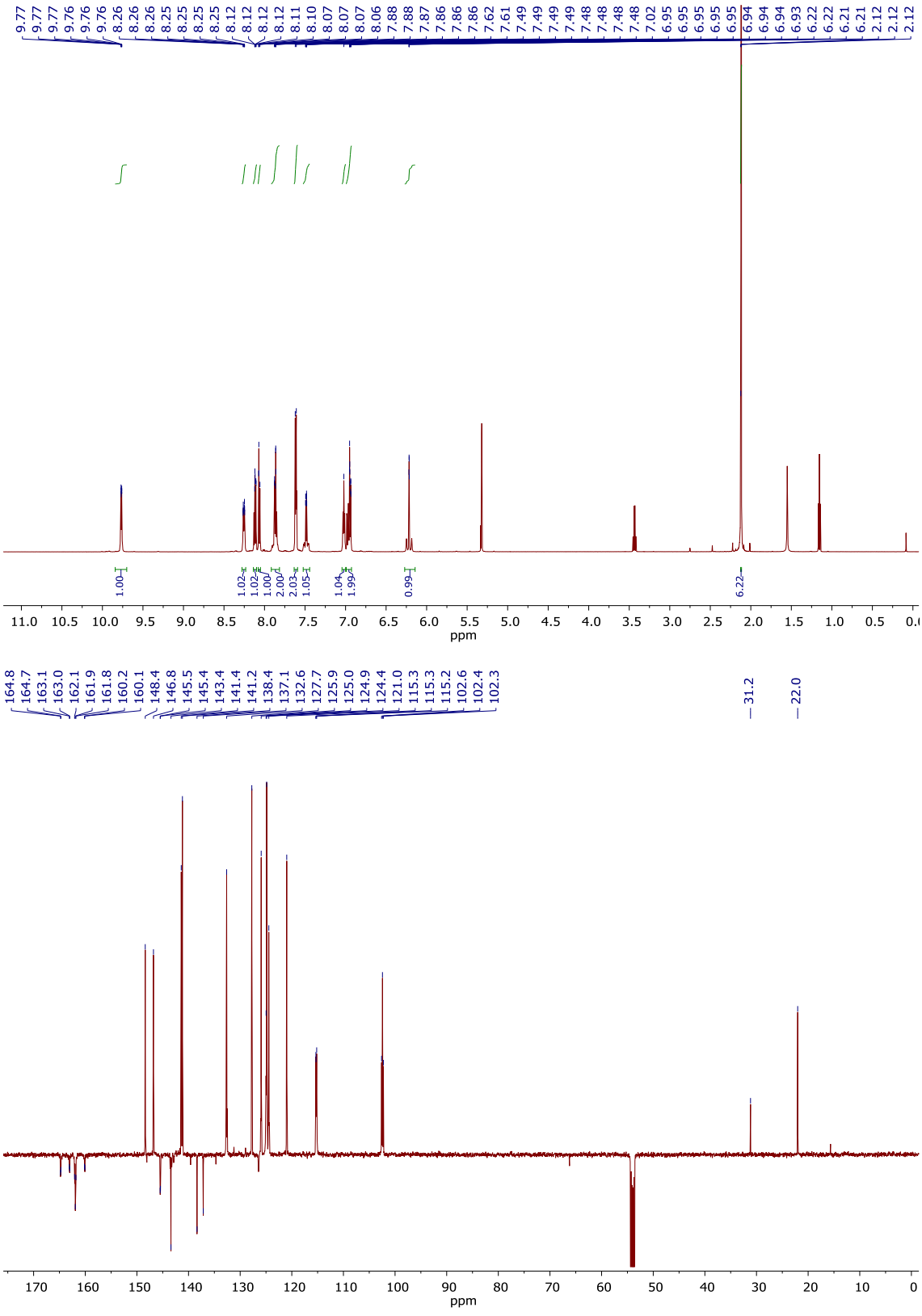


Figure S8. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3cd** (CD_2Cl_2, 600 and 151 MHz, respectively)

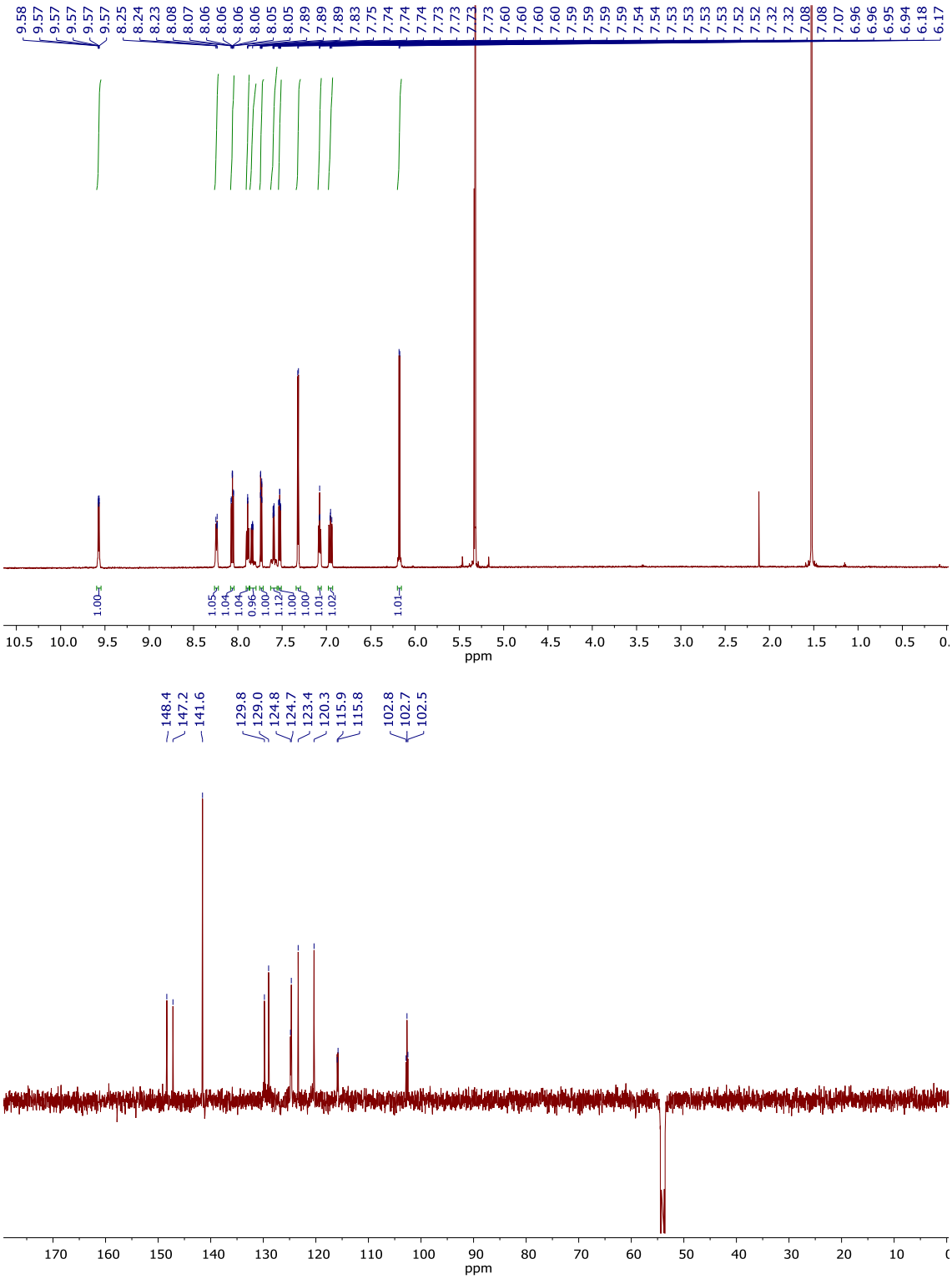


Figure S9. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3ce** (CD_2Cl_2, 400 and 100 MHz, respectively)

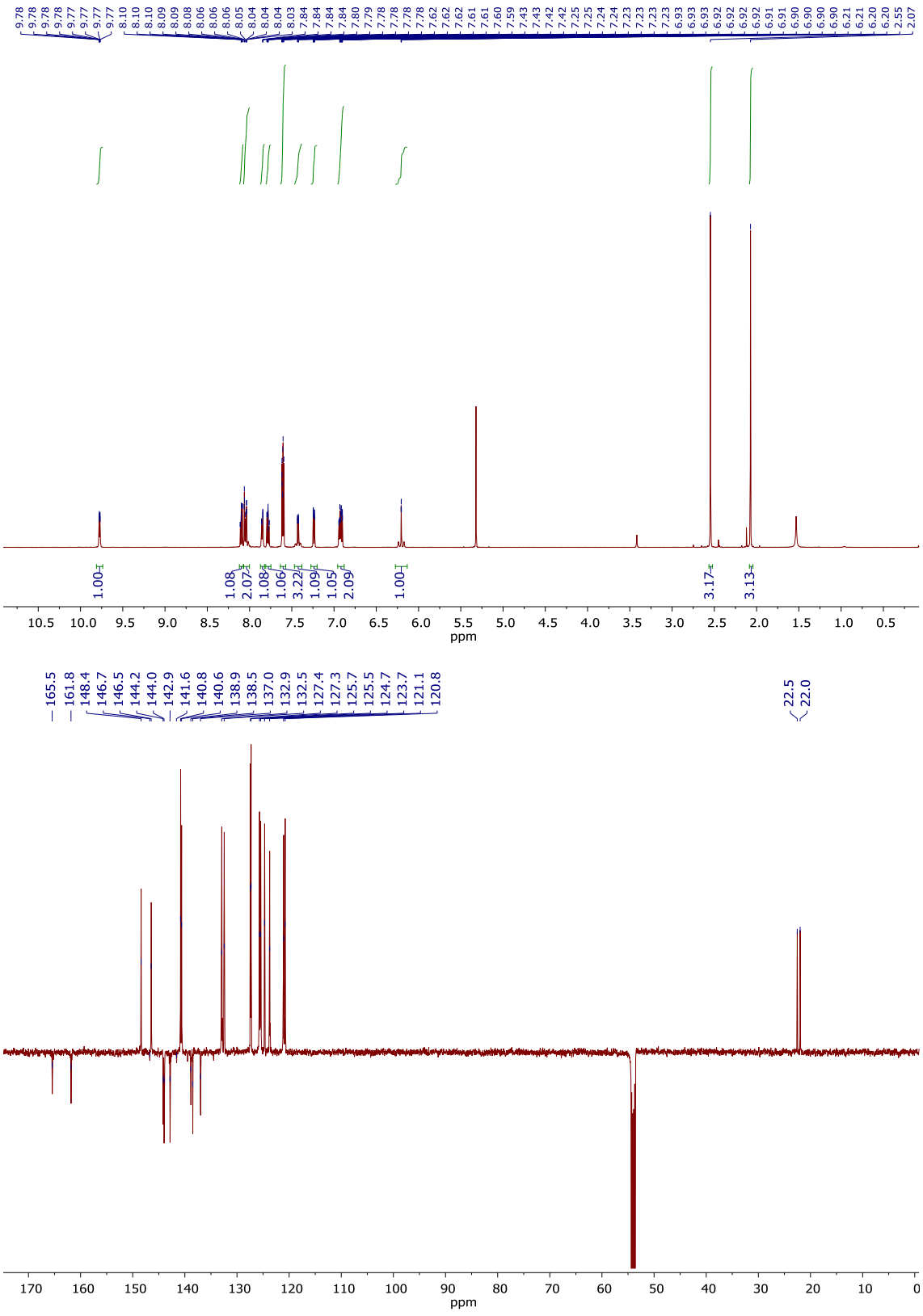


Figure S10. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3dd** (CD_2Cl_2, 600 and 151 MHz, respectively)

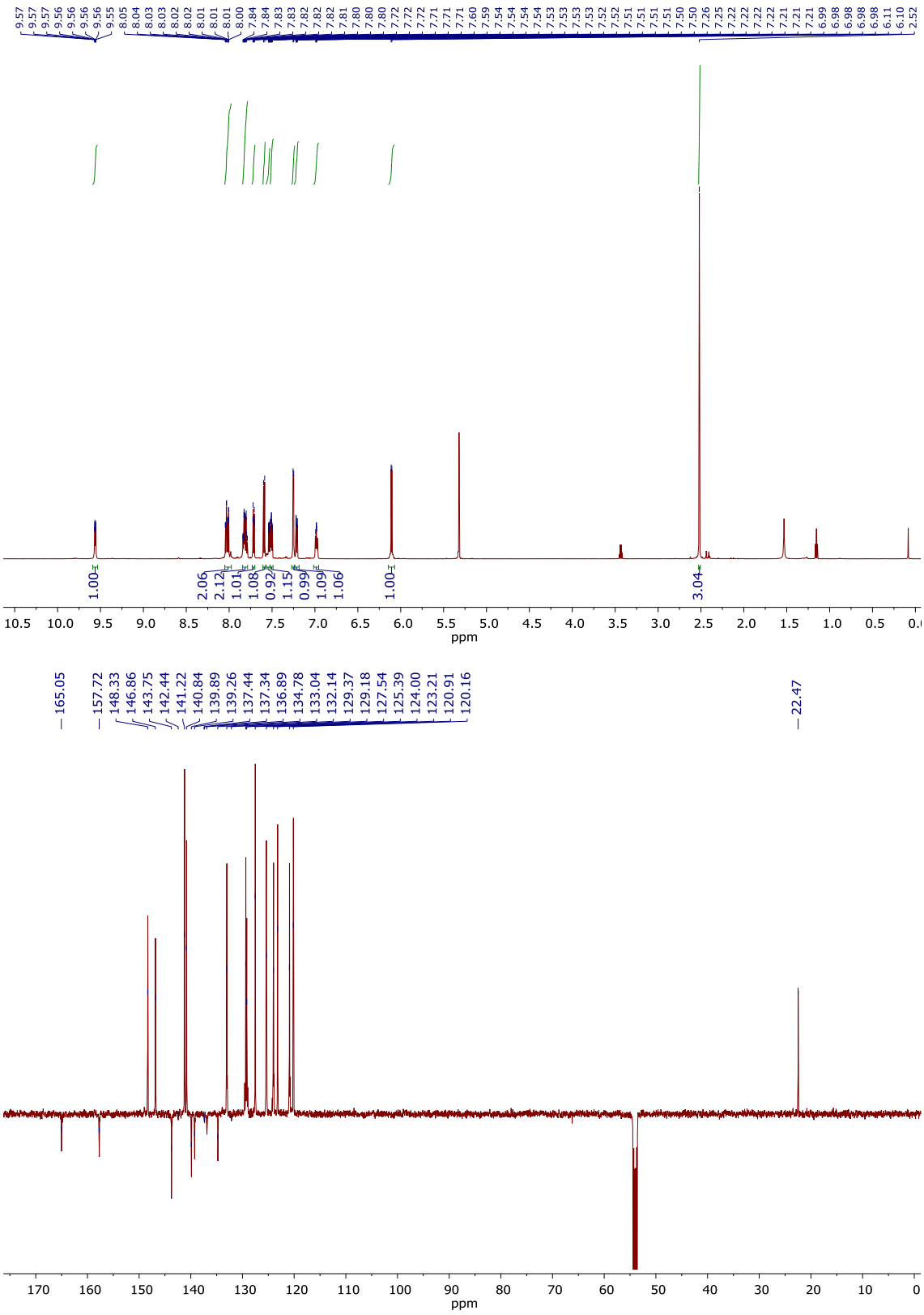


Figure S11. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3de** (CD_2Cl_2, 600 and 151 MHz, respectively)

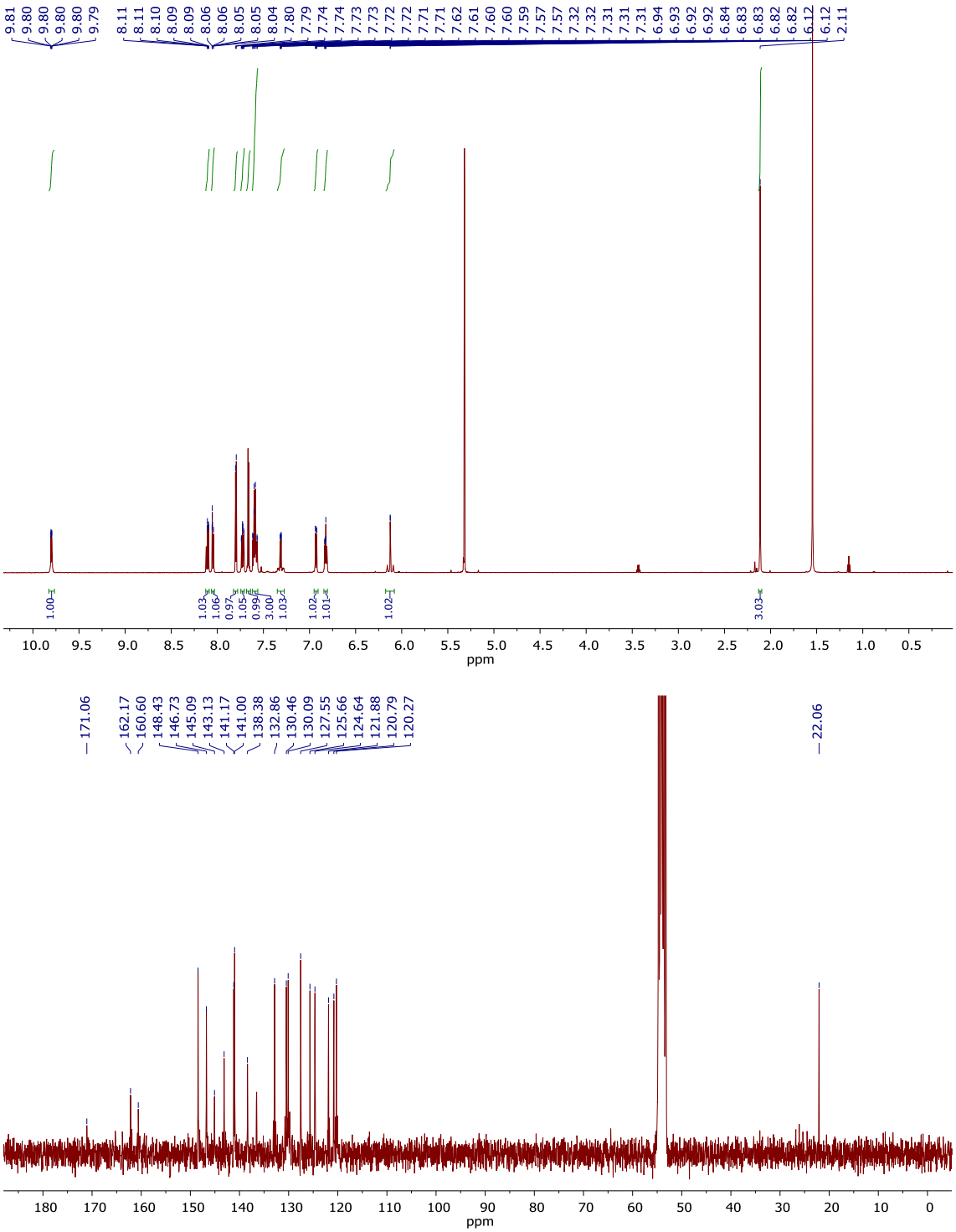


Figure S12. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3ed** (CD_2Cl_2, 600 and 75 MHz, respectively)

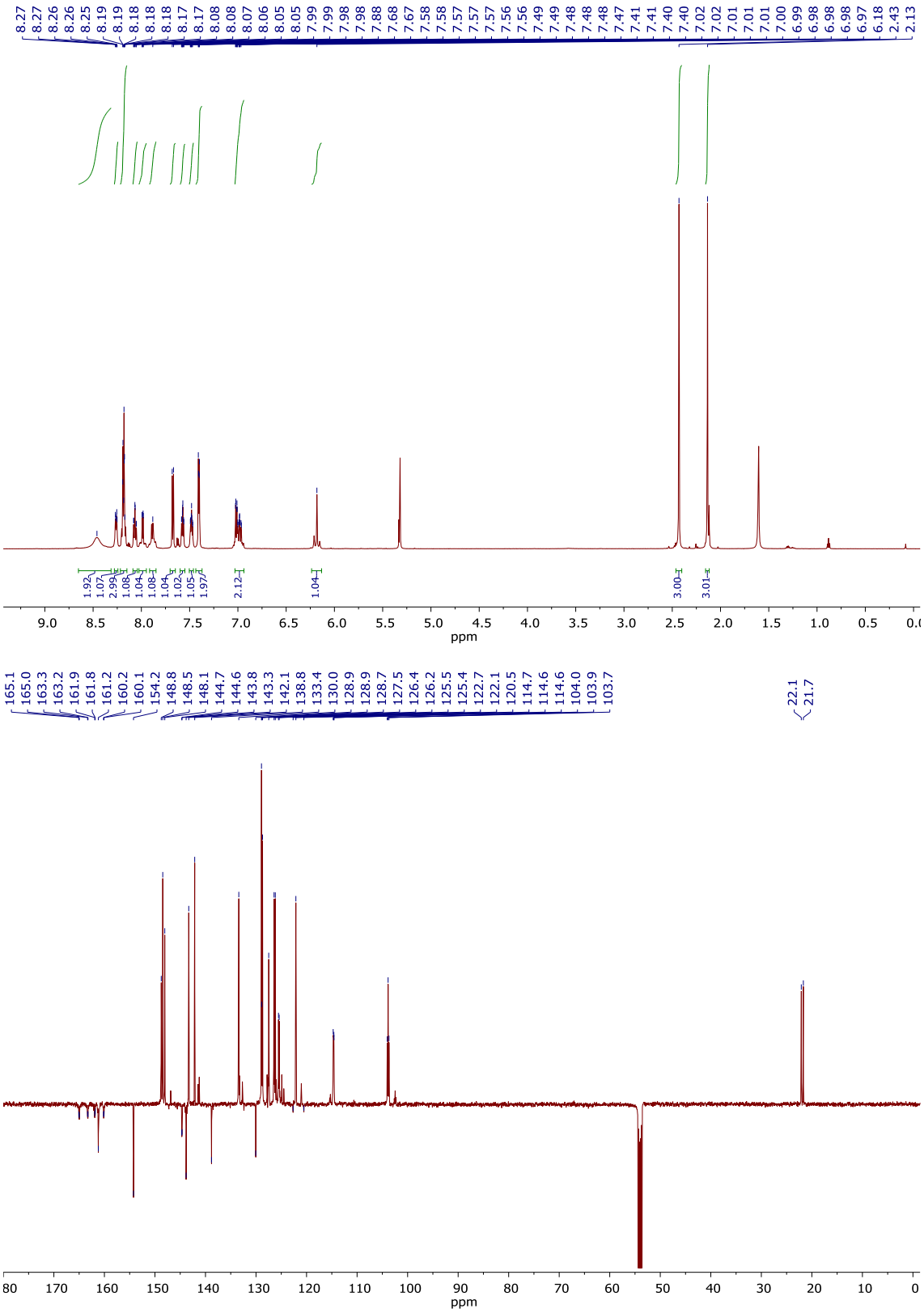


Figure S13. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **4** (CD_2Cl_2, 600 and 151 MHz, respectively)

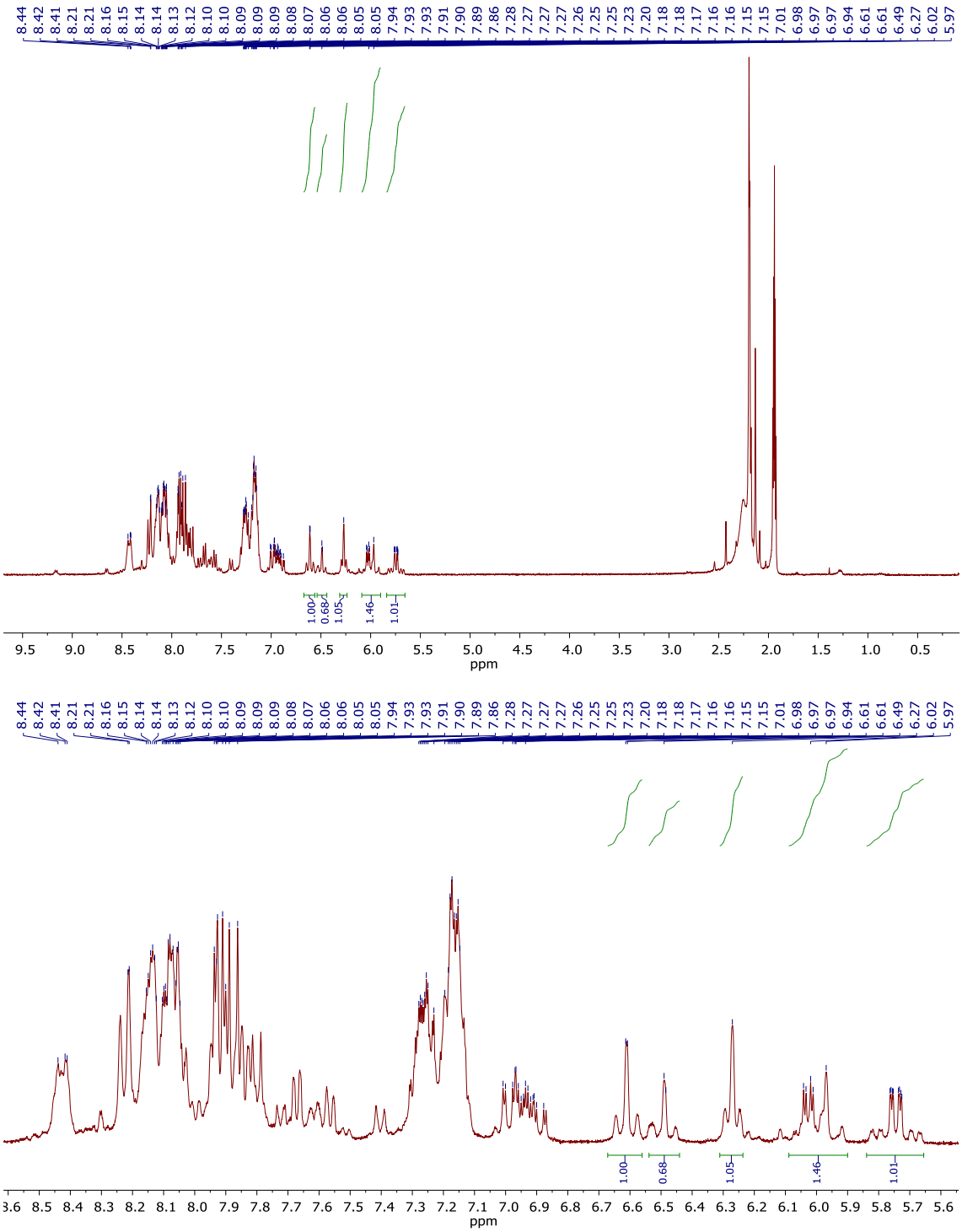


Figure S14. ^{1}H NMR spectrum of complex *mer*-**5cd** (mixture of *mer* isomers) (CD_3CN, 300 MHz). Top: Complete spectrum. Bottom: Aromatic region.

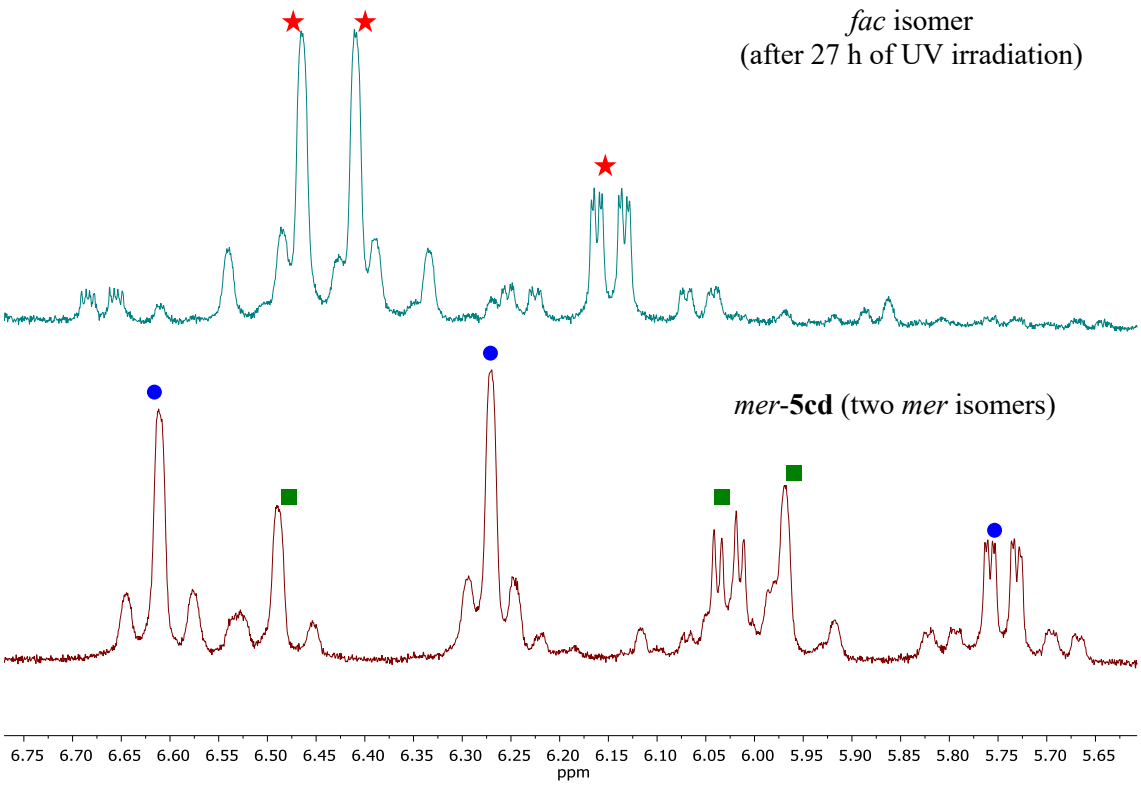


Figure S15. Bottom: Detail of the aromatic region of the ^{1}H NMR spectrum of *mer*-**5cd** (CD_3CN, 300 MHz). The six identifiable signals correspond the protons ortho to the metalated carbon atoms, which are shielded by the ring current of orthogonal aromatic rings. Two sets of three signals can be observed in a 1:0.7 ratio, corresponding to two of the four possible *mer* isomers. **Top:** ^{1}H NMR spectrum of the same sample after irradiation with UV light for 27 h. A new set of three resonances arises, which can be assigned to the *fac* isomer.

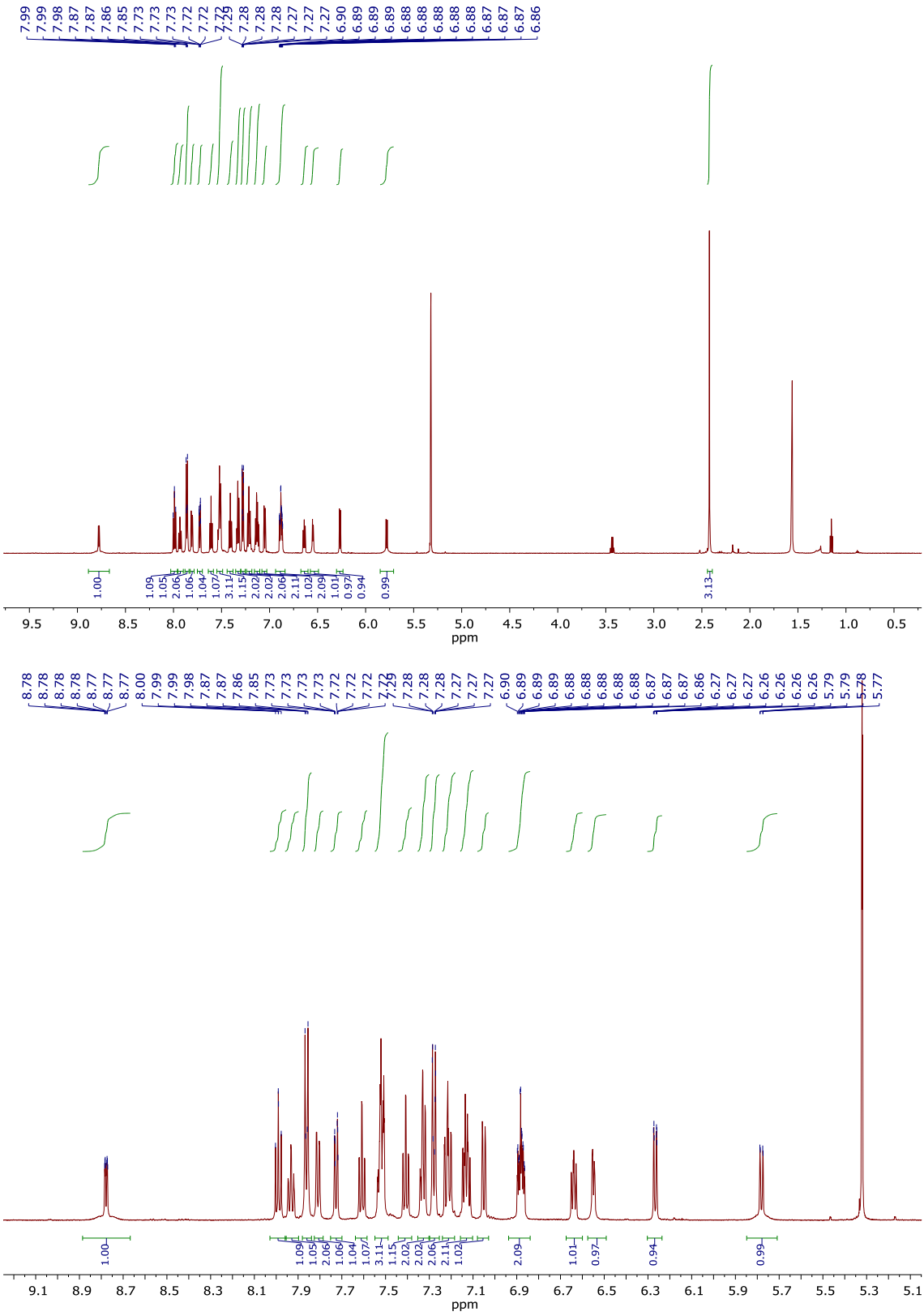


Figure S16. ^{1}H NMR spectrum of complex **6** (CD_2Cl_2, 600 MHz). Top: Complete spectrum. Bottom: Aromatic region.

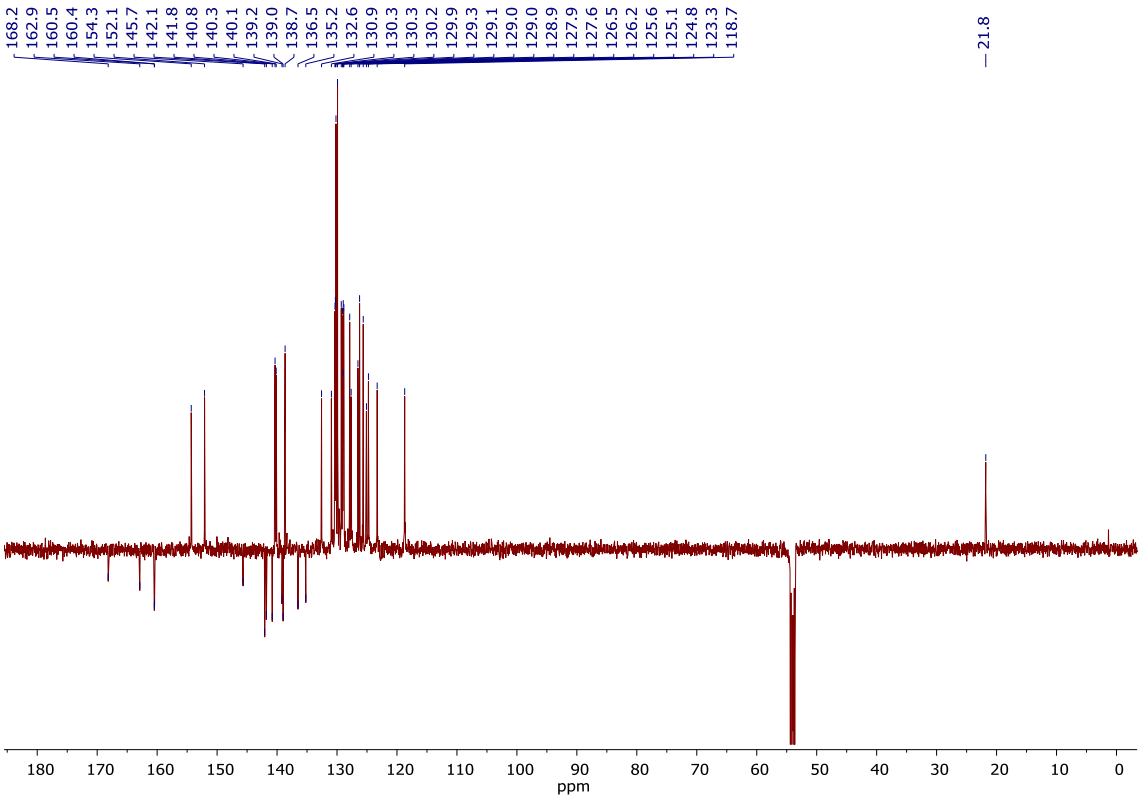


Figure S17. $^{13}C\{^{1}H\}$ APT NMR spectrum of complex **6** (CD_2Cl_2, 151 MHz).

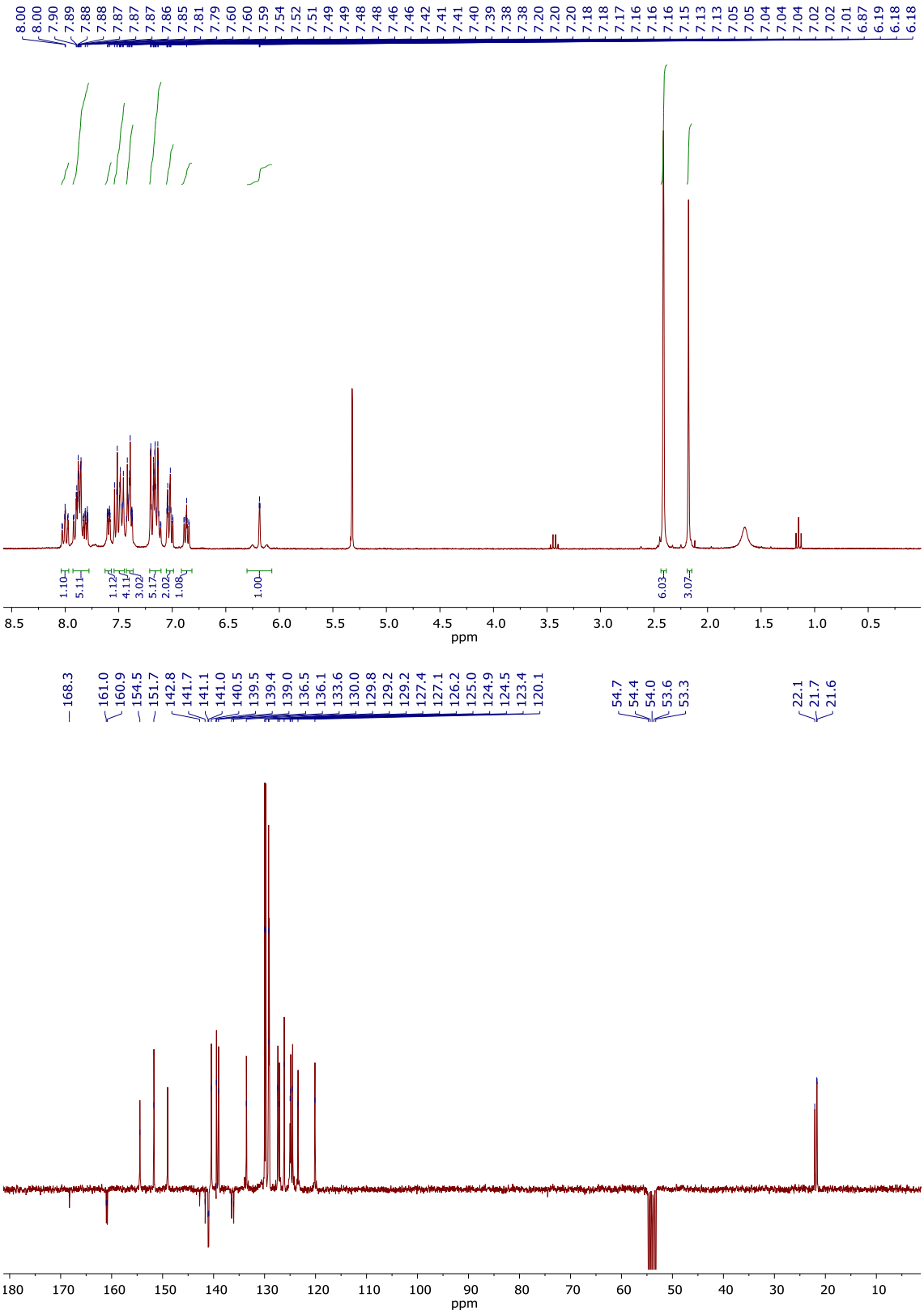


Figure S18. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **7** (CD_2Cl_2, 300 and 75 MHz respectively).

2. Excitation and emission spectra at 77 K

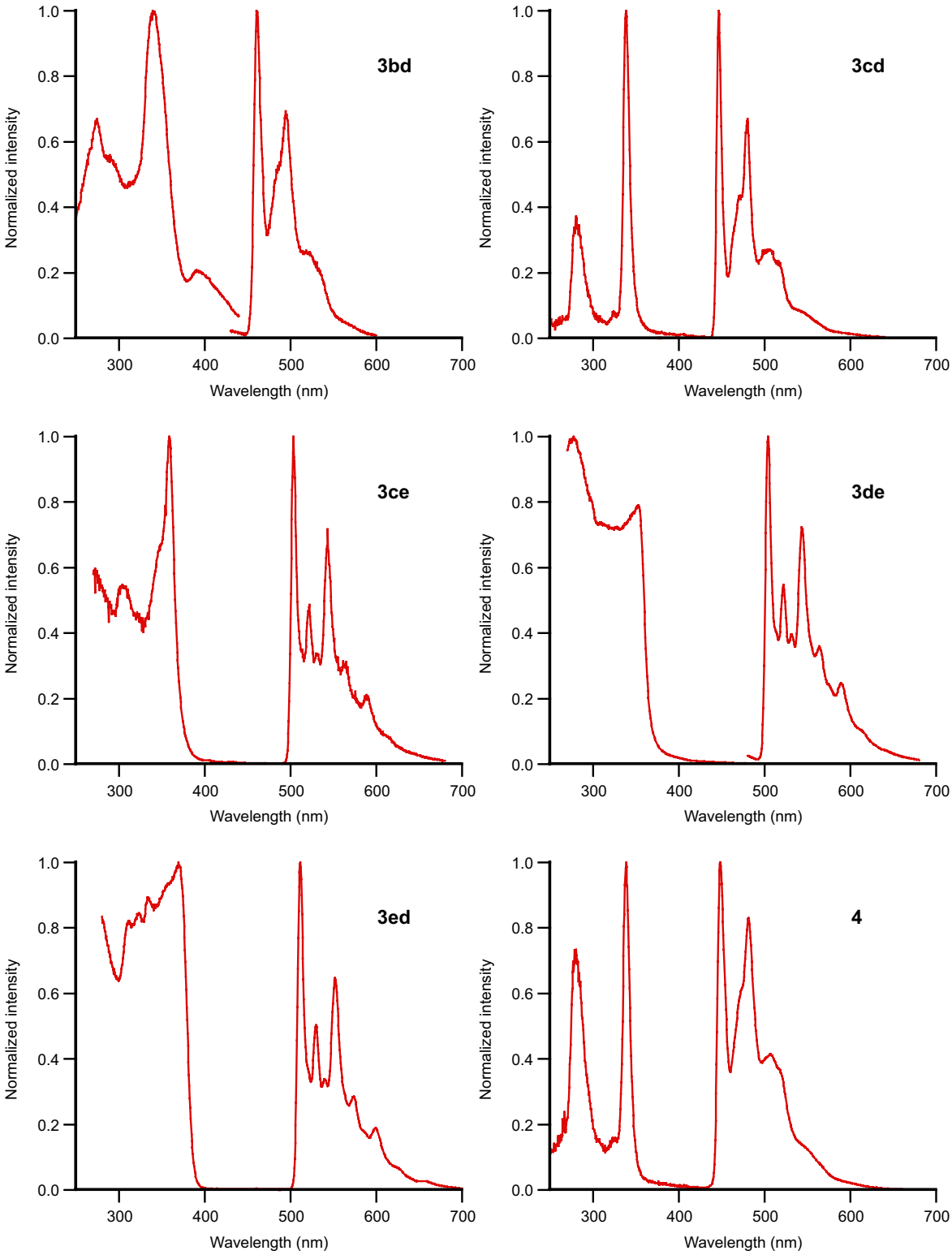


Figure S19. Excitation (left) and emission (right) spectra of complexes **3bd**, **3cd**, **3ce**, **3de**, **3ed** and **4** in PrCN glass at 77 K.

3. Crystallographic data

Table S1. Crystallographic data for **2af**, **2ed**, **3af** and **3bd**.

	2af	**2ed**	**3af**	**3bd**
formula	$C_{28}H_{21}ClN_2Pt$	$C_{21}H_{17}ClN_2PtS$	$C_{28}H_{20}Cl_2N_2Pt$	$C_{31}H_{26}Cl_2N_2Pt$
fw	616.01	559.97	650.45	692.53
T (K)	100(2)	100(2)	100(2)	100(2)
λ	0.71073	0.71073	0.71073	0.71073
cryst syst	tetragonal	triclinic	monoclinic	triclinic
space group	I-4	P-1	$P2_1/n$	P-1
a (Å)	18.1592(16)	12.4660(5)	10.0122(9)	9.9516(6)
b (Å)	18.1592(16)	13.3210(6)	23.216(2)	11.5955(6)
c (Å)	13.5259(12)	13.8989(5)	11.0117(11)	14.6959(9)
α (°)	90	115.7670(10)	90	107.911(2)
β (°)	90	105.4290(10)	108.420(3)	105.371(2)
γ (°)	90	99.361(2)	90	96.812(2)
V (Å^3)	4460.3(9)	1897.89(13)	2428.4(4)	1518.44(15)
Z	8	4	4	2
ρ_{calcd} (Mg m^{-3})	1.835	1.960	1.779	1.515
μ (mm^{-1})	6.431	7.651	6.017	4.817
R1[a]	0.0115	0.0183	0.0188	0.0188
wR2[b]	0.0243	0.0411	0.0367	0.0486

Table S2. Crystallographic data for **3cd**, **4**·Et_2O and **6**·0.5CH_2Cl_2.

	3cd	**4**·Et_2O	**6**·0.5CH_2Cl_2
formula	$C_{23}H_{16}Cl_2F_2N_2Pt$	$C_{34}H_{33}ClF_5N_3O_4PtS$	$C_{41.5}H_{31}ClF_3N_3O_3PtS$
fw	624.37	905.23	939.29
T (K)	100(2)	100(2)	100(2)
λ	0.71073	0.71073	0.71073
cryst syst	monoclinic	triclinic	monoclinic
space group	$P2_1/n$	P-1	C2/c
a (Å)	11.4079(5)	10.6722(14)	24.4833(11)
b (Å)	12.6215(5)	13.0588(17)	15.2726(7)
c (Å)	15.1221(6)	13.3512(16)	21.6707(15)
α (°)	90	74.425(4)	90°
β (°)	106.659(2)	89.412(4)	119.3470(10)
γ (°)	90	69.723(4)	90°
V (Å^3)	2085.96(15)	1674.2(4)	7063.3(7)
Z	4	2	8
ρ_{calcd} (Mg m^{-3})	1.988	1.796	1.767
μ (mm^{-1})	7.013	4.404	4.170
R1[a]	0.0173	0.0209	0.0232
wR2[b]	0.0337	0.0498	0.0593

[a]R1 = $\Sigma||F_o| - |F_c||/\Sigma|F_o|$ for reflections with $I > 2\sigma(I)$. [b]wR2 = $[\Sigma[w(F_o^2 - F_c^2)^2/\Sigma[w(F_o^2)^2]]^{0.5}$ for all reflections; $w^{-1} = \sigma^2(F^2) + (aP)^2 + bP$, where $P = (2F_c^2 + F_o^2)/3$ and a and b are constants set by the program.

4. Computational data

4.1. Complex 3bd

Table S3. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **3bd** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	L4	Pt
–0.032	145 (LUMO+5)	24	41	6	0	29
–0.037	144 (LUMO+4)	13	78	2	0	7
–0.051	143 (LUMO+3)	91	7	0	0	1
–0.060	142 (LUMO+2)	3	94	0	0	2
–0.067	141 (LUMO+1)	78	5	0	5	13
–0.087	140 (LUMO)	42	8	3	15	32
–0.228	139 (HOMO)	55	39	3	0	4
–0.231	138 (HOMO–1)	43	55	1	0	1
–0.244	137 (HOMO–2)	82	4	9	0	4
–0.246	136 (HOMO–3)	26	39	27	0	8
–0.249	135 (HOMO–4)	75	8	14	0	2
–0.252	134 (HOMO–5)	15	12	66	0	6

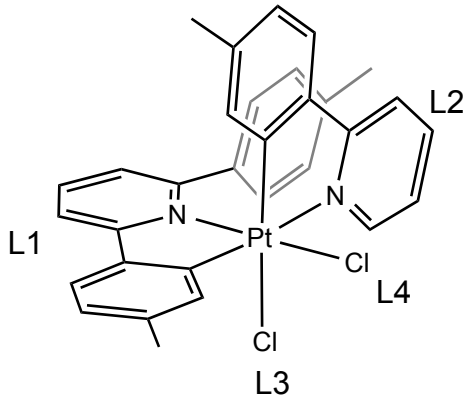
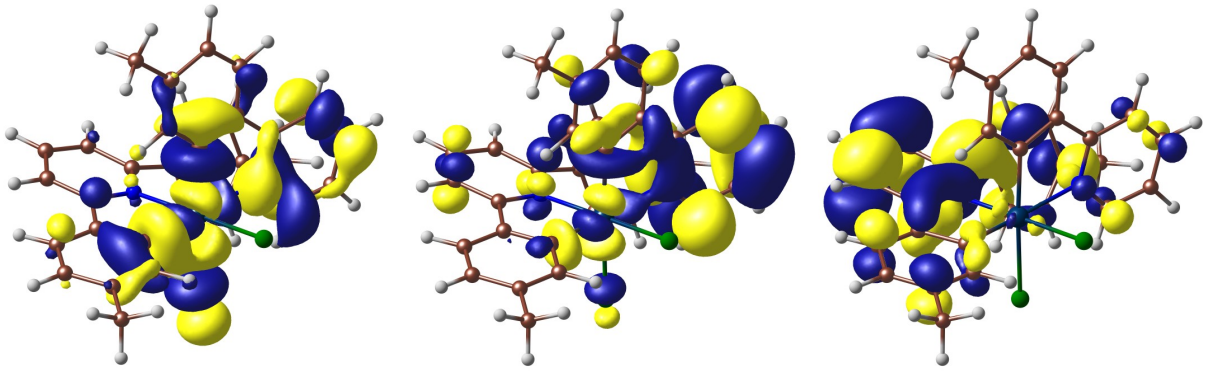
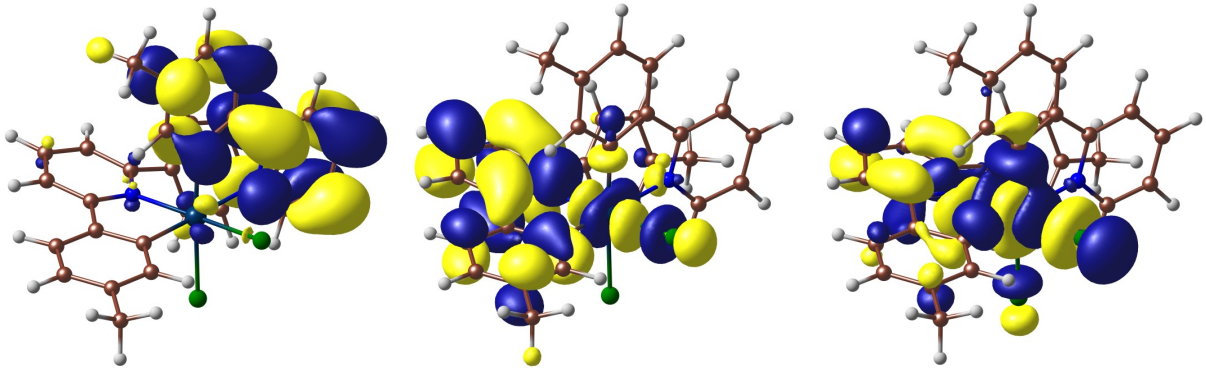


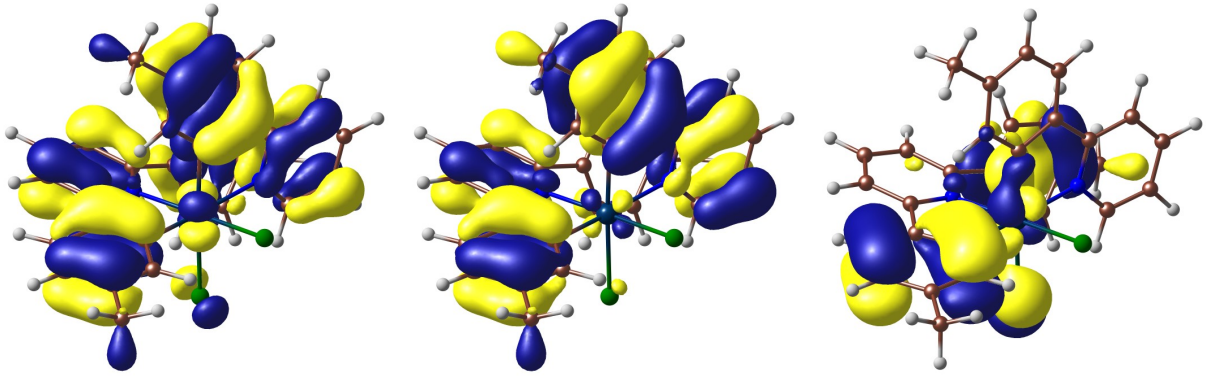
Figure S20. Ligand numbering in complex **3bd**.



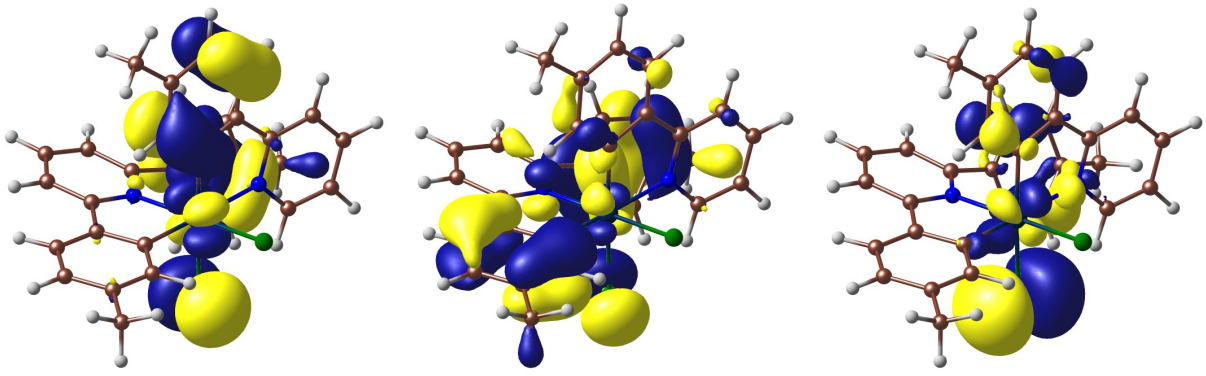
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S21. Molecular orbital isosurfaces of **3bd** (0.03 e bohr^{-3}).

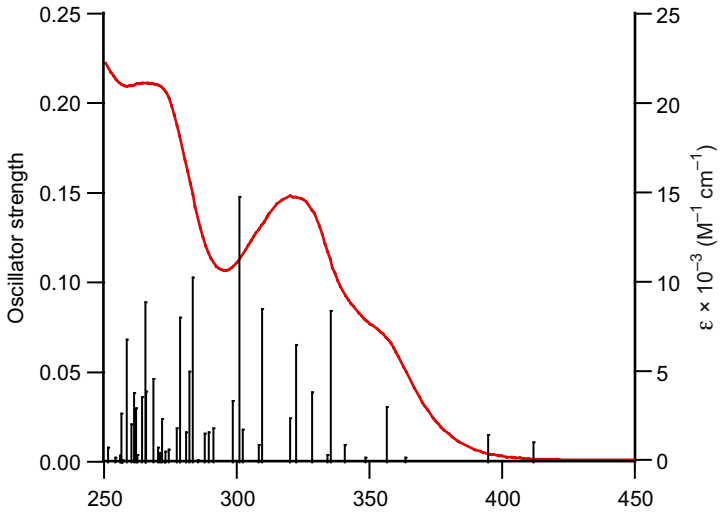


Figure S22. Calculated stick absorption spectrum of **3bd** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S4. Selected vertical singlet excitations of **3bd** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	oscillator strength
S1	H–3 ->L (8%) H ->L (84%) H ->L+1 (2%)	3.015	411.3	0.0113
S2	H–3 ->L (3%) H–2 ->L (3%) H–1 ->L (87%) H–1 ->L+1 (2%)	3.144	394.4	0.0151
S3	H–8 ->L (6%) H–5 ->L (2%) H–3 ->L (64%) H–2 ->L (3%) H–1 ->L (8%) H ->L (9%)	3.416	363.0	0.0027
S4	H–6 ->L (2%) H–5 ->L (9%) H–4 ->L (10%) H–2 ->L (65%) H–1 ->L (2%) H ->L (4%)	3.483	356.0	0.0311
S5	H–8 ->L (6%) H–7 ->L (5%) H–5 ->L (57%) H–4 ->L (7%) H–2 ->L (19%)	3.562	348.1	0.0027
S6	H–10 ->L (2%) H–8 ->L (16%) H–7 ->L (3%) H–6 ->L (17%) H–5 ->L (14%) H–4 ->L (33%) H ->L+1 (7%)	3.644	340.2	0.0095
S7	H–8 ->L (22%) H–6 ->L (7%) H–4 ->L (11%)	3.701	335.0	0.0844

	H–3 ->L (4%) H–1 ->L+1 (3%) H ->L+1 (44%)			
S8	H–9 ->L (46%) H–9 ->L+1 (5%) H–7 ->L (12%) H–6 ->L (14%) H–4 ->L (7%) H–3 ->L (3%) H ->L+1 (5%)	3.717	333.6	0.0041
S9	H–9 ->L (12%) H–8 ->L (9%) H–5 ->L (2%) H–4 ->L (21%) H–3 ->L (8%) H–2 ->L (2%) H–1 ->L+1 (3%) H ->L+1 (34%)	3.782	327.9	0.0392
S10	H–9 ->L (3%) H–5 ->L (2%) H–4 ->L (3%) H–1 ->L+1 (81%)	3.851	322.0	0.0656
S11	H–9 ->L (20%) H–8 ->L (26%) H–7 ->L (7%) H–6 ->L (34%) H–5 ->L (5%) H–1 ->L+1 (4%)	3.879	319.7	0.0245
S12	H–7 ->L (8%) H–6 ->L (2%) H ->L+2 (78%)	4.012	309.0	0.0858
S13	H–9 ->L (2%) H–7 ->L (60%) H–6 ->L (16%) H–5 ->L (5%) H ->L+2 (12%)	4.029	307.7	0.0095
S14	H–2 ->L+1 (22%) H–1 ->L+2 (64%) H ->L+2 (3%)	4.108	301.8	0.0183
S15	H–4 ->L+1 (4%) H–3 ->L+1 (2%) H–2 ->L+1 (59%) H–1 ->L+2 (20%) H ->L+3 (5%)	4.125	300.6	0.1482
S16	H–4 ->L+1 (5%) H–3 ->L+1 (81%) H–1 ->L+2 (3%)	4.162	297.9	0.0341
S17	H–10 ->L (3%) H–5 ->L+1 (2%) H–4 ->L+1 (22%) H–3 ->L+1 (2%) H–2 ->L+1 (6%) H–1 ->L+2 (3%) H–1 ->L+3 (6%) H ->L+3 (48%)	4.266	290.7	0.0189
S18	H–5 ->L+1 (13%) H–4 ->L+1 (35%) H–3 ->L+2 (2%) H–2 ->L+1 (3%)	4.291	288.9	0.0166

	H–1 ->L+3 (19%) H ->L+3 (18%)			
S19	H–10 ->L (4%) H–6 ->L+1 (5%) H–5 ->L+1 (69%) H–4 ->L+1 (7%) H–1 ->L+3 (6%)	4.315	287.4	0.0162
S20	H–10 ->L (30%) H–8 ->L (2%) H–4 ->L+1 (9%) H–3 ->L+2 (7%) H–2 ->L+2 (6%) H–1 ->L+3 (5%) H ->L+4 (9%) H ->L+5 (17%)	4.353	284.9	0.0012

[a] H = HOMO; L = LUMO.

Table S5. Lowest-energy vertical triplet excitations of **3bd** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**
T1	H–3 ->L (3%) H–2 ->L (2%) H–1 ->L (14%) H–1 ->L+1 (8%) H ->L(51%) H ->L+1 (6%) H ->L+3 (2%)	2.7109	457.36
T2	H–8 ->L (8%) H–4 ->L (3%) H–3 ->L (16%) H–3 ->L+1 (2%) H–1 ->L (22%) H–1 ->L+1 (2%) H ->L (13%) H ->L+1 (17%)	2.9014	427.33
T3	H–1 ->L+2 (40%) H–1 ->L+4 (3%) H ->L+2 (36%) H ->L+4 (2%)	2.9395	421.78

[a] H = HOMO; L = LUMO.

4.2. Complex 3cd

Table S6. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **3cd** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	L4	Pt
–0.040	125 (LUMO+5)	27	32	7	0	33
–0.043	124 (LUMO+4)	19	79	0	0	1
–0.052	123 (LUMO+3)	79	19	0	0	1
–0.068	122 (LUMO+2)	1	97	0	0	2
–0.075	121 (LUMO+1)	69	5	0	8	18
–0.081	120 (LUMO)	51	7	4	11	27
–0.236	119 (HOMO)	0	94	3	0	3
–0.243	118 (HOMO–1)	91	4	2	0	3
–0.252	117 (HOMO–2)	6	57	30	1	5
–0.255	116 (HOMO–3)	68	7	14	1	9
–0.259	115 (HOMO–4)	6	3	86	1	4
–0.263	114 (HOMO–5)	4	27	47	18	4

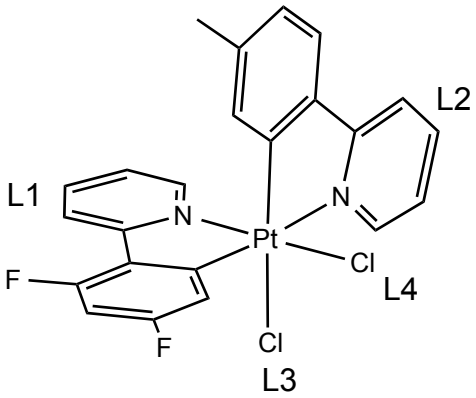


Figure S23. Ligand numbering in complex **3cd**.

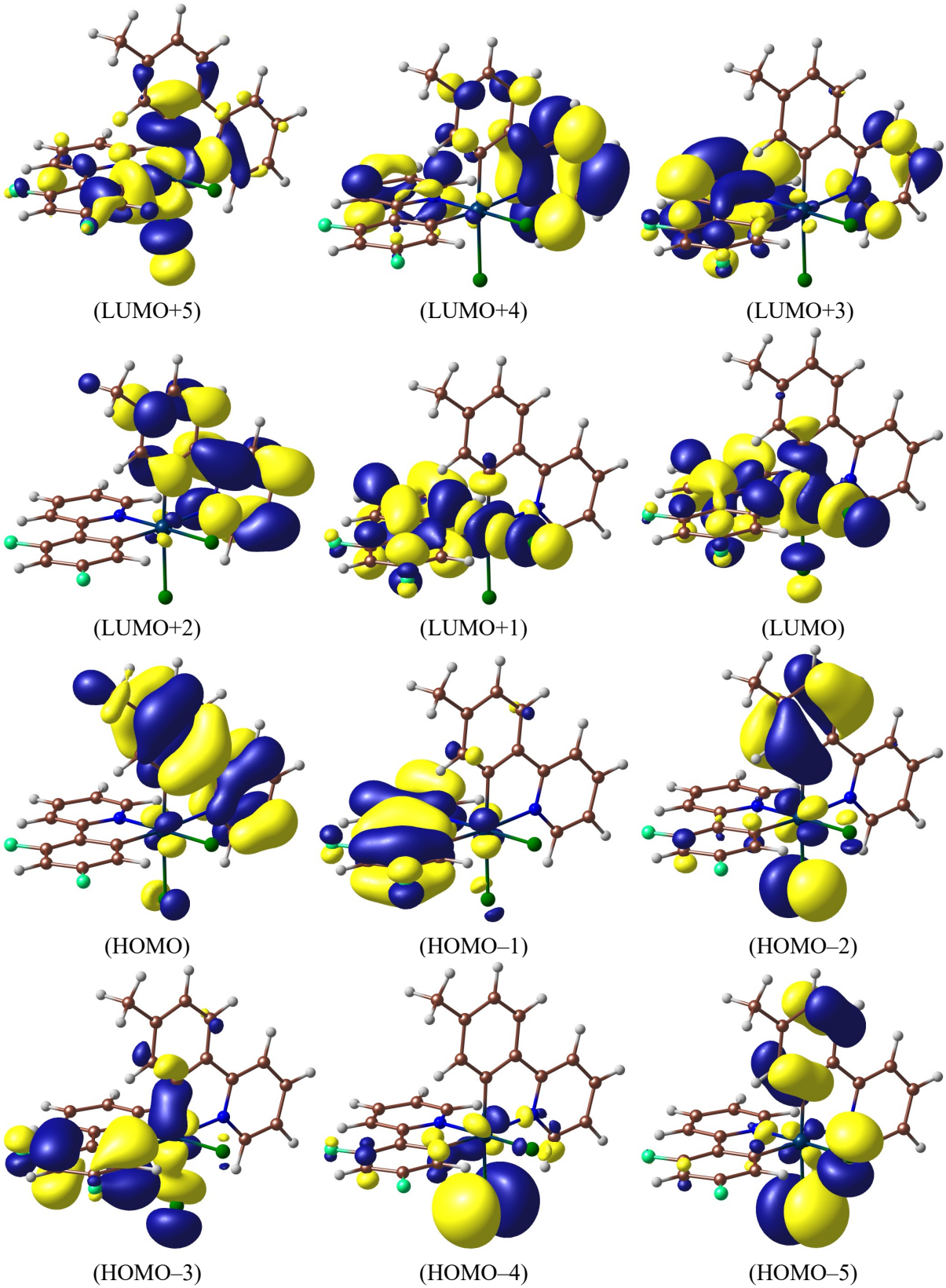


Figure S24. Molecular orbital isosurfaces of **3cd** (0.03 e bohr^{-3}).

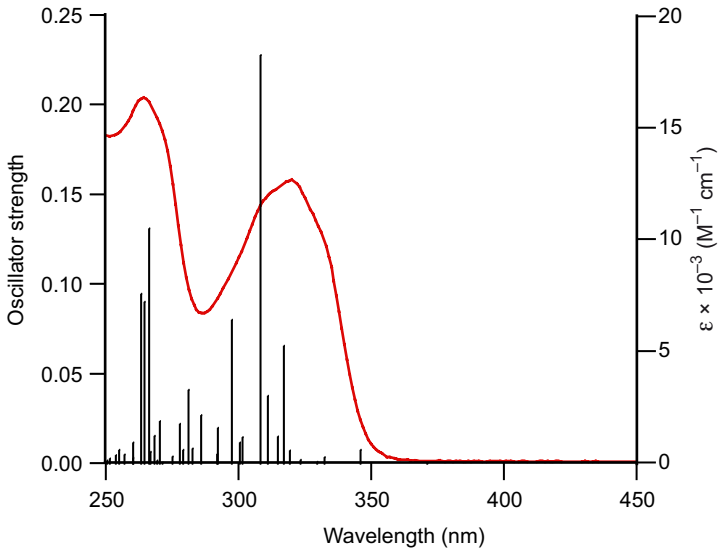


Figure S25. Calculated stick absorption spectrum of **3cd** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S7. Selected vertical singlet excitations of **3cd** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	oscillator strength
S1	H–6 ->L (2%) H–2 ->L (7%) H–1 ->L (6%) H ->L (62%) H ->L+1 (13%)	3.346	370.6	0.0008
S2	H–3 ->L (5%) H–1 ->L (63%) H–1 ->L+1 (13%) H ->L (12%)	3.589	345.5	0.0082
S3	H–6 ->L (3%) H–2 ->L (31%) H–2 ->L+1 (11%) H–1 ->L (3%) H ->L (22%) H ->L+1 (24%)	3.735	331.9	0.0043
S4	H–6 ->L (2%) H–2 ->L (31%) H–2 ->L+1 (2%) H ->L+1 (57%)	3.767	329.2	0.0017
S5	H–4 ->L (35%) H–4 ->L+1 (5%) H–3 ->L (37%) H–3 ->L+1 (8%) H–1 ->L (7%) H–1 ->L+1 (3%)	3.838	323.0	0.0025
S6	H–6 ->L (28%) H–6 ->L+1 (12%) H–5 ->L (22%) H–5 ->L+1 (6%) H–4 ->L (6%) H–2 ->L (9%) H ->L+2 (6%)	3.888	318.9	0.0078

S7	H–7 ->L (20%) H–7 ->L+1 (10%) H–5 ->L (10%) H–3 ->L+1 (3%) H–1 ->L (10%) H–1 ->L+1 (38%) H ->L+1 (2%)	3.916	316.6	0.0661
S8	H–7 ->L (15%) H–7 ->L+1 (6%) H–6 ->L (3%) H–4 ->L (26%) H–4 ->L+1 (4%) H–3 ->L (27%) H–1 ->L+1 (11%)	3.944	314.4	0.0156
S9	H–7 ->L (16%) H–7 ->L+1 (6%) H–5 ->L (8%) H–5 ->L+1 (2%) H–4 ->L (13%) H–3 ->L (3%) H–3 ->L+1 (6%) H–1 ->L (4%) H–1 ->L+1 (18%) H ->L+2 (17%)	3.992	310.6	0.0385
S10	H–7 ->L (6%) H–4 ->L (6%) H–3 ->L (4%) H–3 ->L+1 (3%) H ->L+2 (65%)	4.029	307.8	0.2284
S11	H–6 ->L (5%) H–5 ->L (3%) H–3 ->L+1 (4%) H–2 ->L (9%) H–2 ->L+1 (71%)	4.117	301.1	0.0154
S12	H–7 ->L (8%) H–7 ->L+1 (3%) H–6 ->L (23%) H–6 ->L+1 (7%) H–5 ->L (40%) H–5 ->L+1 (3%) H–2 ->L (7%) H–2 ->L+1 (5%)	4.132	300.1	0.0122
S13	H–5 ->L (2%) H–4 ->L+1 (5%) H–3 ->L (14%) H–3 ->L+1 (60%) H–2 ->L+1 (4%) H–1 ->L+1 (6%)	4.176	296.9	0.0806
S14	H–4 ->L+1 (12%) H–3 ->L+2 (2%) H–1 ->L+2 (77%)	4.249	291.8	0.0206
S15	H–4 ->L (7%) H–4 ->L+1 (70%) H–3 ->L+1 (4%) H–1 ->L+2 (13%)	4.255	291.4	0.0059
S16	H–2 ->L+2 (55%) H–1 ->L+2 (4%) H ->L+3 (28%) H ->L+4 (3%)	4.345	285.3	0.0274

	H ->L+7 (3%)			
S17	H–6 ->L+1 (12%) H–5 ->L (7%) H–5 ->L+1 (56%) H–2 ->L+2 (3%) H ->L+5 (10%)	4.395	282.1	0.0091
S18	H–5 ->L+1 (17%) H–2 ->L+2 (13%) H ->L+3 (21%) H ->L+5 (39%)	4.419	280.6	0.0418
S19	H–6 ->L (23%) H–6 ->L+1 (59%) H–5 ->L (3%) H–5 ->L+1 (8%)	4.447	278.8	0.0084
S20	H–3 ->L+2 (5%) H–2 ->L+2 (10%) H ->L+3 (40%) H ->L+4 (2%) H ->L+5 (30%)	4.468	277.5	0.0226

[a] H = HOMO; L = LUMO.

Table S8. Lowest-energy vertical triplet excitations of **3cd** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**
T1	H–2 ->L+7 (3%) H ->L+2 (77%) H ->L+4 (6%)	2.9251	423.86
T2	H–3 ->L+6 (3%) H–1 ->L (45%) H–1 ->L+1 (32%) H–1 ->L+3 (7%)	2.9549	419.59
T3	H–8 ->L (2%) H–6 ->L (10%) H–6 ->L+1 (4%) H–5 ->L (2%) H–3 ->L (6%) H–2 ->L (9%) H–2 ->L+1 (2%) H–1 ->L (4%) H–1 ->L+1 (10%) H ->L (30%) H ->L+1 (10%)	3.1434	394.43

[a] H = HOMO; L = LUMO.

4.3. Complex 3ce

Table S9. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **3ce** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	L4	Pt
–0.044	122 (LUMO+5)	11	84	0	0	4
–0.046	121 (LUMO+4)	33	32	6	0	29
–0.053	120 (LUMO+3)	83	15	0	0	2
–0.071	119 (LUMO+2)	0	97	0	0	2
–0.077	118 (LUMO+1)	80	3	0	5	12
–0.085	117 (LUMO)	39	9	5	15	33
–0.229	116 (HOMO)	0	95	2	0	3
–0.245	115 (HOMO–1)	94	2	1	0	3
–0.256	114 (HOMO–2)	7	51	35	1	5
–0.257	113 (HOMO–3)	65	8	16	0	10
–0.262	112 (HOMO–4)	10	3	82	1	4
–0.265	111 (HOMO–5)	5	27	37	26	5

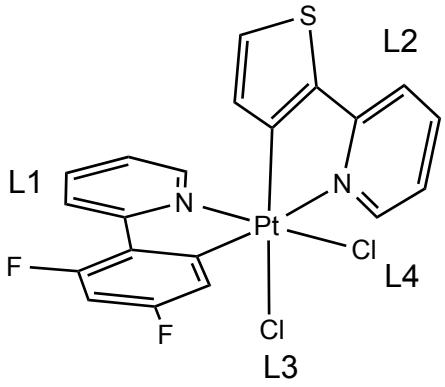


Figure S26. Ligand numbering in complex **3ce**.

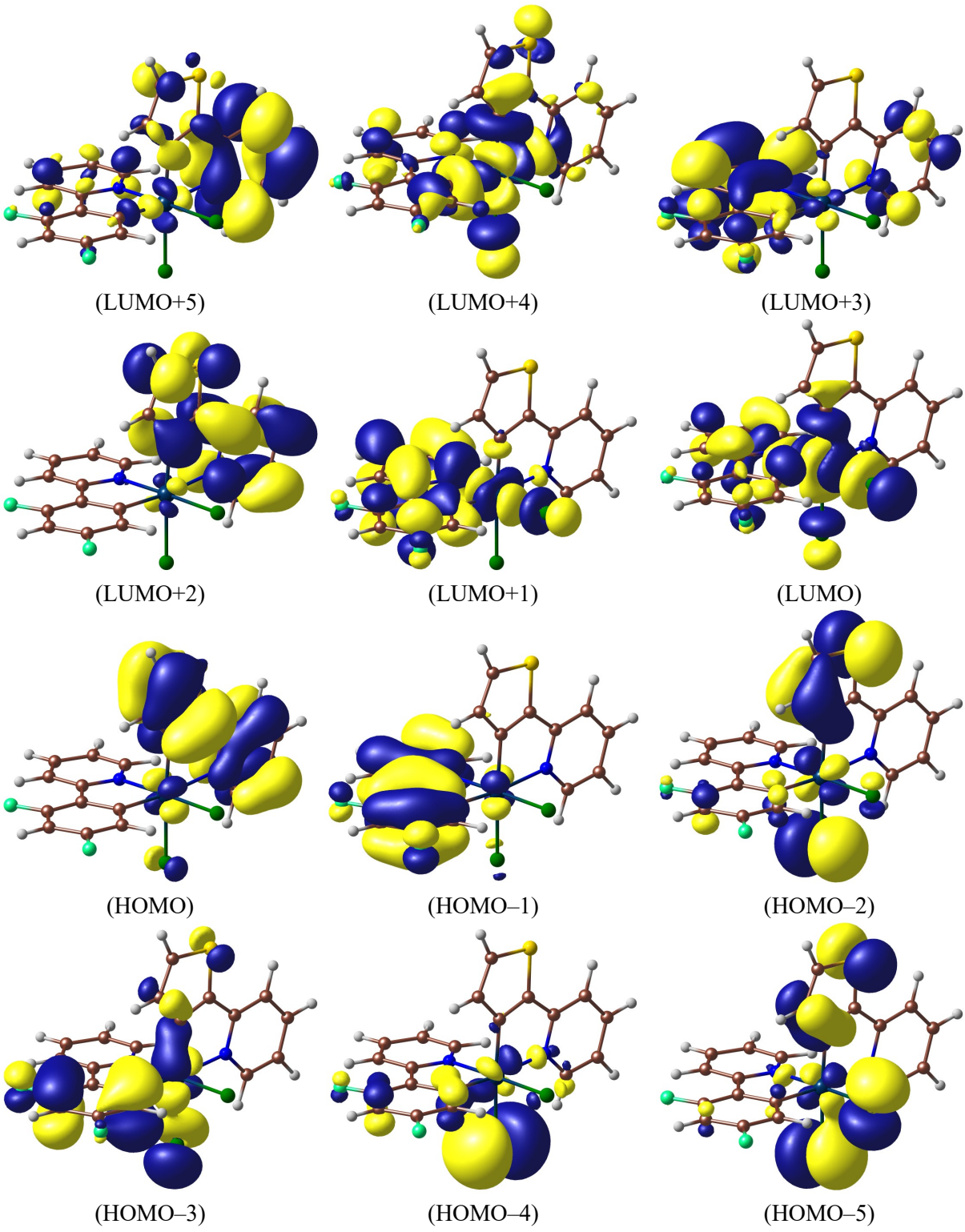


Figure S27. Molecular orbital isosurfaces of **3ce** (0.03 e bohr^{-3}).

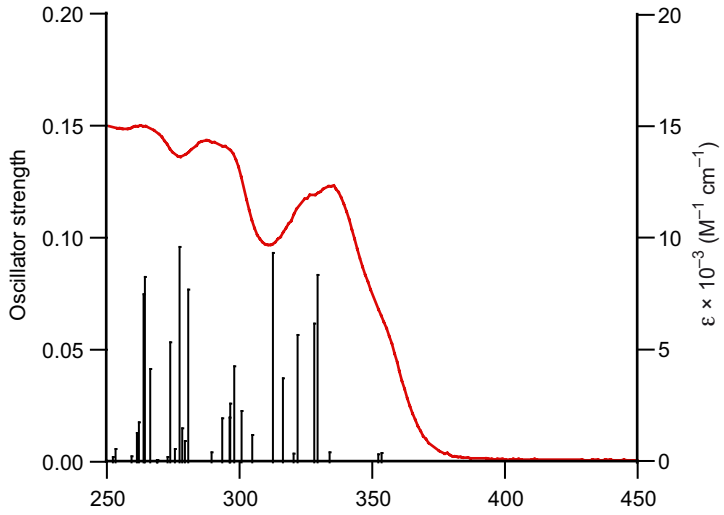


Figure S28. Calculated stick absorption spectrum of **3ce** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S10. Selected vertical singlet excitations of **3ce** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**oscillator strength**
S1	H–2 ->L (2%) H ->L (85%) H ->L+1 (7%)	3.053	406.1	0.0006
S2	H–3 ->L (4%) H–1 ->L (48%) H–1 ->L+1 (5%) H ->L (8%) H ->L+1 (28%)	3.513	352.9	0.0041
S3	H–3 ->L (3%) H–1 ->L (29%) H ->L (2%) H ->L+1 (62%)	3.526	351.7	0.0036
S4	H–6 ->L (11%) H–4 ->L (6%) H–2 ->L (64%) H–2 ->L+1 (5%) H ->L (3%)	3.717	333.5	0.0045
S5	H–6 ->L (4%) H–4 ->L (4%) H–3 ->L (22%) H–1 ->L (5%) H ->L+2 (51%)	3.768	329.0	0.0836
S6	H–5 ->L (3%) H–4 ->L (24%) H–3 ->L (31%) H–3 ->L+1 (2%) H–2 ->L (8%) H–1 ->L (3%) H ->L+2 (23%)	3.784	327.7	0.0618
S7	H–7 ->L (3%) H–6 ->L (13%) H–6 ->L+1 (3%) H–5 ->L (44%)	3.858	321.4	0.057

	H–5 ->L+1 (5%) H–2 ->L (10%) H–1 ->L (3%) H ->L+2 (11%)			
S8	H–7 ->L (53%) H–7 ->L+1 (10%) H–6 ->L (13%) H–6 ->L+1 (2%) H–4 ->L (5%) H–3 ->L (4%) H–1 ->L+1 (4%) H ->L+2 (3%)	3.875	320.0	0.004
S9	H–5 ->L (2%) H–4 ->L (37%) H–4 ->L+1 (2%) H–3 ->L (18%) H–2 ->L (2%) H–1 ->L+1 (31%) H ->L+2 (2%)	3.924	315.9	0.0376
S10	H–7 ->L (13%) H–5 ->L (3%) H–4 ->L (17%) H–3 ->L (4%) H–3 ->L+1 (9%) H–1 ->L (5%) H–1 ->L+1 (40%)	3.972	312.1	0.0936
S11	H ->L+3 (10%) H ->L+4 (75%) H ->L+5 (6%)	4.074	304.3	0.0121
S12	H–7 ->L (11%) H–6 ->L (38%) H–6 ->L+1 (2%) H–5 ->L (34%) H–2 ->L (2%) H–2 ->L+1 (4%)	4.128	300.3	0.0228
S13	H–6 ->L+1 (2%) H–5 ->L (2%) H–3 ->L (3%) H–3 ->L+1 (23%) H–2 ->L (6%) H–2 ->L+1 (52%) H–1 ->L+1 (4%)	4.167	297.6	0.043
S14	H–3 ->L (4%) H–3 ->L+1 (38%) H–2 ->L+1 (20%) H–1 ->L+2 (24%) H ->L+3 (4%)	4.187	296.1	0.0262
S15	H–3 ->L+1 (12%) H–2 ->L+1 (9%) H–1 ->L+2 (70%)	4.193	295.7	0.02
S16	H ->L+3 (81%) H ->L+4 (12%)	4.231	293.1	0.0196
S17	H–4 ->L (3%) H–4 ->L+1 (89%) H–3 ->L+1 (3%)	4.292	288.9	0.0045
S18	H–2 ->L+2 (91%) H ->L+5 (4%)	4.424	280.3	0.077
S19	H–6 ->L+1 (4%) H–5 ->L (5%)	4.444	279.0	0.0095

	H–5 ->L+1 (79%) H–3 ->L+2 (3%) H–2 ->L+1 (3%)			
S20	H–5 ->L+1 (2%) H–4 ->L+2 (9%) H–3 ->L+2 (64%) H–1 ->L+2 (2%) H ->L+4 (2%) H ->L+5 (14%)	4.462	277.9	0.0151

[a] H = HOMO; L = LUMO.

Table S11. Lowest-energy vertical triplet excitations of **3ce** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**
T1	H ->L+2 (88%) H ->L+5 (6%)	2.5507	486.08
T2	H–6 ->L (2%) H–3 ->L (2%) H–2 ->L (3%) H–1 ->L (11%) H–1 ->L+1 (3%) H ->L (61%) H ->L+1 (6%)	2.9092	426.18
T3	H–3 ->L+6 (2%) H–1 ->L (22%) H–1 ->L+1 (45%) H–1 ->L+3 (7%) H ->L (9%) H ->L+1 (2%)	2.9671	417.87

[a] H = HOMO; L = LUMO.

4.4. Complex 3de

Table S12. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **3de** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	L4	Pt
–0.040	118 (LUMO+5)	26	37	6	0	31
–0.042	117 (LUMO+4)	15	81	0	0	4
–0.052	116 (LUMO+3)	87	12	0	0	2
–0.069	115 (LUMO+2)	0	97	0	0	2
–0.072	114 (LUMO+1)	78	3	0	6	13
–0.080	113 (LUMO)	40	9	5	14	32
–0.227	112 (HOMO)	0	94	2	0	3
–0.235	111 (HOMO–1)	93	2	1	0	4
–0.250	110 (HOMO–2)	81	4	8	0	7
–0.253	109 (HOMO–3)	3	52	38	0	6
–0.258	108 (HOMO–4)	5	3	85	2	5
–0.262	107 (HOMO–5)	3	21	30	39	6

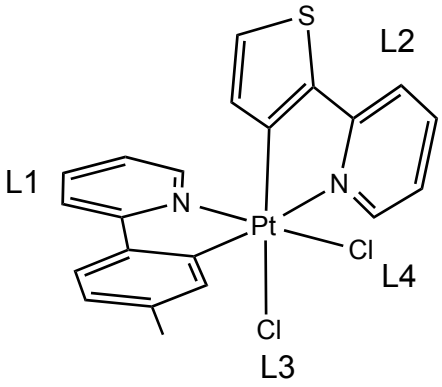
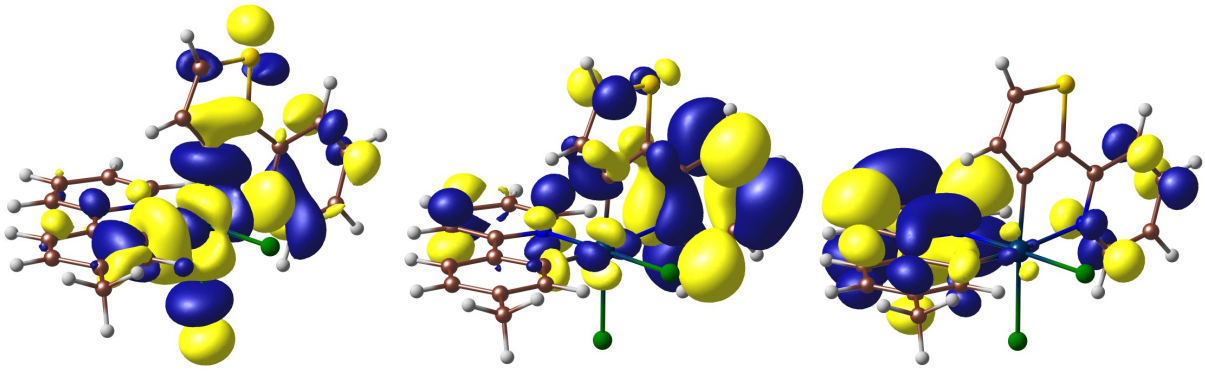
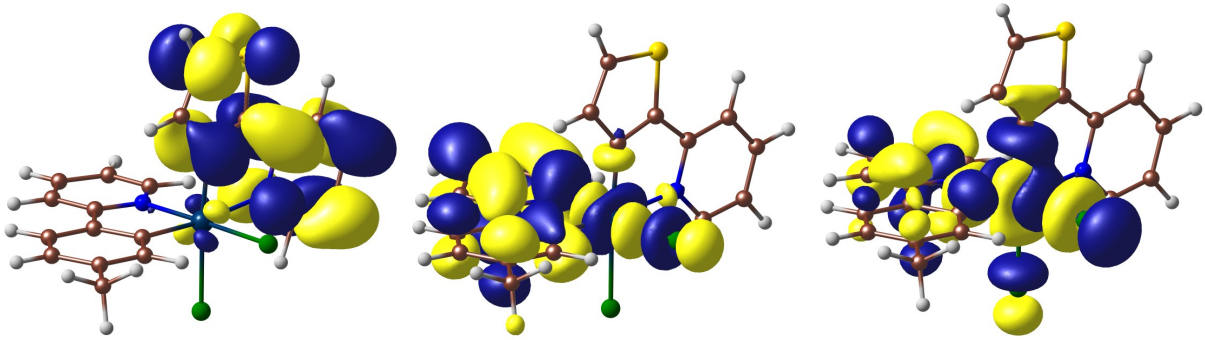


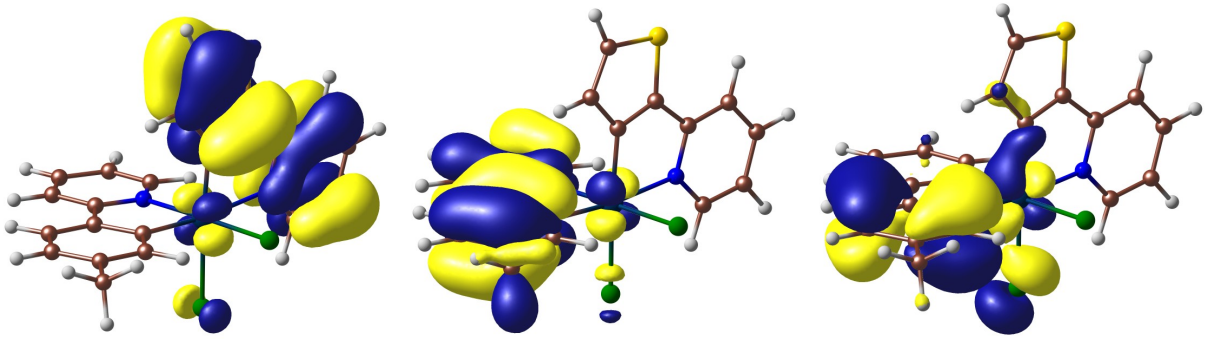
Figure S29. Ligand numbering in complex **3de**.



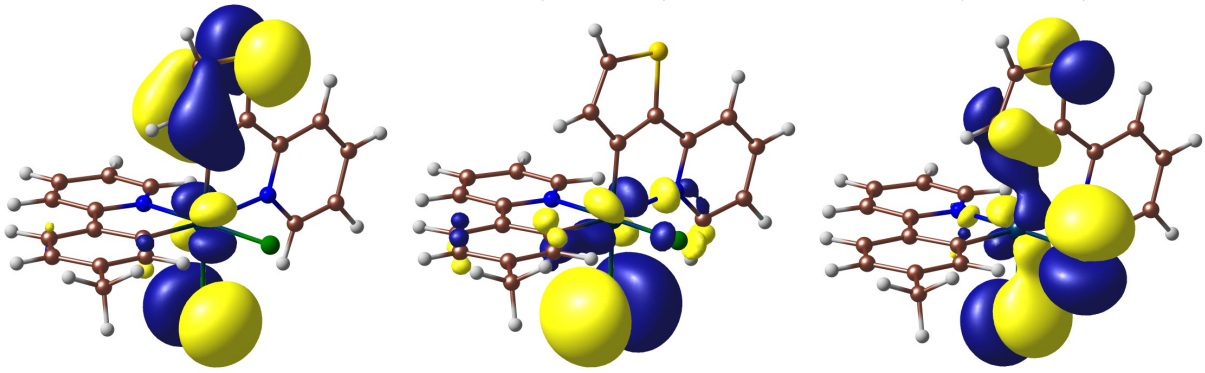
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S30. Molecular orbital isosurfaces of **3de** (0.03 e bohr^{-3}).

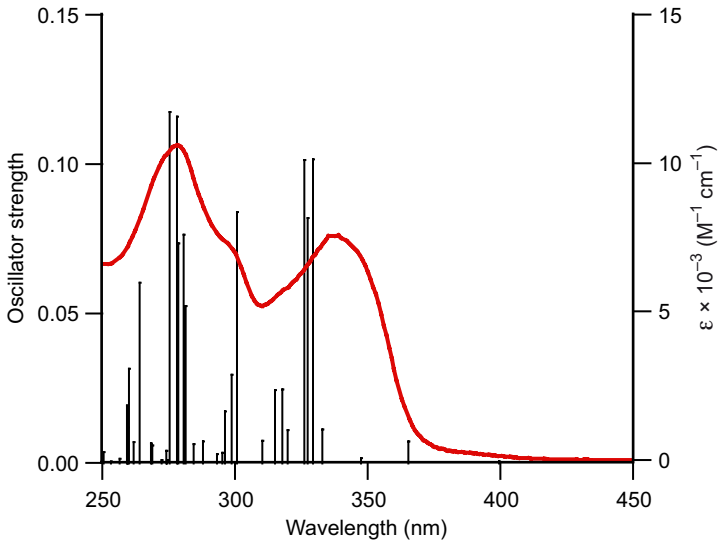


Figure S31. Calculated stick absorption spectrum of **3de** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S13. Selected vertical singlet excitations of **3de** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**	**oscillator strength**
S1	H–3 ->L (3%) H ->L (82%) H ->L+1 (9%)	3.107	399.0	0.0008
S2	H–2 ->L (3%) H–1 ->L (82%) H–1 ->L+1 (8%)	3.399	364.8	0.0074
S3	H ->L (11%) H ->L+1 (87%)	3.573	347.0	0.0019
S4	H–6 ->L (10%) H–5 ->L (6%) H–4 ->L (5%) H–3 ->L (22%) H–2 ->L (37%) H–2 ->L+1 (5%) H ->L (3%)	3.730	332.4	0.0114
S5	H–6 ->L (5%) H–4 ->L (3%) H–3 ->L (7%) H–2 ->L (20%) H–1 ->L+1 (18%) H ->L+2 (37%)	3.768	329.0	0.1019
S6	H–5 ->L (5%) H–2 ->L+1 (2%) H–1 ->L (7%) H–1 ->L+1 (53%) H ->L+2 (25%)	3.794	326.8	0.0821
S7	H–7 ->L (2%) H–4 ->L (11%) H–3 ->L (35%) H–3 ->L+1 (4%) H–2 ->L (8%) H–2 ->L+1 (3%)	3.807	325.7	0.1015

	H–1 ->L (6%) H–1 ->L+1 (3%) H ->L+2 (19%)			
S8	H–7 ->L (38%) H–7 ->L+1 (7%) H–6 ->L (15%) H–6 ->L+1 (3%) H–4 ->L (18%) H–4 ->L+1 (2%) H–3 ->L (4%) H–2 ->L (2%) H ->L+2 (3%)	3.882	319.4	0.0112
S9	H–7 ->L (5%) H–6 ->L (3%) H–5 ->L (49%) H–5 ->L+1 (7%) H–4 ->L (3%) H–3 ->L (13%) H–2 ->L (6%) H ->L+2 (5%)	3.907	317.3	0.0249
S10	H–7 ->L (14%) H–7 ->L+1 (3%) H–6 ->L (5%) H–5 ->L (2%) H–4 ->L (51%) H–3 ->L (2%) H–2 ->L (9%) H–2 ->L+1 (3%) H–1 ->L+1 (2%)	3.941	314.6	0.0246
S11	H–1 ->L+2 (97%)	4.002	309.8	0.0075
S12	H–2 ->L (8%) H–2 ->L+1 (74%) H–1 ->L+1 (3%) H–1 ->L+3 (5%) H–1 ->L+6 (2%)	4.129	300.3	0.0841
S13	H ->L+3 (34%) H ->L+4 (6%) H ->L+5 (49%)	4.156	298.3	0.0298
S14	H–7 ->L (16%) H–6 ->L (44%) H–6 ->L+1 (2%) H–5 ->L (21%) H–3 ->L (2%) H–3 ->L+1 (4%) H ->L+5 (2%)	4.194	295.6	0.0174
S15	H–3 ->L+1 (10%) H ->L+3 (57%) H ->L+4 (3%) H ->L+5 (25%)	4.208	294.6	0.0035
S16	H–6 ->L+1 (3%) H–3 ->L (7%) H–3 ->L+1 (71%) H ->L+3 (4%) H ->L+5 (8%)	4.234	292.8	0.0032
S17	H–4 ->L (4%) H–4 ->L+1 (86%) H–1 ->L+5 (3%)	4.312	287.5	0.0073
S18	H–4 ->L+2 (4%) H–2 ->L+2 (92%)	4.368	283.9	0.0065

S19	H–5 ->L+1 (2%) H–4 ->L+1 (5%) H–2 ->L+5 (8%) H–1 ->L+3 (6%) H–1 ->L+4 (8%) H–1 ->L+5 (53%) H ->L+4 (4%)	4.415	280.8	0.0527
S20	H–3 ->L+2 (81%) H–1 ->L+5 (3%) H ->L+4 (10%)	4.425	280.2	0.0767

[a] H = HOMO; L = LUMO.

Table S14. Lowest-energy vertical triplet excitations of **3de** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**
T1	H ->L+2 (88%) H ->L+4 (6%)	2.5517	485.89
T2	H–2 ->L+6 (3%) H–1 ->L (36%) H–1 ->L+1 (39%) H–1 ->L+3 (7%) H ->L (3%)	2.8434	436.04
T3	H–6 ->L (2%) H–5 ->L (4%) H–3 ->L (7%) H–1 ->L+1 (6%) H ->L(62%) H ->L+1 (10%)	2.9607	418.77

[a] H = HOMO; L = LUMO.

4.5. Complex 3ed

Table S15. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **3ed** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	L4	Pt
–0.039	118 (LUMO+5)	26	33	7	0	33
–0.043	117 (LUMO+4)	17	81	0	0	2
–0.051	116 (LUMO+3)	82	17	0	0	1
–0.067	115 (LUMO+2)	0	97	0	0	2
–0.074	114 (LUMO+1)	73	4	0	7	16
–0.081	113 (LUMO)	45	8	4	13	30
–0.228	112 (HOMO)	93	1	1	0	4
–0.235	111 (HOMO–1)	0	94	3	0	3
–0.250	110 (HOMO–2)	5	57	31	0	6
–0.253	109 (HOMO–3)	72	7	12	0	8
–0.257	108 (HOMO–4)	6	3	85	1	5
–0.261	107 (HOMO–5)	3	28	47	18	4

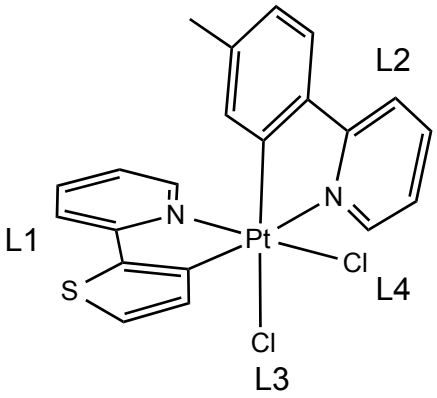


Figure S32. Ligand numbering in complex **3ed**.

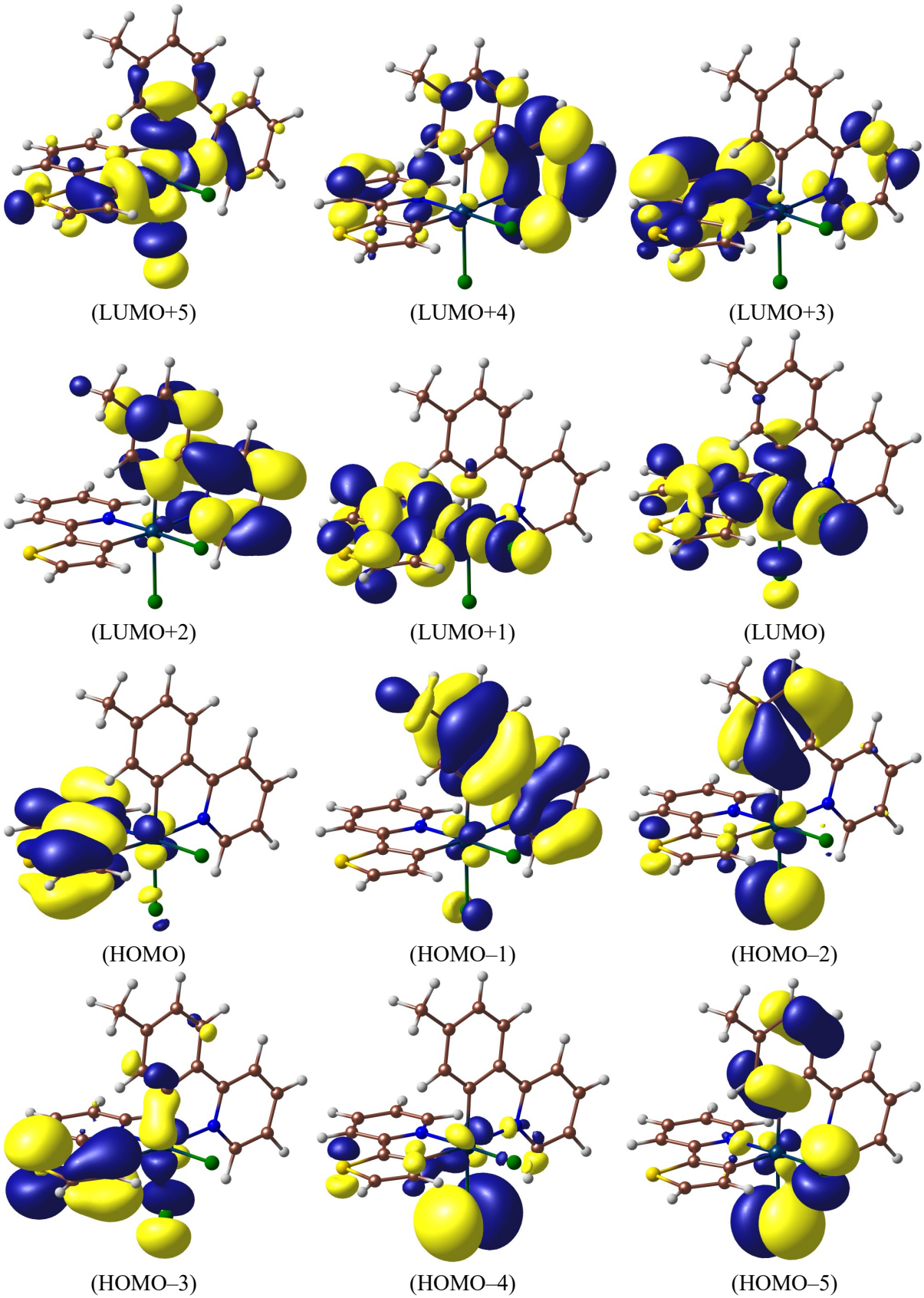


Figure S33. Molecular orbital isosurfaces of **3ed** (0.03 e bohr^{-3}).

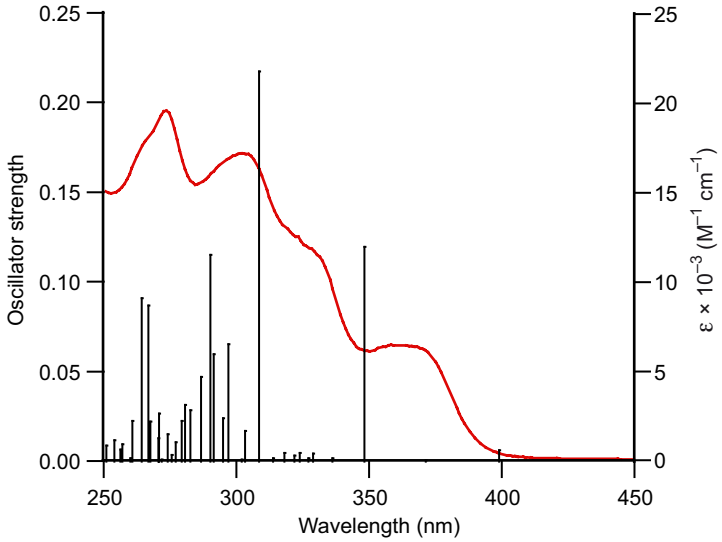


Figure S34. Calculated stick absorption spectrum of **3ed** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S16. Selected vertical singlet excitations of **3ed** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	oscillator strength
S1	H ->L (79%) H ->L+1 (15%)	3.112	398.4	0.0062
S2	H–2 ->L (10%) H–1 ->L (70%) H–1 ->L+1 (10%) H ->L (2%)	3.343	370.9	0.0006
S3	H ->L (14%) H ->L+1 (75%) H ->L+3 (4%)	3.565	347.8	0.1198
S4	H–6 ->L (7%) H–2 ->L (53%) H–2 ->L+1 (8%) H–1 ->L (21%)	3.694	335.7	0.002
S5	H–2 ->L (7%) H–1 ->L (6%) H–1 ->L+1 (84%)	3.775	328.4	0.0044
S6	H–4 ->L (45%) H–4 ->L+1 (4%) H–3 ->L (33%) H–3 ->L+1 (5%) H ->L+2 (3%)	3.796	326.7	0.002
S7	H–4 ->L (3%) H ->L+2 (91%)	3.835	323.3	0.0049
S8	H–6 ->L (30%) H–6 ->L+1 (9%) H–5 ->L (25%) H–5 ->L+1 (5%) H–4 ->L (7%) H–2 ->L (11%) H–1 ->L+2 (3%) H ->L+2 (4%)	3.859	321.3	0.0033
S9	H–7 ->L (54%) H–7 ->L+1 (16%)	3.905	317.5	0.005

	H–6 ->L (3%) H–5 ->L (7%) H–4 ->L (3%) H–3 ->L (7%)			
S10	H–7 ->L (4%) H–5 ->L (10%) H–4 ->L (32%) H–3 ->L (35%) H–3 ->L+1 (7%) H–1 ->L+2 (4%)	3.955	313.5	0.0018
S11	H–3 ->L (2%) H–2 ->L+2 (3%) H–1 ->L+2 (81%)	4.023	308.2	0.2176
S12	H–7 ->L (11%) H–7 ->L+1 (2%) H–6 ->L (28%) H–6 ->L+1 (2%) H–5 ->L (35%) H–2 ->L+1 (15%)	4.096	302.7	0.0172
S13	H–6 ->L (2%) H–6 ->L+1 (3%) H–5 ->L (7%) H–5 ->L+1 (3%) H–2 ->L (11%) H–2 ->L+1 (67%)	4.111	301.6	0.0013
S14	H–4 ->L+1 (32%) H–3 ->L (9%) H–3 ->L+1 (43%) H ->L+3 (4%) H ->L+5 (3%)	4.181	296.6	0.0654
S15	H–3 ->L+1 (7%) H ->L+4 (3%) H ->L+5 (77%)	4.209	294.6	0.0241
S16	H–4 ->L (2%) H–4 ->L+1 (32%) H–3 ->L+1 (4%) H ->L+3 (50%) H ->L+5 (2%)	4.261	291.0	0.06
S17	H–5 ->L+1 (3%) H–4 ->L (3%) H–4 ->L+1 (27%) H–3 ->L (4%) H–3 ->L+1 (24%) H ->L+3 (32%)	4.278	289.8	0.1153
S18	H–2 ->L+2 (64%) H–1 ->L+3 (20%) H–1 ->L+4 (5%) H–1 ->L+6 (4%)	4.333	286.2	0.0474
S19	H–6 ->L+1 (18%) H–5 ->L (5%) H–5 ->L+1 (65%) H–2 ->L+1 (3%) H ->L+3 (3%)	4.395	282.1	0.0288

[a] H = HOMO; L = LUMO.

Table S17. Lowest-energy vertical triplet excitations of **3ed** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm
T1	H ->L (43%) H ->L+1 (43%) H ->L+3 (8%)	2.4677	502.43
T2	H–2 ->L+2 (2%) H–2 ->L+6 (3%) H–1 ->L+2 (74%) H–1 ->L+4 (6%)	2.9244	423.97
T3	H–6 ->L (2%) H–3 ->L (6%) H–1 ->L (3%) H–1 ->L+2 (4%) H ->L (38%) H ->L+1 (34%)	2.9541	419.7

[a] H = HOMO; L = LUMO.

4.6. Complex 4

Table S18. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **4** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	L3	Cl	Pt
–0.057	141 (LUMO+5)	12	85	0	0	3
–0.066	140 (LUMO+4)	3	5	87	0	5
–0.068	139 (LUMO+3)	84	12	3	0	0
–0.081	138 (LUMO+2)	2	96	0	0	2
–0.092	137 (LUMO+1)	75	3	0	6	15
–0.100	136 (LUMO)	46	7	2	14	31
–0.248	135 (HOMO)	0	98	0	0	1
–0.259	134 (HOMO–1)	95	3	0	0	2
–0.267	133 HOMO–2)	4	91	0	0	4
–0.274	132 (HOMO–3)	88	2	3	1	7
–0.288	131 (HOMO–4)	5	4	9	69	12
–0.291	130 (HOMO–5)	4	4	9	72	11

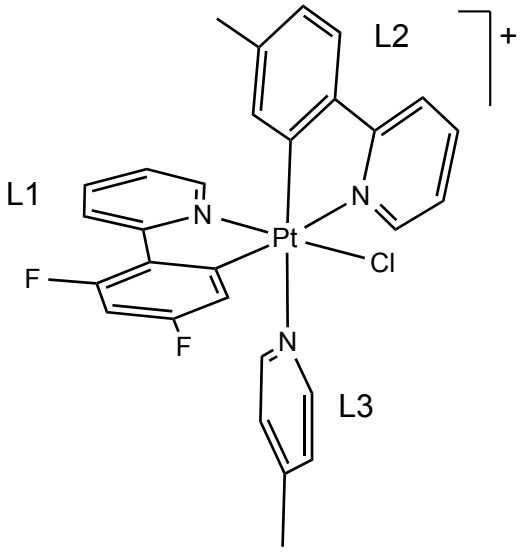
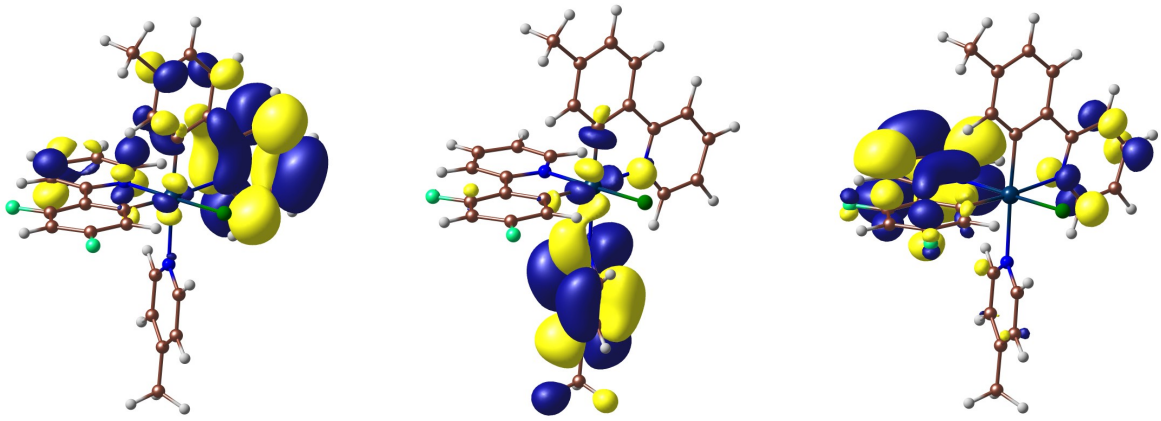
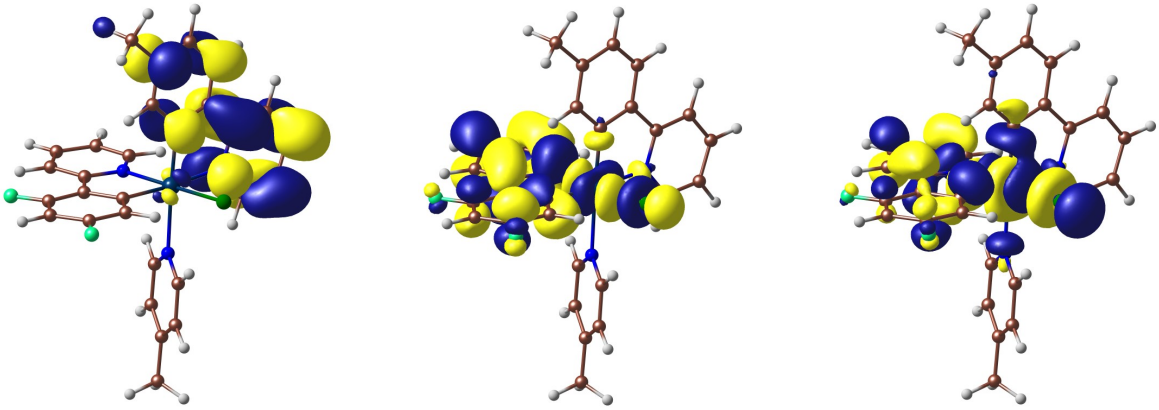


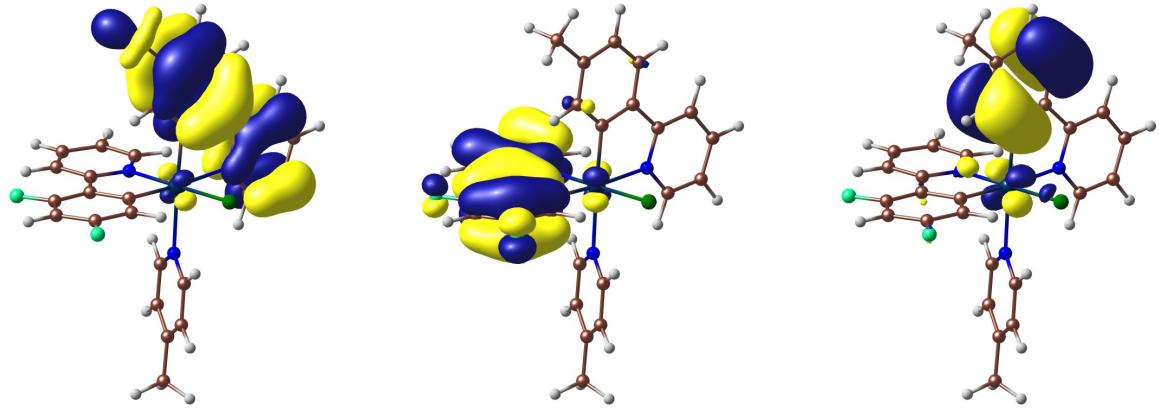
Figure S35. Ligand numbering in complex **4**.



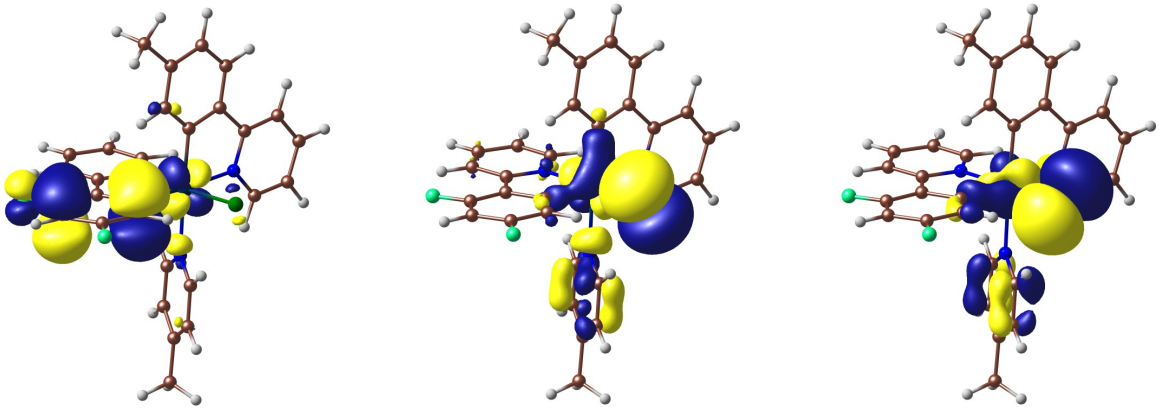
(LUMO+5) (LUMO+4) (LUMO+3)



(LUMO+2) (LUMO+1) (LUMO)



(HOMO) (HOMO–1) (HOMO–2)



(HOMO–3) (HOMO–4) (HOMO–5)

Figure S36. Molecular orbital isosurfaces of **4** (0.03 e bohr^{-3}).

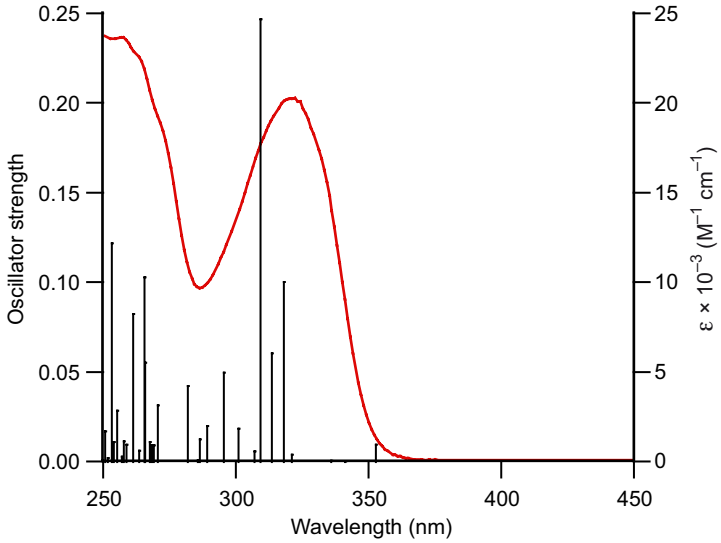


Figure S37. Calculated stick absorption spectrum of **4** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S19. Selected vertical singlet excitations of **4** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	oscillator strength
S1	H–2 ->L (2%) H ->L (85%) H ->L+1 (8%)	3.252	381.2	0.0007
S2	H–1 ->L (80%) H–1 ->L+1 (11%) H ->L (3%)	3.520	352.3	0.0095
S3	H–2 ->L (4%) H ->L (10%) H ->L+1 (82%)	3.638	340.8	0.0004
S4	H–2 ->L (72%) H–2 ->L+1 (6%) H ->L+1 (9%)	3.697	335.4	0.0009
S5	H–3 ->L (81%) H–3 ->L+1 (9%) H–2 ->L (3%)	3.868	320.6	0.0043
S6	H–5 ->L (7%) H–5 ->L+1 (2%) H–4 ->L (23%) H–4 ->L+1 (5%) H–1 ->L (3%) H–1 ->L+1 (50%) H ->L+2 (4%)	3.902	317.7	0.1005
S7	H–5 ->L (7%) H–4 ->L (22%) H–4 ->L+1 (5%) H–1 ->L (8%) H–1 ->L+1 (29%) H ->L+2 (18%)	3.961	313.0	0.0606

S8	H–5 ->L (6%) H–4 ->L (10%) H–4 ->L+1 (2%) H ->L+2 (68%)	4.017	308.7	0.2472
S9	H–6 ->L (5%) H–5 ->L (49%) H–5 ->L+1 (12%) H–4 ->L (13%) H–4 ->L+1 (3%) H–2 ->L (9%) H–2 ->L+1 (2%)	4.043	306.6	0.006
S10	H–5 ->L (3%) H–4 ->L (2%) H–2 ->L (5%) H–2 ->L+1 (86%)	4.127	300.4	0.0188
S11	H–3 ->L (10%) H–3 ->L+1 (81%) H–1 ->L+8 (3%)	4.201	295.1	0.0499
S12	H–2 ->L+2 (21%) H–1 ->L+2 (27%) H ->L+3 (46%)	4.294	288.7	0.0201
S13	H–1 ->L+2 (60%) H ->L+3 (33%) H ->L+4 (3%)	4.336	285.9	0.0125
S14	H–1 ->L+2 (3%) H ->L+3 (3%) H ->L+4 (56%) H ->L+5 (3%) H ->L+6 (33%)	4.346	285.3	0.001
S15	H–2 ->L+2 (63%) H–1 ->L+2 (8%) H ->L+3 (17%) H ->L+5 (5%) H ->145 (4%)	4.406	281.4	0.0425
S16	H ->L+4 (35%) H ->L+5 (22%) H ->L+6 (35%)	4.592	270.0	0.0316
S17	H–4 ->L (6%) H–4 ->L+1 (27%) H–1 ->L+3 (28%) H–1 ->L+4 (25%) H–1 ->L+6 (4%)	4.616	268.6	0.0094
S18	H–6 ->L (24%) H–4 ->L (10%) H–4 ->L+1 (17%) H–1 ->L+4 (34%) H–1 ->L+6 (5%)	4.627	268.0	0.0092
S19	H–6 ->L (58%) H–5 ->L (7%) H–5 ->L+1 (2%) H–4 ->L+1 (11%) H–1 ->L+3 (5%) H–1 ->L+4 (10%)	4.642	267.1	0.0113

[a] H = HOMO; L = LUMO.

Table S20. Lowest-energy vertical triplet excitations of **4** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm
T1	H–2 ->L+9 (4%) H ->L+2 (79%) H ->L+5 (8%)	2.9132	425.6
T2	H–3 ->L+8 (3%) H–1 ->L (40%) H–1 ->L+1 (40%) H–1 ->L+3 (7%)	2.9297	423.2
T3	H–4 ->L (5%) H–2 ->L (9%) H–1 ->L+1 (4%) H ->L (62%) H ->L+1 (9%)	3.1517	393.39

[a] H = HOMO; L = LUMO.

4.7. Spin density distributions

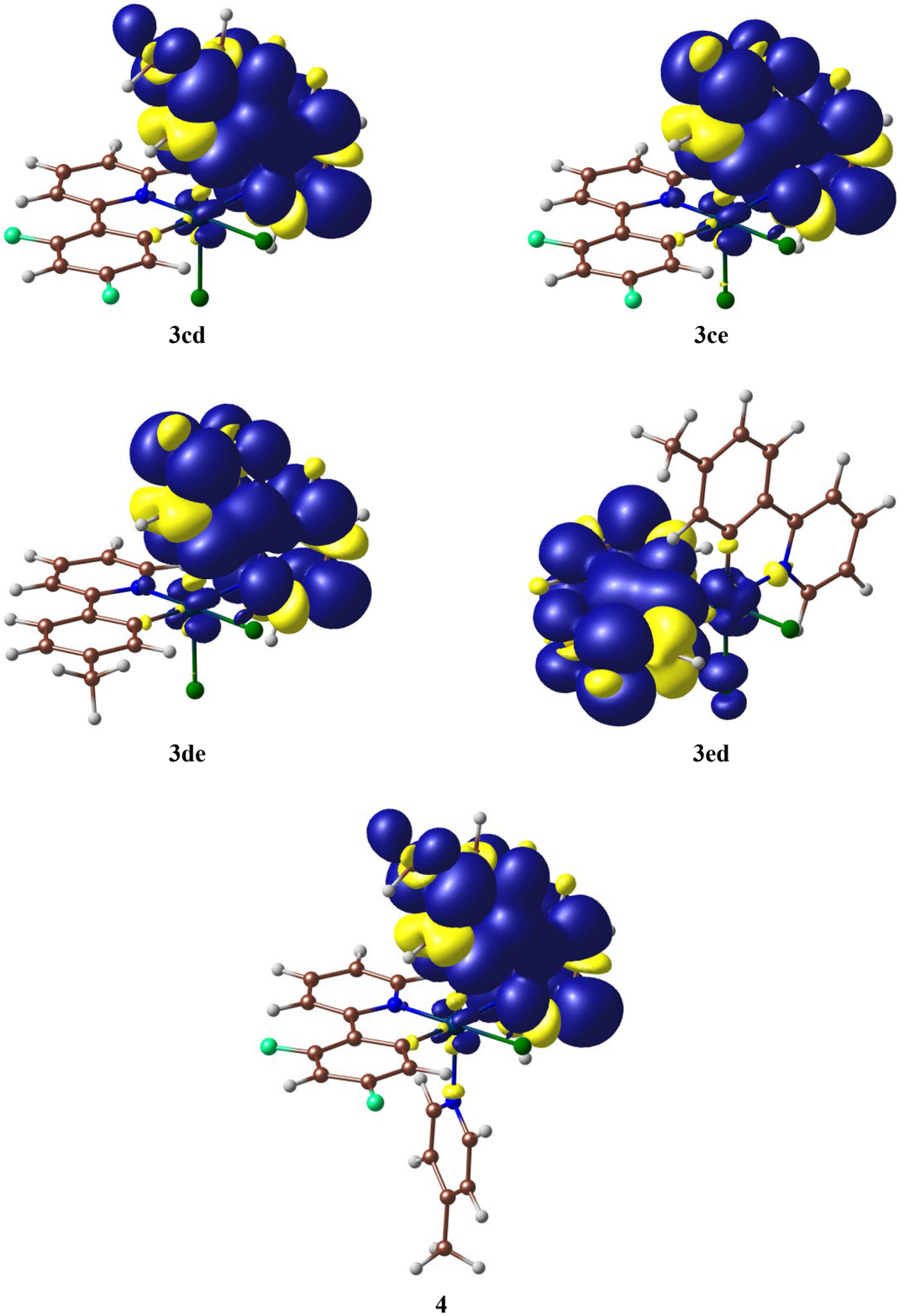


Figure S38. Spin density distributions (0.001 e bohr^{-3}) for the lowest triplet excited state of complexes **3cd**, **3ce**, **3de**, **3ed** and **4**.

4.8. Supplementary computational data

Table S21. Energies, free energies, enthalpies and entropies of the optimized structures in CH_2Cl_2 solution.[a]

Structure	E_0 [b]	ZPE [c]	G [d]	H [e]	S [f]
3bd (S_0)	-2346.1760916	-2345.688972	-2345.756211	-2345.654580	213.901
3cd (S_0)	-2234.9532205	-2234.617434	-2234.675676	2234.589905	180.520
3cd (T_1)	-2234.8501293	-2234.518999	-2234.578519	-2234.490822	184.575
3ce (S_0)	-2516.3816864	-2516.106862	-2516.161669	-2516.081558	168.607
3ce (T_1)	-2516.2942802	-2516.023642	-2516.080393	-2515.997588	174.277
3de (S_0)	-2357.2417314	-2356.923253	-2356.978881	-2356.897721	170.817
3de (T_1)	-2357.1543016	-2356.839917	-2356.897311	-2356.813665	176.048
3ed (S_0)	-2357.2406577	-2356.922205	-2356.978345	-2356.896638	171.965
3ed (T_1)	-2357.1555708	-2356.841226	-2356.899383	-2356.814899	177.811
4 (S_0)	-2062.1978756	-2061.744050	-2061.809564	-2061.710999	207.448
4 (T_1)	-2062.0952872	-2061.646038	-2061.712892	-2061.612342	211.626

[a] Thermal corrections from vibrational calculations at 298.15 K. [b] Electronic energy (Hartrees). [c] Sum of electronic and zero-point energies (Hartrees). [d] Free Energy (Hartrees). [e] Enthalpy (Hartrees). [f] Entropy (cal mol^{-1} K^{-1}).

Table S22. Cartesian coordinates (Å) of the optimized structures at the B3LYP(6-31G**+LANL2DZ) level in CH_2Cl_2 solution.

3bd (S_0)

C	49.853452759	-12.380960595	42.243526565
C	49.576379627	-12.926221181	40.992776026
C	48.254398707	-13.166636036	40.585533598
C	47.207854546	-12.856025766	41.467971374
C	47.471221670	-12.311089089	42.717797336
C	48.796794433	-12.066197395	43.116937213
C	49.162608527	-11.479940177	44.401244364
C	48.250272183	-11.254867440	45.437269170
C	48.683943998	-10.699988687	46.629916682
C	50.016747280	-10.320877534	46.744990562
C	50.907115466	-10.528178487	45.685778426
C	52.264995082	-9.939780166	45.832937486
C	52.642474889	-8.841969365	45.046566071
C	53.827766890	-8.160784417	45.318114170
C	54.672584081	-8.555686908	46.364971816
C	54.284650060	-9.653658419	47.146335785
C	53.091767064	-10.329445125	46.896312923
C	51.839780631	-13.680581024	44.124144296
C	50.829067431	-14.618247919	44.308333486
C	51.015567115	-15.740623656	45.133834331
C	52.252386323	-15.903033340	45.770669305
C	53.273741065	-14.977213030	45.586571292
C	53.089510123	-13.857078147	44.760267473
C	54.149375951	-12.873452261	44.497661570
C	55.490002060	-13.010278500	44.880410288
C	56.412806748	-12.040033919	44.503971003
C	55.989697787	-10.945783053	43.747930388
C	54.644565733	-10.859797359	43.406228731
Cl	52.843646859	-13.089048015	41.213048014
Cl	51.691104420	-9.786004697	41.714245174
H	50.389275152	-13.171941620	40.320171739
H	46.179672994	-13.039490301	41.168787311
H	46.640855940	-12.068970866	43.373206484
H	47.213513726	-11.535175010	45.304706088
H	47.991067302	-10.539613108	47.449423219
H	50.383186333	-9.823943478	47.634650232
H	52.008320039	-8.525595879	44.225980753
H	54.099412094	-7.304597113	44.705932083
H	54.918049827	-9.976589047	47.968471328
H	52.800221780	-11.163941612	47.527555234
H	49.874942965	-14.496363264	43.808079955
H	52.418287518	-16.763334362	46.413130015
H	54.221624521	-15.131735380	46.092479612
H	55.810916841	-13.878440980	45.442836220
H	57.455497070	-12.144219024	44.787289592
H	56.681391719	-10.177146008	43.423104458
H	54.244860165	-10.044053908	42.815002698
N	50.486305463	-11.153897193	44.553690328
N	53.757958886	-11.788302502	43.785377351
Pt	51.688375982	-11.979710041	43.001589062
C	47.966674718	-13.722163931	39.211996526
H	47.042106336	-14.306791283	39.202847369
H	47.847192581	-12.911431047	38.482378524
H	48.782882046	-14.358645414	38.858990956
C	55.973980693	-7.837613648	46.627368535
H	56.249274573	-7.879763728	47.685237037
H	56.792706799	-8.297119156	46.059334859
H	55.919515125	-6.787367310	46.326884971
C	49.894109818	-16.729089609	45.343853351
H	49.293184019	-16.849538924	44.437638635
H	50.277266691	-17.710769129	45.635925749
H	49.217700377	-16.391288572	46.139126956

3cd (S_0)

C	49.757700147	-12.445874292	42.298133583
C	49.434177476	-13.043550149	41.085477931
C	48.089837812	-13.185432994	40.751819081
C	47.055352171	-12.758309642	41.576377620
C	47.407984883	-12.164573562	42.777259766

C	48.742318705	-11.988776435	43.176066474
C	49.186189406	-11.363878112	44.418877926
C	48.379329306	-10.822420988	45.430136760
C	48.964627813	-10.248731148	46.552154403
C	50.355195343	-10.212537064	46.666262269
C	51.115037039	-10.759708880	45.644001311
C	51.812080318	-13.881866873	44.006451942
C	50.861278556	-14.894157973	44.051048143
C	51.085304104	-16.069036137	44.790167046
C	52.296479329	-16.202373722	45.481552256
C	53.255527843	-15.196046344	45.441341982
C	53.033042677	-14.021459333	44.704975542
C	54.016681052	-12.933779049	44.611669898
C	55.292730603	-12.935740921	45.190736549
C	56.131849083	-11.841649178	45.008968450
C	55.695379455	-10.753948415	44.249132417
C	54.420792020	-10.803250907	43.698464221
Cl	52.763170006	-13.106685757	41.129416418
Cl	51.605085652	-9.820654588	41.910502781
H	50.198387583	-13.393490301	40.403633205
H	46.016167013	-12.878918926	41.297727963
H	47.305737096	-10.854789966	45.323530775
H	48.337715866	-9.830388698	47.332599298
H	50.848945657	-9.772001556	47.523922327
H	49.930831226	-14.792860906	43.503310320
H	52.491642174	-17.104350999	46.054564326
H	54.184774734	-15.333502780	45.984916504
H	55.627183325	-13.787159492	45.770347724
H	57.121965117	-11.839724296	45.453457284
H	56.324560621	-9.887699493	44.081589396
H	54.010344154	-10.001642574	43.093520326
N	50.543294624	-11.314900006	44.561908980
N	53.612619825	-11.857952653	43.887023992
Pt	51.626127856	-12.118076450	42.997988963
C	50.030396032	-17.146608924	44.849240849
H	49.506235648	-17.244527565	43.893972619
H	50.465192402	-18.116610348	45.105100007
H	49.275717254	-16.913273931	45.610691773
F	46.400337896	-11.748961825	43.576853098
F	47.771045932	-13.764689832	39.579839062
H	52.196096416	-10.758629200	45.670187118

3cd (T_1)

$\langle S^2 \rangle = 2.02851$

C	1.756700352	-0.063511130	-0.613063522
C	2.456977529	0.450810760	-1.698422813
C	3.835972318	0.607755721	-1.587396362
C	4.546063346	0.275825315	-0.439266688
C	3.822675601	-0.234780319	0.626152621
C	2.431924325	-0.420161517	0.582056672
C	1.608997568	-0.959036819	1.661667246
C	2.043676106	-1.393205441	2.922467053
C	1.126136198	-1.892097226	3.839057548
C	-0.225782917	-1.960928506	3.499217379
C	-0.612677117	-1.522161037	2.242247091
C	-0.736056015	1.434062211	0.193130658
C	0.114315144	2.474585002	0.446176369
C	-0.353380170	3.721847396	0.954335894
C	-1.762221756	3.868968122	1.202833101
C	-2.644854625	2.859998551	0.966404834
C	-2.186578856	1.576872657	0.447036084
C	-3.025048290	0.501657253	0.179437639
C	-4.459990549	0.478620911	0.339783075
C	-5.177505400	-0.639635554	0.002593313
C	-4.497348405	-1.777968605	-0.505787707
C	-3.098218612	-1.727118751	-0.638330968
Cl	-0.707415757	0.408061558	-2.748033901
Cl	0.136352545	-2.766913691	-1.358328824
H	1.955865365	0.725237441	-2.617785319
H	5.618797256	0.406364343	-0.373687552
H	3.093354394	-1.337190558	3.167586214
H	1.465911575	-2.226961372	4.813575373
H	-0.970724529	-2.345002110	4.185549999
H	1.176053361	2.371313385	0.250216164
H	-2.124232886	4.817660880	1.590310012
H	-3.699912338	3.008176854	1.165415432
H	-4.964362340	1.357663622	0.722416773
H	-6.255912535	-0.655351097	0.118901393
H	-5.028643294	-2.677587804	-0.791178578
H	-2.531989537	-2.572343826	-1.019283685
N	0.279379062	-1.039095584	1.361079419
N	-2.385824361	-0.663440704	-0.305785800
Pt	-0.239527067	-0.396338715	-0.532426127
C	0.581807070	4.862741115	1.213287876
H	0.341247026	5.723967160	0.574625007
H	0.500296365	5.216586399	2.249578201
H	1.621812765	4.584764946	1.026895032
F	4.515941963	-0.556272712	1.741544488
F	4.518268591	1.106217956	-2.634945384
H	-1.642649796	-1.552986030	1.914124276

3ce (S_0)

C	49.759594231	-12.460554145	42.284596594
C	49.442348713	-13.052449005	41.068162246
C	48.098858961	-13.235941111	40.750739401
C	47.062174007	-12.857310450	41.595759584
C	47.410363376	-12.270572633	42.801365853
C	48.743148719	-12.054415263	43.185302945
C	49.183187701	-11.437167256	44.433173490
C	48.374254814	-10.939556489	45.464717064
C	48.958087500	-10.368548254	46.589041867
C	50.348387901	-10.291777389	46.685223537
C	51.110646561	-10.796557344	45.643028789
C	51.835104979	-13.867710694	43.909602663
C	50.997499364	-15.009762353	44.029237732
C	51.572893684	-15.993722943	44.793810696
C	53.032090687	-13.999064182	44.585240669
C	54.034104213	-12.952364918	44.565572633
C	55.302362687	-12.997667730	45.158409111
C	56.153340559	-11.905752811	45.022729176
C	55.734960855	-10.786251405	44.298221968
C	54.463651673	-10.798127519	43.734119285
Cl	52.767840789	-12.983143190	41.056827058
Cl	51.595017420	-9.775528734	41.965185788
H	50.208847406	-13.365205354	40.371206916
H	46.024018469	-13.010037407	41.329266027
H	47.300720179	-11.003171108	45.372190105
H	48.329887958	-9.983798823	47.385533480
H	50.840230319	-9.852100258	47.544392808

H	50.021786212	-15.109107496	43.571164496
H	55.612230363	-13.879386143	45.708224273
H	57.139456542	-11.929217853	45.475337440
H	56.376000883	-9.922304034	44.168692871
H	54.070258661	-9.967842859	43.156721235
N	50.539659600	-11.348546736	44.559107410
N	53.639148010	-11.845538631	43.875021088
Pt	51.624347122	-12.088413790	42.965930188
F	46.401222521	-11.903399136	43.621573338
F	47.784501428	-13.808497400	39.574825108
H	52.191462834	-10.763787143	45.653926348
S	53.143283527	-15.550410577	45.381900984
H	51.166940807	-16.963204662	45.049744733

3ce (T_1)

$\langle S^2 \rangle = 2.034291$

C	-1.820553181	-0.547958099	-0.211095481
C	-2.492655247	-1.742646812	-0.437992067
C	-3.854612290	-1.801665438	-0.152896782
C	-4.570516023	-0.721960220	0.350861374
C	-3.872504371	0.454792269	0.567913680
C	-2.500302863	0.585196402	0.302312041
C	-1.704208441	1.793699007	0.498300357
C	-2.150638518	3.036351770	0.970397836
C	-1.257817009	4.094771748	1.087933532
C	0.080147575	3.916746187	0.732595238
C	0.479433893	2.672355612	0.269811733
C	0.728851092	-0.786161999	1.288135087
C	0.096262894	-1.282350438	2.399372738
C	0.968686382	-1.548146227	3.475491812
C	2.191376837	-0.643850821	1.481378468
C	3.005918014	-0.159347181	0.468844420
C	4.427467316	-0.001797430	0.517858656
C	5.099176652	0.465436582	-0.589083569
C	4.375998711	0.784266660	-1.760155525
C	2.983718303	0.623924028	-1.761332754
Cl	0.640061283	-2.419660368	-1.355234751
Cl	-0.350767034	0.618190091	-2.872546741
H	-1.985835509	-2.614634270	-0.830466141
H	-5.629400222	-0.789825752	0.565936716
H	-3.189671326	3.158664900	1.236023521
H	-1.606310046	5.054880818	1.453848450
H	0.805115418	4.718100557	0.808330911
H	-0.967796993	-1.472281102	2.470735799
H	4.957728045	-0.260781369	1.427923586
H	6.177267059	0.584394752	-0.564012543
H	4.873487477	1.146793251	-2.651447199
H	2.381254075	0.855487854	-2.634677482
N	-0.388936419	1.652973589	0.161349163
N	2.314350227	0.186167678	-0.701142821
Pt	0.144714447	-0.212020390	-0.549813236
F	-4.570478949	1.502902604	1.058251129
F	-4.511751419	-2.955105404	-0.370270460
H	1.498972760	2.468323259	-0.027647135
S	2.671395494	-1.168500335	3.102998813
H	0.719930497	-1.944629683	4.450013034

3de (S_0)

C	49.762792208	-12.462081615	42.278295098
C	49.419590493	-13.062303079	41.072624057
C	48.072455133	-13.267573527	40.727306586
C	47.073812202	-12.862969312	41.626456045
C	47.403645206	-12.261290706	42.835348981
C	48.749852495	-12.054623759	43.174539427
C	49.196604990	-11.432891504	44.415836903
C	48.377983661	-10.934512741	45.437893599
C	48.947216400	-10.355732216	46.564142543
C	50.338609499	-10.273178078	46.668607424
C	51.111502241	-10.778901768	45.635072715
C	51.838972630	-13.861167258	43.905927527
C	50.996556793	-15.000547789	44.024262990
C	51.562780313	-15.985394963	44.794113280
C	53.031572093	-13.996290658	44.589165418
C	54.041384633	-12.956018887	44.576124268
C	55.305400165	-13.012413466	45.177879024
C	56.166275768	-11.927430133	45.048496668
C	55.761923494	-10.804333233	44.321612978
C	54.493816364	-10.806619226	43.749375994
Cl	52.782526569	-12.987880491	41.051921267
Cl	51.619973684	-9.770440800	41.955980803
H	50.198676514	-13.376046449	40.387091124
H	46.029101164	-13.021871186	41.374737963
H	47.301643170	-11.001448901	45.339791069
H	48.313152516	-9.969272590	47.355188499
H	50.821461990	-9.827077794	47.529591667
H	50.023173450	-15.095131396	43.560297365
H	55.604676887	-13.896732838	45.729534823
H	57.149116672	-11.959142085	45.507826224
H	56.410909118	-9.945551373	44.196817319
H	54.110902119	-9.972734150	43.169764714
N	50.549973529	-11.338709278	44.549171419
N	53.659811853	-11.846620005	43.883526660
Pt	51.633757005	-12.086367303	42.956841992
H	52.192236439	-10.741469304	45.653665146
S	53.131835836	-15.546969549	45.390327391
H	51.151345742	-16.952604395	45.049993446
H	46.610701145	-11.957838246	43.511957182
C	47.713496002	-13.890524054	39.400485864
H	46.726370719	-14.359963436	39.432860029
H	47.690642053	-13.131115543	38.609029743
H	48.447042510	-14.645246278	39.102345021

3de (T_1)

$\langle S^2 \rangle = 2.034702$

C	-1.992018511	-0.303358995	-0.129468699
C	-2.801587930	-1.390500689	-0.436756291
C	-4.163784796	-1.396205030	-0.090108517
C	-4.695127407	-0.286084107	0.584547954
C	-3.896303916	0.807097838	0.898733070
C	-2.537826150	0.811068350	0.545151576
C	-1.621567655	1.910582170	0.825970918
C	-1.940924977	3.116808482	1.463539374
C	-0.962028125	4.082783804	1.653888076
C	0.339353145	3.844661900	1.202799916
C	0.612588056	2.638841314	0.576130855
C	0.588847064	-0.929845539	1.188169414
C	-0.041043892	-1.495974113	2.267446469
C	0.844291992	-1.955185578	3.264723996
C	2.065499249	-0.933242449	1.325923084

C	2.885029360	-0.408109655	0.337138698
C	4.316135529	-0.379431588	0.342904587
C	4.990286865	0.151438300	-0.733734377
C	4.260649866	0.661110387	-1.830663795
C	2.859781372	0.620732602	-1.788705892
Cl	0.239853043	-2.243962429	-1.605783451
Cl	-0.516147516	1.025461126	-2.736755477
H	-2.380369015	-2.245699427	-0.953218546
H	-5.744710961	-0.280524384	0.864571086
H	-2.954899728	3.289220060	1.802497087
H	-1.209662736	5.016249788	2.148388287
H	1.130592453	4.573464302	1.330218262
H	-1.114438322	-1.602810311	2.366319052
H	4.851144603	-0.783911778	1.195402314
H	6.075018479	0.174609334	-0.741546107
H	4.758983500	1.078683853	-2.697124536
H	2.251640389	0.999606928	-2.605060241
N	-0.342447016	1.709098943	0.400064961
N	2.189053770	0.124639314	-0.756264532
Pt	-0.016714786	-0.103842537	-0.541354062
H	1.596782951	2.394416724	0.199768770
S	2.558721148	-1.677491430	2.855853019
H	0.599058237	-2.439036388	4.199882453
H	-4.333759164	1.652509453	1.420653913
C	-5.039964401	-2.566902318	-0.462982841
H	-5.891626441	-2.661878050	0.216522099
H	-5.441448952	-2.442906288	-1.476489436
H	-4.479040047	-3.505769180	-0.450142453

3ed (S_0)

C	49.744531148	-12.409694655	42.342411008
C	49.186620527	-12.986533946	41.169331517
C	47.813782922	-12.959750540	41.184180760
C	48.781285624	-11.956897739	43.223307397
C	49.191162296	-11.334233815	44.453212004
C	48.369390511	-10.795318170	45.452855821
C	48.944146537	-10.216248978	46.575764969
C	50.337145319	-10.173959038	46.697063401
C	51.110104049	-10.719650850	45.682837947
C	51.797969542	-13.866801197	44.006821837
C	50.838577328	-14.871107012	44.054702324
C	51.057466312	-16.049766148	44.788880193
C	52.272322970	-16.195968455	45.471514187
C	53.240085392	-15.198271852	45.427118862
C	53.022662865	-14.019463700	44.695720761
C	54.014400827	-12.939714037	44.598032101
C	55.293773082	-12.953242241	45.169576656
C	56.140656180	-11.865610800	44.985318038
C	55.708189249	-10.772743997	44.230707312
C	54.429903923	-10.810692250	43.687516602
Cl	52.658385978	-13.107733423	41.097503908
Cl	51.615772546	-9.798800997	41.922014450
H	49.768372594	-13.398075199	40.354990862
H	47.292575876	-10.834153482	45.333571861
H	48.313420068	-9.797110169	47.352756347
H	50.821009649	-9.728092491	47.557496930
H	49.905471624	-14.758169051	43.513927732
H	52.463408028	-17.101329714	46.040634264
H	54.172016270	-15.345639302	45.963507421
H	55.624476583	-13.808523012	45.745694890
H	57.133383704	-11.872665474	45.423942529
H	56.343114633	-9.910969428	44.061655078
H	54.022126815	-10.004228716	43.087156176
N	50.551566670	-11.282539389	44.598399667
N	53.614412149	-11.859500391	43.877291047
Pt	51.618967400	-12.100289639	43.004716658
C	49.993113960	-17.117824804	44.853100191
H	49.452997718	-17.200273794	43.905326540
H	50.422120813	-18.094784168	45.091945560
H	49.252813457	-16.885401689	45.628852924
H	52.191540147	-10.711811248	45.718338385
S	47.165323088	-12.232756728	42.621875545
H	47.132192518	-13.326015016	40.428006897

3ed (T_1)

$\langle S^2 \rangle = 2.032977$

C	1.835272029	-0.139580696	-0.922578787
C	2.572086477	0.144005765	-2.053333554
C	3.944418416	0.291588140	-1.806237598
C	2.682266308	-0.218792898	0.285976004
C	2.081600821	-0.472256554	1.509523871
C	2.707487234	-0.532302438	2.790691667
C	1.961045994	-0.808605311	3.911109883
C	0.568109788	-1.023887437	3.778644641
C	-0.017696952	-0.941909362	2.515981020
C	-0.606810801	1.446818865	-0.113599204
C	0.241150896	2.545414266	-0.193615584
C	-0.216758047	3.838835182	0.111551616
C	-1.555013964	4.001116710	0.494372230
C	-2.411430185	2.908570906	0.575720664
C	-1.955157876	1.615394522	0.273791625
C	-2.813028615	0.424482999	0.330872462
C	-4.180702926	0.417202745	0.634406193
C	-4.876621212	-0.786925633	0.641226790
C	-4.205587470	-1.974830405	0.342357101
C	-2.849255560	-1.910762535	0.047800345
Cl	-0.806876325	-0.218001387	-2.776585395
Cl	0.335594947	-3.001711081	-0.833054998
H	2.150302009	0.246962076	-3.045329595
H	3.775282424	-0.353643961	2.856827261
H	2.431513573	-0.858809753	4.886812827
H	-0.053348148	-1.255143589	4.634984597
H	1.271492012	2.416351179	-0.506351924
H	-1.930059735	4.993258836	0.729046475
H	-3.442625909	3.069088130	0.873940815
H	-4.694777123	1.344514483	0.854844004
H	-5.936753883	-0.797738434	0.873468900
H	-4.716863494	-2.930228718	0.332559285
H	-2.258856530	-2.786483544	-0.200291937
N	0.692737618	-0.686984366	1.416446366
N	-2.181815821	-0.746281741	0.052910652
Pt	-0.083862441	-0.484530847	-0.500592933
C	0.724116342	5.017128762	0.048705000
H	1.470033146	4.890905505	-0.741311819
H	0.183202357	5.949920871	-0.132939243
H	1.268394352	5.132701560	0.994390283
H	-1.080911430	-1.096269545	2.380172378
S	4.377117466	0.064561878	-0.085778004

H	4.729753935	0.518772080	-2.513936115

4 (S_0)

C	49.808116134	-12.430092480	42.344615613
C	49.496350458	-13.003744907	41.118895051
C	48.154190475	-13.101477013	40.754271818
C	47.116811717	-12.651461082	41.561658820
C	47.459484625	-12.087169007	42.779962909
C	48.789841785	-11.959495205	43.211220036
C	49.222642310	-11.397702381	44.487549734
C	48.406741905	-10.907195130	45.517242087
C	48.979759796	-10.426102048	46.688196825
C	50.368104781	-10.434657098	46.836127319
C	51.138719097	-10.925247642	45.794185995
C	51.828317117	-13.907003798	44.063498414
C	50.858182128	-14.901086279	44.087873588
C	51.056188613	-16.087819231	44.815409912
C	52.259923659	-16.249879022	45.514311027
C	53.236861115	-15.261350256	45.492895171
C	53.040784011	-14.074415159	44.768001769
C	54.044214673	-13.005504210	44.690557896
C	55.319336577	-13.043802037	45.271189483
C	56.186500393	-11.970720484	45.103048492
C	55.779400102	-10.864647956	44.352764161
C	54.505679989	-10.877670638	43.801802801
Cl	52.826628148	-13.114966217	41.215587112
H	50.261850487	-13.377421040	40.451069976
H	46.080713408	-12.735957142	41.259116915
H	47.334856821	-10.913173351	45.390535939
H	48.344959614	-10.049984979	47.483376660
H	50.851267316	-10.073648039	47.735812676
H	49.933726990	-14.778164596	43.535175892
H	52.434803511	-17.161497696	46.078286654
H	54.159144034	-15.422105838	46.041288804
H	55.631578142	-13.909866276	45.841012096
H	57.175525263	-11.998822812	45.548446664
H	56.430293939	-10.013414122	44.192641687
H	54.135315712	-10.053361024	43.203863149
N	50.578985037	-11.378956806	44.656484596
N	53.665452882	-11.911126870	43.977853404
Pt	51.678331033	-12.134523597	43.073824243
C	49.983143096	-17.147416819	44.857064999
H	49.402129073	-17.164609894	43.930778590
H	50.411254688	-18.140960122	45.015384037
H	49.281703465	-16.958573091	45.679294523
F	46.449979537	-11.651793717	43.562196688
F	47.846682877	-13.655262062	39.570041557
H	52.218754569	-10.958042555	45.845801150
N	51.634603847	-10.100024562	42.028781411
C	51.545487858	-8.949152630	42.723365921
C	51.648402091	-10.027618826	40.682869667
C	51.476313120	-7.706232379	42.108029355
H	51.531822703	-9.027374076	43.804130440
C	51.578092374	-8.820661832	40.001738483
H	51.730032444	-10.968700238	40.153428359
C	51.487545331	-7.614958511	40.710573578
H	51.413201643	-6.815066617	42.723466517
H	51.596311788	-8.826729484	38.916829924
C	51.386392729	-6.292802645	40.000991497
H	52.062514298	-6.253790534	39.142349974
H	50.368949083	-6.146618859	39.619640441
H	51.616426926	-5.460231358	40.669363529

4 (T_1)

$\langle S^2 \rangle = 2.027044$

C	0.754010665	1.528145936	-0.482478361
C	1.130794360	2.148167620	-1.667012180
C	1.775664176	3.382077401	-1.595550851
C	2.056747186	4.019319942	-0.393198044
C	1.666749391	3.377931583	0.771585922
C	1.012888695	2.135065038	0.772470807
C	0.562545679	1.409824009	1.957626763
C	0.672999587	1.820342722	3.293977687
C	0.173928839	1.016016376	4.311426635
C	-0.436416280	-0.200314453	3.999281973
C	-0.523668083	-0.571088579	2.666728018
C	-2.054463263	0.425283462	-0.350412144
C	-2.437292813	1.728601585	-0.499204934
C	-3.812053585	2.111447540	-0.501711545
C	-4.804264647	1.083354006	-0.336231408
C	-4.465723709	-0.225694154	-0.183355905
C	-3.067213350	-0.637230523	-0.183885545
C	-2.643448754	-1.953819253	-0.046512872
C	-3.495606622	-3.110378502	0.085536046
C	-2.956348250	-4.368451532	0.151387268
C	-1.545742948	-4.523814099	0.088726120
C	-0.744279154	-3.377229651	-0.018129564
Cl	-0.318601720	-0.686349777	-2.679807433
H	0.932225842	1.702421885	-2.633394699
H	2.558831084	4.977933387	-0.359753080
H	1.144278849	2.764901648	3.519389652
H	0.258645835	1.338902426	5.343597305
H	-0.840092749	-0.852086842	4.764409499
H	-1.694274905	2.507320611	-0.629854443
H	-5.852392181	1.369653731	-0.335647007
H	-5.240805566	-0.973173381	-0.062214066
H	-4.569371254	-2.972845415	0.122945179
H	-3.597672102	-5.237925419	0.244830820
H	-1.078436415	-5.500110949	0.123751836
H	0.336427567	-3.463944789	-0.063641304
N	-0.030840550	0.208728188	1.685716474
N	-1.240552225	-2.149012081	-0.062329809
Pt	-0.154461458	-0.282586439	-0.321859241
C	-4.226815453	3.538891199	-0.676206317
H	-3.365915338	4.202224962	-0.785424262
H	-4.865382037	3.658193760	-1.561906863
H	-4.822063561	3.885010538	0.179553633
F	1.941293586	3.999759825	1.937512117
F	2.142476002	3.985755419	-2.738088967
H	-0.981481131	-1.501209227	2.356716342
N	1.934330200	-1.200895592	-0.259194249
C	2.451873461	-1.707416615	0.876700204
C	2.709171812	-1.200182785	-1.362708364
C	3.736628222	-2.230254034	0.946449951
H	1.816812988	-1.696745660	1.754395553
C	4.002289774	-1.702865225	-1.364227870
H	2.261692301	-0.793649333	-2.261102549
C	4.553145923	-2.236636235	-0.190916177
H	4.093307356	-2.629851740	1.889892393

H	4.575816702	-1.677500309	-2.285113242	H	6.679335404	-1.950774775	-0.212882582
C	5.957470325	-2.773818629	-0.158766185	H	6.152256608	-3.334686282	0.757675832
H	6.146564301	-3.425396300	-1.016966826				