ELECTRONIC SUPPLEMENTARY INFORMATION

Luminescent halido(aryl) Pt(IV) complexes obtained via oxidative addition of iodobenzene or diaryliodonium salts to bis-cyclometalated Pt(II) precursors

Juan-Carlos López-López, Delia Bautista and Pablo González-Herrero*

Departamento de Química Inorgánica, Facultad de Química, Universidad de Murcia, Campus de Espinardo, 19, 30100 Murcia, Spain.

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1. Additional experimental procedures and data

1.1. Synthesis of *cis*-[Pt(bppy)$_2$] (1a)

A solution of [$Pt_2Me_4(\mu\text{-}SMe_2)_2$] (200 mg, 0.35 mmol) and 4-(*tert*-butyl)-2-phenylpyridine[1] (2.78 mmol) in acetone (15 mL) was refluxed for 4 h. The solvent was removed under reduced pressure and the residue was subjected to three successive dissolution/evaporation cycles using acetone (10 mL). A solution of the crude mixture in Et_2O (60 mL) was irradiated under N_2 for 24 h. Then, solvent was evaporated and crude was passed through a silica gel column using a mixture of AcOEt/hexane (1:15) as the eluent. The solvent was removed under reduced pressure and the residue was vaccum-dried to give **1a** as a yellow solid (156 mg, 40%). ^{1}H NMR (400 MHz, $(CD_3)_2CO$): 8.87 (d, J = 5.9 Hz, 1H), 8.09 (d with satellites, J_{PtH} = 49.6 Hz, J_{HH} = 7.8 Hz, 1H), 8.06 (d, J = 2.0 Hz, 1H), 7.79 (dd, J = 7.7, 1.4 Hz, 1H), 7.48 (dd, J = 6.0, 2.1 Hz, 1H), 7.18 (td, J = 7.4, 1.4 Hz, 1H), 7.07 (td, J = 7.4, 1.2 Hz, 1H), 1.45 (s, 9H). ^{13}C{^{1}H} NMR (150.8 MHz, $(CD_3)_2CO$): 166.7 (C), 163.4 (C), 150.4 (C), 148.7 (CH), 147.8 (C), 138.0 (J_{PtC} = 104.7 Hz, CH), 124.2 (J_{PtC} = 38.5 Hz, CH), 123.3 (CH), 120.6 (CH), 116.9 (CH), 36.0 (C), 30.6 (CH_3). Elemental analysis calcd (%) for $C_{30}H_{32}N_2Pt$: C 58.52, H 5.24, N 4.55; found: C 58.51, H 5.06, N 4.31.

1.2. Photophysical characterization

UV-vis absorption spectra were recorded on a Perkin-Elmer Lambda 750S spectrophotometer. Excitation and emission spectra were recorded on a Jobin Yvon Fluorolog 3-22 spectrofluorometer. Solution measurements were carried out using 10 mm quartz fluorescence cells (298 K) or 5 mm quartz NMR tubes (77 K). For the low-temperature measurements, a liquid nitrogen Dewar with quartz windows was employed. The photophysical data in PMMA thin films were measured using quartz slides as sample holders. Lifetimes were measured using an IBH FluoroHub controller in MCS mode and the Fluorolog's FL-1040 phosphorimeter pulsed xenon lamp as excitation source; the estimated uncertainty is ±10% or better. Emission quantum yields (Φ) were measured using a Hamamatsu C11347 Absolute PL Quantum Yield Spectrometer; the estimated uncertainty is ±5% or better. Emission data were obtained under rigorous exclusion of oxygen, by bubbling argon through the solutions for 30 min or placing the PMMA films under argon.

1.3. X-ray structure determinations

Single crystals of **2b**, **4b**·0.5CH_2Cl_2, **5b**, **5b'**·CH_2Cl_2 and **6b**·CH_2Cl_2·H_2O suitable for X-ray diffraction were obtained by slow diffusion of Et_2O into solutions of the complexes in CH_2Cl_2. The data were collected on a Bruker D8 QUEST diffractometer with monochromated Mo-*K*α radiation performing φ and ω scans. The structures were solved by direct methods and refined anisotropically on F^2 using the program SHELXL-2018, except for **5b**, which was solved using SHELXL-2016 (G. M. Sheldrick, University of Göttingen).[2,3] Numerical details are given in Tables S1 and S2. Methyl hydrogens were included as part of rigid idealized methyl groups allowed to rotate but not tip; the water hydrogen atoms in **6b**·CH_2Cl_2·H_2O were located in a difference Fourier map and refined freely, using DFIX 0.82 0.02 instruction; other hydrogens were included using a riding model. *Special features of refinement:* In **4b**, the structure contains one resolved CH_2Cl_2 molecule; additionally, there is a poorly-resolved region of residual electron density that could not be adequately modelled and was "removed" using the program SQUEEZE,[4] which is part of the PLATON system; the void volume per cell was 375 Å^3, with a void electron count per cell of 87; this additional solvent was not taken into account when calculating derived parameters such as the formula weight, because its nature was uncertain.

Table S1. Crystallographic data for **2b**, **4b**·0.5CH_2Cl_2 and **5b**.

	2b	**4b**·0.5CH_2Cl_2	**5b**
formula	$C_{30}H_{25}IN_2Pt$	$C_{36.50}H_{33}ClF_6N_3PPt$	$C_{30}H_{25}ClN_2Pt$
fw	735.51	889.17	644.06
T (K)	100(2)	100(2)	100(2)
λ (Å)	0.71073	0.71073	0.71073
cryst syst	Monoclinic	Triclinic	Monoclinic
space group	$P2_1/n$	P-1	$P2_1/n$
a (Å)	9.442(2) Å	12.0157(8)	9.3492(3)
b (Å)	18.463(4) Å	14.6749(11)	18.3426(7)
c (Å)	14.194(3) Å	21.5970(15)	13.7398(5)
α (°)	90	82.664(3)	90
β (°)	96.155(8)	77.421(3)	97.0630(10)
γ (°)	90	73.664(3)	90
V (Å^3)	2460.1(9)	3557.7(4)	2338.34(14)
Z	4	4	4
ρ_{calcd} (Mg m^{-3})	1.986	1.660	1.829
μ (mm^{-1})	6.980	4.126	6.137
R1[a]	0.224	0.0295	0.0160
wR2[b]	0.0451	0.0700	0.0365

[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.

Table S2. Crystallographic data for **5b'** and **6b**.

	5b'·CH_2Cl_2	**6b**·CH_2Cl_2·H_2O
formula	$C_{35}H_{35}Cl_3N_2Pt$	$C_{31}H_{29}Cl_2FN_2OPt$
fw	785.09	730.55
T (K)	100(2)	100(2)
λ (Å)	0.71073	0.71073
cryst syst	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1/c$
a (Å)	12.4548(10)	13.1925(10)
b (Å)	11.0478(9)	9.5664(7)
c (Å)	23.525(2)	22.7013(18)
α (°)	90	90
β (°)	99.262(3)	104.895(3)
γ (°)	90	90
V (Å^3)	3194.8(5)	2768.7(4)
Z	4	4
ρ_{calcd} (Mg m^{-3})	1.632	1.753
μ (mm^{-1})	4.670	5.295
R1[a]	0.0293	0.0278
wR2[b]	0.0634	0.0669

[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.

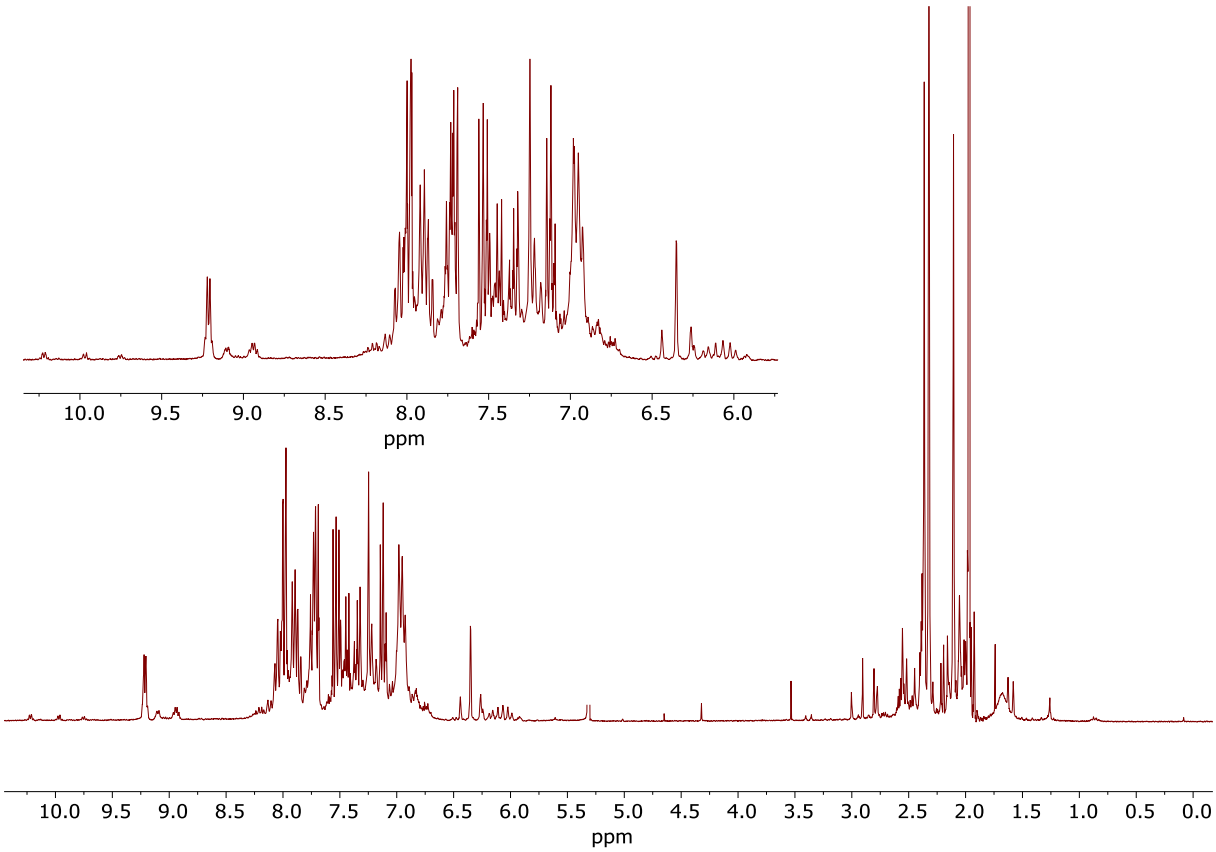

Figure S1. ^{1}H NMR spectrum (CD_2Cl_2, 300 MHz) of the crude product mixture resulting from the reaction of **1b** with $(Ph_2I)PF_6$ in MeCN.

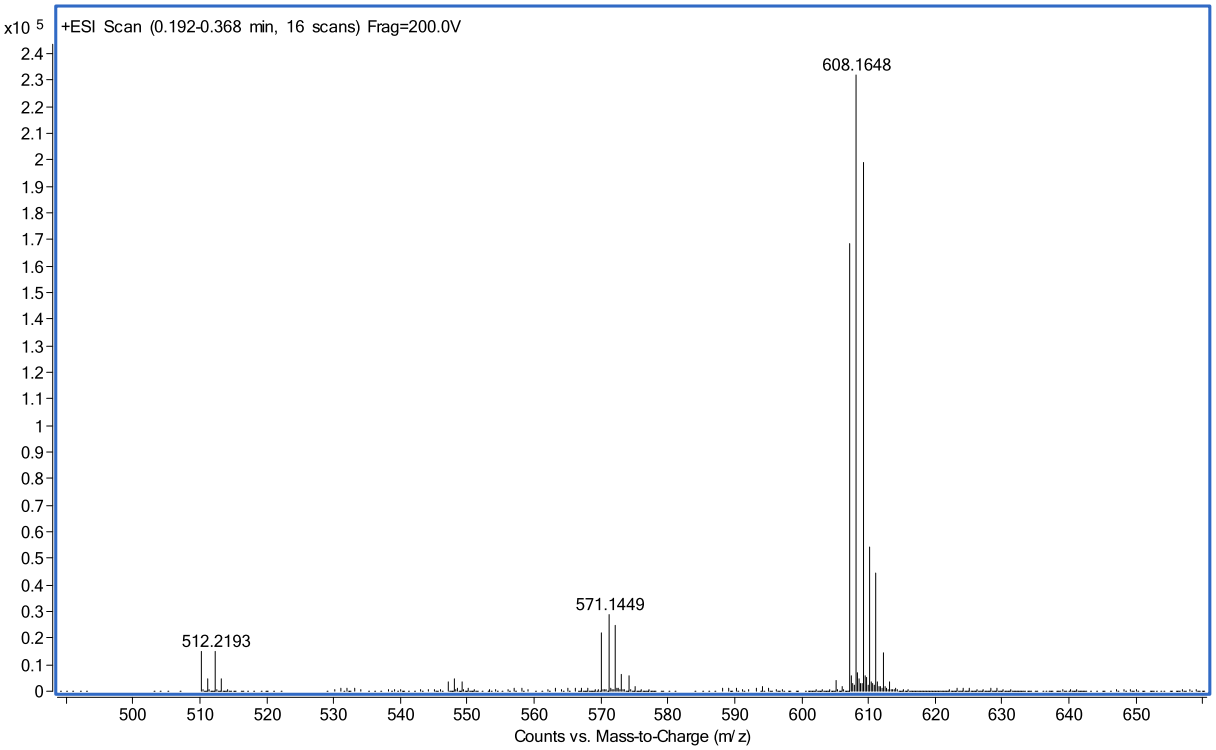

Figure S2. ESI(+) mass spectrum of the crude product mixture resulting from the reaction of **1b** with $(Ph_2I)PF_6$ in MeCN. The most abundant ion at *m/z* 608.1648 corresponds to $[Pt(Ph)(tpy)_2]^+$ and the ion at *m/z* 571.1449 to $[Pt(CH_2CN)(tpy)_2]^+$.

2. Additional photophysical data

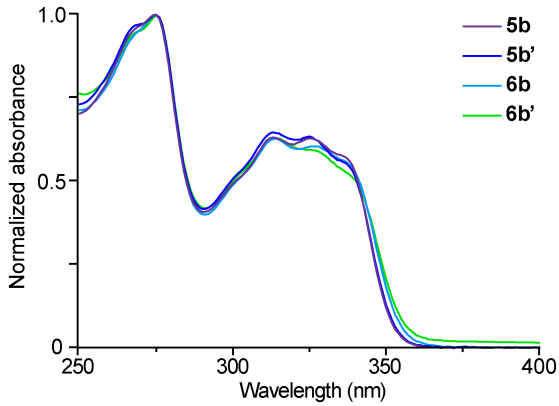

Figure S3. Electronic absorption spectra of complexes **5b**, **5b'**, **6b** and **6b'** in a CH_2Cl_2 solution at 298 K

Table S3. Emission data for the series of complexes **5** and **6** in 2-MeTHF glasses at 77 K.

Complex	λ_{em}/nm[a]	τ/μs[b]
5a	442, *472*, 500, 538 (sh)	227
5b	*450*, 466, 473, 483, 508, 520	317
5b'	*450*, 465, 472, 482, 501, 509, 521	301
5c	*509*, 528, 539,550, 571, 595	353
5d	*552*, 598, 655	83.7
6a	*443*, 472, 503	175
6b	*450*, 475, 484, 508, 522	242
6b'	*451*, 484, 510, 522	255
6c	*512*, 530, 552, 573, 599	260
6d	*552*, 597, 656	61.8

[a] The most intense peak is italicized. [b] Emission lifetime.

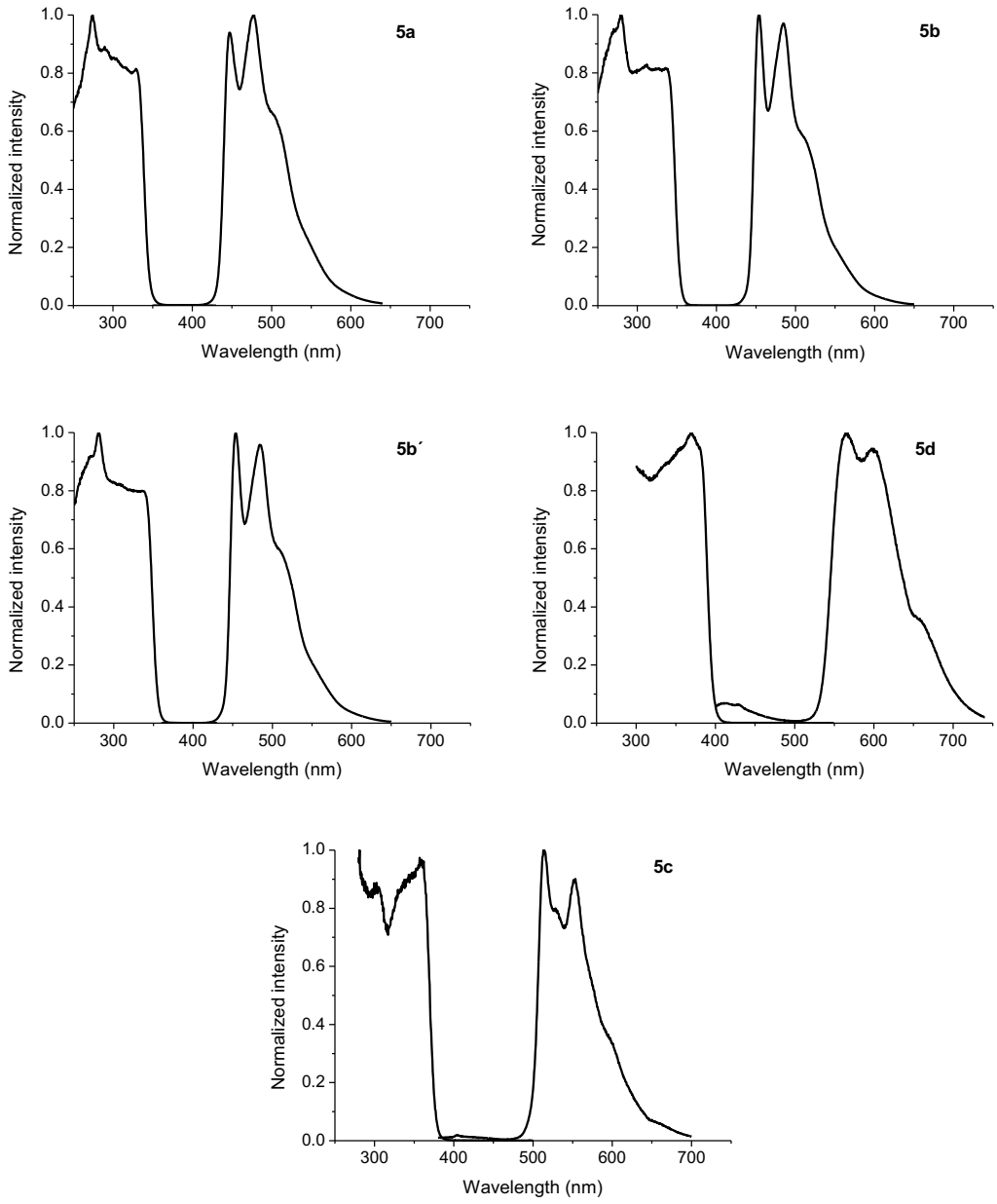

Figure S4. Excitation and emission spectra of the series of complexes **5** in CH_2Cl_2 at 298 K.

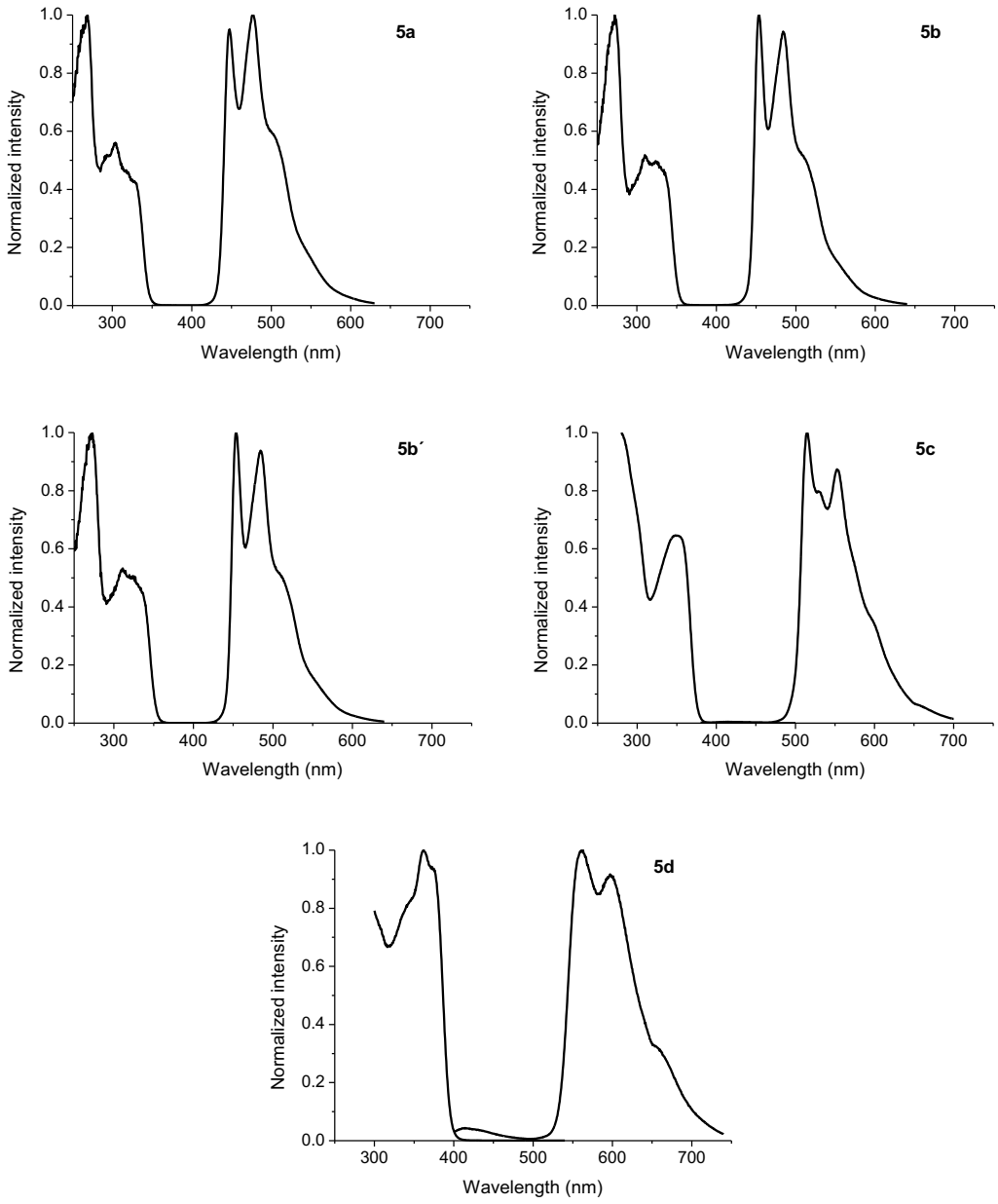

Figure S5. Excitation and emission spectra of the series of complexes **5** in PMMA films at 298 K.

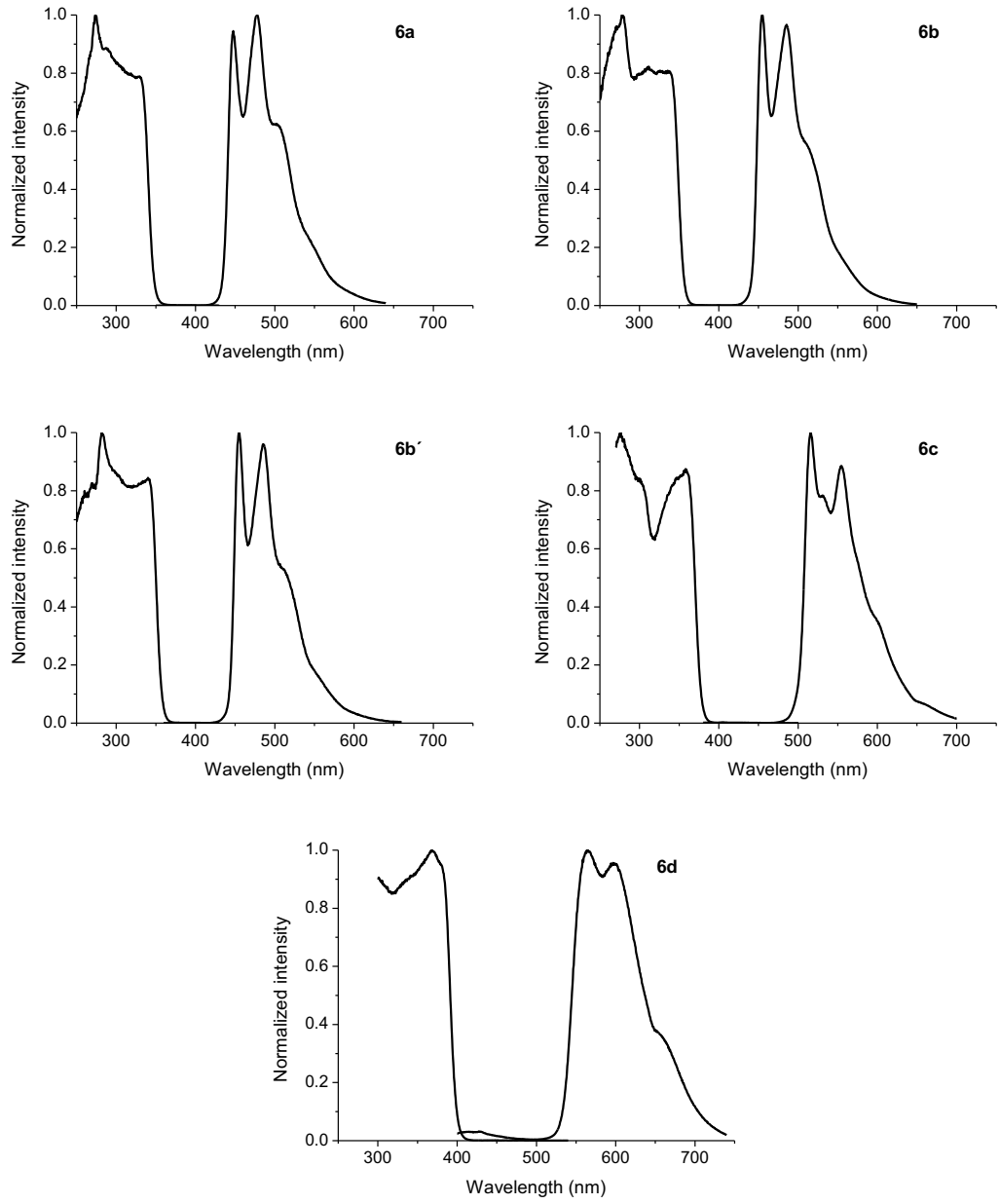

Figure S6. Excitation and emission spectra of the series of complexes **6** in CH_2Cl_2 at 298 K.

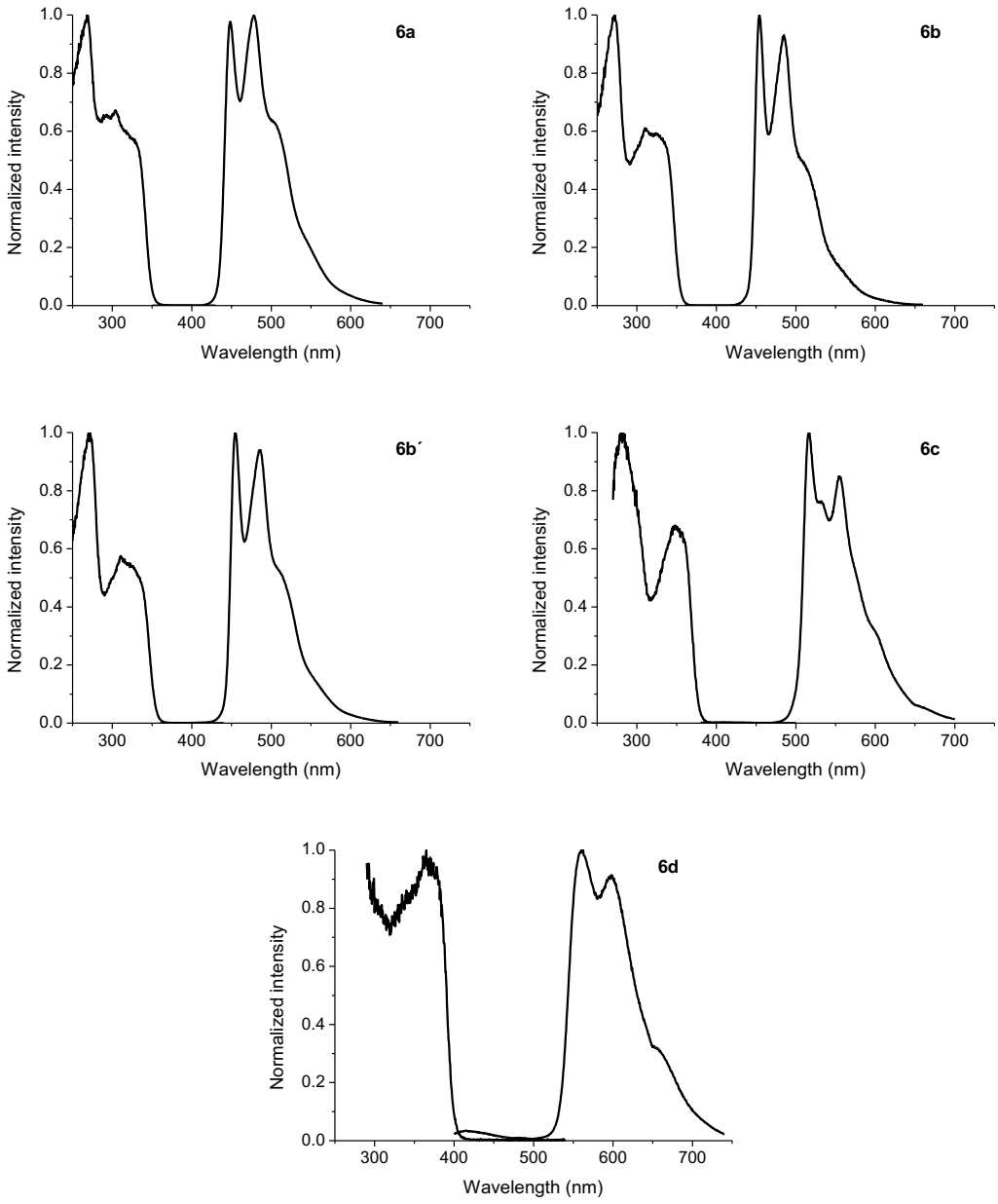

Figure S7. Excitation and emission spectra of the series of complexes **6** in PMMA films at 298 K.

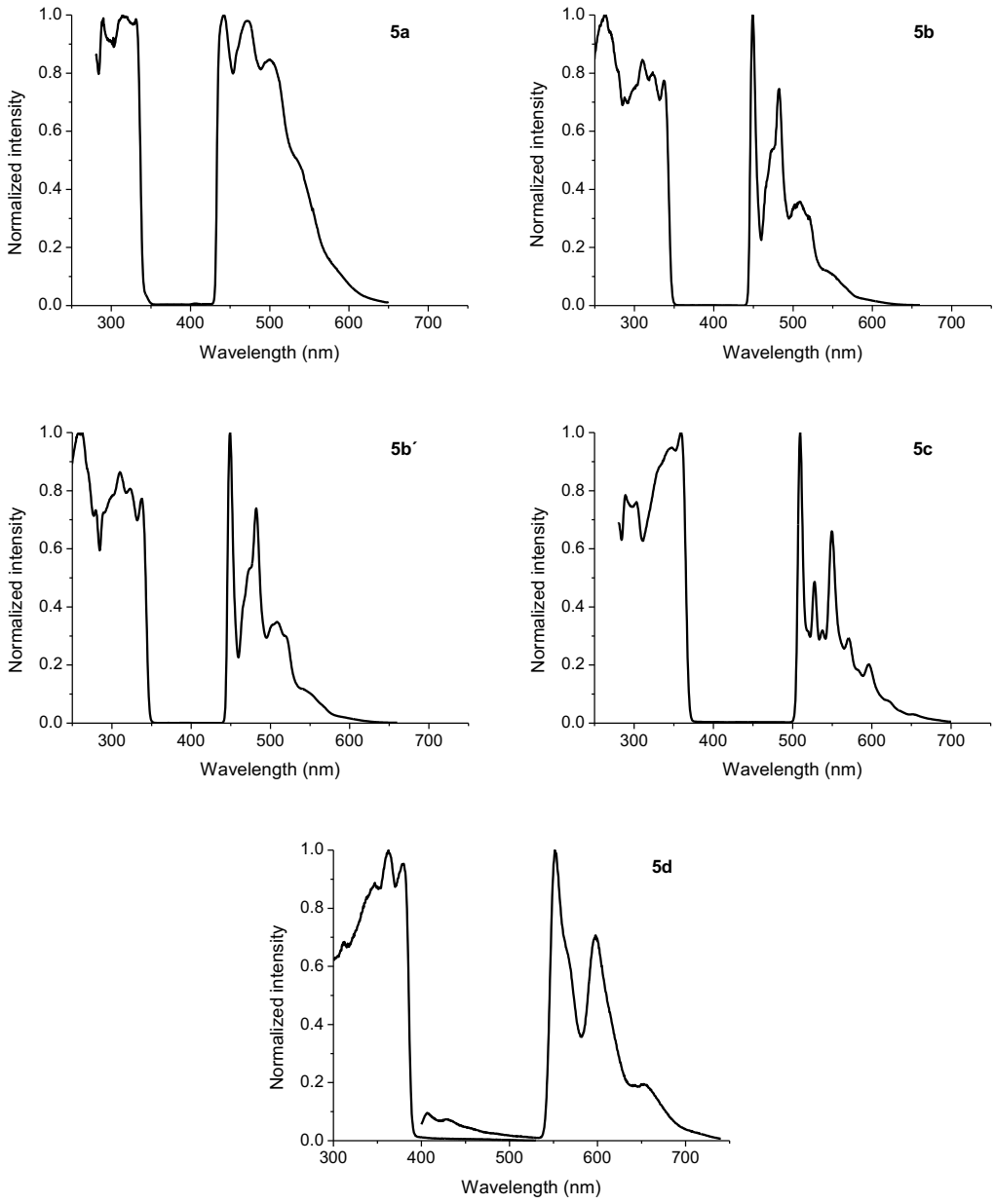

Figure S8. Excitation and emission spectra of the series of complexes **5** in 2-MeTHF glasses at 77 K.

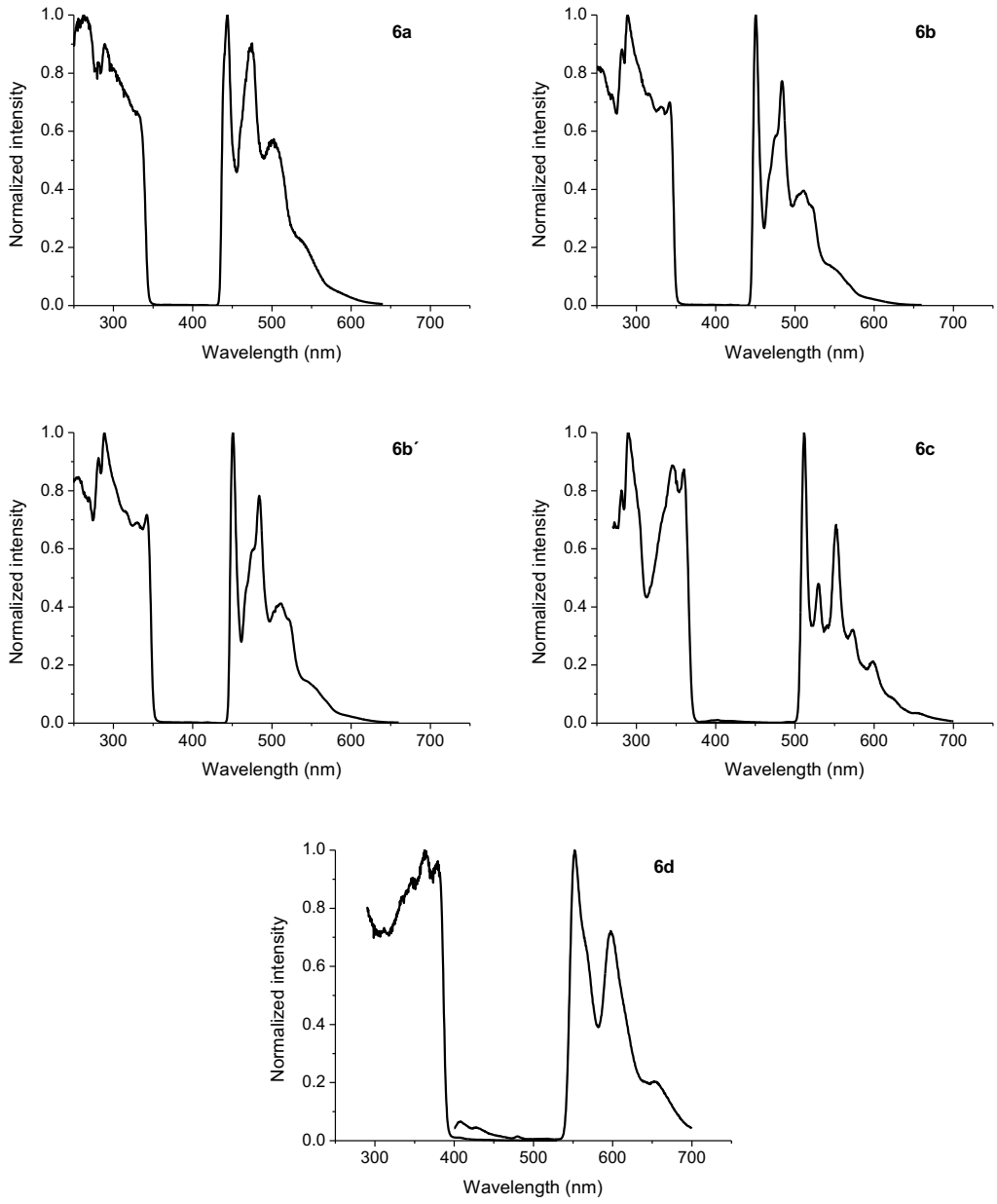

Figure S9. Excitation and emission spectra of the series of complexes **6** in 2-MeTHF glasses at 77 K.

3. NMR spectra of new compounds

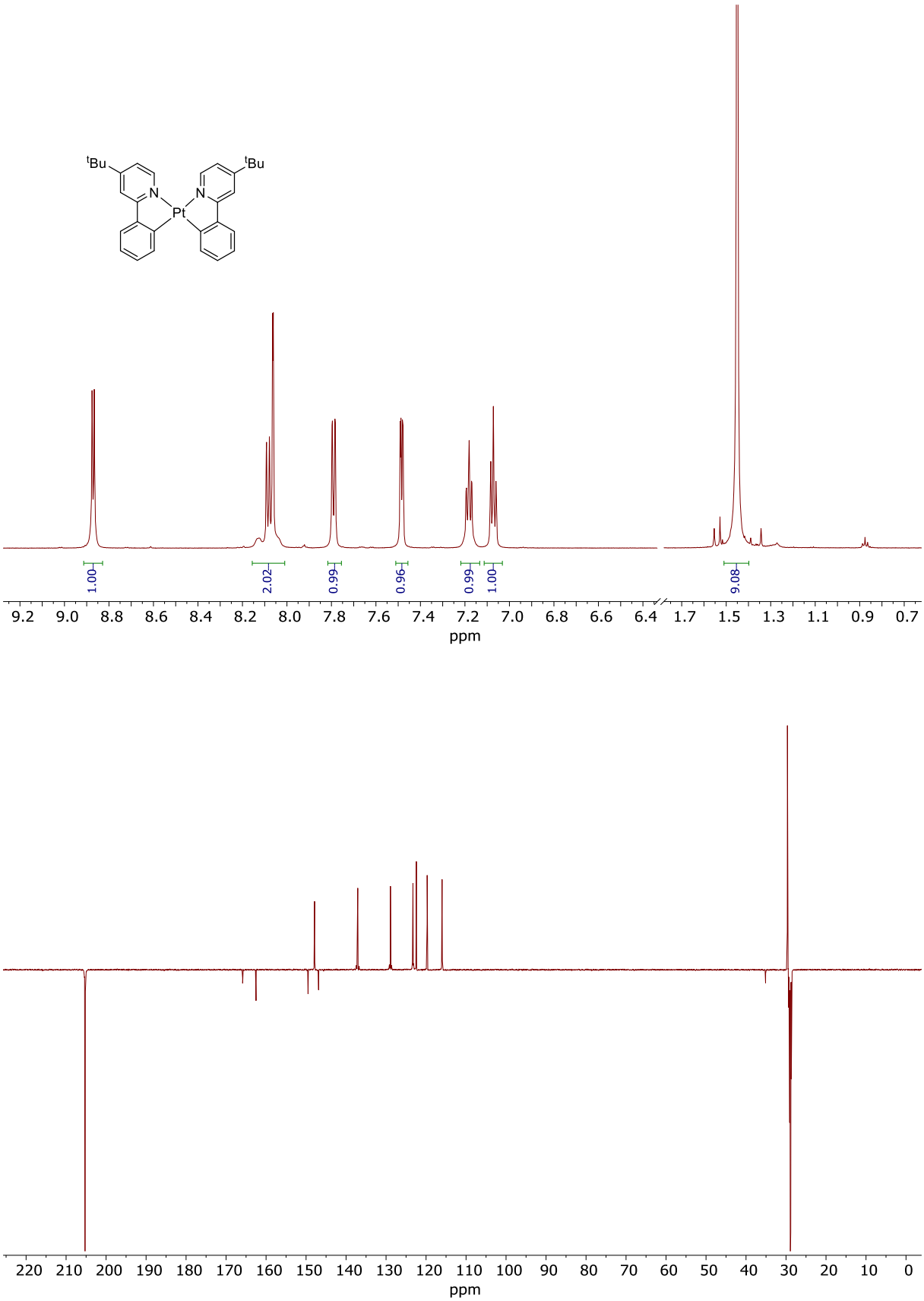

Figure S10. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **1a** (CD_2Cl_2, 600 and 151 MHz, respectively).

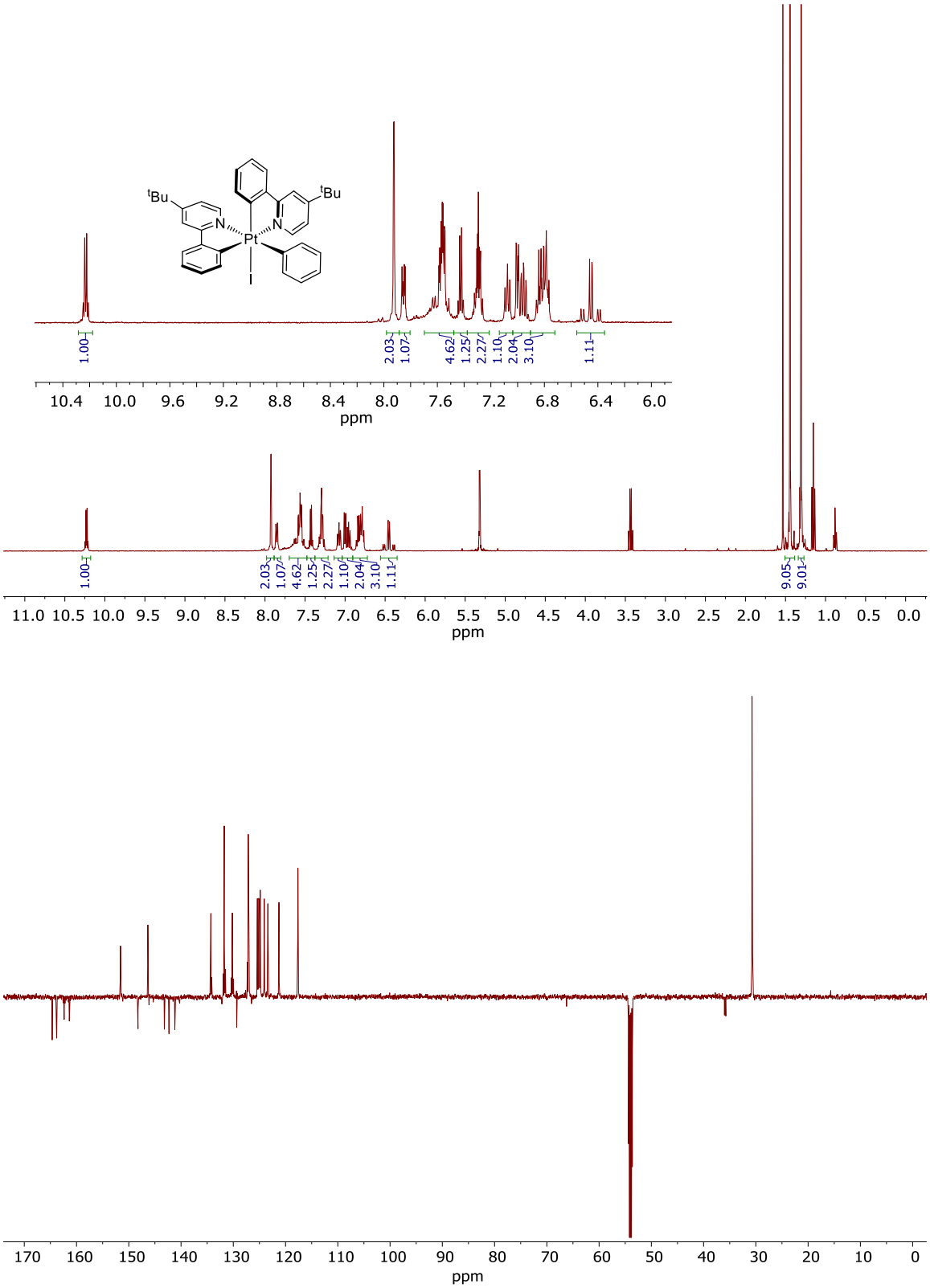

Figure S11. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2a** (CD_2Cl_2, 400 and 151 MHz, respectively).

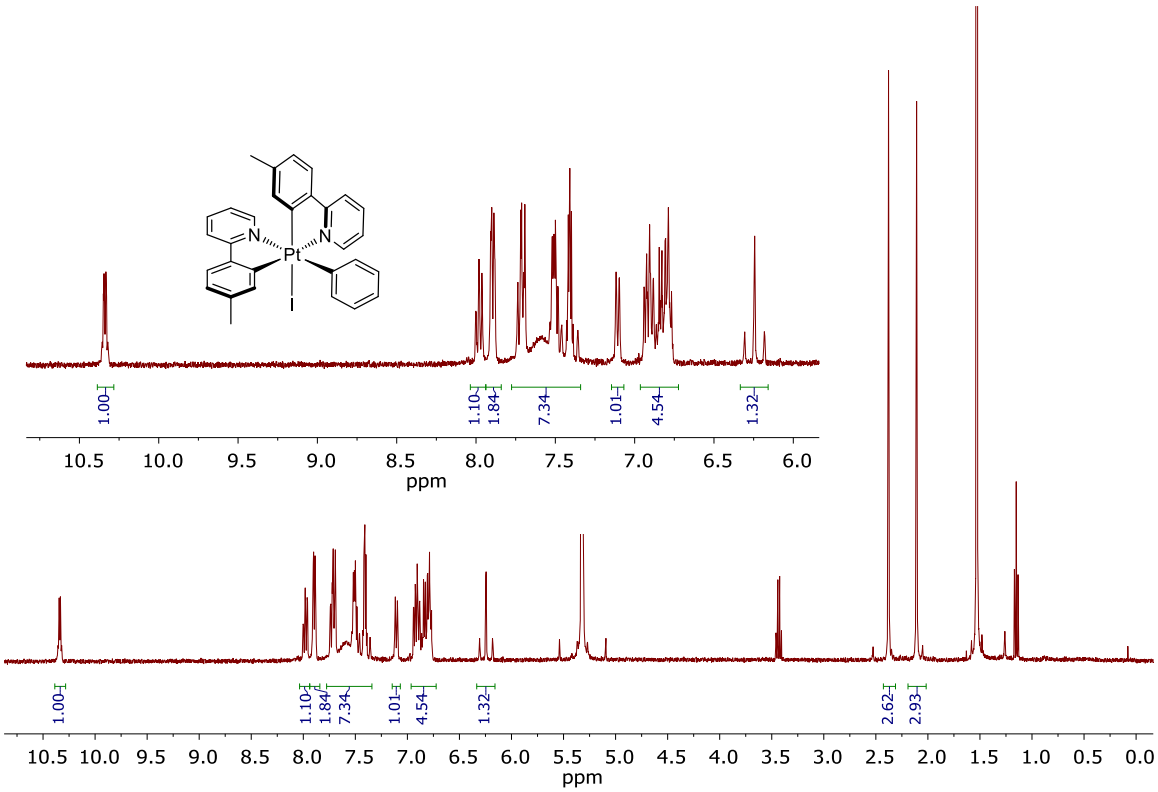

Figure S12. ^{1}H-NMR spectra of complex **2b** (CD_2Cl_2, 400 MHz).

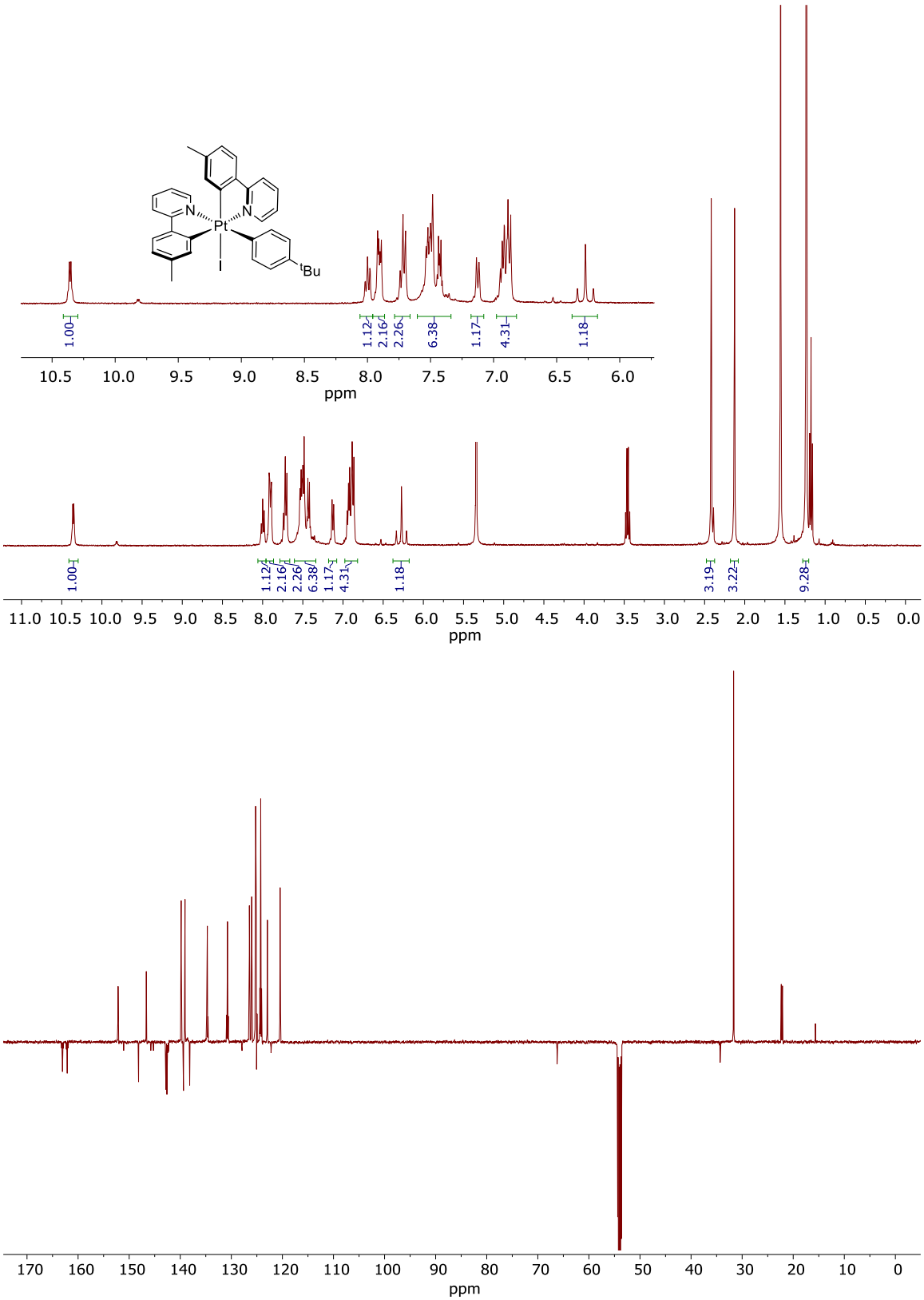

Figure S13. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **2b'** (CD_2Cl_2, 400 and 151 MHz, respectively).

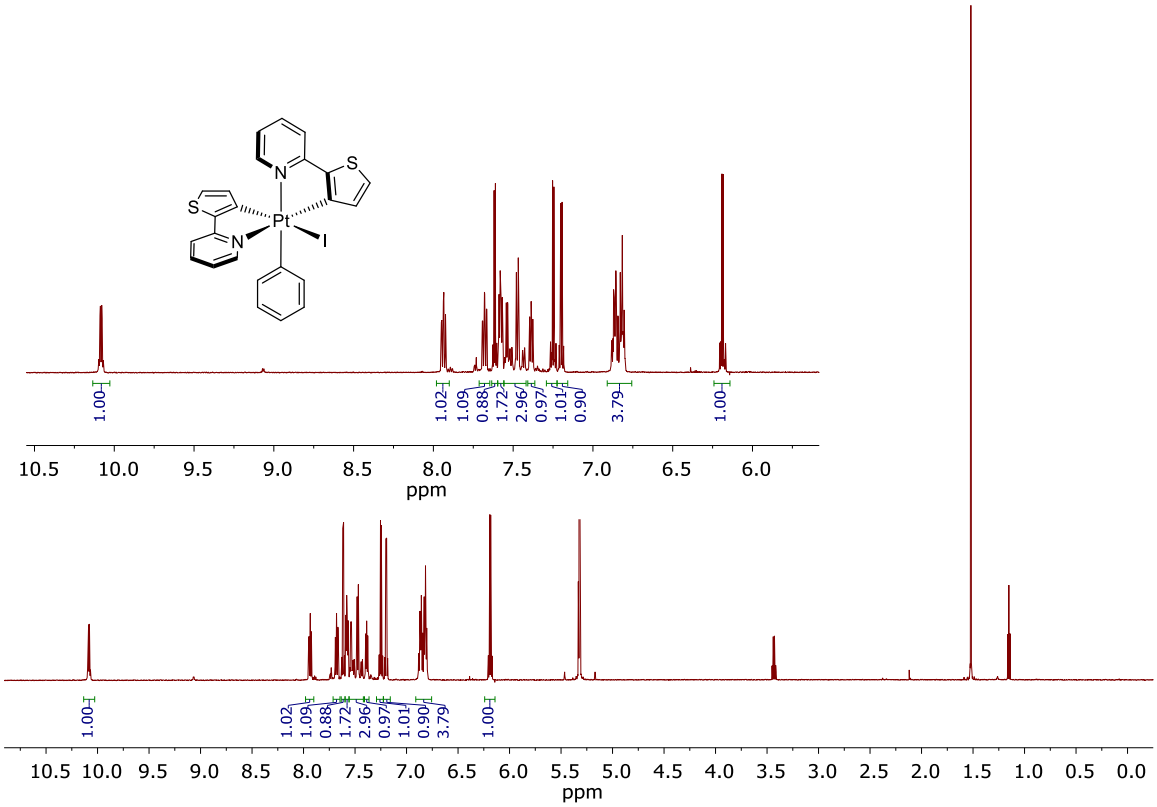

Figure S14. ^{1}H NMR spectrum of complex **2c** (CD_2Cl_2, 600 MHz).

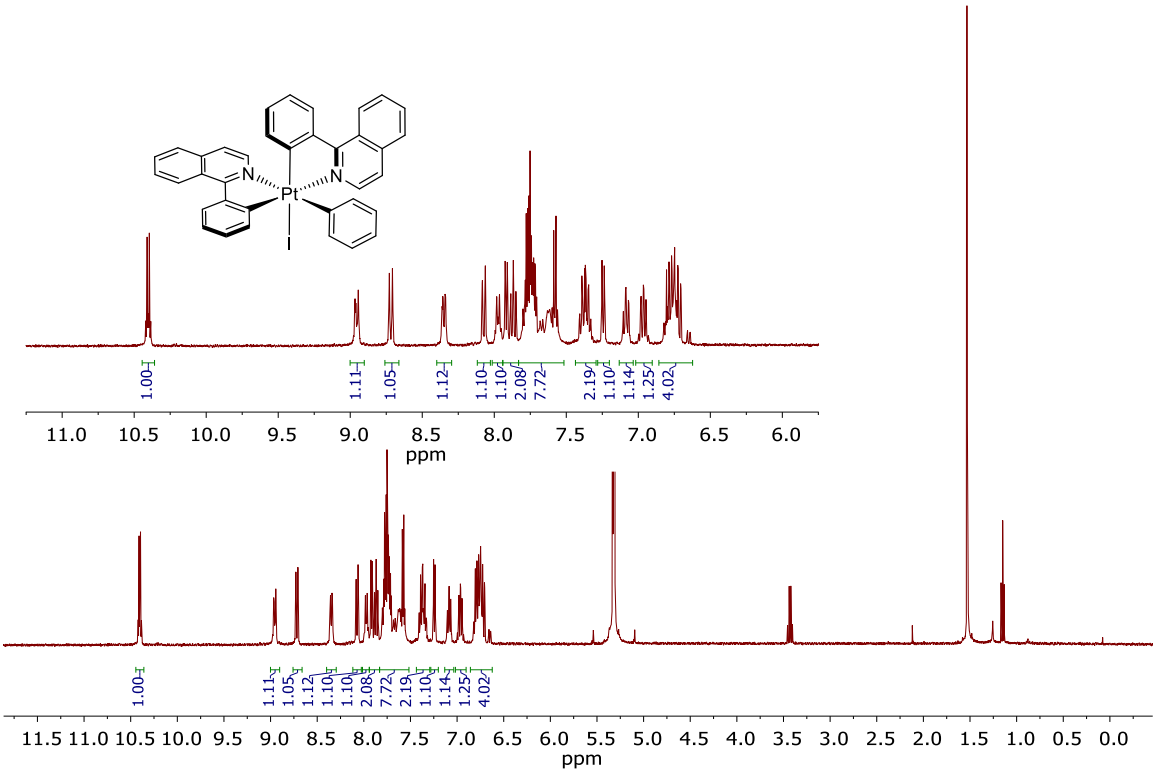

Figure S15. ^{1}H NMR spectrum of complex **2d** (CD_2Cl_2, 400 MHz).

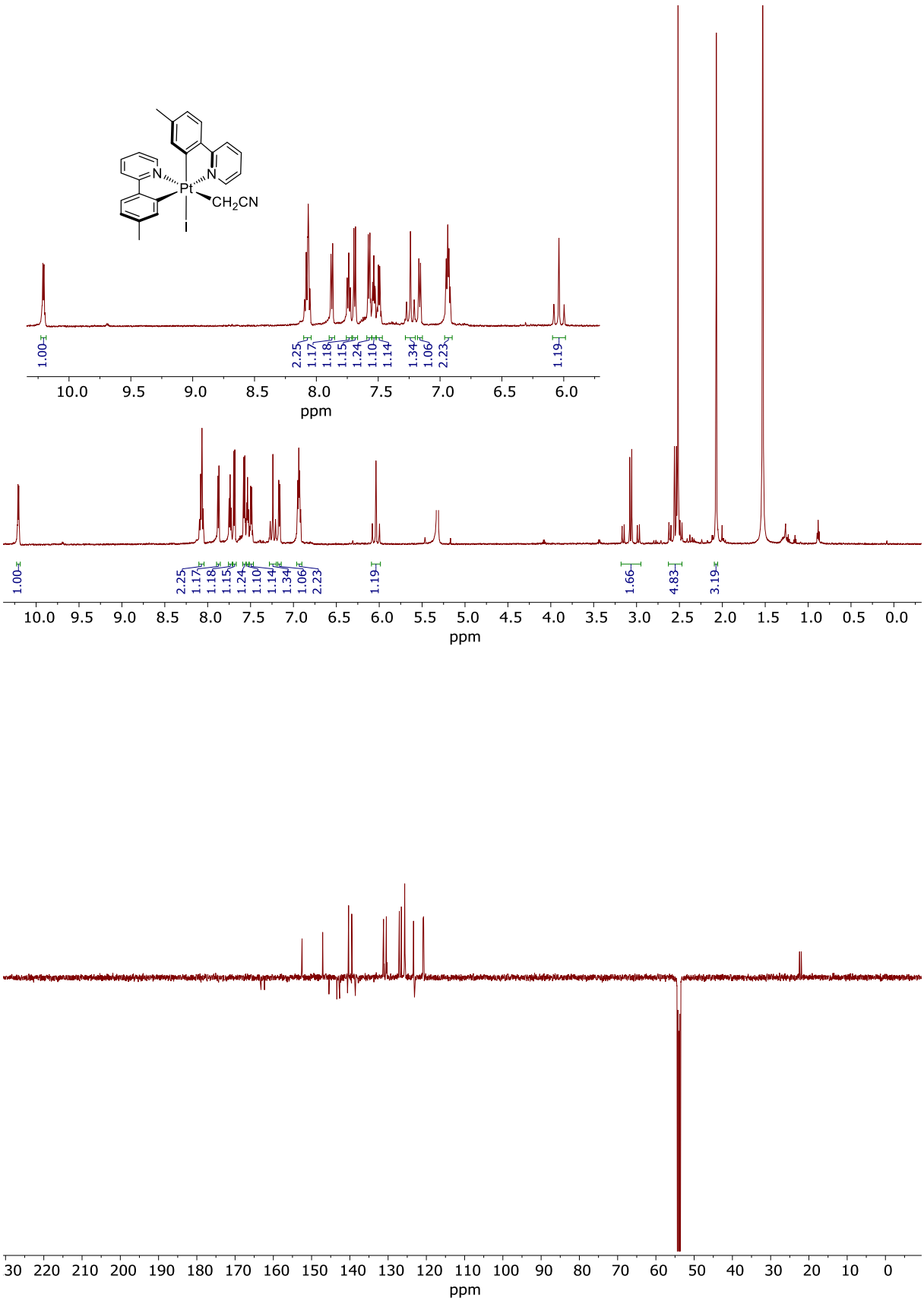

Figure S16. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **3b** (CD_2Cl_2, 600 and 151 MHz, respectively).

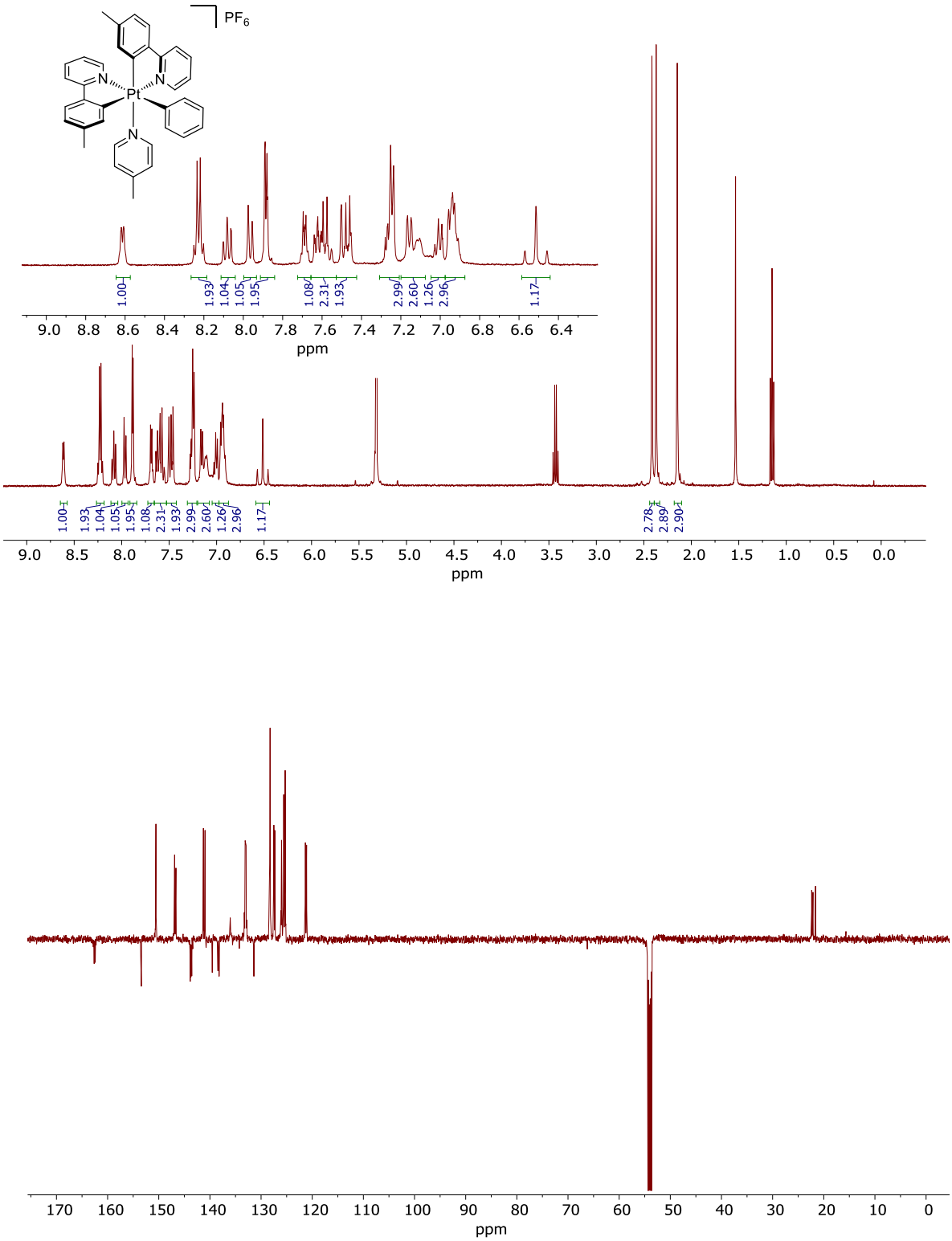

Figure S17. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **4b** (CD_2Cl_2, 400 and 151 MHz, respectively).

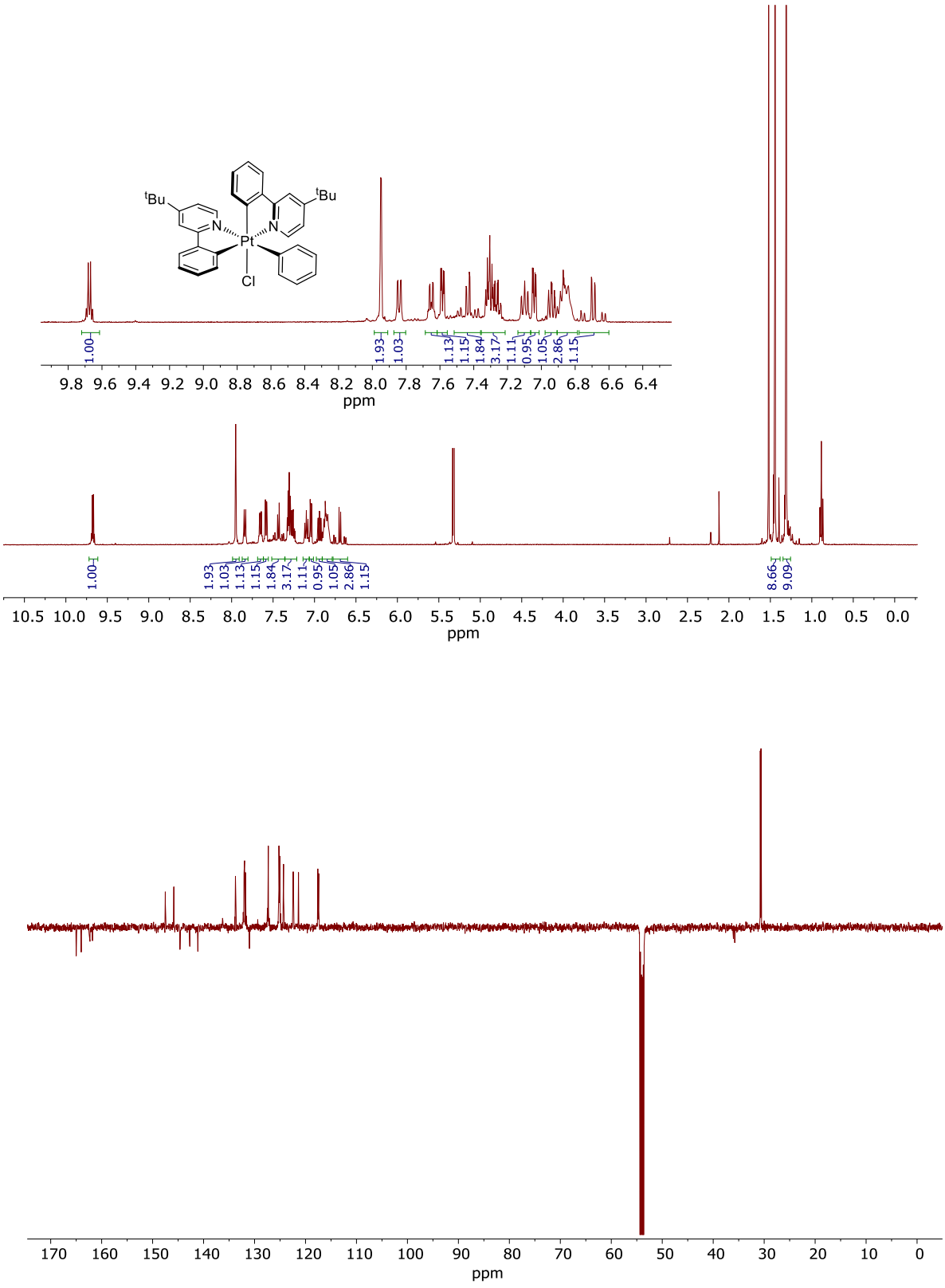

Figure S18. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **5a** (CD_2Cl_2, 400 and 151 MHz, respectively).

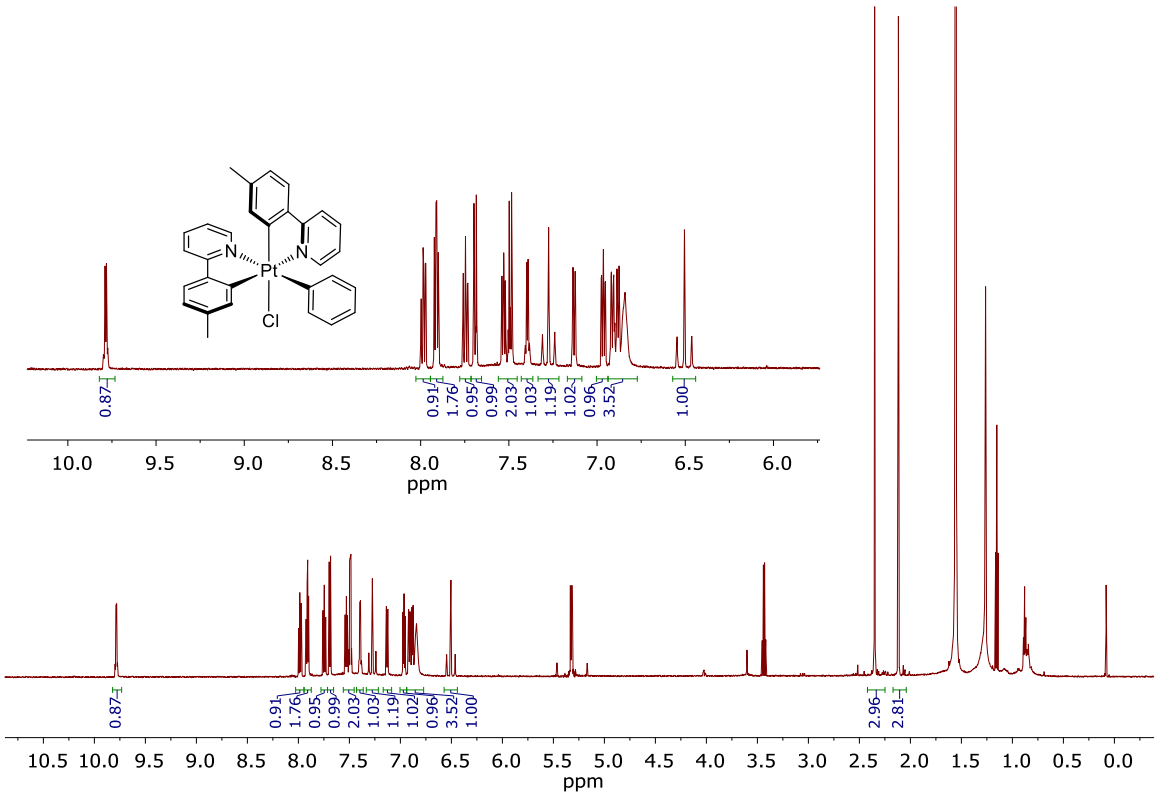

Figure S19. ^{1}H NMR spectrum of complex **5b** (CD_2Cl_2, 600 MHz).

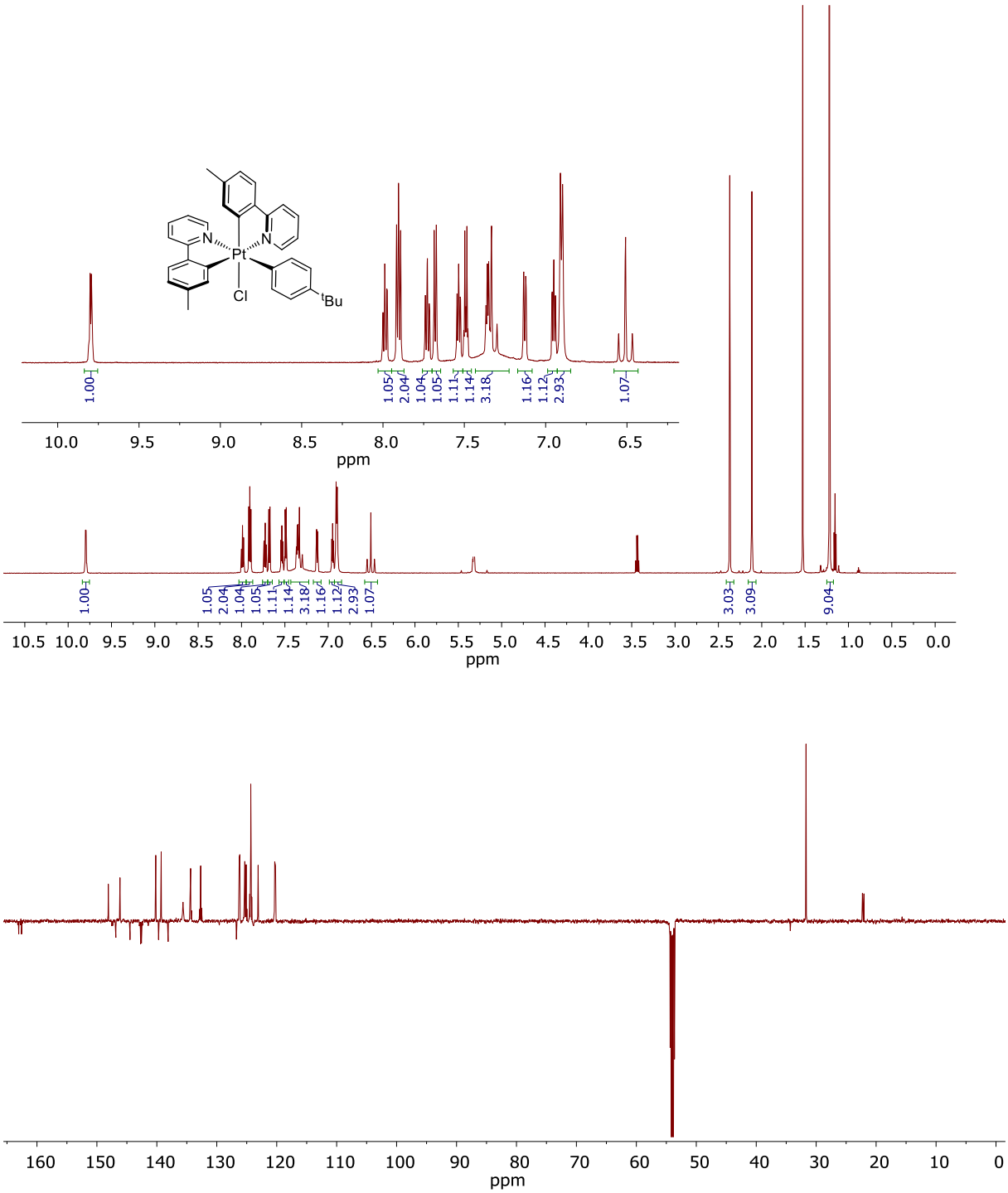

Figure S20. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **5b'** (CD_2Cl_2, 600 and 151 MHz, respectively).

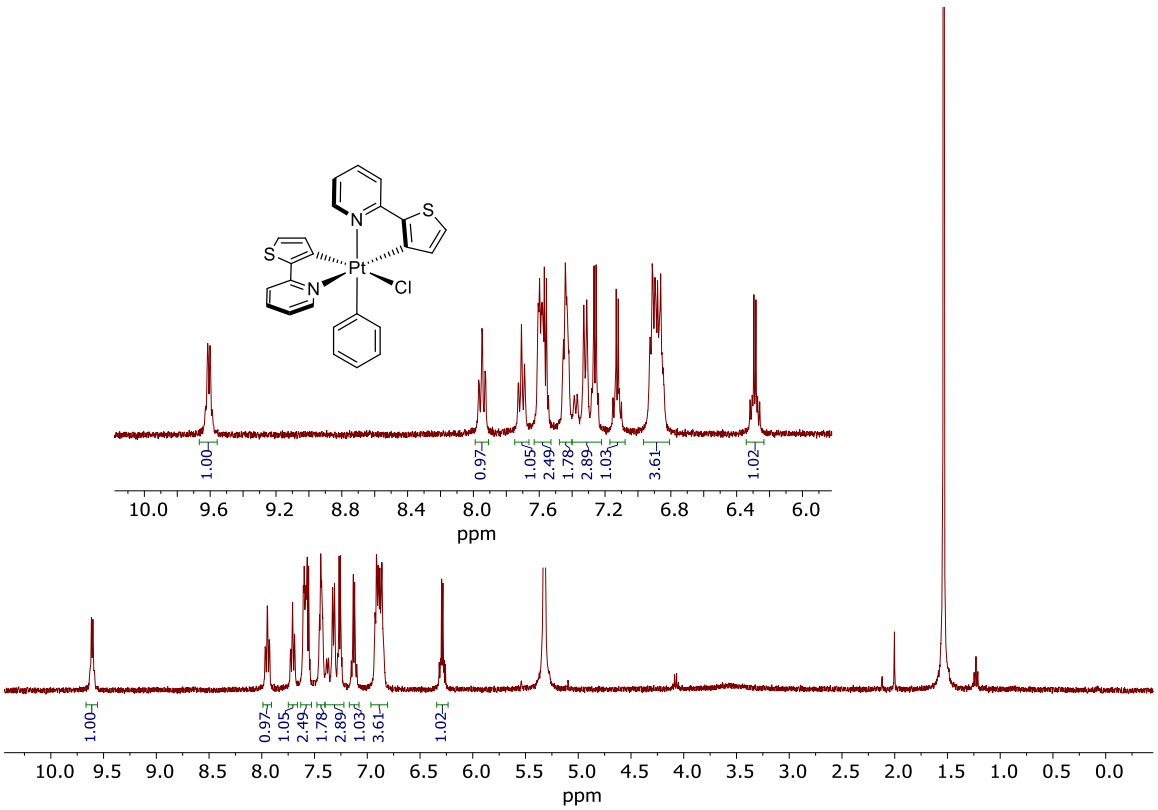

Figure S21. ^{1}H NMR spectrum of complex **5c** (CD_2Cl_2, 600 MHz).

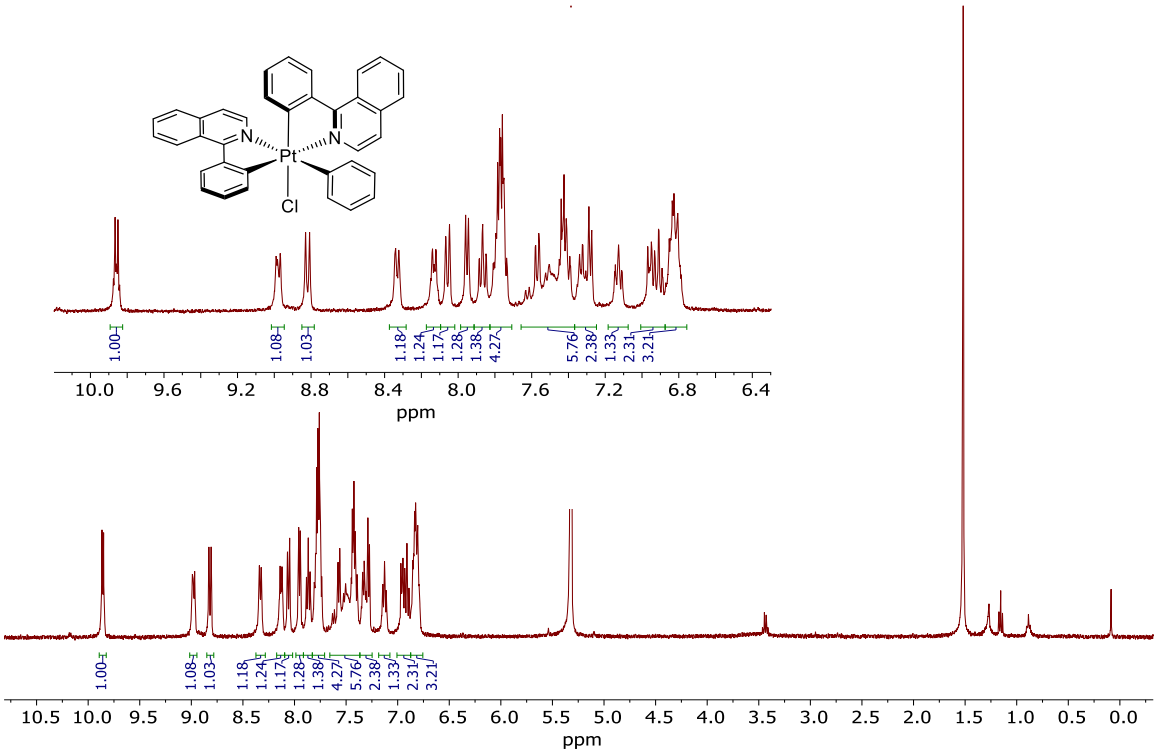

Figure S22. ^{1}H NMR spectrum of complex **5d** (CD_2Cl_2, 600 MHz).

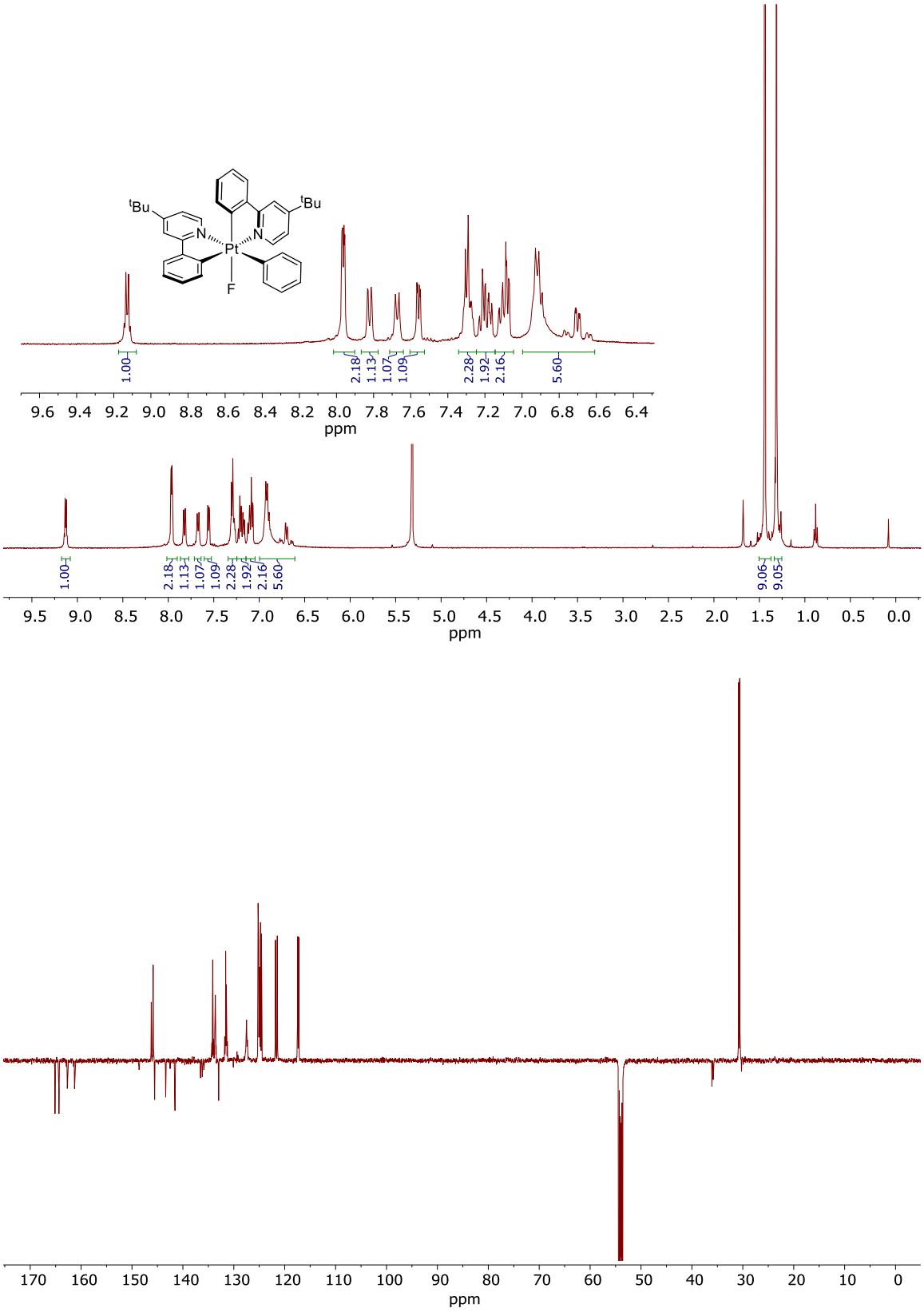

Figure S23. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **6a** (CD_2Cl_2, 400 and 151 MHz, respectively).

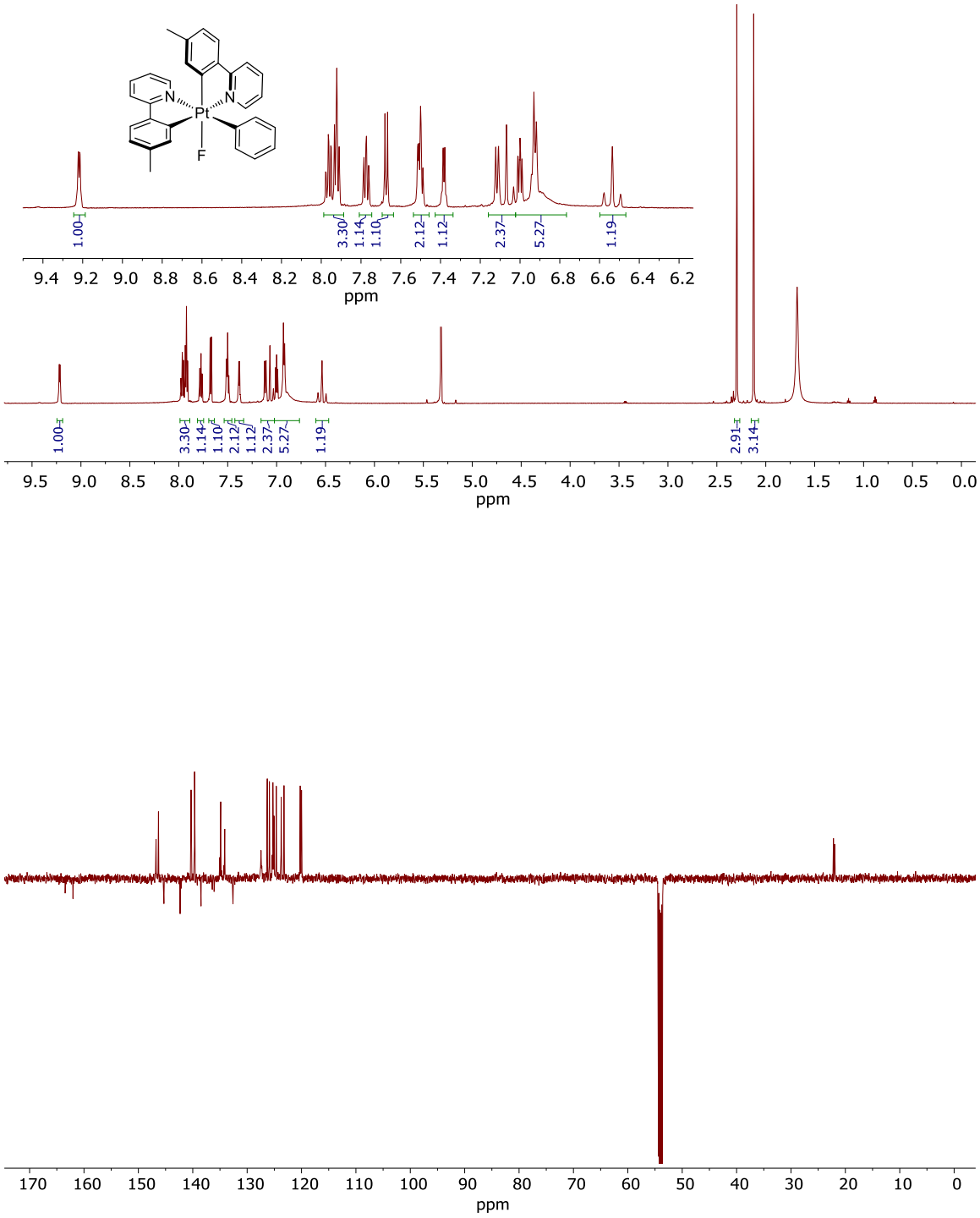

Figure S24. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **6b** (CD_2Cl_2, 600 and 151 MHz, respectively).

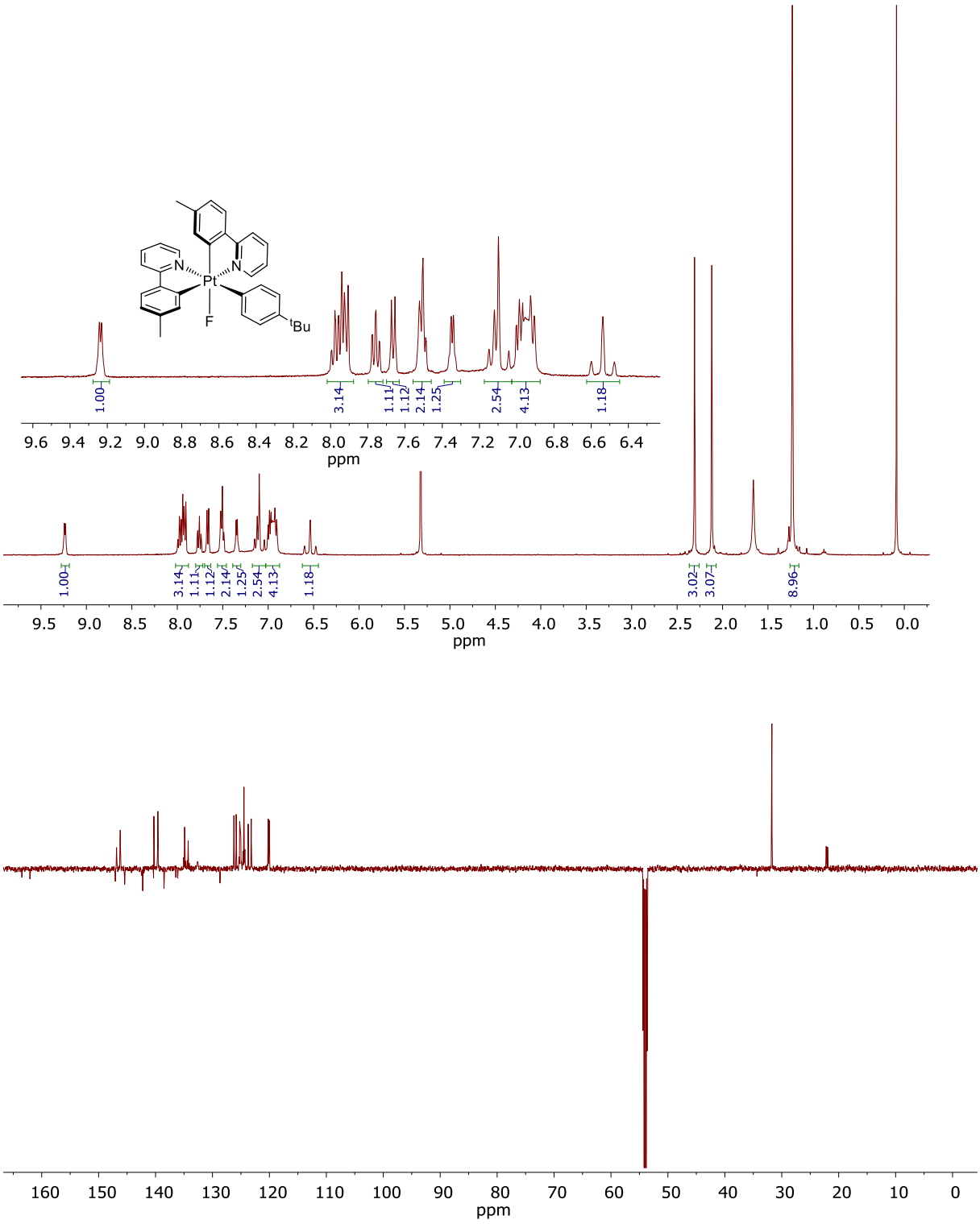

Figure S25. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **6b'** (CD_2Cl_2, 400 and 150.8 MHz, respectively).

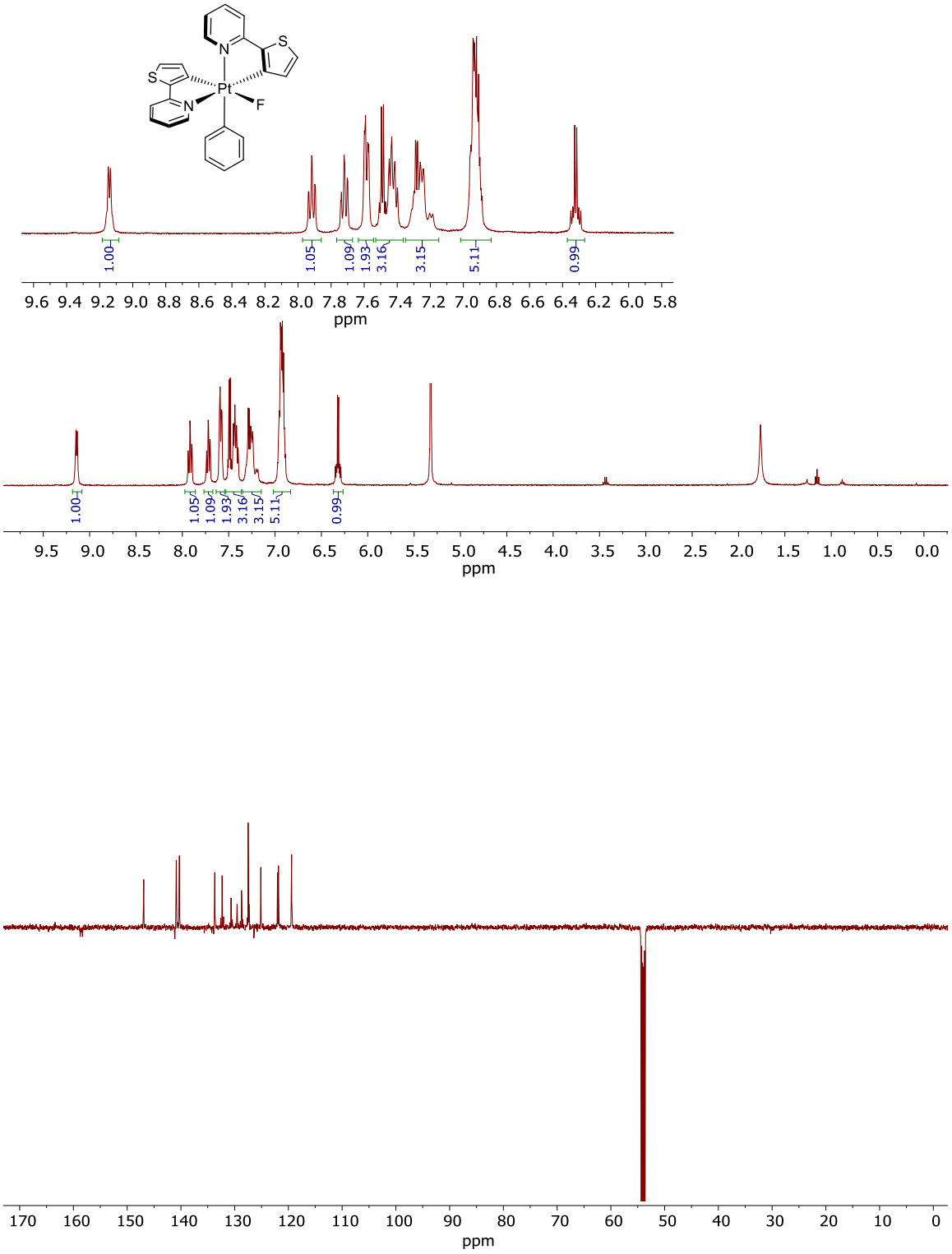

Figure S26. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **6c** (CD_2Cl_2, 400 and 151 MHz, respectively).

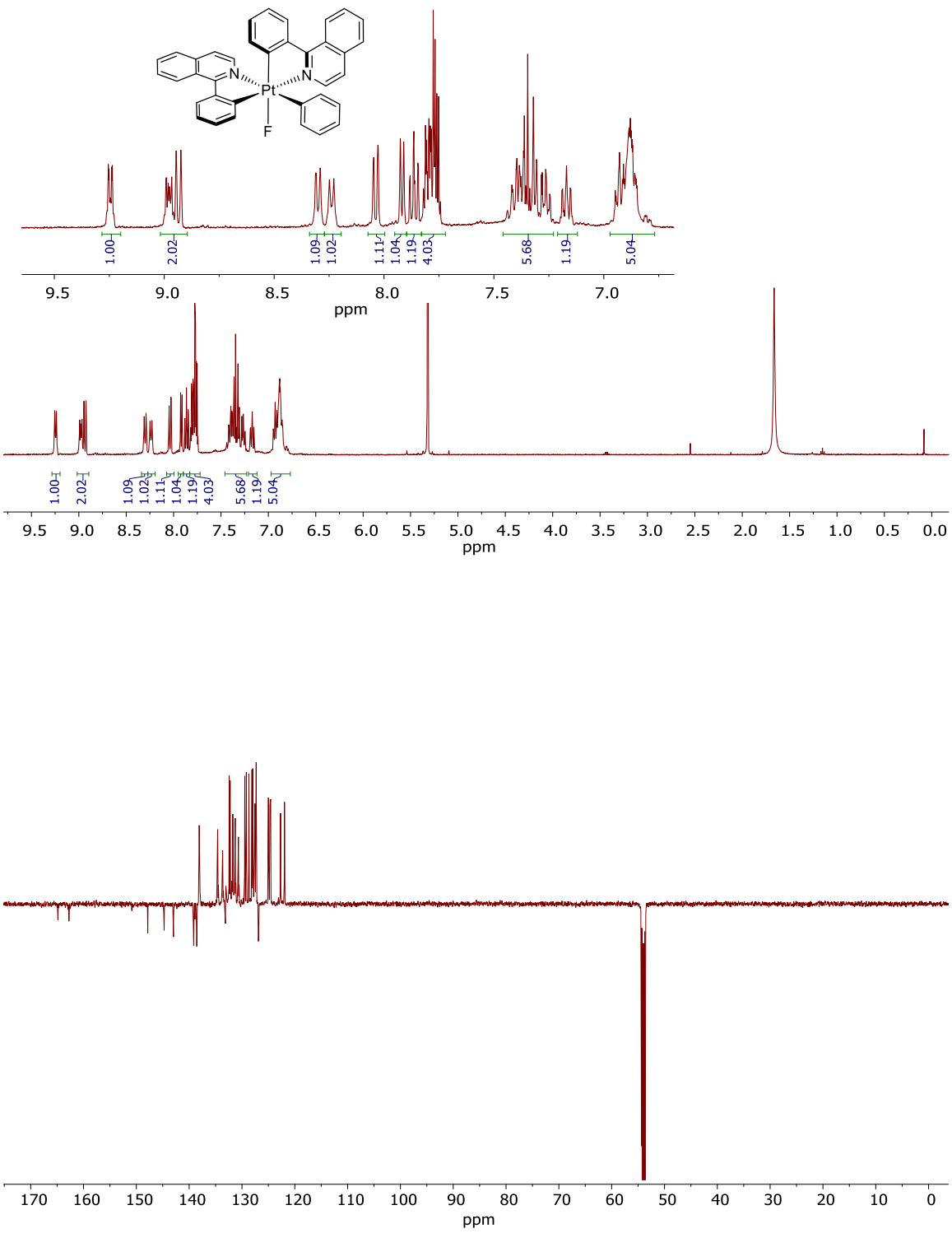

Figure S27. ^{1}H (top) and $^{13}C\{^{1}H\}$ APT (bottom) NMR spectra of complex **6d** (CD_2Cl_2, 400 and 151 MHz, respectively).

4. Computational methods

DFT calculations were carried out with Gaussian 09,[5] using the hybrid B3LYP functional[6,7] together with the 6-31G**[8,9] basis set for the light atoms and the LANL2DZ[10] basis set and effective core potential for the Pt atom. Optimizations were carried out without symmetry restrictions, using "tight" convergence criteria and "ultrafine" integration grid. Vertical excitation energies were obtained from TDDFT calculations at the ground-state optimized geometries. Triplet state geometries were obtained through a spin-unrestricted DFT optimization, using a previously described strategy.[11] The solvent effect (CH_2Cl_2) was accounted for in all cases by using the integral equation formalism variant of the polarizable continuum solvation model (IEFPCM).[12] All the optimized structures were confirmed as minima on the potential energy surface by performing frequency calculations (zero imaginary frequencies). Natural spin densities were obtained from natural population analyses using the NBO 5.9 program.[13]

5. Computational data

5.1. Complex 5b

Table S4. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **5b** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	Ph	Cl	Pt
–0.013	133 (LUMO+5)	28	22	19	0	31
–0.027	132 (LUMO+4)	33	19	8	8	32
–0.036	131 (LUMO+3)	26	70	0	0	2
–0.043	130 (LUMO+2)	70	26	1	0	2
–0.059	129 (LUMO+1)	5	90	0	1	3
–0.062	128 (LUMO)	92	5	0	0	3
–0.224	127 (HOMO)	3	86	3	2	6
–0.228	126 (HOMO–1)	69	0	21	4	5
–0.229	125 (HOMO–2)	18	8	63	1	9
–0.238	124 (HOMO–3)	1	24	66	7	2
–0.241	123 (HOMO–4)	2	61	22	9	7
–0.243	122 (HOMO–5)	63	2	6	22	8

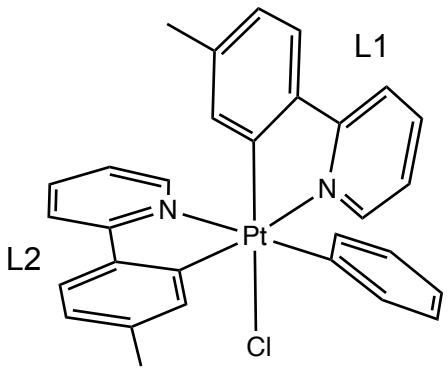

Figure S28. Ligand numbering in complex **5b**.

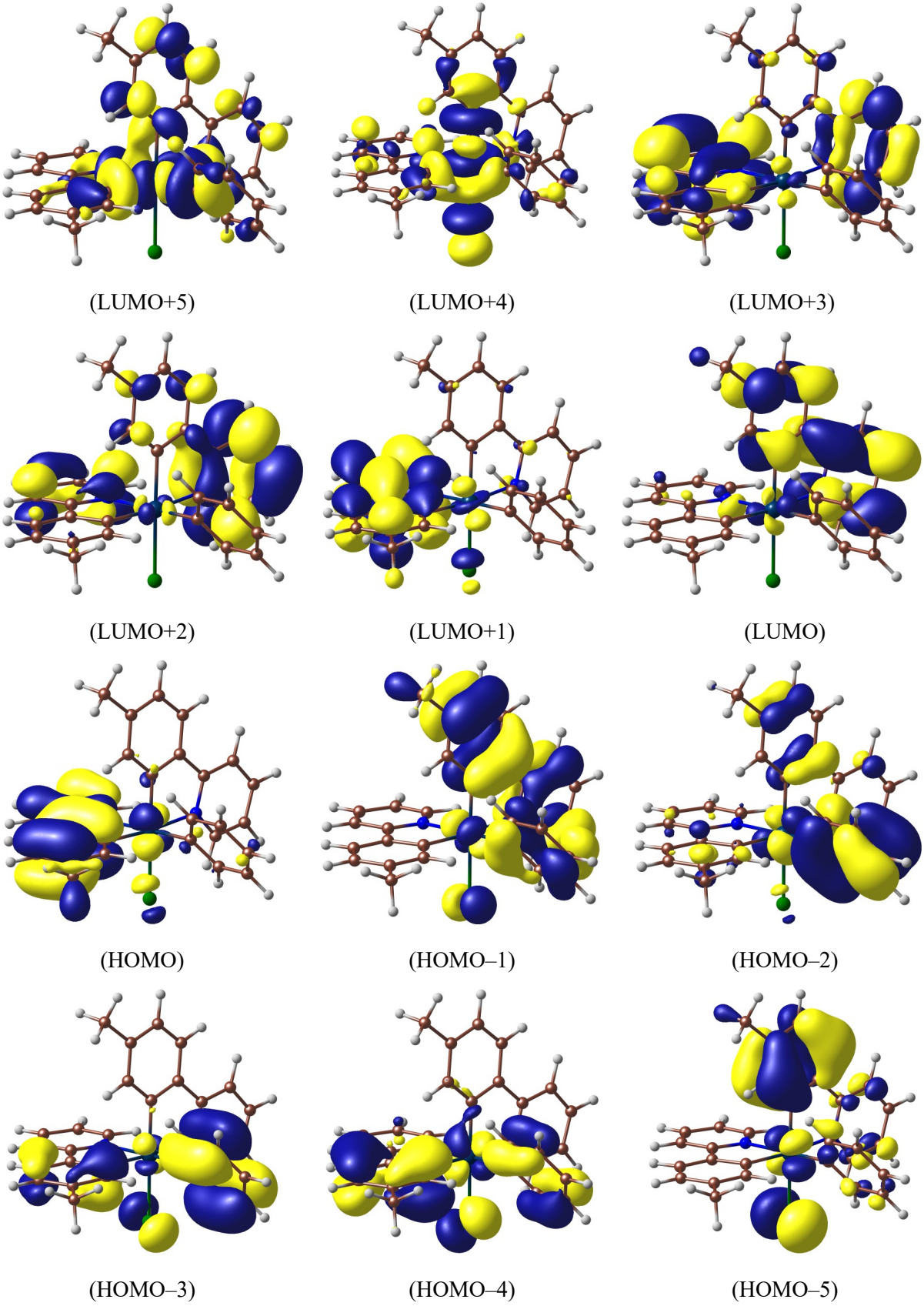

Figure S29. Molecular orbital isosurfaces of **5b** (0.03 e bohr^{-3}).

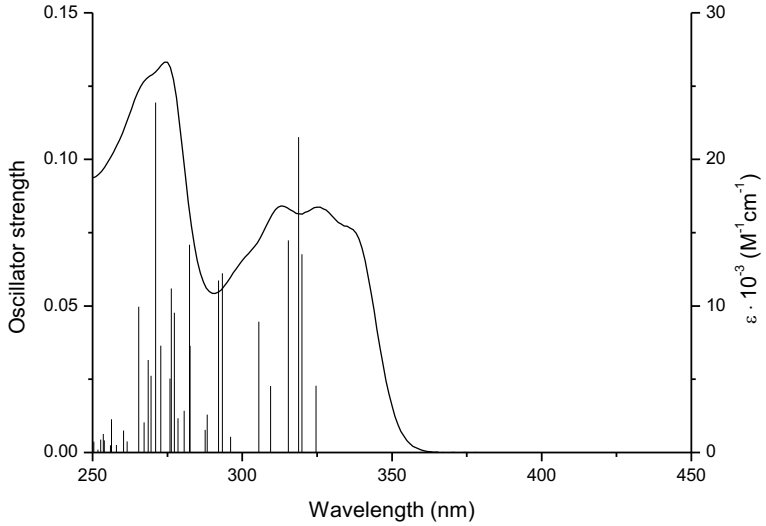

Figure S30. Calculated stick absorption spectrum of **5b** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S5. Selected vertical singlet excitations of **5b** 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 (11%) H -> L (72%) H -> L+1 (12%)	3.823	324.4	0.0231
S2	H–2 -> L (24%) H–1 -> L (17%) H -> L+1 (49%)	3.879	319.6	0.0680
S3	H–2 -> L (6%) H–1 -> L (54%) H -> L (11%) H -> L+1 (23%)	3.893	318.5	0.1079
S4	H–2 -> L (55%) H–1 -> L (21%) H–1 -> L+1 (3%) H -> L (12%)	3.935	315.1	0.0727
S5	H–5 -> L+1 (2%) H–2 -> L+1 (10%) H–1 -> L+1 (77%) H -> L+1 (3%)	4.011	309.1	0.0230
S6	H–2 -> L+1 (82%) H–1 -> L+1 (13%)	4.063	305.2	0.0450
S7	H–4 -> L (4%) H–3 -> L (92%)	4.192	295.8	0.0057
S8	H–4 -> L (16%) H–4 -> L+1 (34%) H–3 -> L+1 (26%) H -> L+2 (9%) H -> L+3 (7%)	4.231	293.1	0.0615
S9	H–5 -> L (60%) H–5 -> L+1 (4%) H–4 -> L (5%) H–3 -> L+1 (5%)	4.250	291.8	0.0590

	H–2 -> L+2 (2%) H–1 -> L+2 (11%)			
S10	H–5 -> L (11%) H–5 -> L+1 (18%) H–4 -> L (26%) H–3 -> L (2%) H–3 -> L+1 (23%) H–1 -> L+2 (4%)	4.305	288.0	0.0133
S11	H–6 -> L (3%) H–5 -> L+1 (19%) H–4 -> L (42%) H–4 -> L+1 (24%) H–3 -> L+1 (3%)	4.315	287.3	0.0081
S12	H–6 -> L (9%) H–6 -> L+1 (25%) H–6 -> L+4 (3%) H–5 -> L+1 (3%) H–4 -> L+1 (10%) H–3 -> L+1 (4%) H–2 -> L+4 (2%) H–1 -> L+4 (3%) H -> L+1 (2%) H -> L+4 (23%)	4.393	282.2	0.0367

[a] H = HOMO; L = LUMO.

Table S6. Lowest-energy vertical triplet excitations of **5b** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations**[a]	**ΔE/eV**	**λ/nm**
T1	H–4 -> L+1 (2%) H–2 -> L+1 (4%) H -> L (3%) H -> L+1 (69%) H -> L+3 (5%)	2.902	427.2
T2	H–5 -> L (6%) H–2 -> L (13%) H–1 -> L (57%) H–1 -> L+2 (3%)	2.921	424.4
T3	H–11 -> L+2 (2%) H–11 -> L+3 (4%) H–4 -> L+1 (10%) H–4 -> L+3 (3%) H–3 -> L+1 (5%) H -> L (11%) H -> L+1 (10%) H -> L+2 (13%) H -> L+3 (25%)	3.638	340.8

[a] H = HOMO; L = LUMO.

5.2. Complex 6b

Table S7. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of **6b** in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	Ph	F	Pt
–0.004	129 (LUMO+5)	36	22	13	0	28
–0.007	128 (LUMO+4)	28	20	12	6	34
–0.035	127 (LUMO+3)	36	62	0	0	1
–0.040	126 (LUMO+2)	61	37	0	0	2
–0.057	125 (LUMO+1)	4	93	0	0	2
–0.059	124 (LUMO)	92	5	0	0	3
–0.221	123 (HOMO)	15	71	0	2	10
–0.224	122 (HOMO–1)	65	13	13	2	8
–0.226	121 (HOMO–2)	9	6	74	0	10
–0.236	120 (HOMO–3)	2	47	43	3	5
–0.238	119 (HOMO–4)	5	33	53	2	7
–0.240	118 (HOMO–5)	78	4	05	5	9

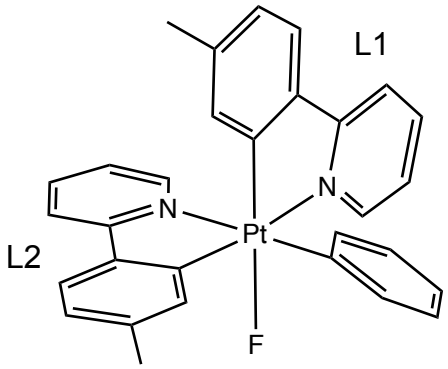

Figure S31. Ligand numbering in complex **6b**.

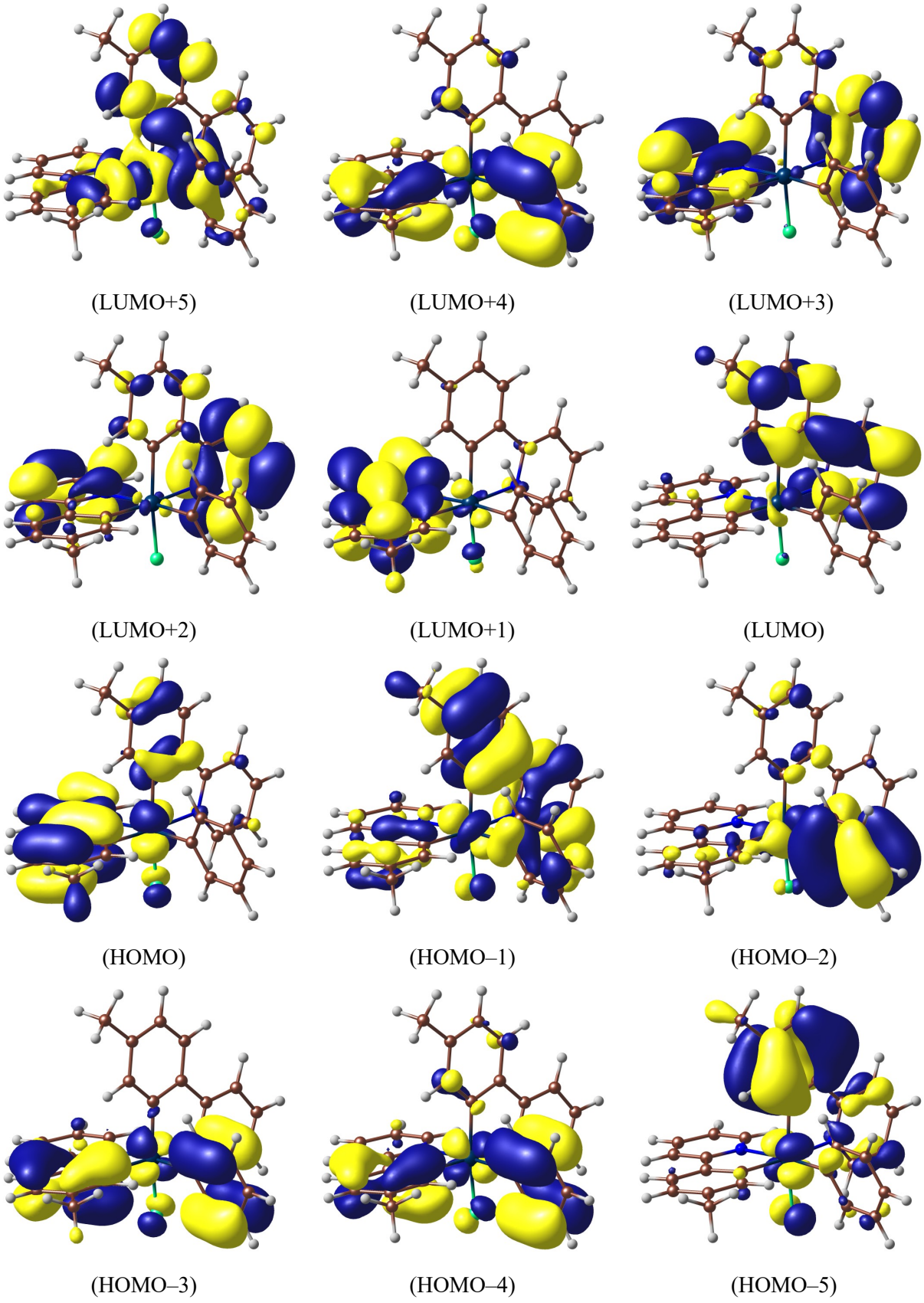

Figure S32. Molecular orbital isosurfaces of **6b** (0.03 e bohr^{-3}).

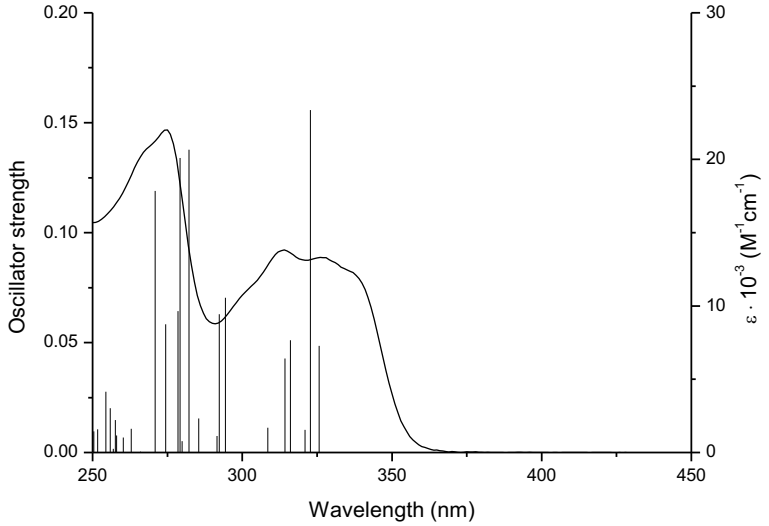

Figure S33. Calculated stick absorption spectrum of **6b** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S8. Selected vertical singlet excitations of **6b** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	monoexcitations[a]	ΔE/eV	λ/nm	Oscillator strength
S1	H–5 -> L (2%) H–1 -> L (9%) H -> L (63%) H -> L+1 (22%)	3.811	325.3	0.0489
S2	H–1 -> L (15%) H -> L (12%) H -> L+1 (63%)	3.846	322.4	0.1562
S3	H–2 -> L (32%) H–1 -> L (48%) H -> L (12%) H -> L+1 (4%)	3.866	320.7	0.0108
S4	H–2 -> L (64%) H–1 -> L (20%) H–1 -> L+1 (4%) H -> L (8%)	3.926	315.8	0.0515
S5	H–1 -> L+1 (87%)	3.950	313.9	0.0432
S6	H–2 -> L+1 (95%) H–1 -> L+1 (3%)	4.023	308.2	0.0117
S7	H–4 -> L+1 (15%) H–3 -> L (18%) H–3 -> L+1 (34%) H -> L+2 (16%) H -> L+3 (6%)	4.216	294.1	0.0709
S8	H–5 -> L (46%) H–4 -> L (2%) H–3 -> L (10%) H–3 -> L+1 (4%) H–1 -> L+2 (21%) H -> L+2 (4%) H -> L+3 (3%)	4.246	292.0	0.0634
S9	H–5 -> L (5%) H–4 -> L (16%)	4.257	291.2	0.0080

	H–3 -> L (63%) H–3 -> L+1 (8%) H -> L+2 (3%)			
S10	H–5 -> L (6%) H–4 -> L (76%) H–4 -> L+1 (2%) H–3 -> L (5%) H–3 -> L+1 (2%)	4.319	287.1	0.0002
S11	H–5 -> L (4%) H–5 -> L+1 (70%) H–4 -> L+1 (13%) H -> L+2 (7%)	4.348	285.2	0.0159
S12	H–5 -> L (4%) H–5 -> L+1 (6%) H–4 -> L+1 (3%) H–3 -> L+1 (21%) H–2 -> L+2 (6%) H -> L+1 (3%) H -> L+2 (50%)	4.398	281.9	0.1382

[a] H = HOMO; L = LUMO.

Table S9. Lowest-energy vertical triplet excitations of **6b** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations[a]**	**ΔE/eV**	**λ/nm**
T1	H–4 -> L+1 (2%) H–3 -> L+1 (3%) H–2 -> L+1 (3%) H–1 -> L+1 (9%) H -> L (4%) H -> L+1 (58%) H -> L+3 (3%)	2.902	427.2
T2	H–5 -> L (7%) H–2 -> L (4%) H–1 -> L (55%) H–1 -> L+3 (2%) H -> L (10%) H -> L+1 (3%)	2.914	425.5
T3	H–11 -> L+2 (3%) H–11 -> L+3 (2%) H–5 -> L (5%) H–5 -> L+3 (2%) H–4 -> L+1 (7%) H–3 -> L+1 (10%) H–3 -> L+2 (2%) H–3 -> L+3 (2%) H–1 -> L+2 (7%) H -> L (13%) H -> L+1 (9%) H -> L+2 (8%) H -> L+3 (16%)	3.631	341.5

[a] H = HOMO; L = LUMO.

5.3. Complex 6b'

Table S10. Fragment contributions (%; from atomic orbital contributions) to the frontier orbitals of ## in CH_2Cl_2 solution.

energy (a.u.)	number	L1	L2	*t*-Bu-Ph	F	Pt
–0.003	145 (LUMO+5)	38	22	12	0	27
–0.006	144 (LUMO+4)	28	20	12	6	34
–0.034	143 (LUMO+3)	37	62	0	0	1
–0.040	142 (LUMO+2)	61	37	0	0	2
–0.057	141 (LUMO+1)	4	93	0	0	2
–0.058	140 (LUMO)	92	5	0	0	3
–0.218	139 (HOMO)	2	2	86	0	9
–0.221	138 (HOMO–1)	18	68	1	3	10
–0.224	137 (HOMO–2)	67	20	3	2	8
–0.234	136 (HOMO–3)	1	16	80	1	2
–0.237	135 (HOMO–4)	4	65	18	4	10
–0.239	134 (HOMO–5)	80	3	3	5	9

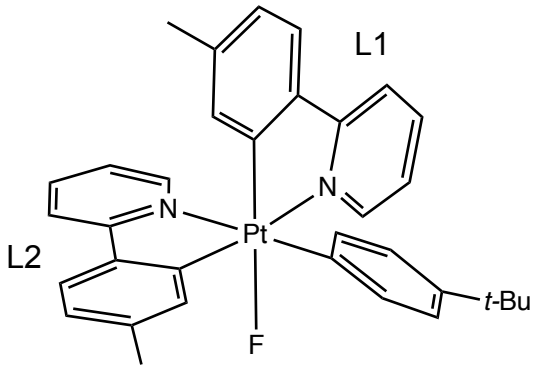

Figure S34. Ligand numbering in complex **6b'**.

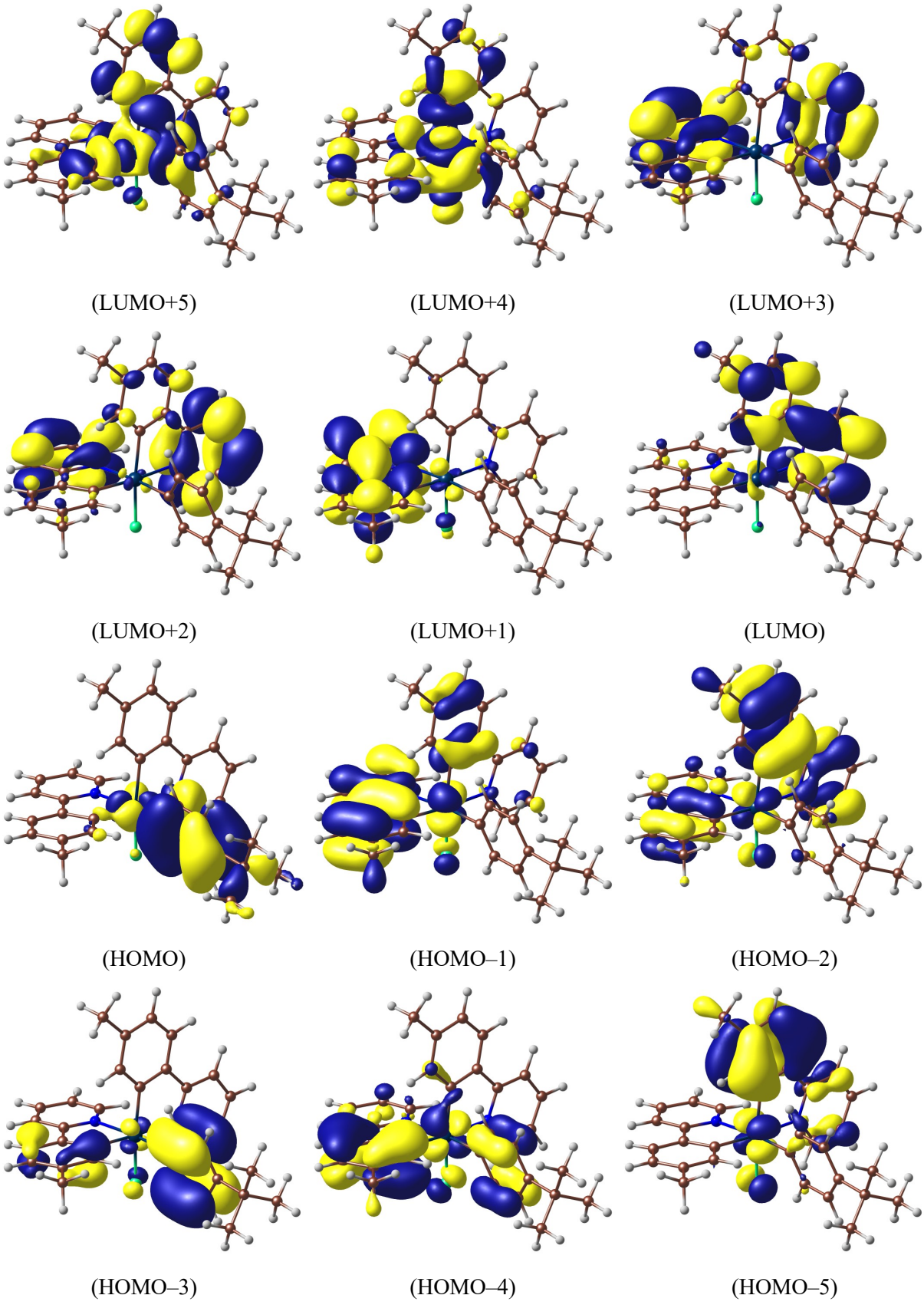

Figure S35. Molecular orbital isosurfaces of **6b'** (0.03 e bohr^{-3}).

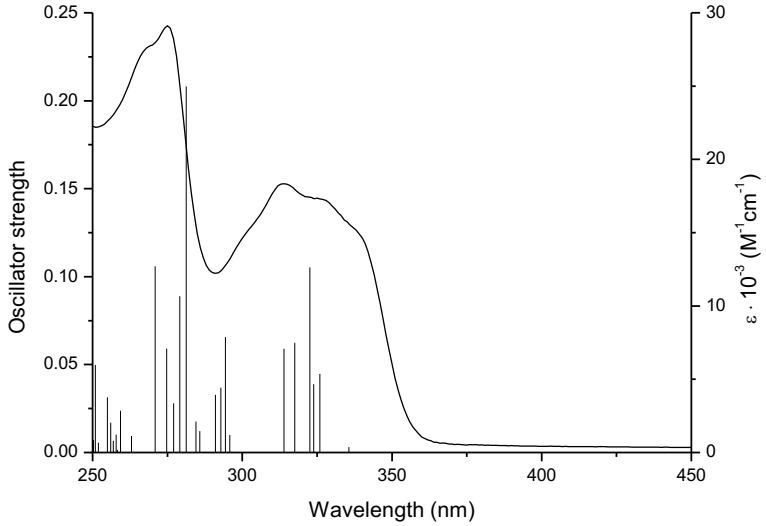

Figure S36. Calculated stick absorption spectrum of **6b'** compared with the experimental spectrum in CH_2Cl_2 solution (*ca.* 1×10^{-5} M) at 298 K.

Table S11. Selected vertical singlet excitations of **6b'** 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 (98%)	3.698	335.3	0.0036
S2	H–2 -> L (6%) H–1 -> L (63%) H–1 -> L+1 (21%) H -> L+1 (3%)	3.807	325.6	0.0453
S3	H–2 -> L (4%) H–1 -> L (9%) H–1 -> L+1 (9%) H -> L+1 (76%)	3.832	323.5	0.0394
S4	H–2 -> L (4%) H–1 -> L (9%) H–1 -> L+1 (59%) H -> L+1 (20%)	3.847	322.3	0.1058
S5	H–2 -> L (77%) H–1 -> L (14%)	3.909	317.2	0.0629
S6	H–4 -> L+1 (3%) H–2 -> L+1 (90%)	3.954	313.6	0.0595
S7	H–4 -> L+1 (3%) H–3 -> L (92%) H–1 -> L+2 (2%)	4.196	295.5	0.0106
S8	H–4 -> L (9%) H–4 -> L+1 (31%) H–3 -> L (3%) H–3 -> L+1 (23%) H–1 -> L+2 (12%) H–1 -> L+3 (6%) H -> L+2 (7%)	4.217	294.1	0.0662
S9	H–5 -> L (40%) H–4 -> L (7%) H–2 -> L+2 (12%) H–1 -> L+2 (9%)	4.238	292.5	0.0374

	H -> L+2 (22%) H -> L+3 (3%)			
S10	H–5 -> L (11%) H–4 -> L+1 (2%) H–3 -> L+1 (3%) H–2 -> L+2 (9%) H -> L+2 (59%) H -> L+3 (6%)	4.265	290.7	0.0333
S11	H–5 -> L (6%) H–4 -> L (77%) H–4 -> L+1 (4%) H–3 -> L+1 (3%) H–1 -> L+2 (2%)	4.307	287.9	0.0007
S12	H–5 -> L (3%) H–5 -> L+1 (69%) H–4 -> L+1 (15%) H–3 -> L+1 (3%) H–2 -> L+1 (3%) H–1 -> L+2 (5%)	4.342	285.5	0.0128

[a] H = HOMO; L = LUMO.

Table S12. Lowest-energy vertical triplet excitations of **6b'** from TDDFT calculations at the ground state geometry in CH_2Cl_2 solution.

state	**monoexcitations[a]**	**ΔE/eV**	**λ/nm**
T1	H–4 -> L+1 (5%) H–2 -> L+1 (14%) H–1 -> L (4%) H–1 -> L+1 (55%) H–1 -> L+3 (3%)	2.902	427.2
T2	H–5 -> L (8%) H–2 -> L (53%) H–2 -> L+3 (2%) H–1 -> L (13%) H–1 -> L+1 (3%)	2.913	425.6
T3	H–11 -> L+2 (2%) H–5 -> L (13%) H–5 -> L+3 (3%) H–4 -> L+1 (7%) H–2 -> L (3%) H–2 -> L+2 (9%) H–1 -> L (16%) H–1 -> L+1 (3%) H–1 -> L+3 (10%) H -> L (16%)	3.625	342.0

[a] H = HOMO; L = LUMO.

5.4. Supplementary computational data

Table S13. 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]
5b (S_0)	-1847.236102	-1846.767708	-1846.830977	-1846.736295	199.275
5b (T_1)	-1847.133817	-1846.669969	-1846.734847	-1846.637901	204.040
6b (S_0)	-1486.852548	-1486.383224	-1486.445768	-1486.352355	196.603
6b (T_1)	-1486.750284	-1486.285324	-1486.348963	-1486.253900	200.075
6b' (S_0)	-1644.115433	-1643.533805	-1643.603109	-1643.497304	222.685
6b' (T_1)	-1644.013154	-1643.435903	-1643.506225	-1643.398848	225.993

[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 S14. Cartesian coordinates (Å) of the optimized structures at the B3LYP(6-31G**+LANL2DZ) level in CH_2Cl_2 solution.

5b (S_0)

C	-0.226156789	-1.675989667	1.065740844
C	0.513514450	-2.065930677	2.181142554
C	0.289813512	-3.296771081	2.819072295
C	-0.710609394	-4.139725070	2.314372225
C	-1.454335214	-3.769454176	1.200017878
C	-1.225499477	-2.540494188	0.558520387
C	-1.970893163	-2.112690366	-0.634029154
C	-3.012537434	-2.826820487	-1.243778481
C	-3.623244069	-2.314993119	-2.383322448
C	-3.191328259	-1.095095301	-2.909204003
C	-2.159357486	-0.427502397	-2.260740925
C	1.125710877	-3.709895526	4.006307156
H	1.276552466	-1.404479182	2.578018448
H	-0.906138657	-5.093206003	2.797253396
H	-2.218767406	-4.446093783	0.830978570
H	-3.342285113	-3.771176987	-0.828503709
H	-4.430509640	-2.863875574	-2.857937660
H	-3.641230751	-0.666802884	-3.797335637
H	-1.768625340	0.523822197	-2.607254575
H	2.014873168	-4.266259976	3.683845061
H	0.564073303	-4.360405450	4.683111961
H	1.474055629	-2.841217691	4.572326899
N	-1.574627416	-0.925409949	-1.160787047
C	1.608192065	0.744019714	1.068022953
C	1.564607884	1.628960076	2.145560528
C	2.729724156	2.066683542	2.796072786
C	3.968452064	1.589321922	2.346869238
C	4.038167812	0.715638256	1.268106553
C	2.871656871	0.286176793	0.614009225
C	2.905645921	-0.616365498	-0.544814072
C	4.065480306	-1.159361745	-1.119628307
C	3.963169838	-1.991325998	-2.227745120
C	2.703655605	-2.279011685	-2.759462113
C	1.591280365	-1.715483805	-2.147906789
C	2.646297670	3.051958191	3.937043431
H	0.608206024	1.995371145	2.499743422
H	4.882294235	1.908211096	2.840895131
H	5.012409343	0.369725052	0.937070565
H	5.038231573	-0.929801083	-0.702745593
H	4.858408434	-2.412037744	-2.674671016
H	2.582201181	-2.921562482	-3.623700781
H	0.587369421	-1.899706461	-2.513341362
H	2.673211842	4.083818001	3.564776322
H	3.485068253	2.934543920	4.629595779
H	1.715142957	2.935673629	4.499299576
N	1.694371136	-0.913599422	-1.078737379
C	-1.449179541	0.951678392	1.121964524
C	-1.622802474	0.717921640	2.494967370
C	-2.651303941	1.338910813	3.212133244
C	-3.538062973	2.203660936	2.569674619
C	-3.382530890	2.439740305	1.202765779
C	-2.352329913	1.819579564	0.488058978
H	-0.952629054	0.048484413	3.022579805
H	-2.756730077	1.139457097	4.275756554
H	-4.337899695	2.685819198	3.124992923
H	-4.061244983	3.112790434	0.684507028
H	-2.241222990	2.034894558	-0.568217650
Pt	0.026212919	0.039461445	0.007188578
Cl	0.286723437	1.997980164	-1.612603123

5b (T_1)

$\langle S^2 \rangle = 2.028923$

C	-0.233304595	-1.678577217	1.060641179
C	0.512036351	-2.069269192	2.171667292
C	0.295892071	-3.304167037	2.804439571
C	-0.702213457	-4.149064202	2.298581560
C	-1.450514538	-3.777681110	1.187489103
C	-1.229033386	-2.545066062	0.550835685
C	-1.974867728	-2.115088825	-0.640280865
C	-3.011966880	-2.831000294	-1.255269549
C	-3.622141565	-2.316878244	-2.394093402
C	-3.193929473	-1.093054058	-2.913711164
C	-2.166539162	-0.423448799	-2.259993743

C	1.137342463	-3.719014853	3.987098297
H	1.271593498	-1.404791259	2.570833533
H	-0.891909838	-5.105594604	2.777679315
H	-2.212021095	-4.456636344	0.816661188
H	-3.338267346	-3.778632322	-0.844737496
H	-4.425900327	-2.867107767	-2.873063753
H	-3.643236375	-0.663022701	-3.801298153
H	-1.778979672	0.531123711	-2.601035108
H	2.032658329	-4.261762990	3.658587045
H	0.583654994	-4.382383769	4.657859205
H	1.476014045	-2.851913988	4.561416847
N	-1.582584083	-0.923492200	-1.160498238
C	1.566465725	0.761924442	1.072791745
C	1.543506153	1.665001719	2.109318607
C	2.721856958	2.104328439	2.767593139
C	3.986130453	1.556551605	2.345684055
C	4.074624658	0.665671186	1.321238606
C	2.880676745	0.243148123	0.602741258
C	2.909023659	-0.603748013	-0.502319413
C	4.088536093	-1.186505358	-1.092814108
C	3.988230249	-1.994150640	-2.196286226
C	2.707921863	-2.254466270	-2.751914416
C	1.581934396	-1.676064889	-2.143413783
C	2.676077982	3.115703629	3.872499253
H	0.595208034	2.066083630	2.447981653
H	4.888385028	1.871307820	2.864176681
H	5.042783016	0.274561773	1.029913840
H	5.057996290	-0.976208387	-0.657345418
H	4.876491489	-2.429385698	-2.641969460
H	2.582427129	-2.883872029	-3.624542495
H	0.587849401	-1.858704141	-2.539871854
H	3.182392916	4.046694799	3.580295181
H	3.195769152	2.752281628	4.768894366
H	1.648778611	3.366073530	4.148307203
N	1.654964137	-0.892377218	-1.080896576
C	-1.469627293	0.944760151	1.137774081
C	-1.620762004	0.722148104	2.515429310
C	-2.649395632	1.332738950	3.241411367
C	-3.559489948	2.176109169	2.603111832
C	-3.426981842	2.401434349	1.231792998
C	-2.396310993	1.791659638	0.509032991
H	-0.932051901	0.068677313	3.039658249
H	-2.736942690	1.142073853	4.308316856
H	-4.359650552	2.650189488	3.164945757
H	-4.124111420	3.058214109	0.717032082
H	-2.302649091	1.999252470	-0.550621136
Pt	0.008742961	0.043070135	0.012884401
Cl	0.242110631	2.034103745	-1.604743332

6b (S_0)

C	-0.213359491	-1.755530749	1.122982397
C	0.520398325	-2.144607787	2.244762244
C	0.299981733	-3.373531659	2.887573147
C	-0.694289653	-4.225053928	2.383826945
C	-1.437126518	-3.862661986	1.265571302
C	-1.210788497	-2.635459437	0.621724434
C	-1.964729597	-2.210305793	-0.568390818
C	-3.006037809	-2.911335418	-1.194282432
C	-3.613961247	-2.370675446	-2.323508539
C	-3.185721918	-1.137891225	-2.826234217
C	-2.152228601	-0.484465273	-2.165836574
C	1.132911842	-3.777281168	4.080454170
H	1.277499322	-1.476876556	2.644574669
H	-0.885909423	-5.177348684	2.870910562
H	-2.199391031	-4.542981544	0.897393728
H	-3.337989649	-3.864755432	-0.801301887
H	-4.421323748	-2.908897561	-2.810333028
H	-3.640744887	-0.693684205	-3.703928904
H	-1.741643307	0.474886687	-2.467487566
H	2.037970120	-4.310976771	3.763632766
H	0.579680925	-4.444901907	4.747540492
H	1.456462094	-2.905045368	4.655975048
N	-1.574998422	-1.017143121	-1.081063621
C	1.575937844	0.713708373	1.059272102
C	1.521335901	1.560866548	2.168020954
C	2.680308325	2.058217177	2.784709118
C	3.928375524	1.680316077	2.269675057
C	4.011224440	0.837550322	1.167406266
C	2.848585315	0.346071233	0.550903489
C	2.891488736	-0.551365032	-0.612981558
C	4.058078757	-1.006471791	-1.247401768
C	3.962671411	-1.852828003	-2.345480502
C	2.703473403	-2.242707634	-2.808100837
C	1.584384301	-1.761185870	-2.140568243
C	2.581535699	2.999424792	3.961233404
H	0.556308077	1.845395000	2.573209243
H	4.838926852	2.047956827	2.735331319
H	4.991988509	0.561141111	0.792675117
H	5.030627910	-0.697398781	-0.884713720
H	4.863341974	-2.205434828	-2.838193607
H	2.587508797	-2.900221446	-3.661810946
H	0.579561744	-2.024429379	-2.451982736
H	2.551811479	4.043819160	3.625683555
H	3.442527371	2.898112919	4.628827858
H	1.671748454	2.820268479	4.541597391
N	1.680062432	-0.945942026	-1.081325955
C	-1.436953752	0.931684657	1.120517801
C	-1.892229620	0.539367314	2.387876558
C	-2.887441435	1.268351197	3.050000013
C	-3.448319899	2.400593201	2.457414280
C	-2.999967855	2.800015315	1.196242933
C	-2.004808307	2.074337626	0.534621790
H	-1.470833796	-0.333018218	2.874876105
H	-3.222227602	0.944767903	4.032784650
H	-4.221727535	2.964921737	2.971629122
H	-3.422152375	3.683664379	0.723004054
H	-1.636676639	2.389530878	-0.435313067
Pt	0.005646653	-0.055526966	0.042792815
F	0.028385335	1.498984142	-1.365835955

6b (T_1)

$\langle S^2 \rangle = 2.028594$

C	-0.216448168	-1.750567003	1.117133427
C	0.524214307	-2.138671180	2.234447298
C	0.313842046	-3.371342982	2.873464869
C	-0.677402786	-4.226640364	2.370494245
C	-1.426464036	-3.864850727	1.256093515
C	-1.209795041	-2.634339047	0.615575585
C	-1.967145667	-2.209923055	-0.572267819
C	-3.004872555	-2.914575205	-1.199706531
C	-3.615734779	-2.373771254	-2.327302597
C	-3.193865950	-1.137382352	-2.826432225
C	-2.163802697	-0.480115629	-2.164409044
C	1.154250570	-3.774347965	4.061312220

H	1.277452511	-1.466796708	2.634965974
H	-0.861492671	-5.181782036	2.854841523
H	-2.185487597	-4.548639328	0.887712695
H	-3.331518113	-3.870915934	-0.809366289
H	-4.420288603	-2.914777271	-2.815679174
H	-3.651140960	-0.693153551	-3.702940554
H	-1.757515238	0.482258336	-2.462212293
H	2.065096598	-4.294202635	3.738205778
H	0.610638826	-4.453919008	4.724150503
H	1.468336064	-2.902849806	4.643230200
N	-1.583840185	-1.013177996	-1.081252723
C	1.536843292	0.732580918	1.061345789
C	1.499678100	1.582483661	2.144121330
C	2.670983423	2.082350184	2.767164230
C	3.950053794	1.668640548	2.248168626
C	4.054956055	0.826328848	1.184122832
C	2.862322428	0.314155559	0.526691893
C	2.897233399	-0.540887740	-0.572950521
C	4.084640428	-1.047527283	-1.216102352
C	3.988157789	-1.874691623	-2.304964982
C	2.703172836	-2.231839576	-2.794815630
C	1.570440560	-1.724754091	-2.137203369
C	2.606198237	3.023934504	3.931736191
H	0.539549578	1.888590040	2.545372530
H	4.851310246	2.045232697	2.725843514
H	5.035088551	0.537089677	0.822014265
H	5.057070627	-0.766058698	-0.829931207
H	4.882285149	-2.253525832	-2.788917331
H	2.580691544	-2.880076790	-3.654012456
H	0.573057844	-1.980290245	-2.482708699
H	3.060368321	3.994082748	3.685783728
H	3.164815802	2.633639464	4.793153507
H	1.575609034	3.205216580	4.246671596
N	1.638678231	-0.924316991	-1.087156764
C	-1.459008553	0.931763330	1.129496145
C	-1.897720184	0.540754689	2.403275172
C	-2.897643014	1.258477385	3.070683181
C	-3.480526838	2.378914095	2.476814966
C	-3.049009325	2.778023788	1.209580814
C	-2.049002646	2.063219167	0.543444312
H	-1.459619112	-0.323167313	2.891108104
H	-3.219110076	0.935565913	4.058168754
H	-4.257751107	2.934599489	2.994742886
H	-3.488252000	3.652978015	0.735618666
H	-1.692767618	2.379153966	-0.430833581
Pt	-0.009968477	-0.045573342	0.043060860
F	-0.012675237	1.515429013	-1.367495180

6b' (S_0)

C	-0.182764344	-1.766424857	1.144921747
C	0.572078691	-2.130223426	2.261235097
C	0.375014173	-3.351227685	2.926193995
C	-0.617223268	-4.221307940	2.450848201
C	-1.380875929	-3.884334377	1.338688183
C	-1.178028383	-2.664784630	0.672825848
C	-1.955172069	-2.266014018	-0.511515323
C	-2.998265925	-2.987713454	-1.110496550
C	-3.629539161	-2.470658523	-2.237996231
C	-3.223037312	-1.240885639	-2.765565284
C	-2.186836417	-0.566335488	-2.131129642
C	1.230120713	-3.727166755	4.112483327
H	1.327635623	-1.448168283	2.639178124
H	-0.790842661	-5.167957920	2.955415755
H	-2.141049879	-4.578442426	0.992602267
H	-3.313608792	-3.938699169	-0.698272637
H	-4.438257393	-3.024885134	-2.704190492
H	-3.696632164	-0.814894984	-3.642473894
H	-1.791691626	0.393031751	-2.452792494
H	2.134025708	-4.259927724	3.790809463
H	0.692808538	-4.386608731	4.800423450
H	1.556138111	-2.842246290	4.666848291
N	-1.586907720	-1.076491831	-1.047905216
C	1.577445084	0.721441065	1.015211248
C	1.530300206	1.584370744	2.112164168
C	2.692739583	2.106245511	2.701372459
C	3.936909549	1.737232144	2.170637561
C	4.012418930	0.879038480	1.079816017
C	2.846193539	0.363083867	0.490580074
C	2.881782868	-0.551260715	-0.660396702
C	4.043749584	-1.001677995	-1.306629810
C	3.941454161	-1.866240170	-2.389821555
C	2.680044679	-2.279029720	-2.825786078
C	1.565853837	-1.800985868	-2.147580122
C	2.601298680	3.064118986	3.864990096
H	0.568213067	1.861832309	2.529027705
H	4.850184802	2.124014764	2.614984299
H	4.990359447	0.610084677	0.692456101
H	5.018048980	-0.675024547	-0.964630857
H	4.838513195	-2.215300507	-2.891581786
H	2.558736573	-2.951326993	-3.667161955
H	0.559524305	-2.081643447	-2.438401370
H	2.551676803	4.102723007	3.514133684
H	3.474841517	2.984651687	4.519127155
H	1.704018630	2.881878750	4.463585912
N	1.668086299	-0.968083850	-1.102845170
C	-1.434704167	0.903244333	1.124056653
C	-1.870599802	0.532158306	2.400278134
C	-2.864204357	1.260718985	3.068506188
C	-3.467395331	2.385825245	2.492980595
C	-3.020274116	2.751013470	1.210972725
C	-2.030414115	2.032452871	0.540141870
H	-1.437577049	-0.327510872	2.900075753
H	-3.160882142	0.926826879	4.057376485
H	-3.448296271	3.620137460	0.716967385
H	-1.688550657	2.345584649	-0.440133639
Pt	0.000256943	-0.080818743	0.036374878
F	-0.020084137	1.454785459	-1.392876627
C	-4.563560020	3.207721933	3.195974409
C	-4.082724727	4.668070500	3.371522447
H	-3.854860458	5.138621535	2.410425658
H	-4.856516757	5.269240657	3.862956013
H	-3.178170881	4.710031128	3.987751068
C	-5.849493877	3.196013896	2.335215707
H	-6.221829022	2.174417019	2.202890014
H	-6.638261354	3.784972066	2.817511000
H	-5.676372482	3.620596299	1.341801619
C	-4.913370651	2.647671107	4.587912598
H	-5.289623559	1.620833310	4.530950567
H	-4.048686114	2.657030437	5.259783064
H	-5.695411644	3.261703420	5.046827205

6b' (T_1)

$\langle S^2 \rangle$ =2.028615

C	-0.185493607	-1.758093052	1.139204992

C	0.573904707	-2.121187439	2.252398504
C	0.382000578	-3.343818135	2.915896237
C	-0.609747517	-4.215206135	2.442281584
C	-1.377398547	-3.878521624	1.332684858
C	-1.179387865	-2.657789664	0.667848581
C	-1.957602315	-2.259472863	-0.515561131
C	-2.999377531	-2.982181049	-1.115267760
C	-3.630876493	-2.465014424	-2.242618605
C	-3.225809909	-1.234251179	-2.768877801
C	-2.190980076	-0.558359369	-2.133554470
C	1.242057364	-3.719505379	4.098651612
H	1.327553775	-1.436758692	2.630199087
H	-0.779584653	-5.163018792	2.945895597
H	-2.136409667	-4.574169971	0.987203918
H	-3.313272658	-3.934017680	-0.703896215
H	-4.438541789	-3.020002109	-2.709722426
H	-3.699492425	-0.808328435	-3.645768456
H	-1.796299972	0.401934145	-2.452996518
H	2.149699578	-4.243001127	3.772401217
H	0.711146462	-4.387038920	4.783684119
H	1.561825930	-2.835137460	4.657588192
N	-1.590962133	-1.068886485	-1.050521563
C	1.547034595	0.737210378	1.014830849
C	1.518743954	1.599955326	2.087828518
C	2.694562540	2.122811833	2.682599515
C	3.969176471	1.719976007	2.144428004
C	4.065605329	0.865431671	1.089352040
C	2.868002098	0.328129472	0.461709061
C	2.894223392	-0.543836856	-0.624900317
C	4.076451912	-1.045789221	-1.281256497
C	3.971289544	-1.893510838	-2.353388733
C	2.682529939	-2.276583047	-2.812835259
C	1.555303254	-1.772253639	-2.143615130
C	2.638939841	3.078509242	3.836146110
H	0.561881197	1.898372966	2.502449799
H	4.874039530	2.114969151	2.599937525
H	5.042685753	0.584653620	0.712613812
H	5.051946662	-0.744455603	-0.918508313
H	4.861500951	-2.268893568	-2.847174227
H	2.553138560	-2.941796283	-3.657936125
H	0.555250320	-2.046603001	-2.466370341
H	3.074968808	4.051456416	3.569270032
H	3.218994530	2.707065856	4.691719246
H	1.612068617	3.249941249	4.168292529
N	1.631804102	-0.952250856	-1.109439968
C	-1.447358224	0.911131381	1.126351557
C	-1.871687843	0.544236072	2.407861160
C	-2.867762756	1.266898865	3.078941373
C	-3.485591551	2.382772956	2.500903252
C	-3.050380354	2.744794717	1.213816524
C	-2.058065277	2.031634598	0.540857265
H	-1.427435203	-0.308796863	2.909642818
H	-3.154812262	0.935992361	4.071688412
H	-3.489917930	3.607116339	0.717922121
H	-1.724721912	2.342806447	-0.443101922
Pt	-0.008216682	-0.070388857	0.033565097
F	-0.047611019	1.468051525	-1.400958015
C	-4.584946549	3.198302138	3.206384125
C	-4.117305692	4.664339753	3.369767098
H	-3.900584685	5.131156638	2.404287737
H	-4.893580289	5.260982523	3.862808880
H	-3.209048797	4.718954337	3.979555737
C	-5.876556161	3.168868712	2.354592130
H	-6.239786970	2.142913509	2.231011657
H	-6.667760605	3.753084920	2.838682636
H	-5.714346241	3.588970031	1.357437917
C	-4.919857395	2.643558987	4.604100813
H	-5.286463514	1.612791795	4.556045444
H	-4.050734385	2.665429375	5.269938160
H	-5.704684682	3.252829324	5.064621177

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