Electronic Supplementary Information

4,5-Substituted C^C* Cyclometalated Thiazol-2-ylidene Platinum(II) Complexes – Synthesis and Photophysical Properties†

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List of Abbreviations

acac	Acetylacetonate
B3LYP	Becke three-parameter exchange, Lee-Yang-Parr correlation functional
BP86	Becke 1988 exchange correction, Perdew86 correlation functional
CIE	Color coordinates, defined by an international commission (*CIE – Commission internationale de l'éclairage*)
COD	1,5-Cyclooctadiene
COSY	Homonuclear correlation spectroscopy
DFT	Density functional theory
DMF	Dimethylformamide
DMSO	Dimethyl sulfoxide
ECP	Effective core potential
FMO	Frontier molecular orbital
HMBC	Heteronuclear multiple-bond correlation spectroscopy
HOMO	Highest occupied molecular orbital
HSQC	Heteronuclear single-quantum correlation spectroscopy
Hz	Hertz
ILCT	Intraligand charge transfer
LUMO	Lowest unoccupied molecular orbital
MLCT	Metal-to-ligand charge transfer
M.p.	Melting point
NHC	N-Heterocyclic carbene
NMR	Nuclear magnetic resonance spectroscopy
NOESY	Nuclear Overhauser effect spectroscopy
OLED	Organic light-emitting diode
PMMA	Poly(methyl methacrylate)
QY	Quantum yield

1D-NMR Spectra

The following section contains all ^{1}H-NMR and ^{13}C-NMR data for the reported compounds.

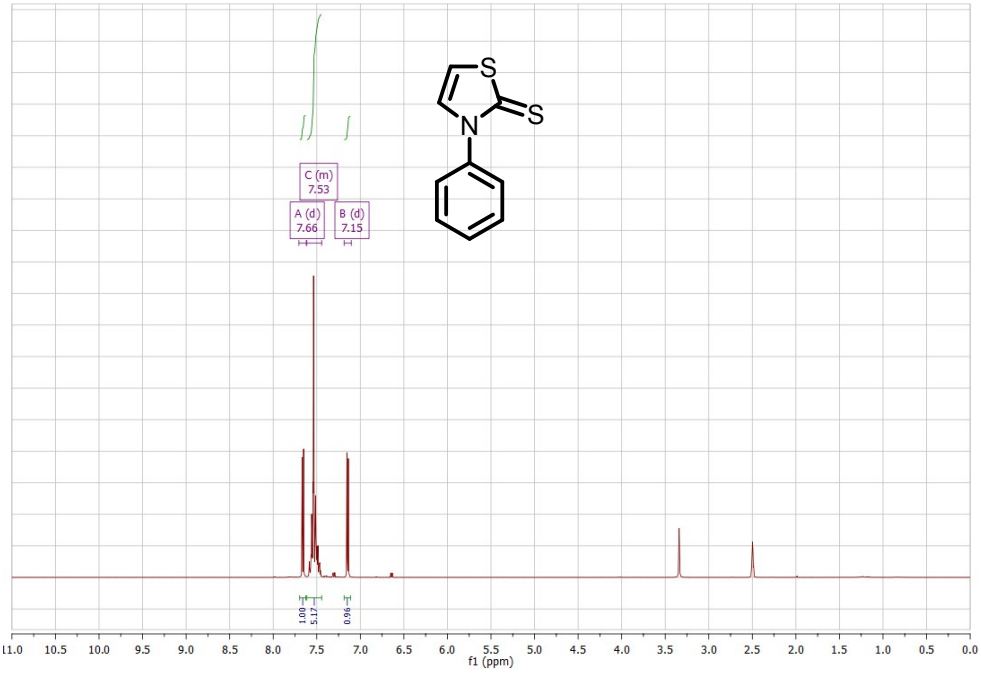


Figure S1. ^{1}H-NMR spectrum of compound **8** in DMSO.

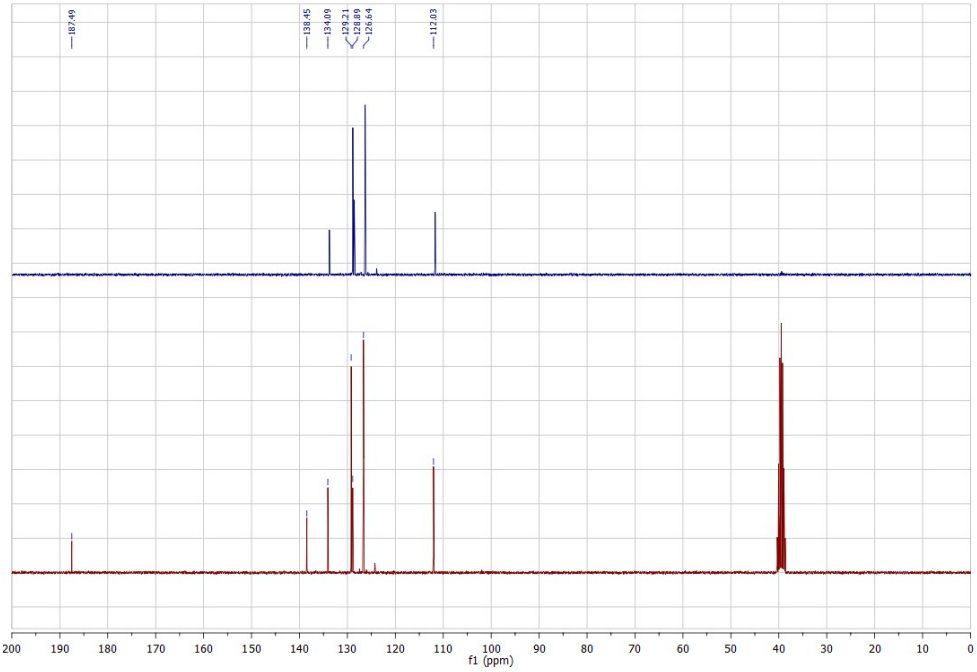


Figure S2. ^{13}C-NMR spectra of compound **8** in DMSO (top: DEPT; bottom: proton decoupled).

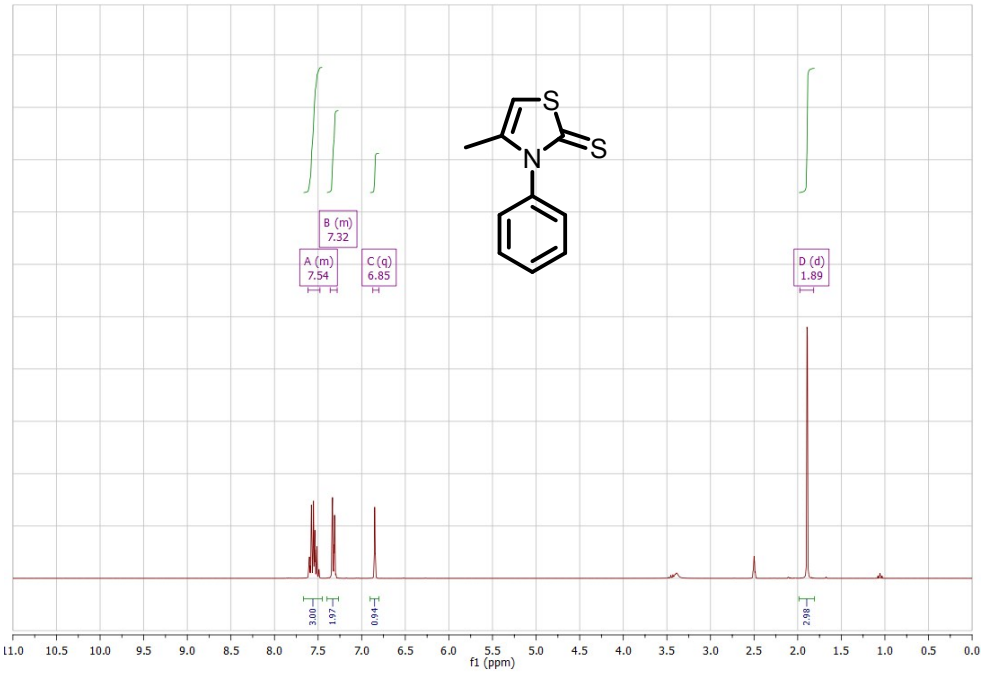


Figure S3. ^{1}H-NMR spectrum of compound **9** in DMSO.

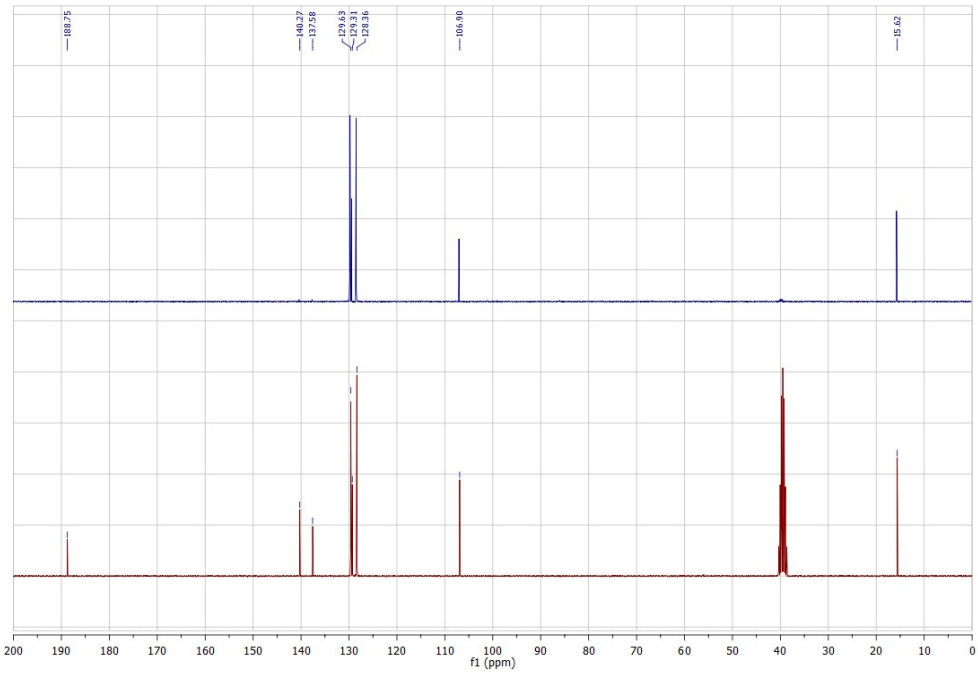


Figure S4. ^{13}C-NMR spectra of compound **9** in DMSO (top: DEPT; bottom: proton decoupled).

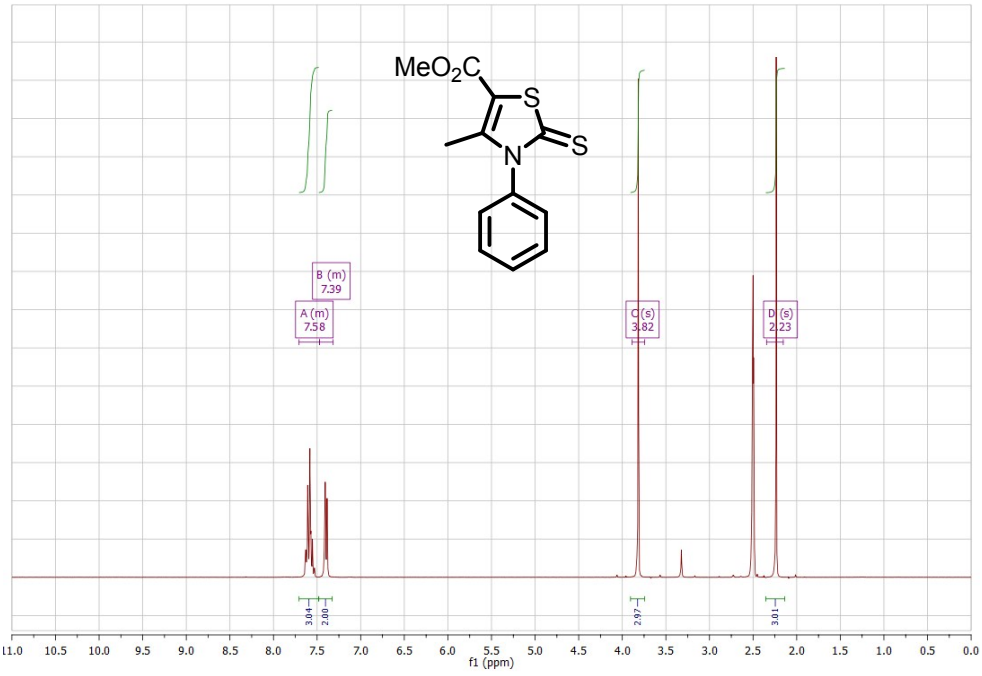


Figure S5. ^{1}H-NMR spectrum of compound **10** in DMSO.

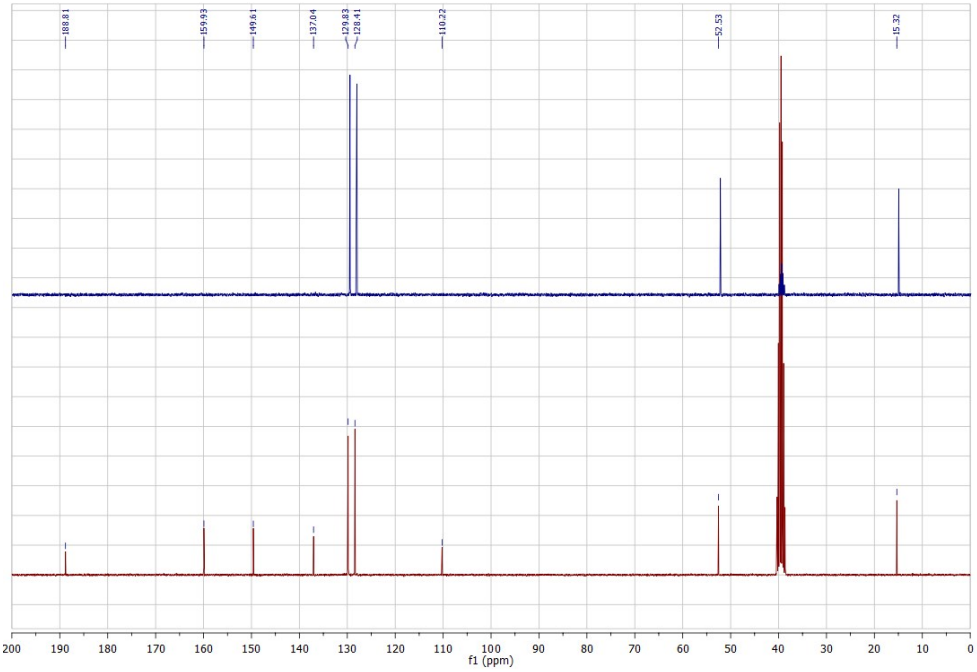


Figure S6. ^{13}C-NMR spectra of compound **10** in DMSO (top: DEPT; bottom: proton decoupled).

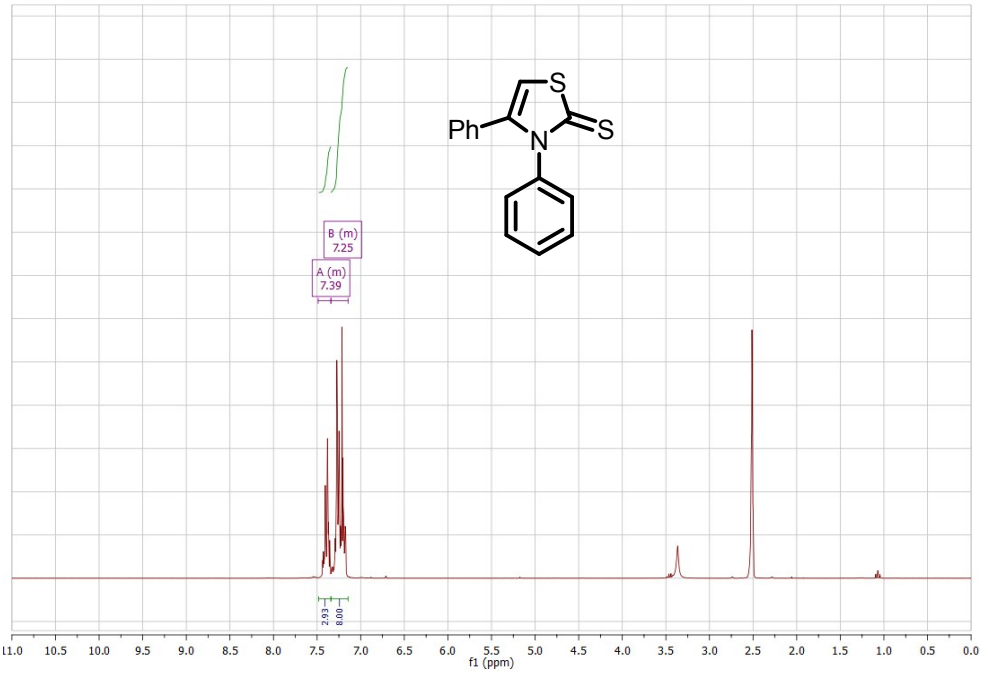


Figure S7. ^{1}H-NMR spectrum of compound **11** in DMSO.

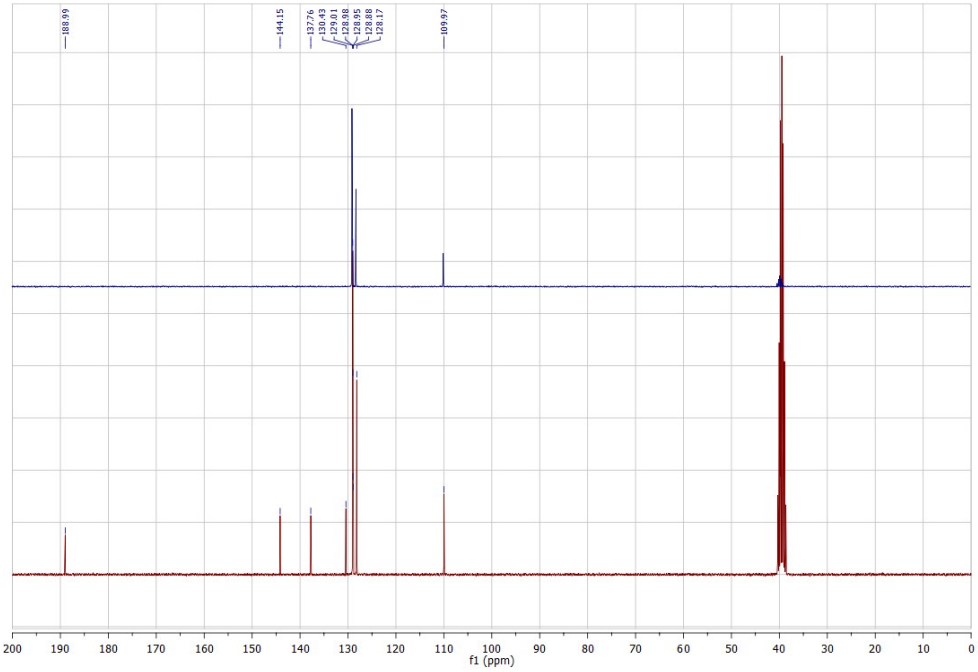


Figure S8. ^{13}C-NMR spectra of compound **11** in DMSO (top: DEPT; bottom: proton decoupled).

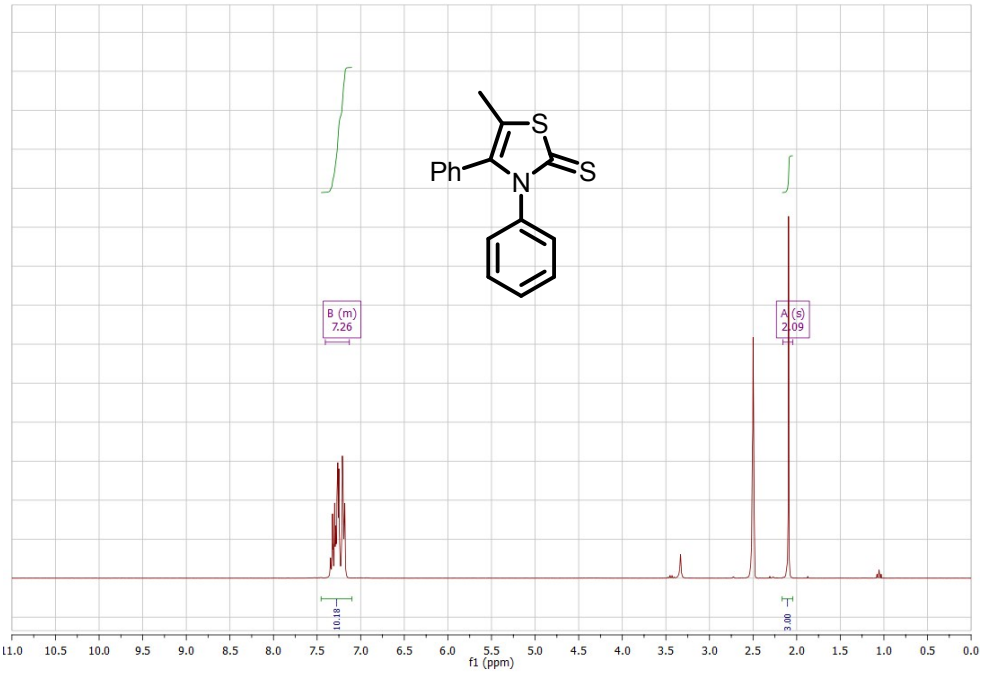


Figure S9. ^{1}H-NMR spectrum of compound **12** in DMSO.

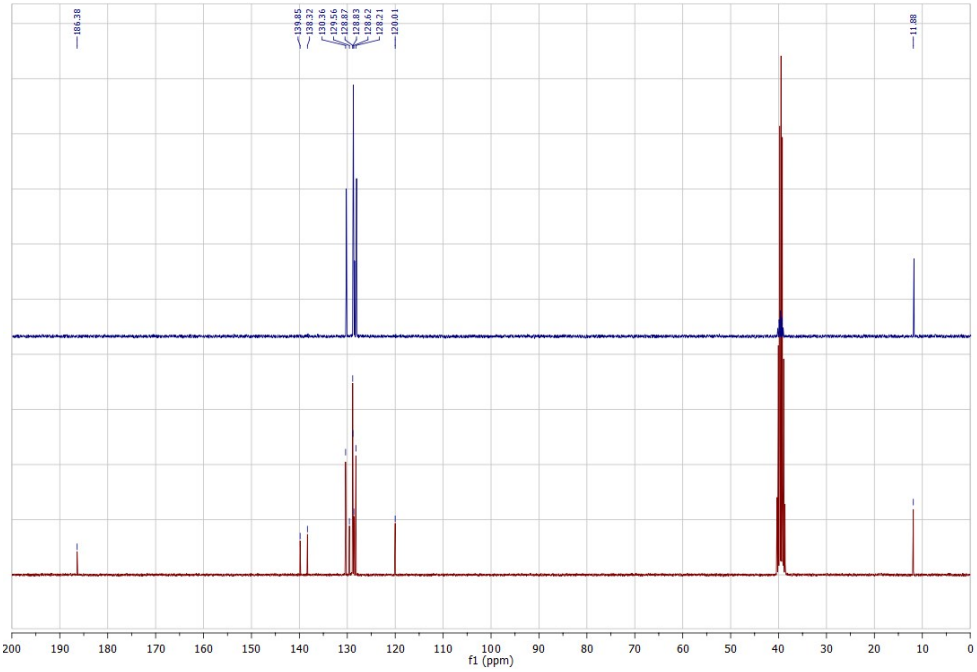


Figure S10. ^{13}C-NMR spectra of compound **12** in DMSO (top: DEPT; bottom: proton decoupled).

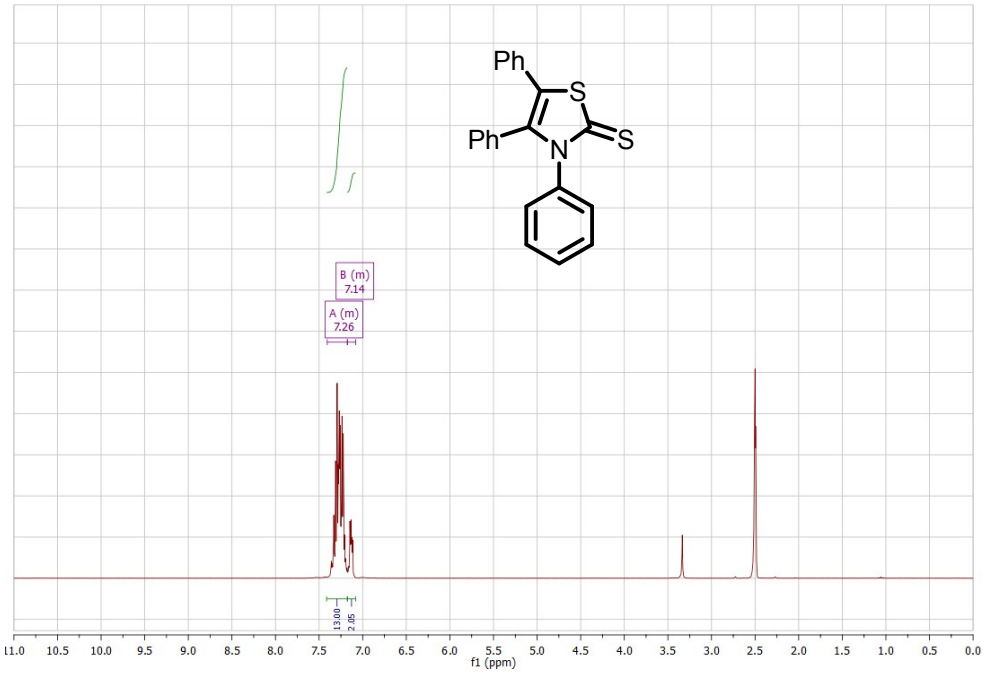


Figure S11. ^{1}H-NMR spectrum of compound **13** in DMSO.

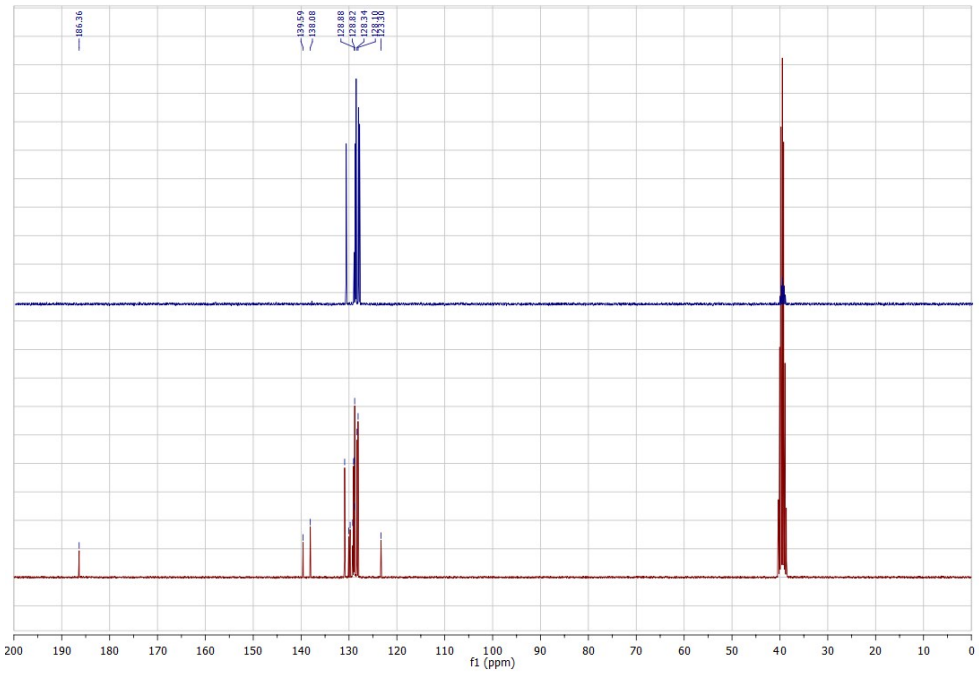


Figure S12. ^{13}C-NMR spectra of compound **13** in DMSO (top: DEPT; bottom: proton decoupled).

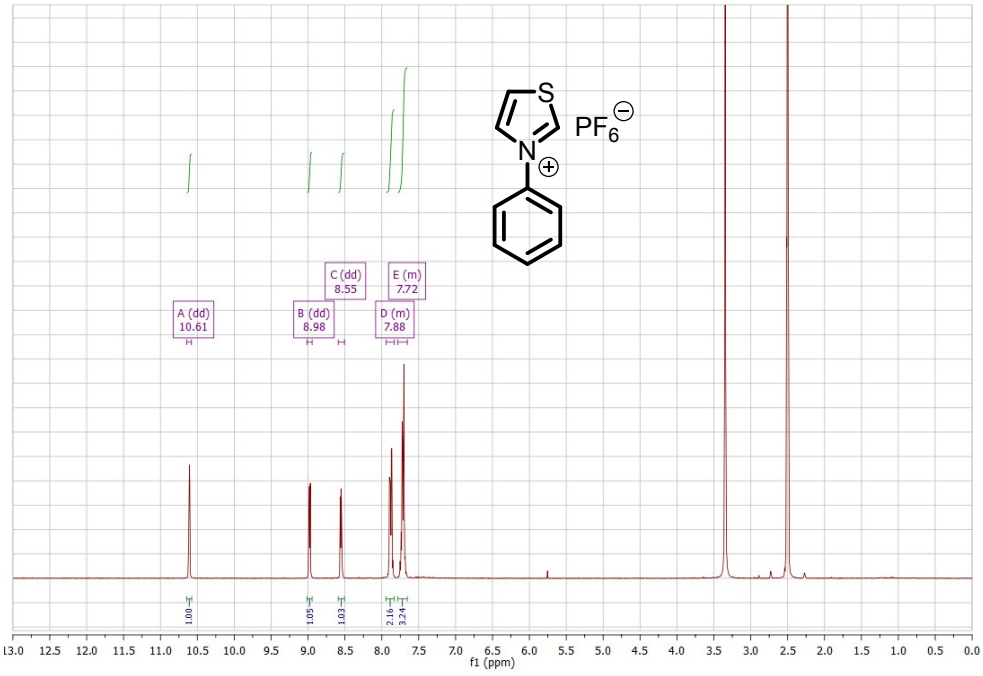


Figure S13. ^{1}H-NMR spectrum of compound **14** in DMSO.

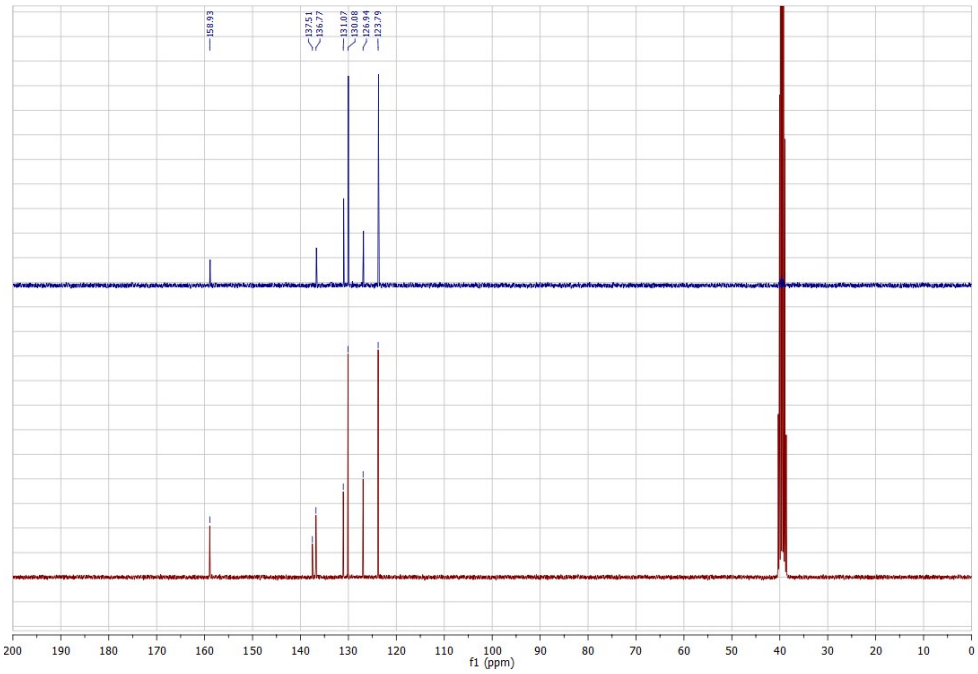


Figure S14. ^{13}C-NMR spectra of compound **14** in DMSO (top: DEPT; bottom: proton decoupled).

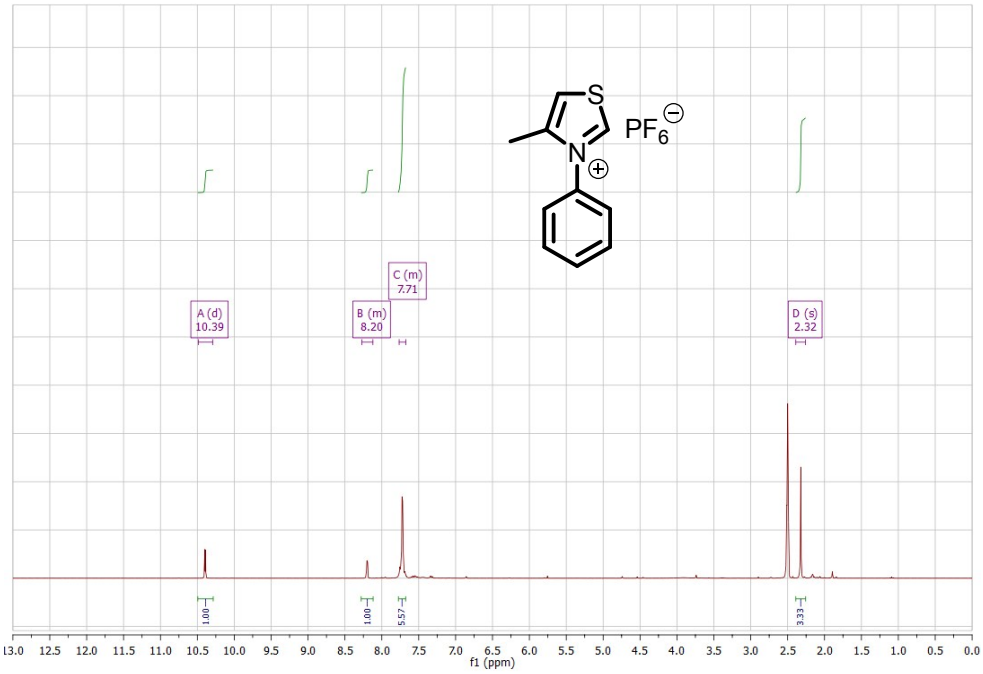


Figure S15. ^{1}H-NMR spectrum of compound **15** in DMSO.

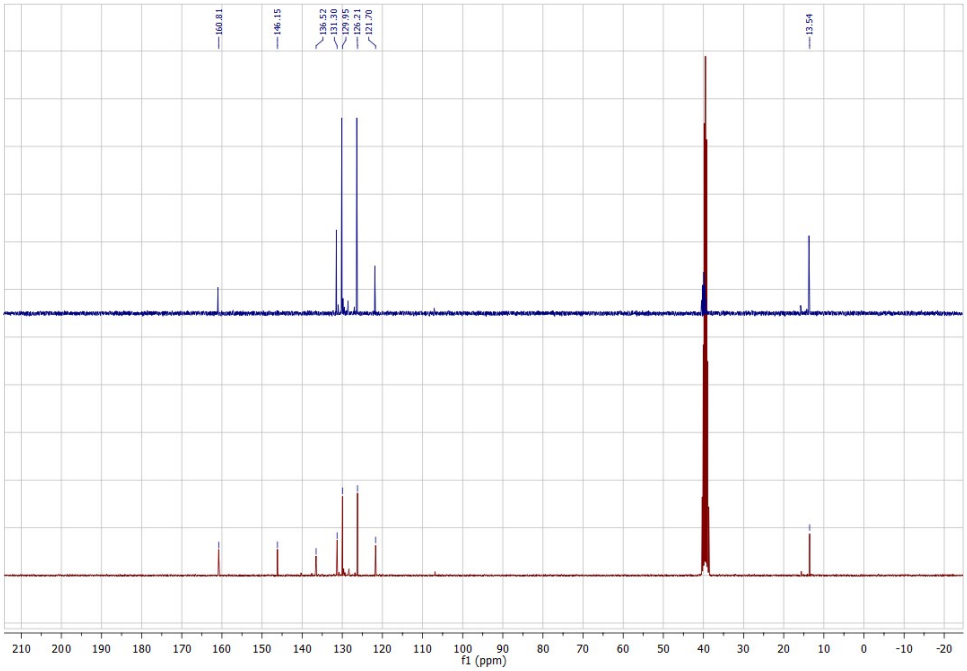


Figure S16. ^{13}C-NMR spectra of compound **15** in DMSO (top: DEPT; bottom: proton decoupled).

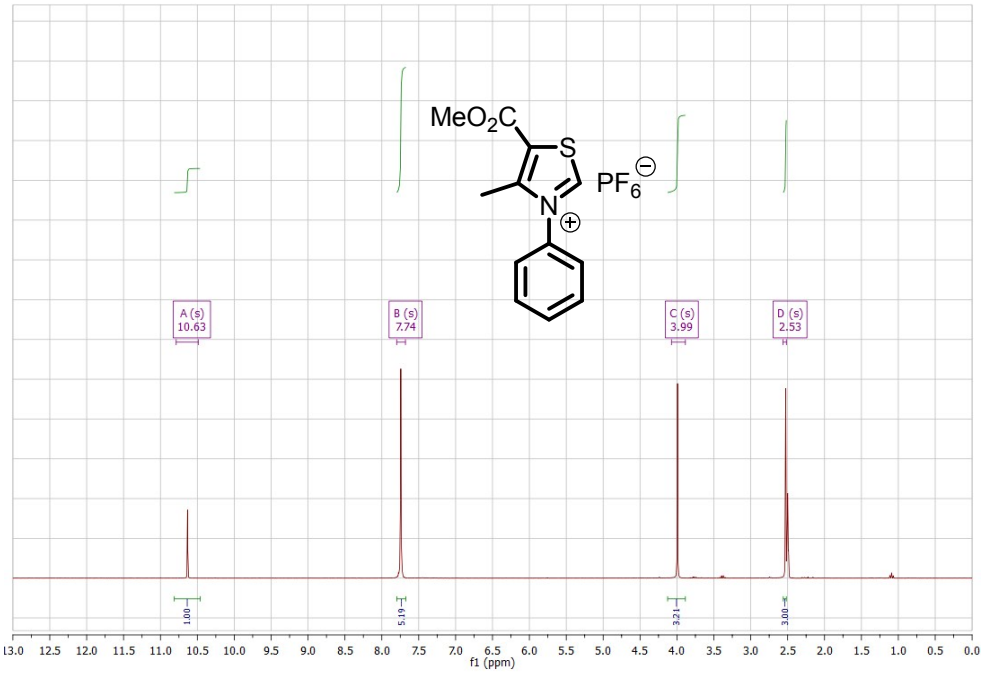


Figure S17. ^{1}H-NMR spectrum of compound **16** in DMSO.

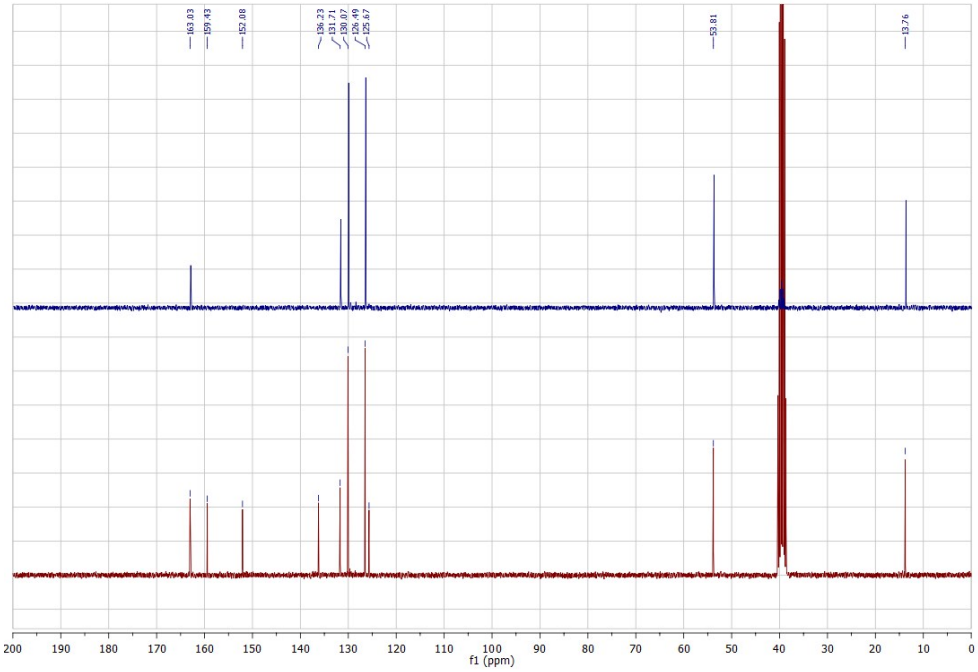


Figure S18. ^{13}C-NMR spectra of compound **16** in DMSO (top: DEPT; bottom: proton decoupled).

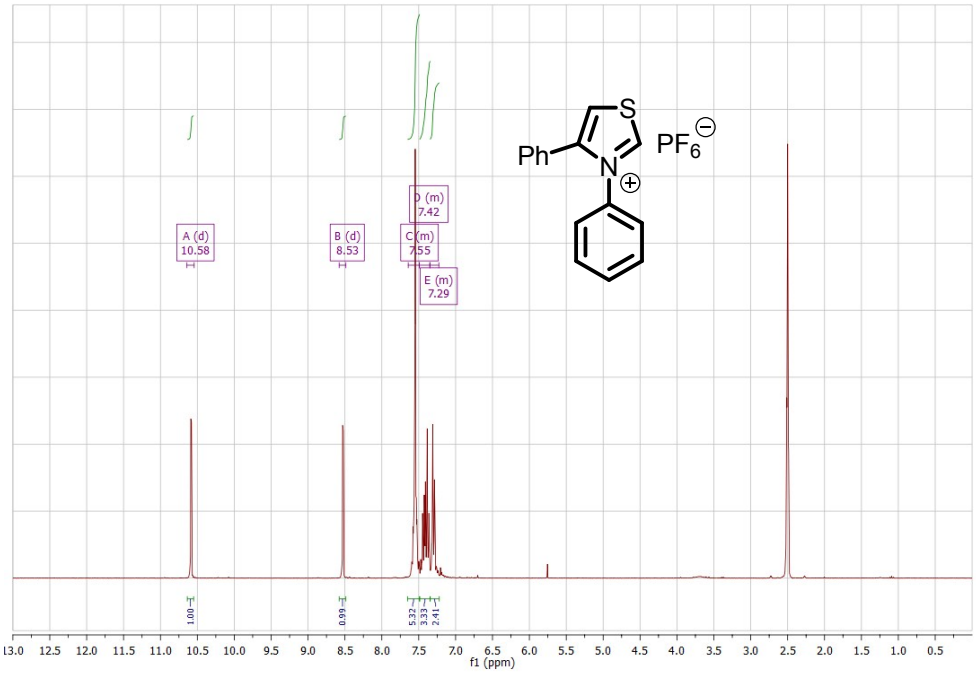


Figure S19. ^{1}H-NMR spectrum of compound **17** in DMSO.

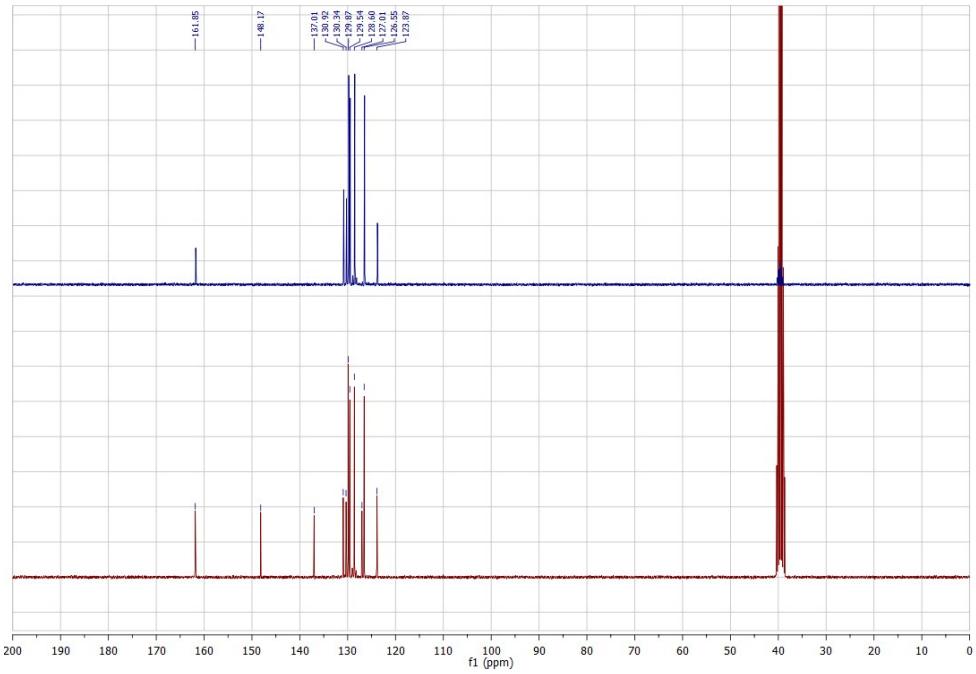


Figure S20. ^{13}C-NMR spectra of compound **17** in DMSO (top: DEPT; bottom: proton decoupled).

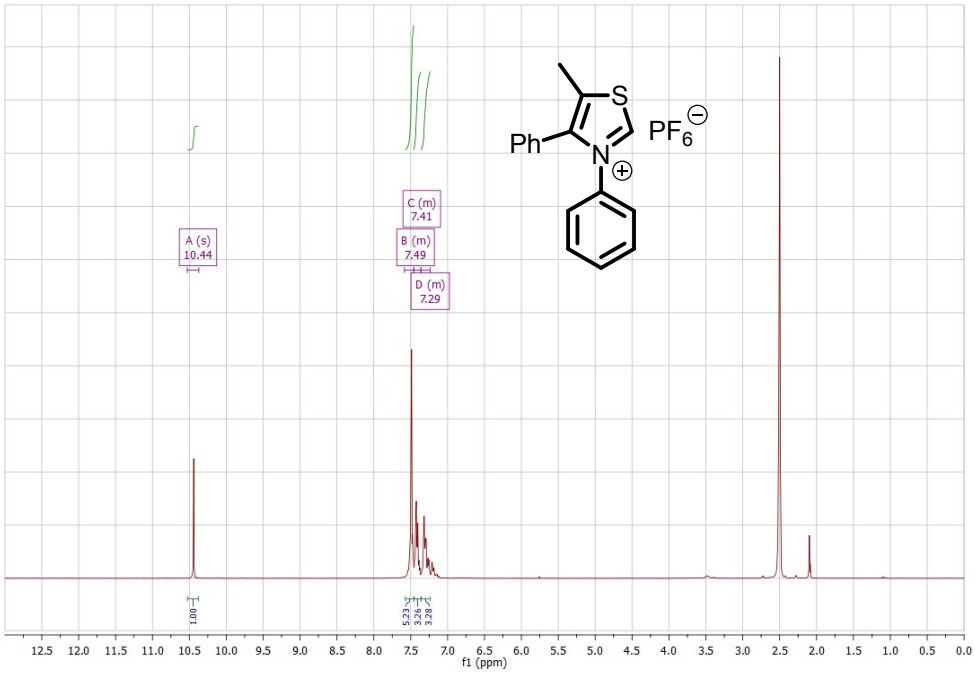


Figure S21. ^{1}H-NMR spectrum of compound **18** in DMSO.

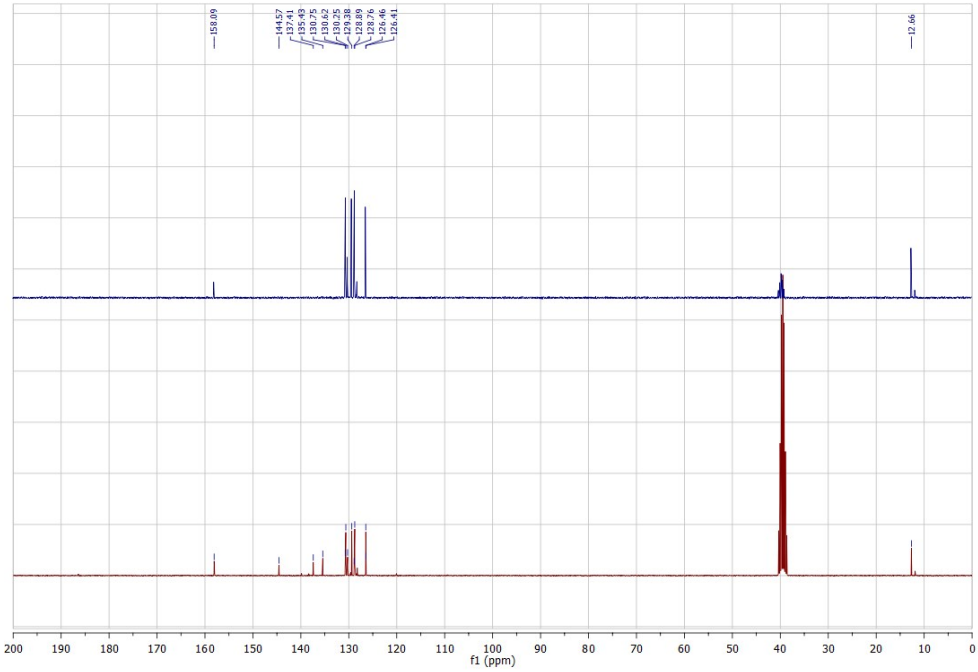


Figure S22. ^{13}C-NMR spectra of compound **18** in DMSO (top: DEPT; bottom: proton decoupled).

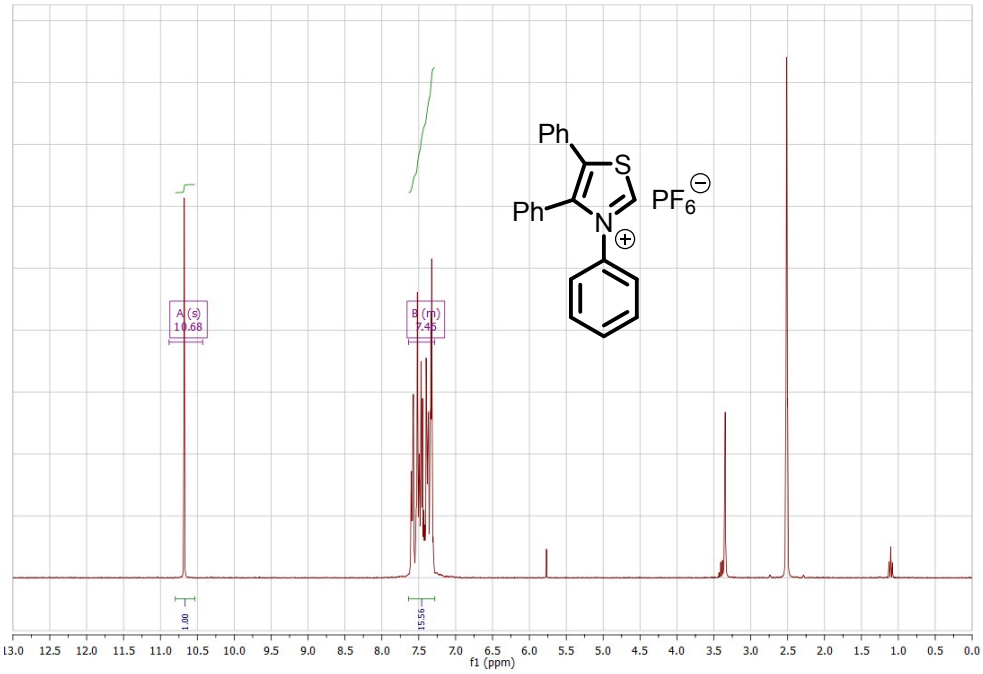


Figure S23. ^{1}H-NMR spectrum of compound **19** in DMSO.

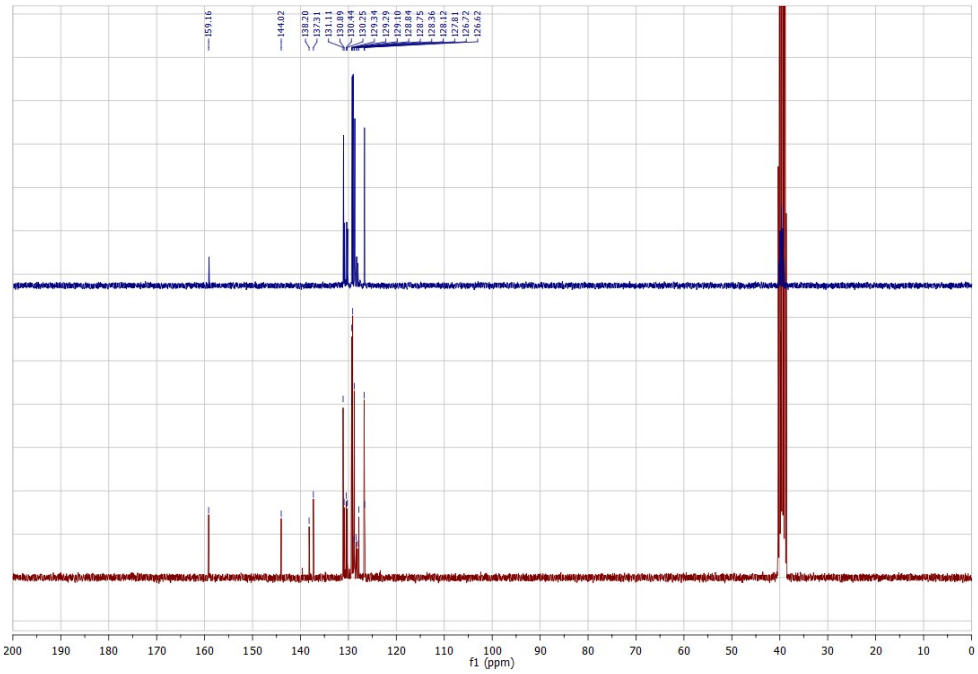


Figure S24. ^{13}C-NMR spectra of compound **19** in DMSO (top: DEPT; bottom: proton decoupled).

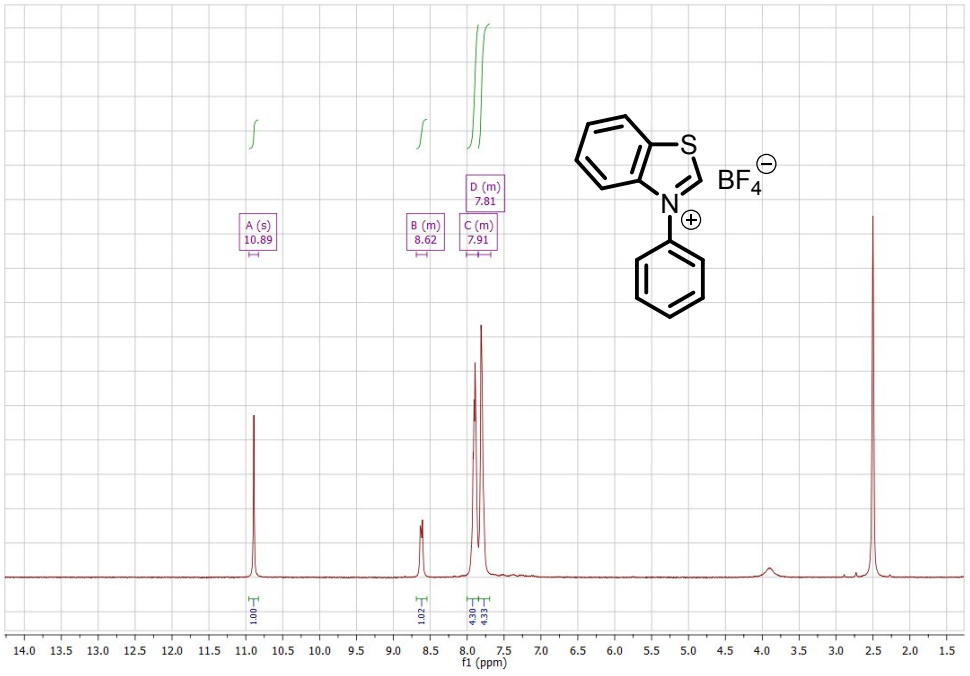


Figure S25. ^{1}H-NMR spectrum of compound **22** in DMSO.

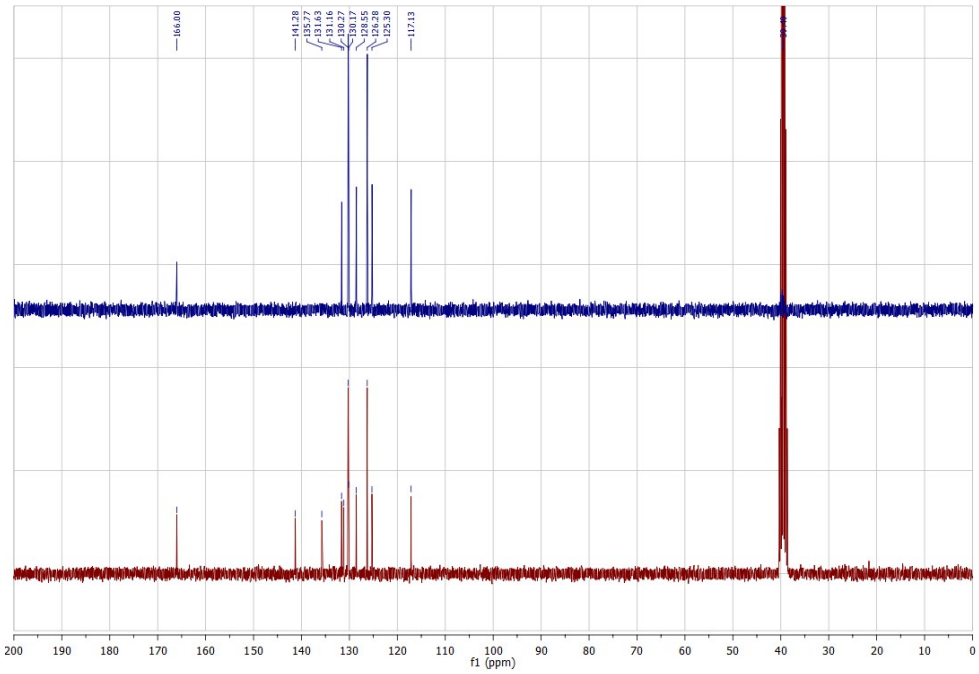


Figure S26. ^{13}C-NMR spectra of compound **22** in DMSO (top: DEPT; bottom: proton decoupled).

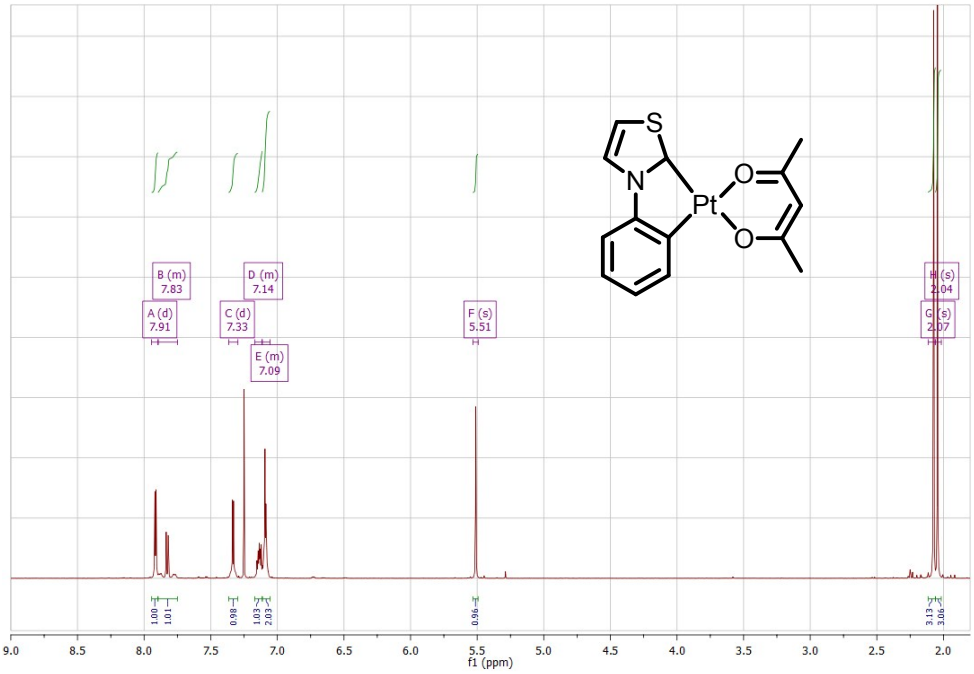


Figure S27. ^{1}H-NMR spectrum of compound **23** in $CDCl_3$.

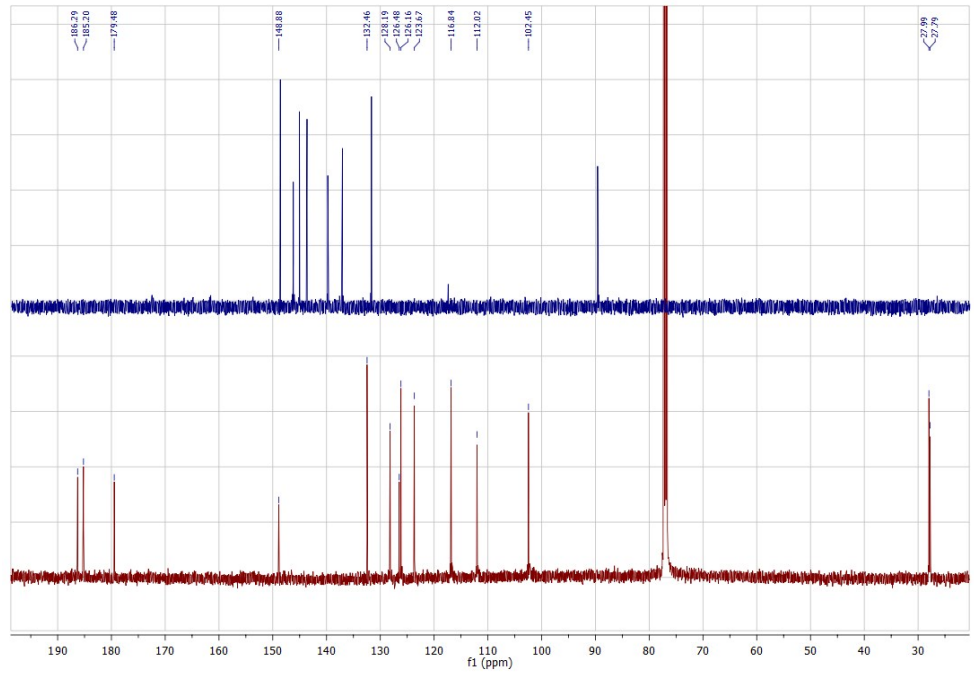


Figure S28. ^{13}C-NMR spectra of compound **23** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

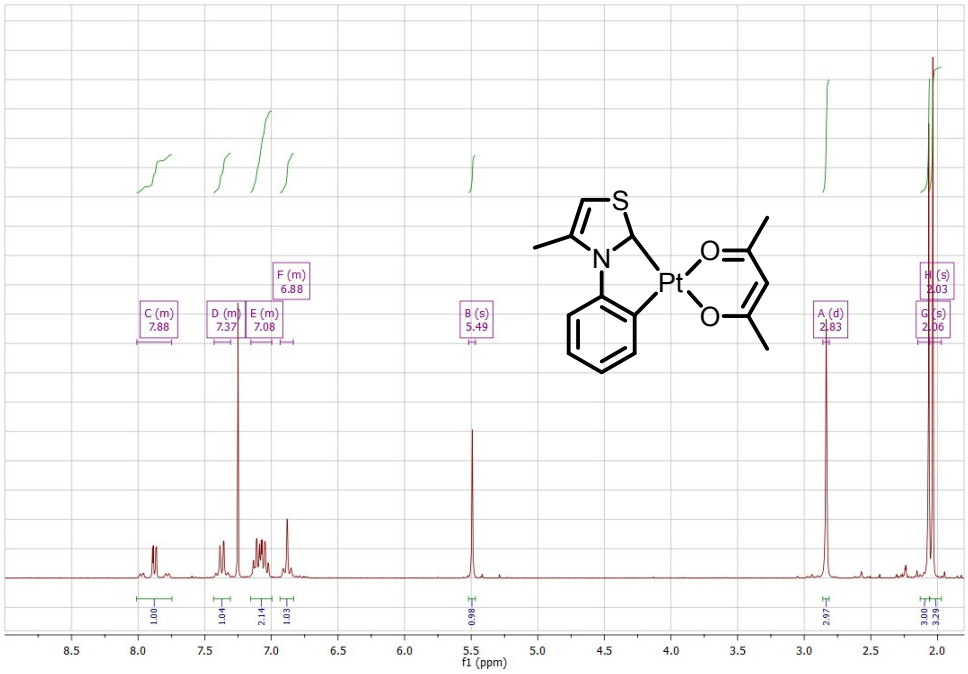


Figure S29. ^{1}H-NMR spectrum of compound **24** in $CDCl_3$.

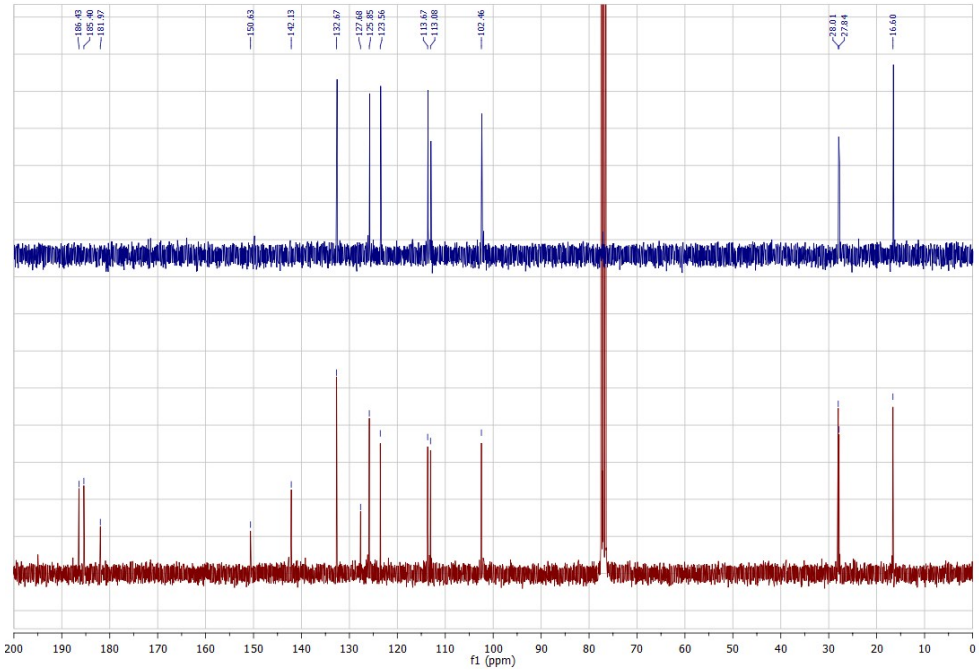


Figure S30. ^{13}C-NMR spectra of compound **24** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

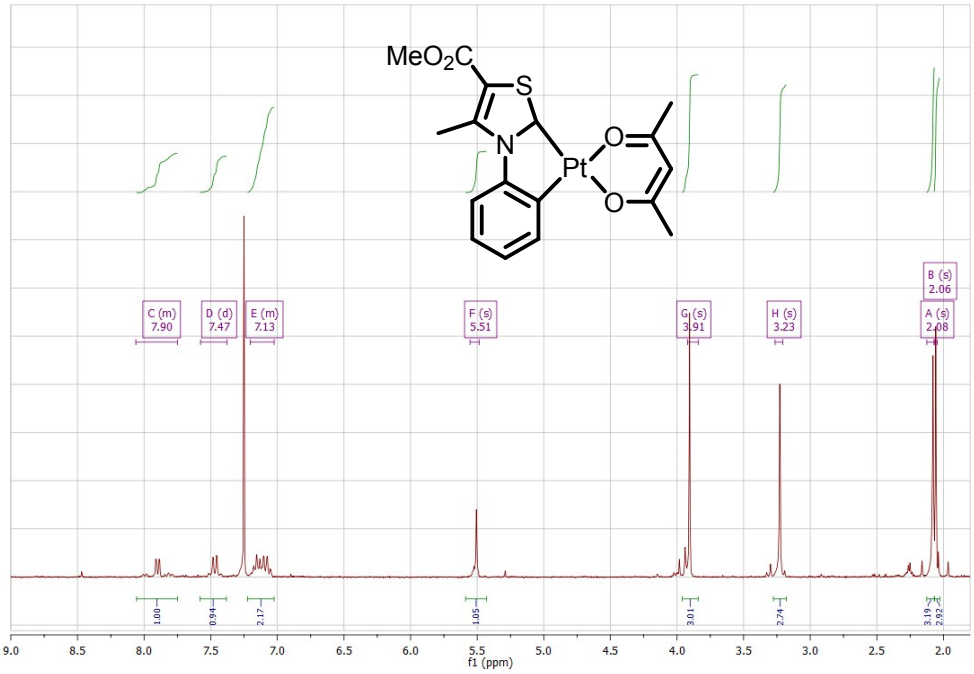


Figure S31. ^{1}H-NMR spectrum of compound **25** in $CDCl_3$.

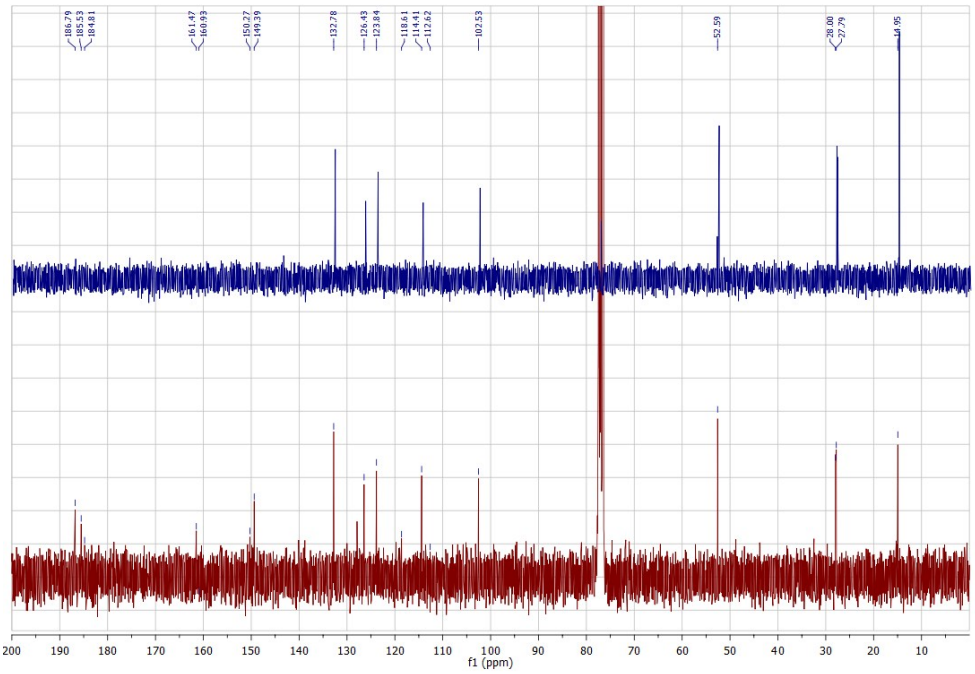


Figure S32. ^{13}C-NMR spectra of compound **25** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

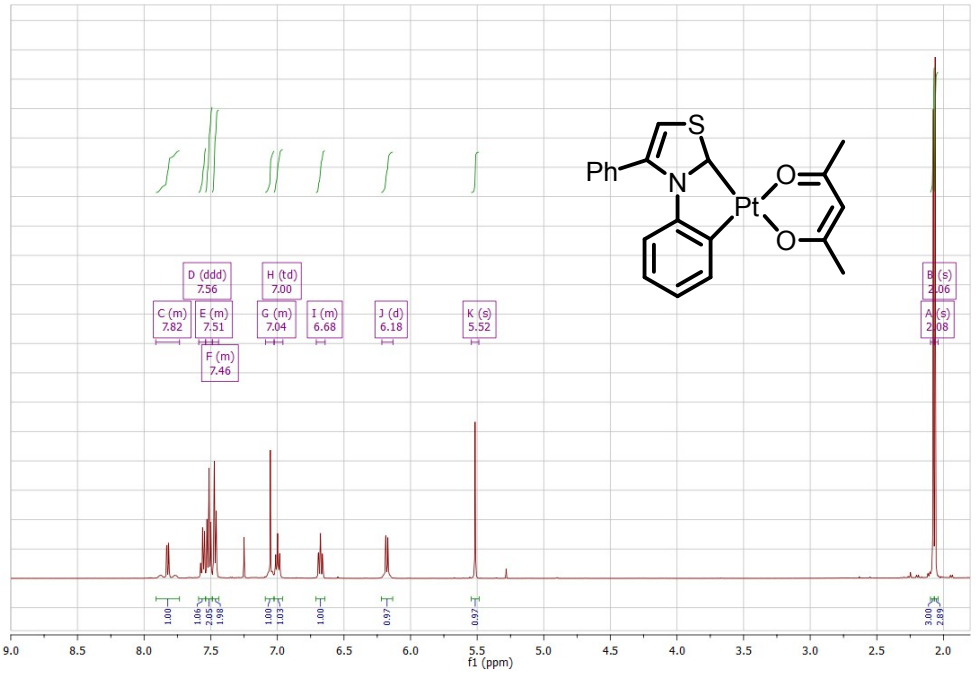


Figure S33. ^{1}H-NMR spectrum of compound **26** in $CDCl_3$.

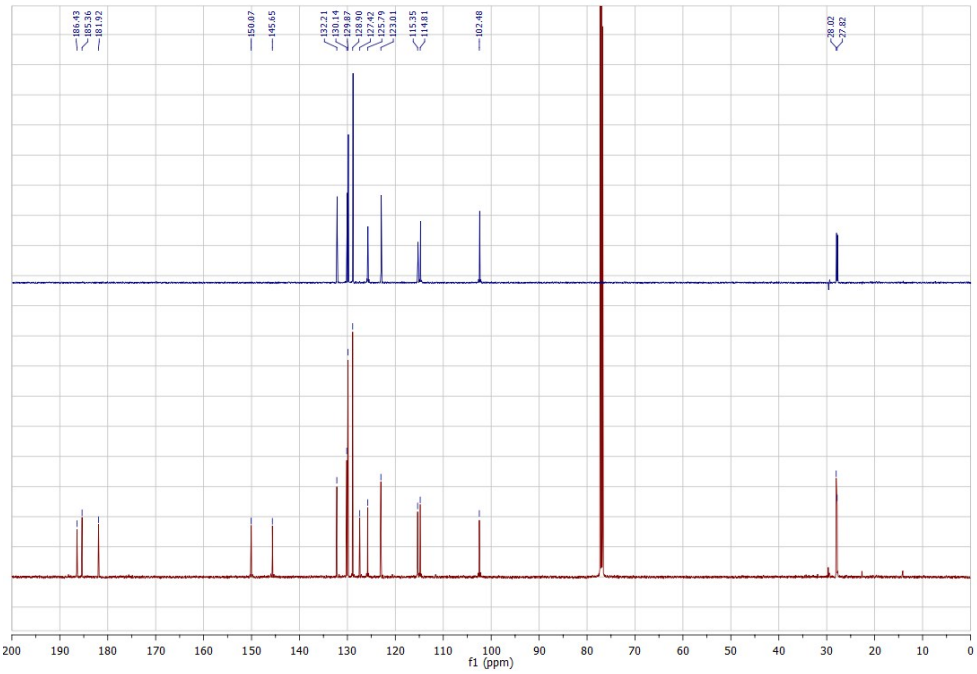


Figure S34. ^{13}C-NMR spectra of compound **26** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

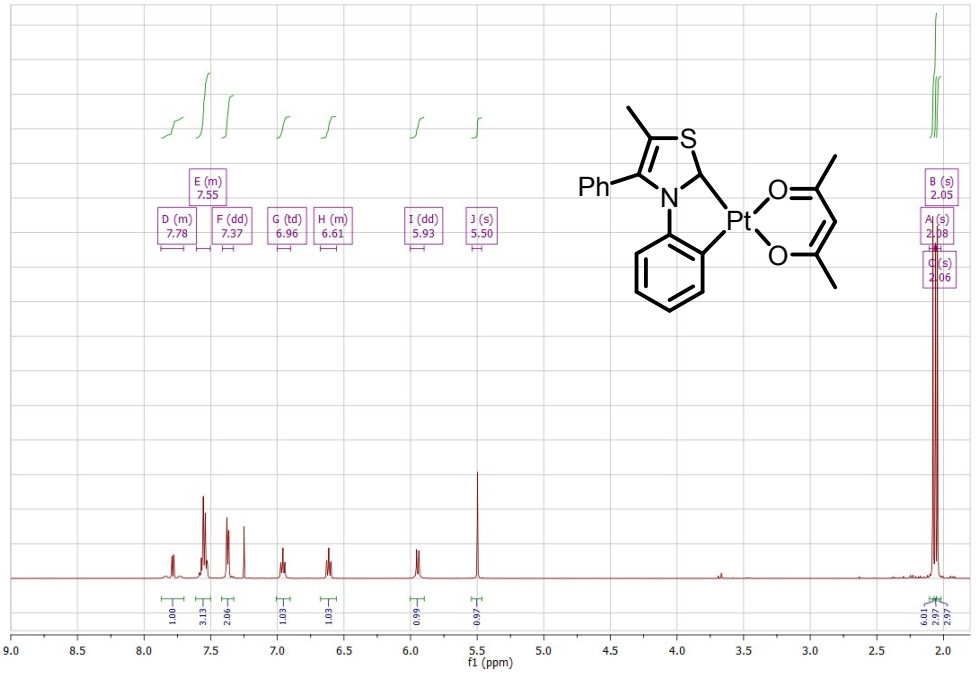


Figure S35. ^{1}H-NMR spectrum of compound **27** in $CDCl_3$.

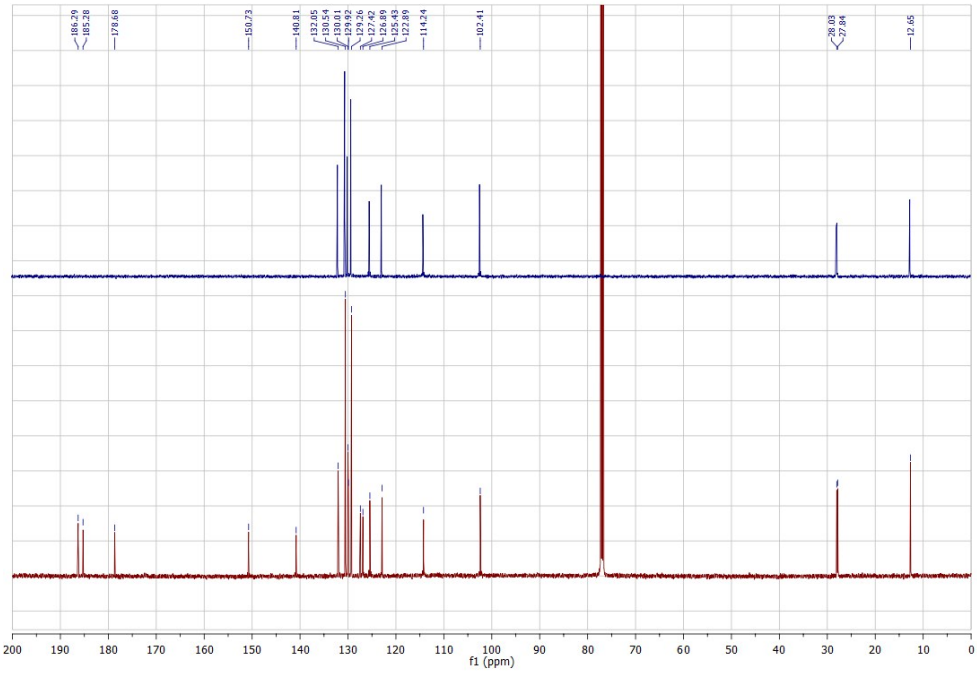


Figure S36. ^{13}C-NMR spectra of compound **27** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

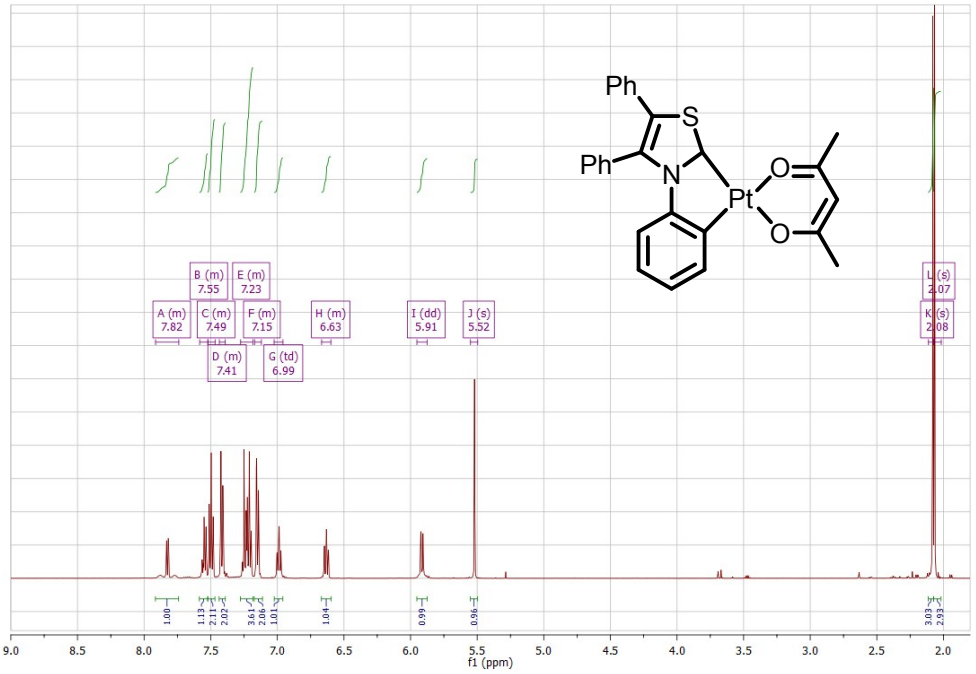


Figure S37. ^{1}H-NMR spectrum of compound **28** in $CDCl_3$.

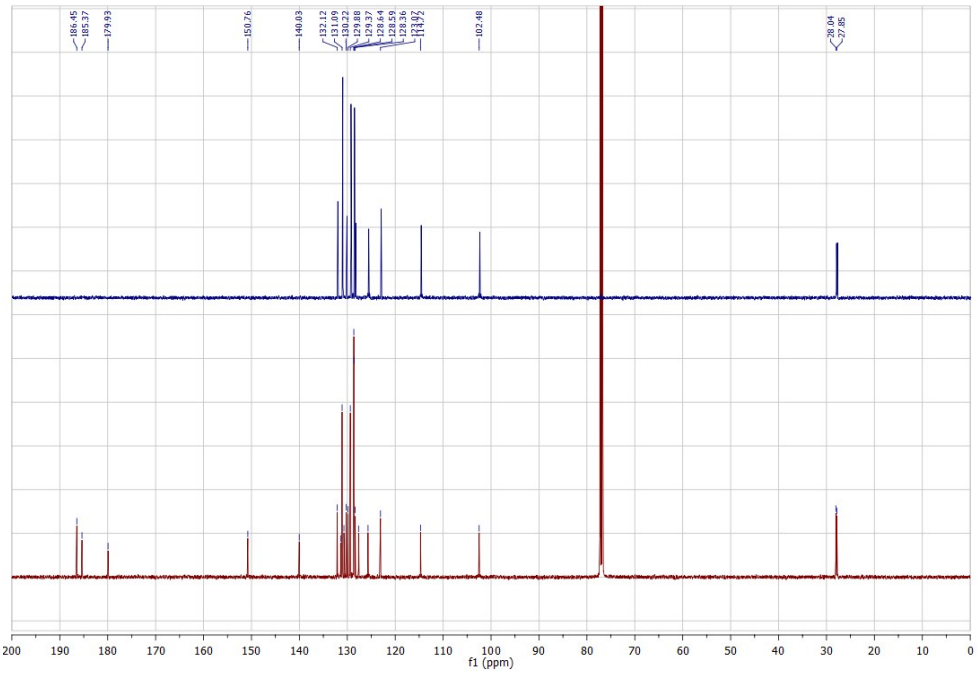


Figure S38. ^{13}C-NMR spectra of compound **28** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

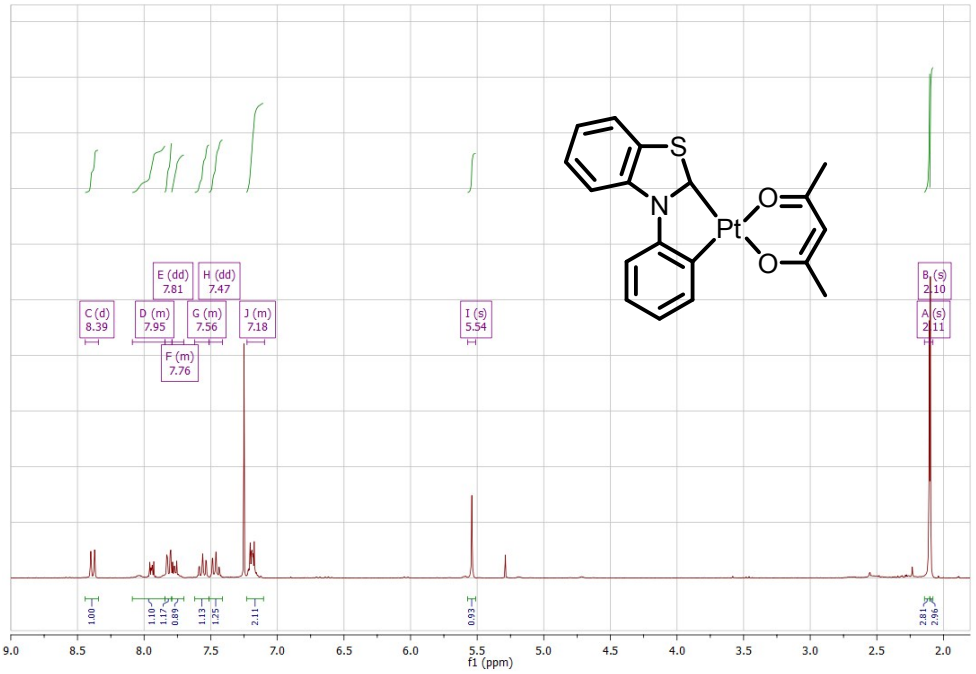


Figure S39. ^{1}H-NMR spectrum of compound **29** in $CDCl_3$.

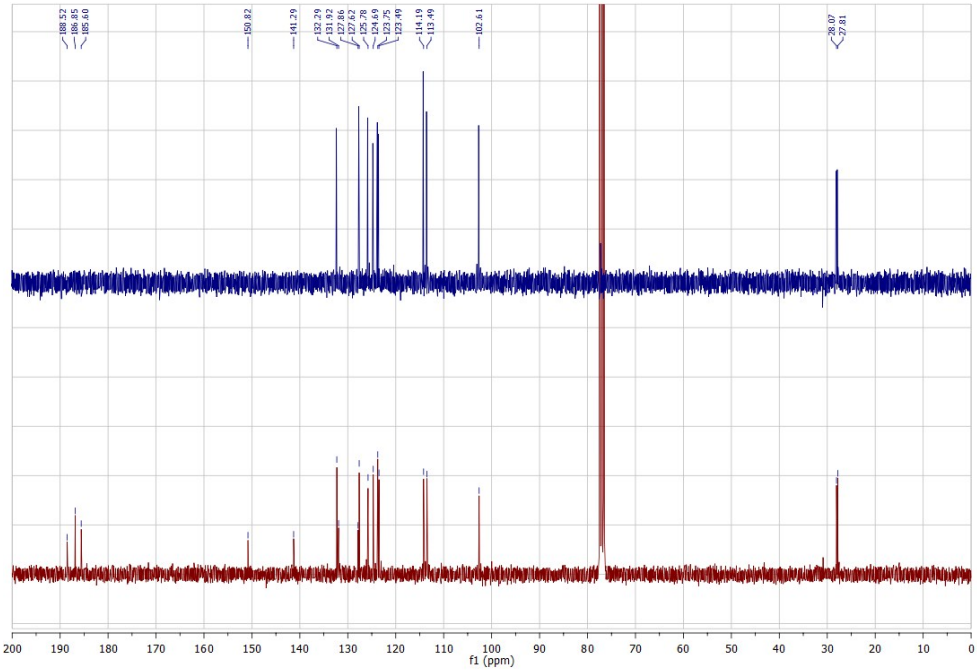


Figure S40. ^{13}C-NMR spectra of compound **29** in $CDCl_3$ (top: DEPT; bottom: proton decoupled).

2D-NMR Spectra

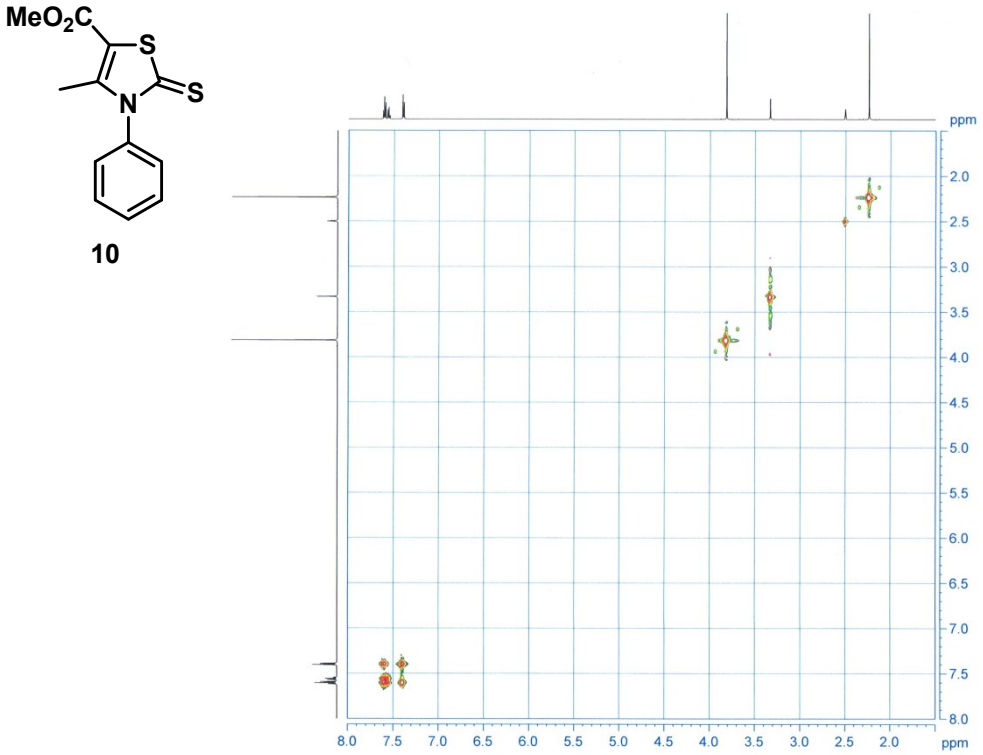


Figure S41. COSY spectrum of compound **10**.

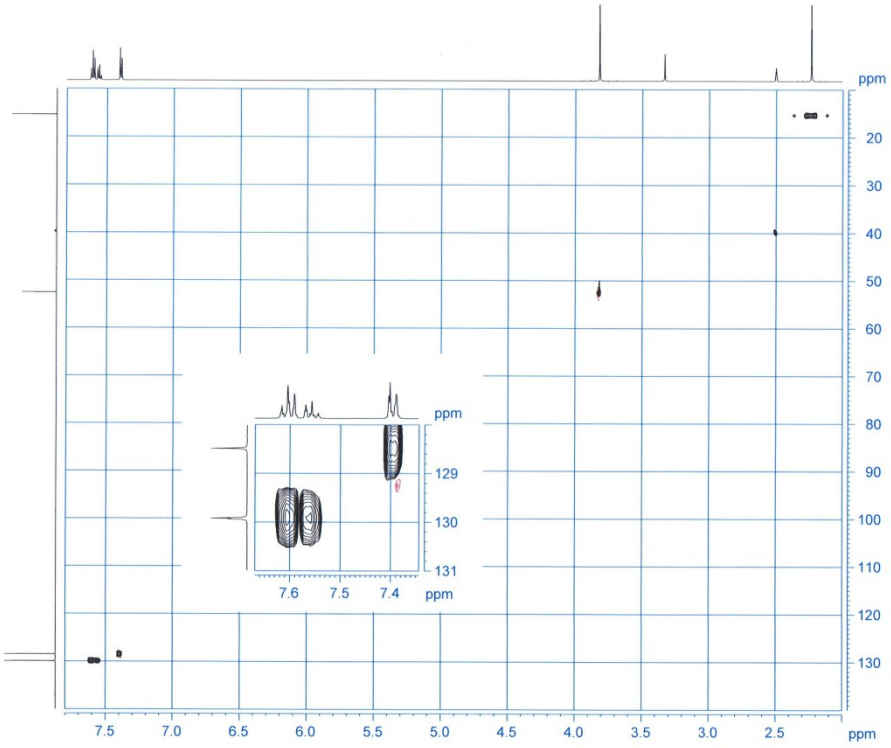


Figure S42. HSQC spectrum of compound **10**.

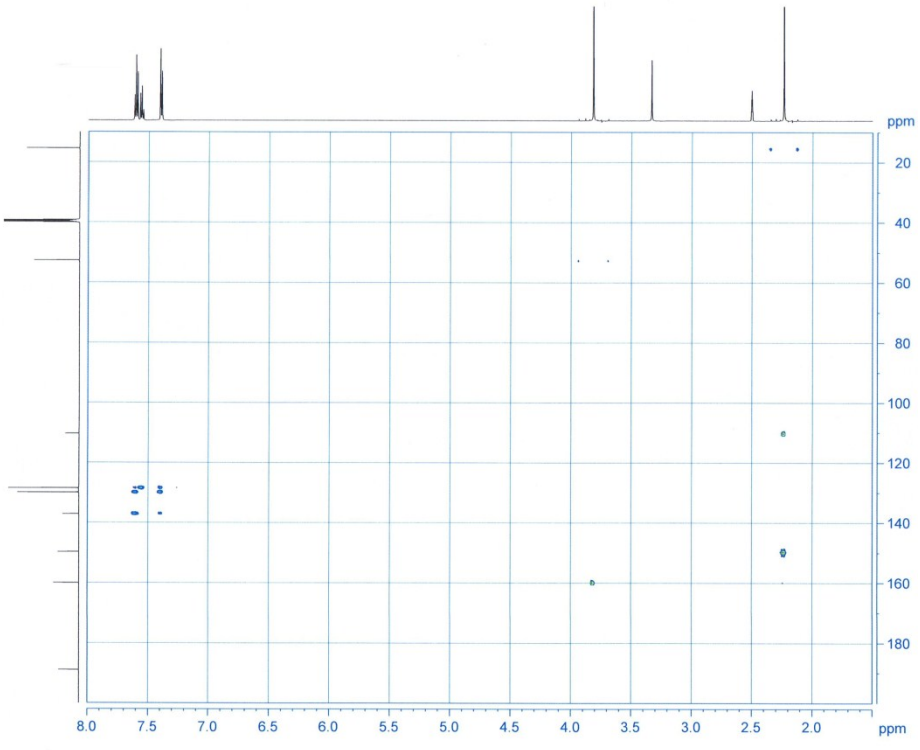


Figure S43. HMBC spectrum of compound **10**.

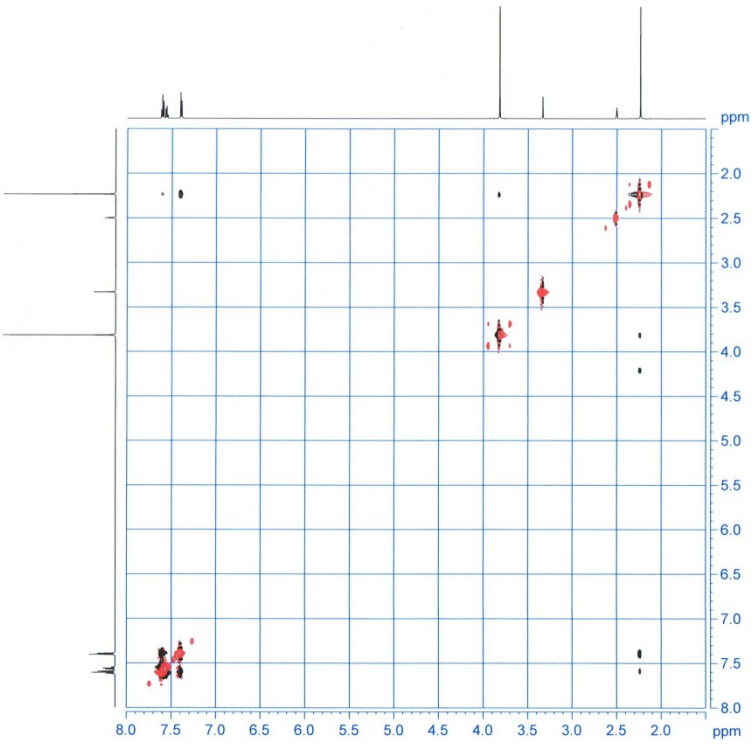


Figure S44. NOESY spectrum of compound **10**.

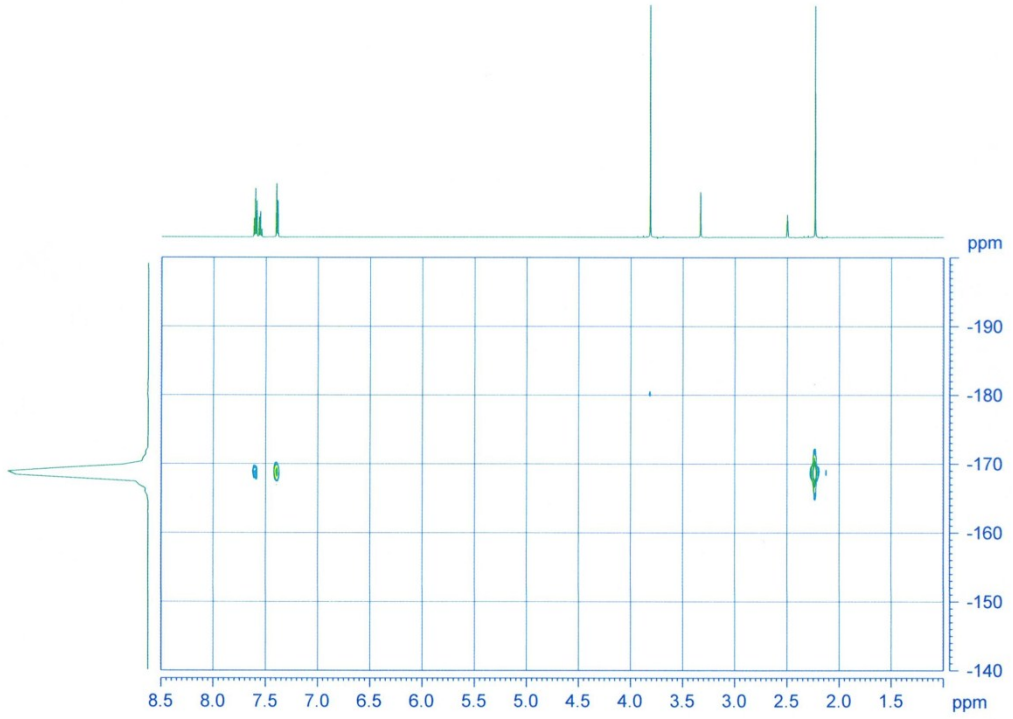


Figure S45. ^{1}H-^{15}N-HMBC spectrum of compound **10**.

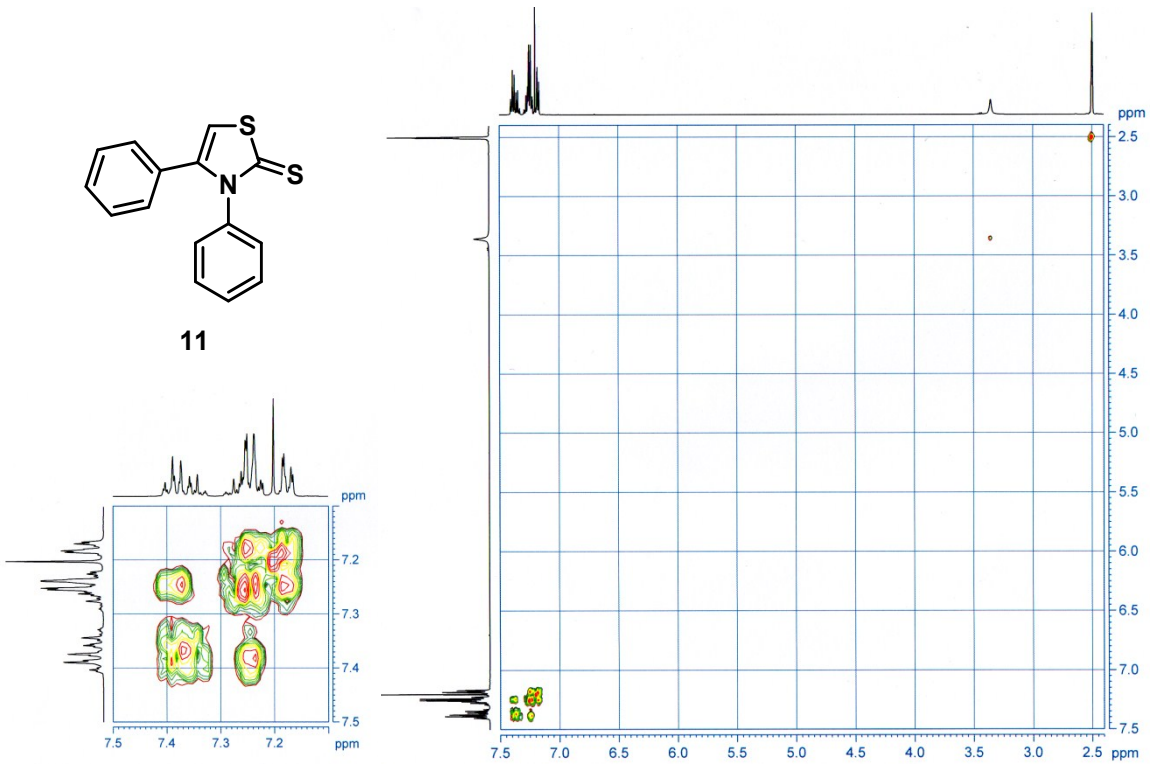


Figure S46. COSY spectra of compound **11**.

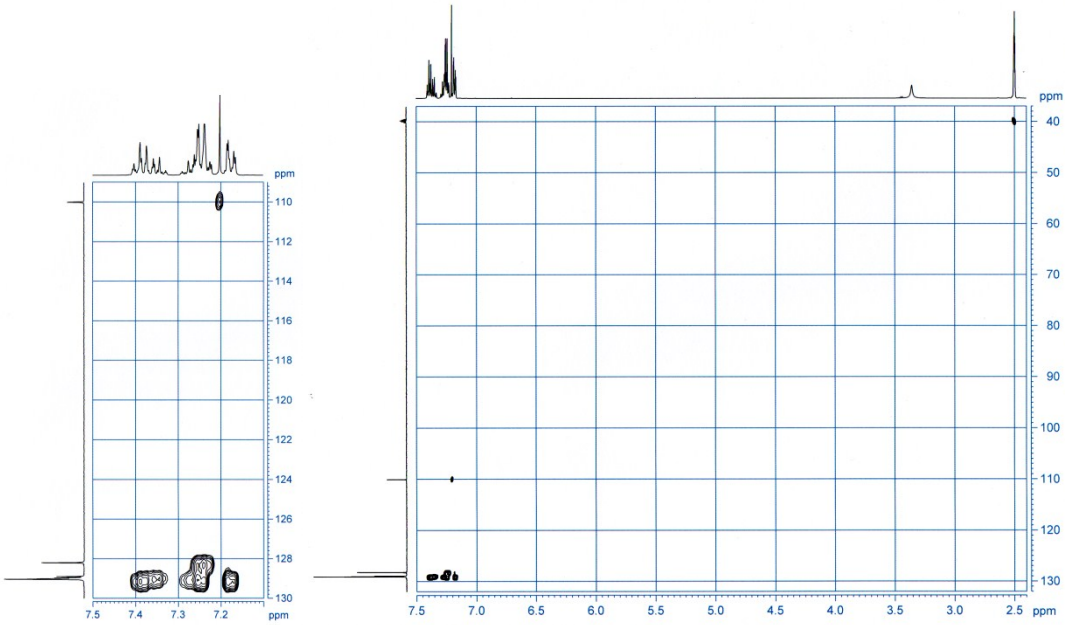


Figure S47. HSQC spectra of compound **11**.

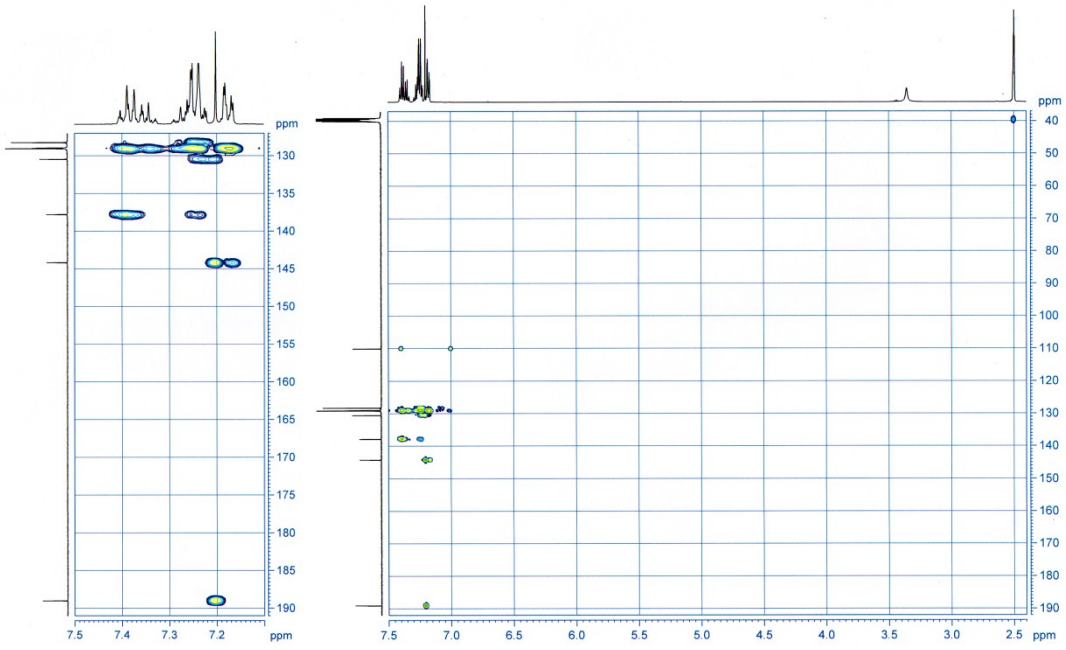


Figure S48. HMBC spectra of compound **11**.

Photoluminescence Data

In the following section additional photophysical data of complexes **23**–**29** are given.

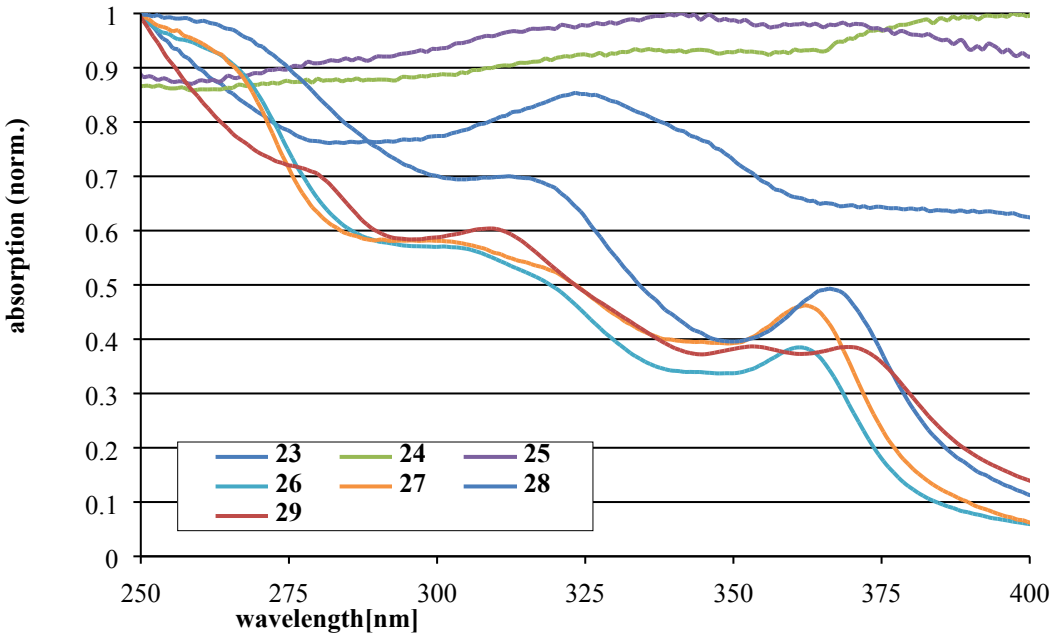


Figure S49. Absorption spectra for complexes **23**–**29** at room temperature (100% amorphous film).

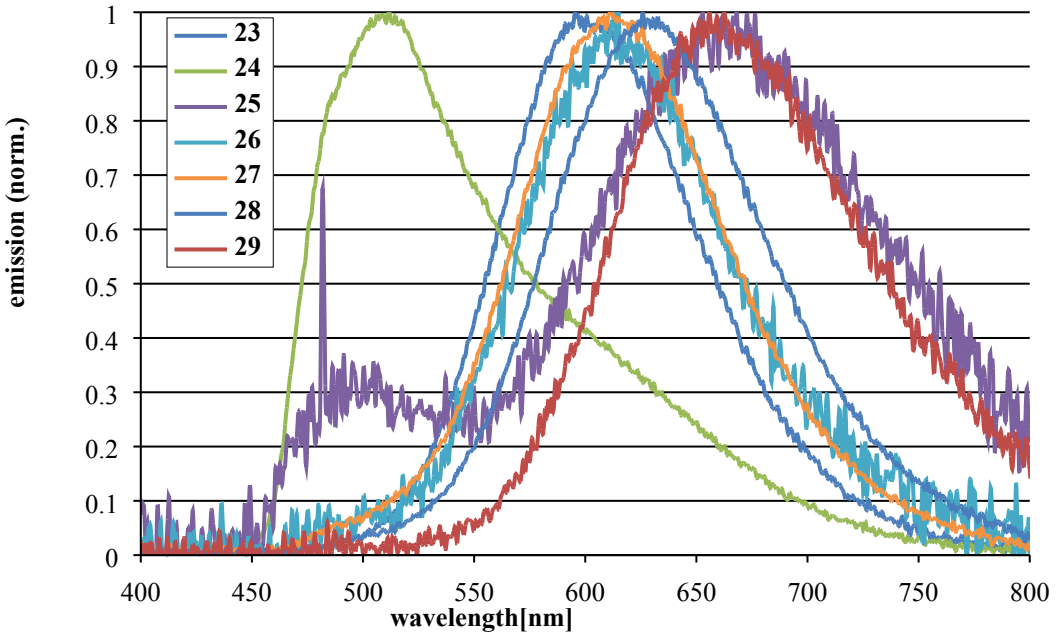


Figure S50. Emission spectra of complexes **23**–**29** at room temperature (100% amorphous film).

Table S1. Additional photoluminescence data (2 wt% in PMMA and neat film, room temperature) of complexes **23**–**29**.

	λ_{exc} (nm)[a]	CIE x;y[b]	λ_{em} (nm)[c]	ϕ[d]	τ_0(µs)[e]	k_r (10^3 s^{-1})[g]	k_{nr} (10^3 s^{-1})[h]
23	370	0.22;0.43	497	0.56	8.76	113.6	2169.2
23 **neat film**	370	0.54;0.45	547	0.40	2.4	421.1	570.0
24	360	0.24;0.47	501	0.72	9.15	109.9	1834.0
24 **neat film**	360	0.32;0.51	510	0.55	5.36	184.6	1341.0
25	370	0.26;0.47	502	0.69	9.11	110.4	1937.5
25 **neat film**	370	0.49;0.40	654	0.21	n.d.[f]	n.d.[f]	n.d.[f]
26	360	0.24;0.47	502	0.52	11.58	85.8	2908.8
26 **neat film**	360	0.56;0.43	611	0.06	n.d.[f]	n.d.[f]	n.d.[f]
27	370	0.27;0.52	509	0.56	10.48	95.2	2587.2
27 **neat film**	370	0.55;0.43	612	0.37	4.28	234.2	995.4
28	370	0.28;0.54	514	0.61	12.26	81.6	2917.2
28 **neat film**	370	0.59;0.40	629	0.40	4.28	232.6	1032.0
29	370	0.34;0.54	522	0.38	10.2	100.0	2356.0
29 **neat film**	370	0.63;0.36	682	0.13	3.4	325.0	348.0

[a]Excitation wavelength. [b]CIE coordinates at room temperature. [c]Maximum emission wavelength. [d]Quantum yield at λ_{exc}; N_2 atmosphere. [e]Decay lifetimes (excited by laser pulses (355 nm, 1 ns)) given as $\tau_0 = \tau_v/\phi$. [f]n.d. = not determined; [g]$k_r = \phi/\tau_v$; [h]$k_{nr} = (1 - \phi)/\tau_v$

Quantum Chemical Calculations

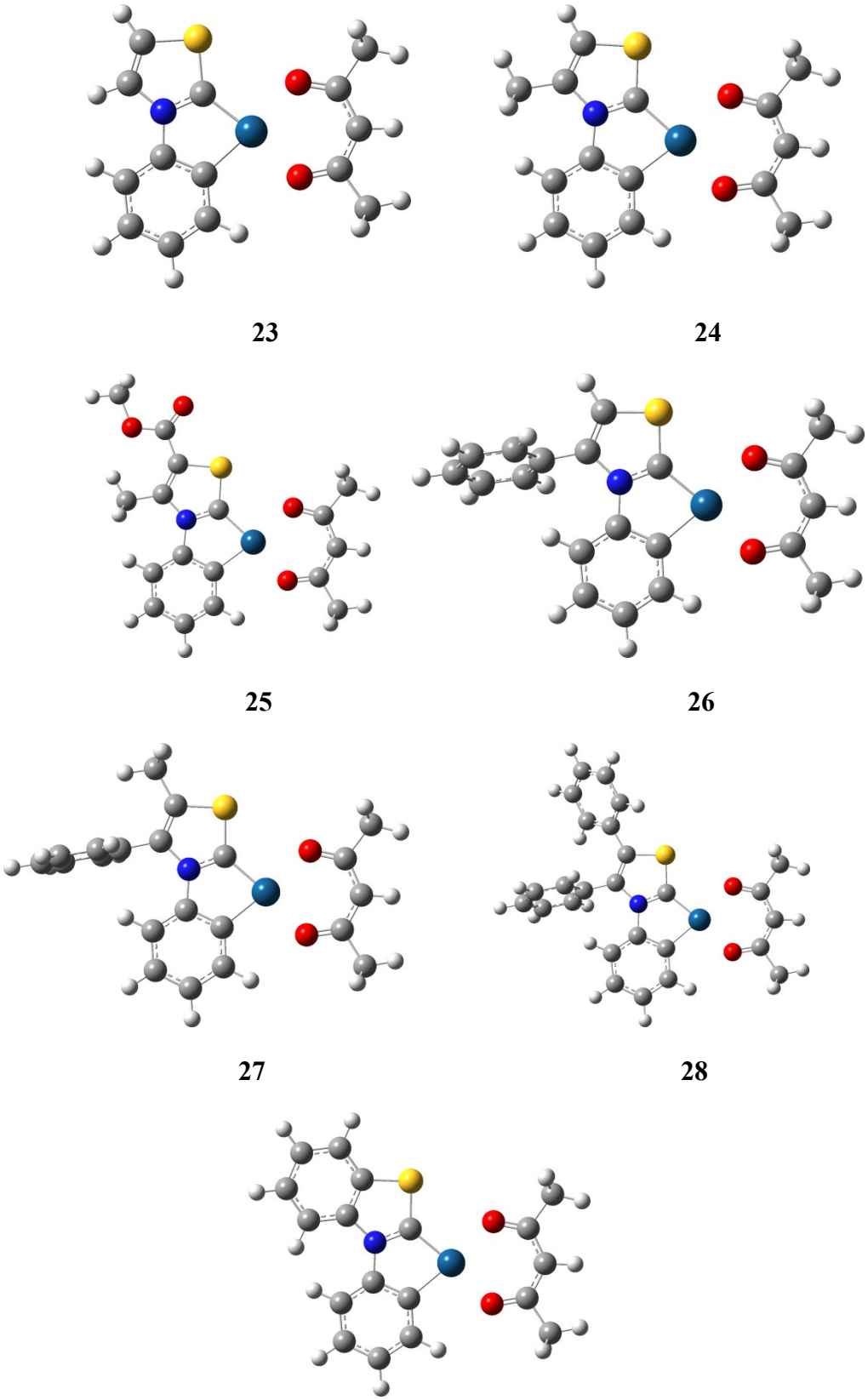


Figure S51. Calculated ground state geometries of complexes **23**–**29** (B3LYP/6-31G(d)).

Table S2. Summary of the prediction of wavelength maxima using the procedure described by Unger and Straßner (BP86/6-31G(d)).[1]

#	S-T gap [eV]	λ_{max} [nm]	S-T gap corr. [eV]	λ_{max} corr. [nm]	λ_{max} exp. [nm]	$\Delta\lambda_{max}$[a] [nm]
23	2.225	557.2	2.617	473.8	497	23.2
24	2.212	560.4	2.604	476.1	501	24.9
25	2.237	554.3	2.629	471.6	502	30.4
26	2.087	594.2	2.475	500.9	522	21.1
27	2.109	587.8	2.499	496.2	502	5.8
28	2.098	591.0	2.487	498.6	509	10.4
29	1.846	671.7	2.229	556.1	514	42.1
					average	**22.6**

[a] $\Delta\lambda_{max} = \left|(\lambda_{max}\ \text{exp.} - \lambda_{max}\ \text{corr.})\right|$

Table S3. Summary of the prediction of wavelength maxima using the procedure described by Unger and Straßner (B3LYP/6-31G(d)).[1]

#	S-T gap [eV]	λ_{max} uncorr. [nm]	S-T gap corr. [eV]	λ_{max} corr. [nm]	λ_{max} exp. [nm]	$\Delta\lambda_{max}$[a] [nm]
23	2.269	546.5	2.560	484.3	497	12.7
24	2.259	548.8	2.551	486.0	501	15.0
25	2.665	465.2	2.944	421.1	502	80.9
26	2.015	615.4	2.314	535.8	522	13.8
27	2.104	589.3	2.401	516.5	502	14.5
28	2.098	591.1	2.394	517.8	509	8.8
29	2.105	589.0	2.401	516.3	514	2.3
					average	**21.1**

[a] $\Delta\lambda_{max} = \left|(\lambda_{max}\ \text{exp.} - \lambda_{max}\ \text{corr.})\right|$

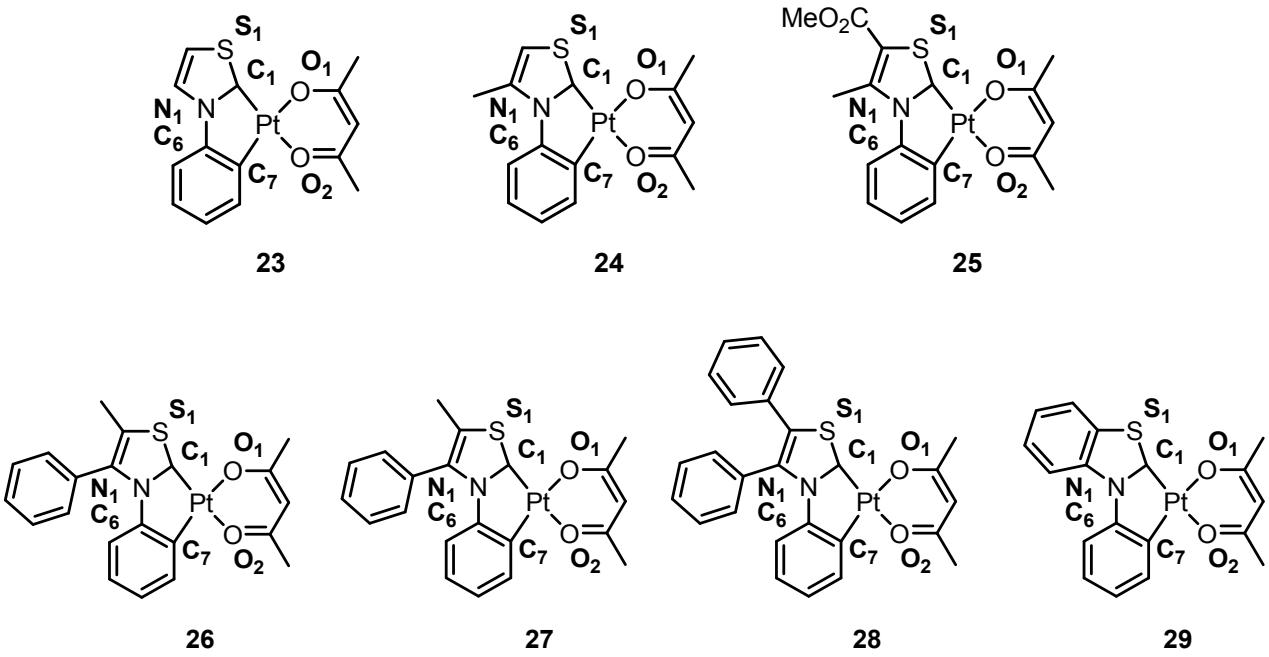


Table S4. Comparison of bond lengths, angles and dihedral angles of structures **23**–**25** from DFT calculations (B3LYP/6-31G(d)).

	23		**24**		**25**	
Bond [Å]/Angles [°]	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.731	1.765	1.724	1.761	1.712	1.711
C(1)-N(1)	1.358	1.443	1.364	1.453	1.373	1.374
N(1)-C(6)	1.434	1.356	1.447	1.364	1.451	1.452
Pt(1)-C(1)	1.934	1.943	1.928	1.934	1.923	1.930
Pt(1)-C(7)	2.003	1.949	1.995	1.944	1.993	1.996
Pt(1)-O(1)	2.133	2.122	2.137	2.127	2.137	2.128
Pt(1)-O(2)	2.086	2.124	2.091	2.129	2.089	2.074
S(1)-C(1)-N(1)	109.0	108.8	110.0	109.8	110.6	110.7
O(1)-Pt(1)-O(2)	89.6	89.5	89.3	89.1	89.2	88.3
C(1)-Pt(1)-C(7)	80.1	81.3	79.7	80.8	79.8	79.8
Pt(1)-C(1)-N(1)-C(6)	0.0	0.0	0.0	1.3	0	-2.6
N(1)-C(1)-Pt(1)-O(2)	-180.0	-180.0	-180.0	178.8	-180.0	-177.8

Table S5. Comparison of bond lengths, angles and dihedral angles of structures **23**–**25** from DFT calculations (BP86/6-31G(d)).

	23		**24**		**25**	
Bond [Å]/Angles [°]	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.744	1.771	1.737	1.767	1.725	1.766
C(1)-N(1)	1.374	1.446	1.380	1.456	1.389	1.444
N(1)-C(6)	1.435	1.369	1.447	1.377	1.450	1.397
Pt(1)-C(1)	1.925	1.934	1.920	1.926	1.990	1.936
Pt(1)-C(7)	2.001	1.953	1.992	1.949	1.915	1.946
Pt(1)-O(1)	2.131	2.124	2.134	2.130	2.134	2.116
Pt(1)-O(2)	2.085	2.122	2.089	2.125	2.088	2.137
S(1)-C(1)-N(1)	108.7	108.9	109.7	109.8	110.3	110.0
O(1)-Pt(1)-O(2)	90.9	90.7	90.6	90.3	90.4	90.0
C(1)-Pt(1)-C(7)	80.4	81.6	79.9	81.1	80.1	80.9
Pt(1)-C(1)-N(1)-C(6)	0.0	0.0	0.0	0.0	0.0	-8.2
N(1)-C(1)-Pt(1)-O(2)	-180.0	-180.0	-180.0	-180.0	-180.0	-173.4

Table S6. Comparison of bond lengths, angles and dihedral angles of structures **26**–**29** from DFT calculations (B3LYP/6-31G(d)).

	26		**27**		**28**		**29**	
Bond [Å]/Angles [°]	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.727	1.771	1.725	1.765	1.720	1.765	1.732	1.761
C(1)-N(1)	1.363	1.454	1.359	1.456	1.361	1.460	1.361	1.451
N(1)-C(6)	1.448	1.365	1.448	1.365	1.450	1.372	1.444	1.364
Pt(1)-C(1)	1.928	1.940	1.929	1.937	1.928	1.935	1.923	1.946
Pt(1)-C(7)	1.996	1.944	1.995	1.946	1.995	1.948	1.996	1.940
Pt(1)-O(1)	2.141	2.126	2.143	2.131	2.143	2.133	2.138	2.117
Pt(1)-O(2)	2.091	2.136	2.093	2.135	2.094	2.136	2.087	2.133
S(1)-C(1)-N(1)	110.0	108.8	109.9	108.7	110.0	108.7	111.4	109.3
O(1)-Pt(1)-O(2)	89.2	88.8	89.1	88.8	89.1	88.8	89.3	88.9
C(1)-Pt(1)-C(7)	79.7	81.1	79.6	80.9	79.6	80.8	79.8	81.0
Pt(1)-C(1)-N(1)-C(6)	4.2	1.5	1.1	-0.3	4.4	0.2	-4.0	-1.0
N(1)-C(1)-Pt(1)-O(2)	178.3	-177.3	179.6	-176.8	178.1	-177.0	-179.1	176.9

Table S7. Comparison of bond lengths, angles and dihedral angles of structures **26**–**29** from DFT calculations (BP86/6-31G(d)).

	26		**27**		**28**		**29**	
Bond [Å]/Angles [°]	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.740	1.771	1.737	1.769	1.732	1.752	1.743	1.758
C(1)-N(1)	1.378	1.455	1.375	1.456	1.377	1.396	1.377	1.449
N(1)-C(6)	1.448	1.377	1.447	1.377	1.449	1.445	1.444	1.378
Pt(1)-C(1)	1.920	1.930	1.921	1.928	1.920	1.910	1.915	1.935
Pt(1)-C(7)	1.994	1.948	1.993	1.950	1.992	1.984	1.994	1.945
Pt(1)-O(1)	2.139	2.130	2.140	2.135	2.141	2.145	2.136	2.119
Pt(1)-O(2)	2.089	2.132	2.091	2.130	2.092	2.091	2.086	2.127
S(1)-C(1)-N(1)	109.7	109.0	109.5	108.9	109.7	111.4	111.1	110.0
O(1)-Pt(1)-O(2)	90.5	90.1	90.4	90.1	90.4	90.1	90.6	90.1
C(1)-Pt(1)-C(7)	80.0	81.2	80.0	81.1	79.9	79.9	80.1	81.1
Pt(1)-C(1)-N(1)-C(6)	4.9	2.8	2.0	1.0	4.6	10.5	-4.0	2.9
N(1)-C(1)-Pt(1)-O(2)	177.8	-178.5	179.2	-177.8	177.9	176.2	-179.1	-179.1

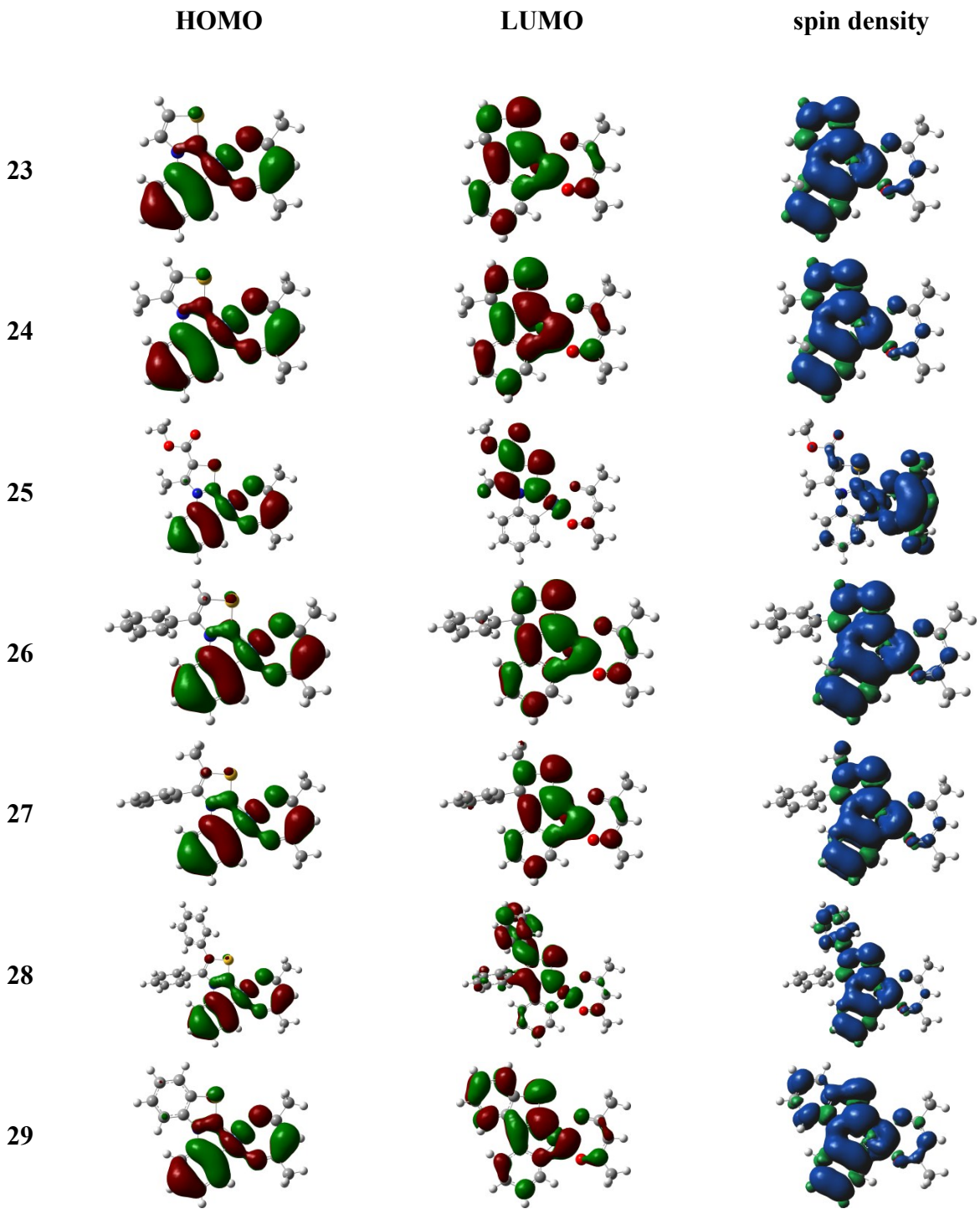
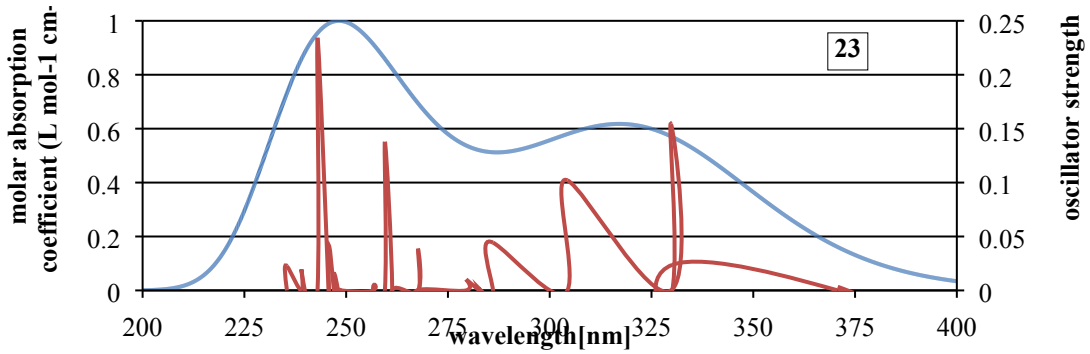


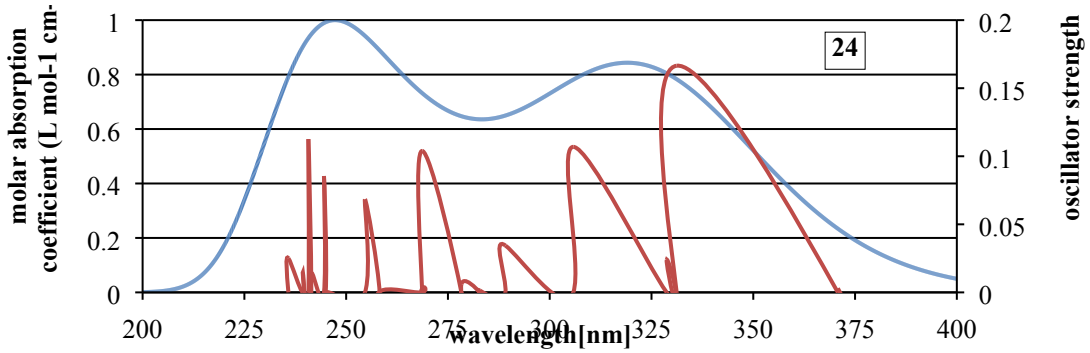
Figure S52. Calculated FMOs for the ground state geometries and calculated spin densities for the triplet state geometries of complexes **23**–**29** (B3LYP/6-31G(d); isovalue 0.02).

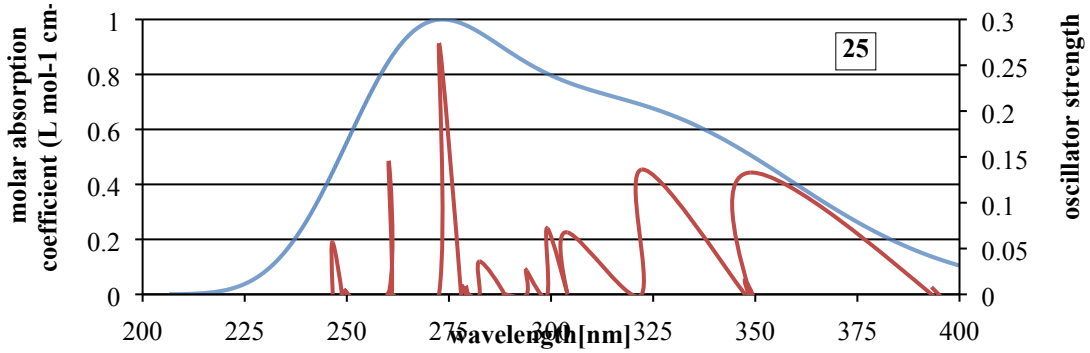
Table S8. Selected singlet exited states (S_n) and calculated transitions for complexes **23**–**29** (TD-B3LYP/6-31G(d)-CPCM(dichloromethane)).

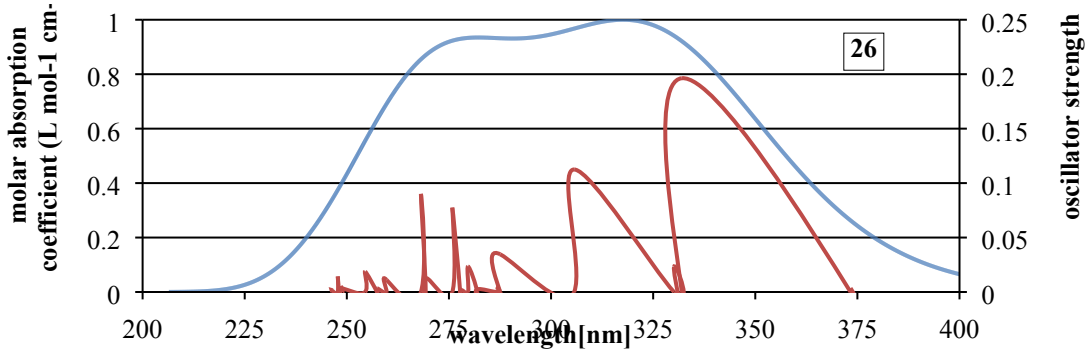
#	Excitation	Coefficient	oscillator strength	Excitation Energy [eV]	Wavelength [nm]	Character
23	HOMO-1 → LUMO	0.65	0.15	3.76	330	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.69	0.10	4.08	304	^{1}MLCT/^{1}LLCT
	HOMO → LUMO+2	0.56	0.14	4.78	259	^{1}MLCT/^{1}ILCT
	HOMO-3 → LUMO+1	0.53	0.23	5.11	243	^{1}MLCT/^{1}LLCT
24	HOMO-1 → LUMO	0.64	0.17	3.75	331	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.69	0.11	4.06	306	^{1}MLCT/^{1}LLCT
	HOMO-4 → LUMO	0.63	0.10	4.62	268	^{1}MLCT/^{1}LLCT
	HOMO → LUMO+2	0.59	0.07	4.87	254	^{1}MLCT/^{1}LLCT
	HOMO-2 → LUMO+1	0.56	0.09	5.07	244	^{1}MLCT
	HOMO-1 → LUMO+2	0.50	0.11	5.15	241	^{1}MLCT/^{1}LLCT
25	HOMO-1 → LUMO	0.62	0.13	3.56	349	^{1}MLCT
	HOMO → LUMO+1	0.63	0.14	3.85	322	^{1}MLCT/^{1}LLCT
	HOMO → LUMO+2	0.60	0.07	4.08	304	^{1}MLCT/^{1}LLCT
	HOMO-1 → LUMO+1	0.55	0.07	4.15	299	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+2	0.34				^{1}MLCT/^{1}LLCT
	HOMO-4 → LUMO	0.54	0.27	4.55	272	^{1}MLCT/^{1}LLCT
	HOMO-3 → LUMO+1	0.62	0.15	4.77	260	^{1}MLCT/^{1}ILCT
	HOMO-4 → LUMO+1	0.60	0.06	5.03	246	^{1}MLCT/^{1}ILCT
26	HOMO-1 → LUMO	0.65	0.20	3.74	332	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.69	0.11	4.06	305	^{1}MLCT/^{1}ILCT
	HOMO-4 → LUMO	0.51	0.08	4.50	276	^{1}MLCT/^{1}ILCT
	HOMO-4 → LUMO	0.35	0.09	4.63	268	^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+2	0.48				^{1}MLCT/^{1}LLCT
27	HOMO-1 → LUMO	0.67	0.20	3.74	332	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.69	0.11	4.04	307	^{1}MLCT/^{1}LLCT
	HOMO-1 → LUMO+1	0.68	0.03	4.27	290	^{1}MLCT/^{1}LLCT
	HOMO-4 → LUMO	0.57	0.06	4.59	270	^{1}MLCT/^{1}ILCT
	HOMO-4 → LUMO	0.30	0.13	4.74	262	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+3	0.56				^{1}MLCT/^{1}ILCT
28	HOMO-1 → LUMO	0.69	0.25	3.65	340	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.62	0.18	3.99	310	^{1}MLCT/^{1}LLCT
	HOMO → LUMO+2	0.65	0.06	4.05	306	^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+1	0.66	0.08	4.17	297	^{1}MLCT/^{1}LLCT
	HOMO-4 → LUMO	0.57	0.10	4.43	280	^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+3	0.35	0.14	4.58	270	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+3	0.56				^{1}MLCT/^{1}ILCT
29	HOMO-1 → LUMO	0.63	0.20	3.65	340	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+1	0.69	0.10	4.06	305	^{1}MLCT/^{1}LLCT
	HOMO-3 → LUMO	0.67	0.08	4.20	295	^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+1	0.47	0.07	4.46	278	^{1}MLCT/^{1}LLCT
	HOMO → LUMO+2	0.51	0.12	4.64	267	^{1}MLCT/^{1}ILCT
	HOMO → LUMO+3	0.36				^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+2	0.47	0.07	4.92	252	^{1}MLCT/^{1}LLCT
	HOMO-3 → LUMO+1	0.51	0.17	5.01	248	^{1}MLCT/^{1}ILCT
	HOMO-1 → LUMO+3	0.36				^{1}MLCT/^{1}ILCT

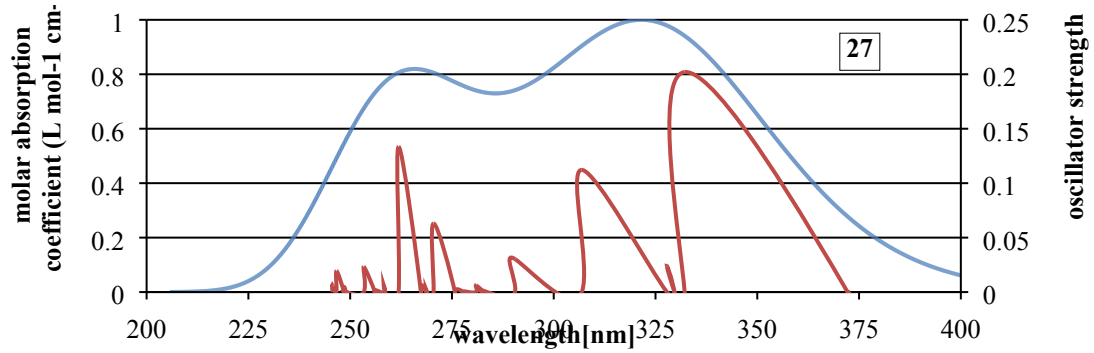
The following sections contains all calculated absorption spectra with plotted oscillator strengths for complexes **23**–**29** (TD-B3LYP/6-31G(d)-CPCM(dichloromethane)):[a]

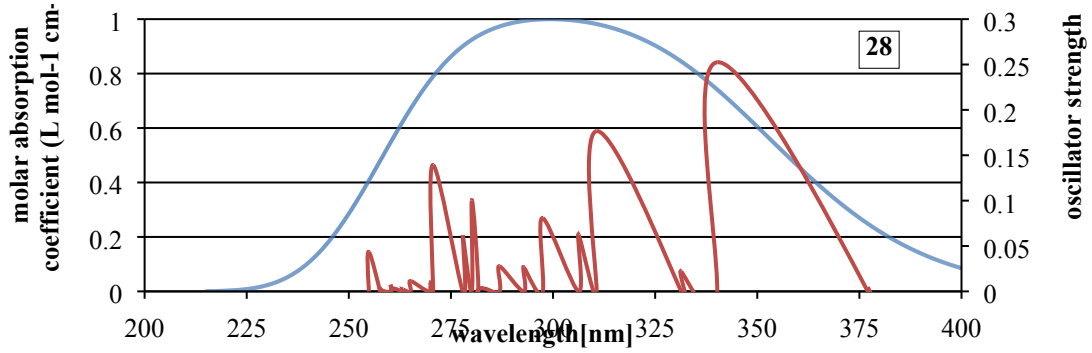


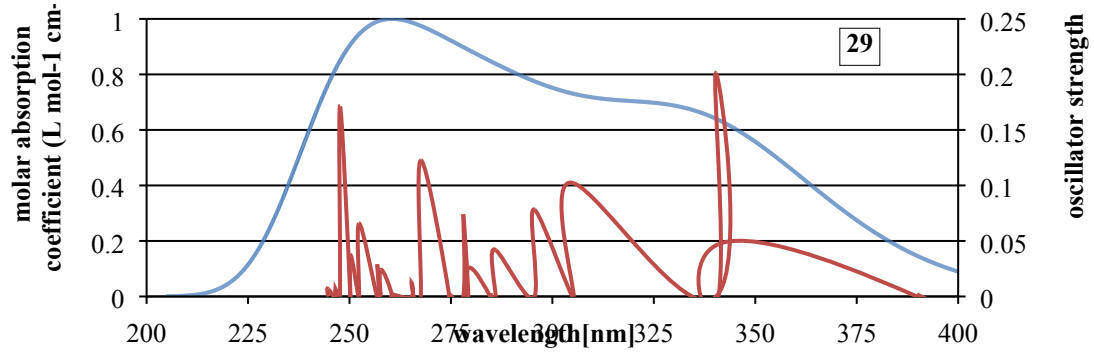












[a] Data were extracted and normalized using Multifwn v3.3.8[2]

In the following section the coordinates of the singlet ground-state structure geometries for **23**–**29** are given (B3LYP/6-31G(d)).

Optimized singlet ground-state structure of **23**.

C	-1.29421	2.65596	0.00003
C	-2.50778	3.35462	-0.00005
C	-3.72590	2.67128	-0.00013
C	-3.74301	1.27356	-0.00013
C	-2.52339	0.60452	-0.00004
C	-1.27518	1.25868	0.00004
H	-0.35251	3.19677	0.00008
H	-2.50257	4.44188	-0.00005
C	-1.10653	-1.27102	0.00001
C	-3.37457	-1.80027	-0.00003
C	-2.86350	-3.05184	0.00000
H	-4.41666	-1.51508	-0.00006
H	-3.40948	-3.98406	0.00001
N	-2.38894	-0.82326	-0.00004
Pt	0.31558	0.04035	0.00007
C	3.15113	-1.06441	-0.00014
C	2.97989	1.44595	-0.00000
O	1.91436	-1.37306	-0.00016
O	1.70702	1.59404	0.00007
C	4.09572	-2.25067	-0.00013
H	5.14721	-1.95321	-0.00025
H	3.89928	-2.87154	0.88145
H	3.89909	-2.87174	-0.88151
C	3.74785	2.75204	-0.00004
H	3.46637	3.33954	0.88144
H	4.83046	2.60406	-0.00021
H	3.46606	3.33965	-0.88134
C	3.69153	0.23659	-0.00006
H	4.77257	0.31231	-0.00008
H	-4.66378	3.21926	-0.00020
H	-4.68960	0.73980	-0.00021
S	-1.11391	-3.00249	0.00003

Optimized singlet ground-state structure of **24**.

C	0.82088	2.79618	-0.00008
C	1.93627	3.63992	-0.00021
C	3.22282	3.10229	-0.00042
C	3.40994	1.71644	-0.00034
C	2.28693	0.88917	-0.00001
C	0.97279	1.40752	-0.00004
H	-0.18204	3.21240	-0.00005
H	1.80004	4.71863	-0.00024
C	1.05111	-1.10524	-0.00011
C	3.36123	-1.48182	0.00043
C	2.90114	-2.75765	0.00057

N	2.30041	-0.55754	0.00001
Pt	-0.49129	0.05201	-0.00001
C	-3.20861	-1.33082	-0.00035
C	-3.28980	1.18373	0.00031
O	-1.94731	-1.51230	-0.00009
O	-2.03832	1.45813	0.00038
C	-4.02931	-2.60612	-0.00079
H	-5.10541	-2.41567	-0.00016
H	-3.77189	-3.20379	-0.88276
H	-3.77102	-3.20502	0.88009
C	-4.18565	2.40601	0.00066
H	-3.96387	3.01972	-0.87998
H	-5.24787	2.14972	-0.00055
H	-3.96554	3.01793	0.88297
C	-3.87724	-0.09079	-0.00010
H	-4.96045	-0.12412	-0.00024
H	4.09198	3.75413	-0.00062
H	4.41749	1.32643	-0.00078
S	1.16037	-2.82611	0.00020
C	4.81202	-1.10688	-0.00005
H	3.50529	-3.65351	0.00107
H	5.08622	-0.52563	0.88694
H	5.41180	-2.02071	-0.00044
H	5.08515	-0.52531	-0.88720

Optimized singlet ground-state structure of **25**.

C	1.51403	3.01211	-0.00023
C	1.01904	4.31918	-0.00012
C	-0.35647	4.54627	0.00016
C	-1.25204	3.47276	0.00031
C	-0.74322	2.17235	0.00014
C	0.64672	1.91673	-0.00008
H	2.58455	2.83063	-0.00042
H	1.70776	5.16042	-0.00024
C	-0.73475	-0.18209	0.00024
C	-2.89785	0.71485	0.00013
C	-3.17660	-0.62996	0.00013
N	-1.51849	0.94576	0.00025
Pt	1.17977	-0.00363	0.00002
C	2.76262	-2.61194	0.00018
C	4.15537	-0.51825	-0.00032
O	1.59604	-2.09939	0.00028
O	3.23408	0.37337	-0.00040
C	2.78617	-4.12781	0.00046
H	3.80074	-4.53366	0.00013
H	2.25132	-4.49936	0.88196
H	2.25060	-4.49968	-0.88047
C	5.55923	0.05146	-0.00051
H	5.69324	0.68882	0.88108
H	6.32850	-0.72454	-0.00082
H	5.69286	0.68920	-0.88188
C	3.98473	-1.91039	-0.00008
H	4.88798	-2.50915	-0.00008

H	-0.74737	5.55985	0.00028
H	-2.31010	3.68476	0.00056
S	-1.70740	-1.59122	0.00017
C	-3.89802	1.82882	0.00034
H	-3.78128	2.46078	0.88728
H	-3.78144	2.46109	-0.88639
H	-4.90267	1.41350	0.00035
C	-4.43251	-1.40003	-0.00016
O	-4.44618	-2.61698	-0.00030
O	-5.55513	-0.64799	-0.00026
C	-6.78654	-1.39407	-0.00055
H	-7.57742	-0.64389	-0.00043
H	-6.85062	-2.02414	-0.89099
H	-6.85078	-2.02461	0.88954

Optimized singlet ground-state structure of **26**.

C	0.24000	2.88812	-0.12668
C	-0.80463	3.81125	-0.24097
C	-2.12616	3.37200	-0.32113
C	-2.42269	2.00641	-0.26883
C	-1.36974	1.10399	-0.12620
C	-0.02076	1.51655	-0.07580
H	1.27066	3.22756	-0.08565
H	-0.58452	4.87544	-0.27952
C	-0.29888	-0.98335	-0.06427
C	-2.63111	-1.17306	-0.07099
C	-2.27697	-2.48349	-0.11643
N	-1.49844	-0.33691	-0.06859
Pt	1.32964	0.04812	-0.00955
C	3.93297	-1.54210	0.08158
C	4.20695	0.95878	0.10037
O	2.66252	-1.62634	0.03453
O	2.98125	1.32895	0.05783
C	4.65294	-2.87680	0.10416
H	5.73999	-2.77000	0.13853
H	4.32226	-3.45335	0.97574
H	4.37755	-3.45363	-0.78619
C	5.19330	2.10876	0.13863
H	4.98523	2.73733	1.01205
H	6.23201	1.77194	0.17948
H	5.05469	2.73605	-0.74946
C	4.69445	-0.35713	0.11369
H	5.77122	-0.47356	0.15262
H	-2.93772	4.08628	-0.42879
H	-3.44990	1.67945	-0.34894
S	-0.54751	-2.69133	-0.11562
C	-4.03629	-0.71168	0.04945
C	-4.49673	-0.12251	1.23852
C	-4.94094	-0.94163	-0.99635
C	-5.83567	0.24096	1.36906
H	-3.80201	0.05073	2.05538
C	-6.28231	-0.57793	-0.86122
H	-4.58673	-1.39711	-1.91657

C	-6.73112	0.01507	0.31950
H	-6.18174	0.69612	2.29281
H	-6.97355	-0.75629	-1.68017
H	-7.77452	0.29939	0.42404
H	-2.95499	-3.32435	-0.09545

Optimized singlet ground-state structure of **27**.

C	0.44727	2.97250	-0.03380
C	-0.56457	3.93790	-0.06436
C	-1.90416	3.55100	-0.08781
C	-2.25092	2.19611	-0.07565
C	-1.22881	1.24865	-0.03708
C	0.13620	1.61087	-0.02199
H	1.49113	3.27157	-0.02131
H	-0.30517	4.99392	-0.07314
C	-0.23452	-0.87458	-0.02036
C	-2.57251	-0.98458	-0.01929
C	-2.28620	-2.31567	-0.02681
N	-1.40715	-0.18785	-0.02234
Pt	1.43338	0.09470	-0.00466
C	3.98119	-1.59024	0.02135
C	4.34692	0.89852	0.03162
O	2.70800	-1.62785	0.00650
O	3.13515	1.31276	0.01776
C	4.65256	-2.95051	0.02561
H	5.74326	-2.88327	0.03902
H	4.31789	-3.51832	0.90135
H	4.33934	-3.51322	-0.86130
C	5.37553	2.01169	0.04711
H	5.21476	2.64292	0.92861
H	6.40196	1.63683	0.05815
H	5.23566	2.64831	-0.83408
C	4.78661	-0.43426	0.03377
H	5.85906	-0.58990	0.04634
H	-2.69225	4.29840	-0.11678
H	-3.29356	1.91384	-0.09924
S	-0.54824	-2.57085	-0.02911
C	-3.95304	-0.43129	0.01635
C	-4.55569	-0.11110	1.24259
C	-4.68487	-0.26945	-1.16923
C	-5.86099	0.37961	1.27930
H	-3.99396	-0.23999	2.16342
C	-5.99116	0.22078	-1.13002
H	-4.22313	-0.52028	-2.11999
C	-6.57977	0.54842	0.09325
H	-6.31670	0.62840	2.23364
H	-6.54768	0.34648	-2.05460
H	-7.59627	0.93106	0.12284
C	-3.24043	-3.47148	-0.01737
H	-3.08765	-4.10838	0.86226
H	-4.27212	-3.11114	-0.00129
H	-3.11351	-4.10213	-0.90562

Optimized singlet ground-state structure of **28**.

C	1.96489	3.04670	-0.17188
C	1.31007	4.27545	-0.30350
C	-0.08169	4.32430	-0.37861
C	-0.83770	3.15026	-0.30359
C	-0.16898	1.93699	-0.14341
C	1.24034	1.85464	-0.09829
H	3.04925	3.00286	-0.13473
H	1.88866	5.19444	-0.35973
C	0.11263	-0.38879	-0.04316
C	-2.14376	0.23931	-0.03281
C	-2.28797	-1.12184	-0.04235
N	-0.79017	0.62997	-0.05826
Pt	1.99816	0.01198	-0.00327
C	3.88525	-2.38678	0.13062
C	5.01523	-0.13910	0.11442
O	2.66562	-2.02311	0.07501
O	3.99633	0.63481	0.05601
C	4.09362	-3.88848	0.17747
H	5.14920	-4.16798	0.22302
H	3.57609	-4.29992	1.05164
H	3.64014	-4.34596	-0.70932
C	6.34122	0.59446	0.14416
H	6.36473	1.26827	1.00831
H	7.19680	-0.08334	0.19569
H	6.43170	1.21832	-0.75252
C	5.01264	-1.54197	0.15155
H	5.98085	-2.02633	0.20147
H	-0.59306	5.27520	-0.50030
H	-1.91358	3.20613	-0.38094
S	-0.70702	-1.90072	-0.04451
C	-3.26932	1.20669	0.03727
C	-3.52462	1.91389	1.22368
C	-4.11901	1.38527	-1.06287
C	-4.60576	2.79087	1.30100
H	-2.86865	1.77949	2.07933
C	-5.20064	2.26408	-0.98242
H	-3.92752	0.83528	-1.97936
C	-5.44515	2.96873	0.19755
H	-4.79311	3.33475	2.22266
H	-5.85082	2.39727	-1.84252
H	-6.28697	3.65287	0.25911
C	-3.51056	-1.94729	-0.01949
C	-3.59794	-3.08915	-0.83643
C	-4.59071	-1.64432	0.82819
C	-4.73307	-3.89775	-0.81278
H	-2.77637	-3.33449	-1.50408
C	-5.72612	-2.45248	0.84474
H	-4.53434	-0.78065	1.48130
C	-5.80323	-3.58125	0.02597
H	-4.78170	-4.77305	-1.45467
H	-6.54961	-2.20316	1.50841
H	-6.68853	-4.21081	0.04433

Optimized singlet ground-state structure of **29**.

C	-0.49277	3.07077	0.00904
C	0.31615	4.20986	-0.06252
C	1.70119	4.08158	-0.15633
C	2.29593	2.81580	-0.15409
C	1.47840	1.69181	-0.04325
C	0.07053	1.79328	0.00981
H	-1.57343	3.16710	0.05382
C	0.90171	-0.57830	-0.06071
C	3.21556	-0.24567	0.02898
C	3.15792	-1.65310	-0.03868
N	1.92525	0.31846	-0.02772
Pt	-0.91240	0.05641	-0.00428
C	-3.07900	-2.09015	-0.02924
C	-3.91948	0.27732	0.10209
O	-1.82282	-1.87762	-0.05751
O	-2.81016	0.91969	0.09625
C	-3.47307	-3.55328	-0.08454
H	-4.55522	-3.70024	-0.04671
H	-3.08319	-4.00004	-1.00642
H	-3.00900	-4.08674	0.75283
C	-5.14259	1.16804	0.17979
H	-5.14393	1.85871	-0.67129
H	-6.07680	0.60132	0.18200
H	-5.09100	1.77813	1.08892
C	-4.09218	-1.11387	0.04545
H	-5.11368	-1.47540	0.06066
H	2.33147	4.96252	-0.23907
H	3.36759	2.74426	-0.27361
S	1.48979	-2.20679	-0.11001
C	4.46009	0.38097	0.17976
H	4.54643	1.45004	0.30099
C	4.31143	-2.43620	-0.00848
H	4.24326	-3.51829	-0.06558
C	5.60941	-0.40570	0.21342
H	6.57307	0.08090	0.33101
C	5.54472	-1.80087	0.10901
H	6.45583	-2.39082	0.13467
H	-0.13754	5.19788	-0.06114

In the following section the coordinates of the triplet-state structure geometries for **23**–**29** are given (B3LYP/6-31G(d)).

Optimized triplet-state structure of **23**.

C	1.15883	2.67423	0.00003
C	2.32312	3.41965	0.00008
C	3.60001	2.77173	0.00009
C	3.71357	1.40039	0.00006
C	2.52419	0.62966	0.00002
C	1.20000	1.26256	0.00000
H	0.18760	3.15897	0.00002
H	2.28299	4.50493	0.00010
C	1.12652	-1.27264	-0.00005
C	3.46734	-1.68211	0.00005
C	2.99361	-2.94623	0.00005
H	4.50520	-1.37930	0.00008
H	3.59430	-3.84565	0.00008
N	2.46150	-0.72442	0.00001
Pt	-0.31213	0.03292	-0.00006
C	-3.11749	-1.13266	0.00009
C	-3.03077	1.38557	0.00002
O	-1.86924	-1.40850	0.00002
O	-1.76971	1.57773	-0.00006
C	-4.02084	-2.34960	0.00013
H	-5.08197	-2.08871	0.00028
H	-3.80151	-2.96330	-0.88105
H	-3.80128	-2.96341	0.88116
C	-3.85315	2.65928	0.00002
H	-3.59652	3.25773	-0.88172
H	-4.92870	2.46672	0.00016
H	-3.59631	3.25786	0.88162
C	-3.69982	0.14626	0.00010
H	-4.78279	0.18407	0.00015
H	4.50046	3.38023	0.00012
H	4.69032	0.92655	0.00007
S	1.23404	-3.03400	0.00000

Optimized triplet-state structure of **24**.

C	-0.71720	2.78664	0.00713
C	-1.78881	3.65762	0.00828
C	-3.12151	3.14632	-0.00093
C	-3.38416	1.79432	-0.00885
C	-2.29429	0.88294	-0.00566
C	-0.91377	1.38804	0.00016
H	0.30319	3.15662	0.01138
H	-1.63054	4.73206	0.01491
C	-1.05409	-1.12224	-0.03073
C	-3.42530	-1.38911	0.00849
C	-2.99251	-2.67434	0.01957

N	-2.35708	-0.47992	-0.01041
Pt	0.48985	0.04284	-0.00813
C	3.18965	-1.36631	0.00192
C	3.32652	1.14889	0.01151
O	1.92236	-1.52910	-0.00764
O	2.08727	1.45084	0.00308
C	3.98152	-2.65885	0.00172
H	5.06168	-2.49335	0.01005
H	3.70224	-3.25481	0.87814
H	3.71470	-3.24688	-0.88390
C	4.25768	2.34564	0.02213
H	4.04785	2.96133	0.90439
H	5.31233	2.06002	0.02884
H	4.06061	2.96719	-0.85893
C	3.88387	-0.14430	0.01152
H	4.96592	-0.20308	0.01899
H	-3.95569	3.84312	-0.00304
H	-4.40960	1.45479	-0.01885
S	-1.25163	-2.87169	0.00808
C	-4.86955	-0.98814	0.02075
H	-3.64405	-3.53797	0.03754
H	-5.48888	-1.88862	0.03934
H	-5.12304	-0.39007	0.90384
H	-5.14466	-0.41209	-0.87049

Optimized triplet-state structure of **25**.

C	-1.58059	2.98838	0.06022
C	-1.10500	4.30035	0.15575
C	0.26633	4.54408	0.18509
C	1.17910	3.48434	0.12836
C	0.69075	2.18020	0.05035
C	-0.69605	1.90852	0.00271
H	-2.64783	2.79255	0.01969
H	-1.80547	5.13043	0.20049
C	0.72394	-0.16429	-0.17043
C	2.86174	0.75106	0.09298
C	3.16305	-0.58693	-0.00447
N	1.48653	0.96795	-0.01445
Pt	-1.19981	-0.01165	-0.20187
C	-2.59983	-2.66601	0.19238
C	-4.13218	-0.58307	0.20422
O	-1.56344	-2.10038	-0.38002
O	-3.25183	0.28682	-0.22419
C	-2.46598	-4.13063	0.51445
H	-3.37658	-4.53800	0.96552
H	-2.23912	-4.71101	-0.39095
H	-1.63407	-4.29833	1.21234
C	-5.52546	-0.05974	0.42465
H	-5.95535	0.32755	-0.51048
H	-6.19726	-0.83254	0.81202
H	-5.51683	0.77648	1.13761
C	-3.82027	-1.96767	0.41125
H	-4.65231	-2.58126	0.75125

H	0.64323	5.56100	0.24828
H	2.23418	3.71131	0.13751
S	1.71360	-1.55921	-0.21689
C	3.83633	1.86734	0.30880
H	3.85385	2.54885	-0.54913
H	3.57372	2.44785	1.19935
H	4.83446	1.45657	0.43932
C	4.42583	-1.34113	0.03992
O	4.45862	-2.55590	-0.03518
O	5.53498	-0.57755	0.16220
C	6.77393	-1.30922	0.20553
H	7.55240	-0.55200	0.30022
H	6.78745	-1.98746	1.06227
H	6.90697	-1.88866	-0.71124

Optimized triplet-state structure of **26**.

C	0.32318	2.85438	-0.20442
C	-0.68089	3.78545	-0.38366
C	-2.03760	3.35937	-0.49508
C	-2.39573	2.03152	-0.40435
C	-1.37755	1.06623	-0.19432
C	0.02847	1.47475	-0.12436
H	1.36288	3.15863	-0.13690
H	-0.44767	4.84383	-0.45663
C	-0.29619	-1.02307	0.04052
C	-2.67826	-1.11288	-0.13773
C	-2.33313	-2.41644	-0.30448
N	-1.54329	-0.28266	-0.06604
Pt	1.32793	0.03726	0.02577
C	3.92538	-1.55359	0.14267
C	4.23942	0.94517	0.11521
O	2.65001	-1.62654	0.10353
O	3.02546	1.33248	0.07070
C	4.62225	-2.89891	0.18825
H	5.71107	-2.81074	0.21750
H	4.28258	-3.45263	1.07102
H	4.33235	-3.48708	-0.68995
C	5.25281	2.07328	0.13279
H	5.06407	2.71776	0.99902
H	6.28399	1.71401	0.17276
H	5.12340	2.69144	-0.76310
C	4.70420	-0.38404	0.14836
H	5.77888	-0.51844	0.18484
H	-2.81336	4.10234	-0.66135
H	-3.43183	1.74055	-0.50369
S	-0.60955	-2.72427	-0.33718
C	-4.07133	-0.65612	0.06245
C	-4.43565	0.06241	1.21537
C	-5.06879	-1.01439	-0.85766
C	-5.76512	0.41640	1.43448
H	-3.67350	0.33472	1.94000
C	-6.40045	-0.66247	-0.63192
H	-4.79180	-1.55949	-1.75554

C	-6.75215	0.05513	0.51231
H	-6.03298	0.96823	2.33134
H	-7.16084	-0.94369	-1.35534
H	-7.78813	0.33252	0.68602
H	-3.04250	-3.23178	-0.35346

Optimized triplet-state structure of **27**.

C	0.50624	2.92770	-0.18337
C	-0.47239	3.89296	-0.32485
C	-1.84447	3.51363	-0.39784
C	-2.24066	2.19708	-0.31432
C	-1.24692	1.19488	-0.15313
C	0.17077	1.55861	-0.10725
H	1.55629	3.19882	-0.13865
H	-0.20602	4.94404	-0.39199
C	-0.22151	-0.92458	0.06442
C	-2.60831	-0.94488	-0.08295
C	-2.32777	-2.27628	-0.19589
N	-1.45014	-0.15054	-0.04467
Pt	1.43211	0.08251	0.02618
C	3.98604	-1.58334	0.12314
C	4.36963	0.90533	0.06827
O	2.70981	-1.62214	0.10267
O	3.16650	1.32713	0.03725
C	4.64810	-2.94666	0.17144
H	5.73924	-2.88715	0.18396
H	4.30717	-3.48315	1.06433
H	4.32983	-3.53489	-0.69683
C	5.41467	2.00463	0.06128
H	5.25791	2.66080	0.92518
H	6.43588	1.61658	0.08827
H	5.28879	2.61959	-0.83734
C	4.79749	-0.43541	0.10718
H	5.86846	-0.59948	0.12995
H	-2.60113	4.28335	-0.52589
H	-3.28845	1.94264	-0.38062
S	-0.59436	-2.62301	-0.24036
C	-3.97556	-0.38755	0.07952
C	-4.37294	0.15925	1.31159
C	-4.90187	-0.43689	-0.97302
C	-5.66518	0.65339	1.48070
H	-3.66277	0.19589	2.13302
C	-6.19740	0.05537	-0.79995
H	-4.59855	-0.85200	-1.93000
C	-6.58070	0.60314	0.42526
H	-5.96000	1.07312	2.43854
H	-6.90383	0.01399	-1.62447
H	-7.58786	0.98814	0.55912
C	-3.30132	-3.41181	-0.23637
H	-3.12111	-4.10612	0.59401
H	-4.33113	-3.05328	-0.17170
H	-3.19246	-3.98636	-1.16517

Optimized triplet-state structure of **28**.

C	1.96556	2.98844	-0.28623
C	1.32258	4.19774	-0.47299
C	-0.09761	4.24756	-0.53024
C	-0.87014	3.11473	-0.38380
C	-0.22371	1.86952	-0.17249
C	1.23296	1.78989	-0.14793
H	3.04891	2.93045	-0.25445
H	1.89404	5.11454	-0.58875
C	0.12604	-0.45322	0.13248
C	-2.15665	0.23896	0.01333
C	-2.29538	-1.12940	-0.05109
N	-0.82360	0.64787	0.00221
Pt	2.00217	0.00984	0.04098
C	3.94249	-2.34046	0.19636
C	5.05264	-0.08504	0.03946
O	2.71317	-1.99608	0.18077
O	4.03063	0.67658	-0.00819
C	4.16653	-3.83690	0.29616
H	5.22537	-4.10746	0.30541
H	3.69113	-4.21392	1.20890
H	3.67612	-4.33340	-0.54898
C	6.37852	0.64979	-0.01358
H	6.43599	1.35669	0.82215
H	7.23728	-0.02458	0.02956
H	6.43120	1.23799	-0.93706
C	5.06004	-1.48955	0.13307
H	6.03294	-1.96612	0.16117
H	-0.59032	5.20194	-0.69652
H	-1.94584	3.18774	-0.44206
S	-0.73377	-1.97475	-0.11088
C	-3.28307	1.20291	0.10758
C	-3.48706	1.93680	1.28830
C	-4.17459	1.36765	-0.96221
C	-4.56042	2.82064	1.39177
H	-2.79988	1.81254	2.12077
C	-5.24731	2.25437	-0.85607
H	-4.02207	0.79975	-1.87501
C	-5.44244	2.98232	0.31925
H	-4.70935	3.38185	2.31013
H	-5.92968	2.37575	-1.69275
H	-6.27808	3.67192	0.40096
C	-3.52978	-1.92698	-0.06666
C	-3.59448	-3.08934	-0.86127
C	-4.64892	-1.59446	0.72191
C	-4.74328	-3.87599	-0.88424
H	-2.74178	-3.36248	-1.47644
C	-5.79316	-2.38825	0.69983
H	-4.61257	-0.72454	1.36719
C	-5.84908	-3.52893	-0.10481
H	-4.77371	-4.76229	-1.51201
H	-6.64196	-2.11825	1.32226
H	-6.74349	-4.14564	-0.11842

Optimized triplet-state structure of **29**.

C	-0.53529	3.01536	-0.04113
C	0.25070	4.14521	-0.14426
C	1.66751	4.02200	-0.23198
C	2.29687	2.79561	-0.17865
C	1.50675	1.62866	-0.03265
C	0.04510	1.72586	-0.00340
H	-1.61746	3.08853	-0.00206
C	0.89770	-0.64836	0.09804
C	3.24781	-0.20707	0.08437
C	3.21673	-1.60672	-0.11599
N	1.95587	0.34412	0.05821
Pt	-0.92025	0.04346	0.04490
C	-3.10898	-2.06903	-0.00110
C	-3.95808	0.30116	0.03838
O	-1.84702	-1.85922	0.01731
O	-2.85542	0.93991	0.06059
C	-3.49360	-3.53423	-0.03215
H	-4.57557	-3.68653	-0.04591
H	-3.05254	-4.00584	-0.91773
H	-3.07016	-4.03856	0.84391
C	-5.19162	1.18263	0.05013
H	-5.16424	1.85750	-0.81312
H	-6.12078	0.60824	0.02517
H	-5.18224	1.80910	0.94952
C	-4.12357	-1.09820	0.00600
H	-5.14372	-1.46332	-0.01134
H	2.27060	4.91782	-0.35435
H	3.37030	2.74212	-0.29069
S	1.56864	-2.23191	-0.28028
C	4.47126	0.43153	0.32080
H	4.51886	1.48277	0.56850
C	4.39333	-2.34754	-0.14875
H	4.35906	-3.42074	-0.30959
C	5.64881	-0.32070	0.28910
H	6.59687	0.17597	0.47236
C	5.61569	-1.69414	0.04313
H	6.53908	-2.26532	0.01931
H	-0.20079	5.13236	-0.18204

In the following section the coordinates of the singlet ground-state structure geometries for **23**–**29** are given (BP86/6-31G(d)).

Optimized singlet ground-state structure of **23**.

C	1.28667	2.66193	-0.00027
C	2.50582	3.36639	-0.00035
C	3.73323	2.68220	-0.00025
C	3.75493	1.27673	-0.00011
C	2.52968	0.60069	-0.00005
C	1.27109	1.25646	-0.00011
H	0.33502	3.20385	-0.00032
H	2.49797	4.46279	-0.00049
C	1.09360	-1.27133	0.00021
C	3.37620	-1.81349	-0.00001
C	2.85201	-3.07223	0.00008
H	4.42887	-1.53262	-0.00014
H	3.39520	-4.01618	0.00002
N	2.39437	-0.82796	0.00010
Pt	-0.31658	0.03937	0.00005
C	-3.15040	-1.06555	-0.00027
C	-2.97196	1.46073	0.00001
O	-1.90253	-1.38438	0.00008
O	-1.68569	1.61196	-0.00004
C	-4.10101	-2.25242	-0.00072
H	-5.15954	-1.94742	-0.00052
H	-3.90815	-2.88038	-0.88899
H	-3.90798	-2.88125	0.88688
C	-3.73892	2.77213	0.00076
H	-3.45528	3.36751	-0.88571
H	-4.83030	2.62332	-0.00113
H	-3.45808	3.36478	0.88996
C	-3.68618	0.24487	-0.00029
H	-4.77690	0.32424	-0.00043
H	4.67746	3.23715	-0.00029
H	4.71065	0.74013	-0.00001
S	1.09756	-3.01529	0.00027

Optimized singlet ground-state structure of **24**.

C	0.80745	2.80388	-0.00006
C	1.92669	3.65545	-0.00005
C	3.22328	3.11952	-0.00001
C	3.41737	1.72678	0.00002
C	2.29065	0.89059	-0.00000
C	0.96539	1.40772	-0.00003
H	-0.20613	3.21844	-0.00009
H	1.78545	4.74272	-0.00007
C	1.04048	-1.10504	0.00001
C	3.36787	-1.48403	0.00003
C	2.89996	-2.76987	0.00003

N	2.30604	-0.55597	0.00002
Pt	-0.49343	0.05024	-0.00003
C	-3.20613	-1.33821	0.00000
C	-3.28614	1.19267	0.00003
O	-1.93239	-1.52571	0.00002
O	-2.02201	1.47377	-0.00000
C	-4.03001	-2.61637	-0.00011
H	-5.11428	-2.42143	0.00045
H	-3.77412	-3.22156	-0.88830
H	-3.77327	-3.22226	0.88735
C	-4.18386	2.41859	0.00018
H	-3.96380	3.03872	-0.88731
H	-5.25418	2.15842	-0.00049
H	-3.96475	3.03779	0.88858
C	-3.87331	-0.08958	0.00001
H	-4.96645	-0.12229	0.00002
H	4.09712	3.78010	0.00000
H	4.43474	1.33491	0.00005
S	1.15398	-2.83823	0.00007
C	4.82140	-1.10823	0.00003
H	3.50637	-3.67494	0.00002
H	5.09807	-0.52170	0.89426
H	5.42758	-2.02841	-0.00001
H	5.09804	-0.52165	-0.89418

Optimized singlet ground-state structure of **25**.

C	1.54681	3.00676	-0.00009
C	1.05862	4.32474	-0.00009
C	-0.32348	4.56550	-0.00001
C	-1.23370	3.49425	0.00006
C	-0.73219	2.18210	0.00003
C	0.66530	1.91232	-0.00003
H	2.62472	2.81359	-0.00015
H	1.76014	5.16729	-0.00014
C	-0.72585	-0.18140	0.00010
C	-2.89860	0.73713	0.00009
C	-3.18538	-0.61916	0.00005
N	-1.51500	0.96180	0.00010
Pt	1.18180	-0.00990	0.00003
C	2.74402	-2.62921	0.00002
C	4.15611	-0.52883	-0.00015
O	1.56649	-2.10892	0.00014
O	3.23261	0.38016	-0.00013
C	2.76058	-4.14934	0.00009
H	3.78224	-4.56118	-0.00036
H	2.22112	-4.52497	0.88798
H	2.22027	-4.52507	-0.88724
C	5.56659	0.03527	-0.00017
H	5.70878	0.67677	0.88810
H	6.33647	-0.75249	-0.00073
H	5.70838	0.67773	-0.88780
C	3.97343	-1.92645	-0.00012
H	4.88209	-2.53497	-0.00019

H	-0.70856	5.59094	0.00001
H	-2.30046	3.71387	0.00013
S	-1.71701	-1.59322	0.00007
C	-3.89864	1.85409	0.00018
H	-3.78314	2.49230	0.89436
H	-3.78330	2.49236	-0.89397
H	-4.91123	1.43180	0.00024
C	-4.44233	-1.39022	-0.00003
O	-4.46243	-2.61938	-0.00003
O	-5.57289	-0.62199	-0.00015
C	-6.80434	-1.38535	-0.00029
H	-7.60665	-0.63433	-0.00060
H	-6.86309	-2.02256	-0.89749
H	-6.86350	-2.02224	0.89711

Optimized singlet ground-state structure of **26**.

C	0.27285	2.89635	-0.15322
C	-0.76894	3.83202	-0.28586
C	-2.10170	3.40152	-0.37728
C	-2.41358	2.03173	-0.31481
C	-1.36406	1.11658	-0.14930
C	-0.00251	1.51975	-0.09228
H	1.31545	3.22823	-0.10650
H	-0.53692	4.90276	-0.33189
C	-0.29060	-0.97888	-0.07701
C	-2.64141	-1.15657	-0.09469
C	-2.28694	-2.47993	-0.15468
N	-1.50289	-0.32300	-0.08265
Pt	1.33391	0.04278	-0.01100
C	3.92542	-1.56228	0.10516
C	4.20860	0.95418	0.11914
O	2.64227	-1.64783	0.04781
O	2.97253	1.33665	0.06753
C	4.64392	-2.90234	0.13890
H	5.73952	-2.79500	0.18143
H	4.30551	-3.48139	1.01693
H	4.37460	-3.48952	-0.75736
C	5.20111	2.10412	0.16091
H	4.99225	2.74162	1.03874
H	6.24613	1.75902	0.20819
H	5.07162	2.73720	-0.73531
C	4.69013	-0.37114	0.13931
H	5.77610	-0.49144	0.18708
H	-2.91205	4.12791	-0.50287
H	-3.45095	1.70653	-0.40569
S	-0.55373	-2.69717	-0.14775
C	-4.04528	-0.69596	0.05135
C	-4.46664	-0.01623	1.21747
C	-4.99772	-1.02478	-0.93638
C	-5.81323	0.33569	1.38041
H	-3.73384	0.23321	1.99232
C	-6.34604	-0.67261	-0.76679
H	-4.67052	-1.54729	-1.84183

C	-6.75598	0.00929	0.38960
H	-6.12906	0.86148	2.28814
H	-7.07520	-0.92827	-1.54344
H	-7.80785	0.28613	0.52069
H	-2.97252	-3.32604	-0.13015

Optimized singlet ground-state structure of **27**.

C	0.46700	2.97723	-0.06675
C	-0.54701	3.95065	-0.12295
C	-1.89619	3.56695	-0.16230
C	-2.25155	2.20643	-0.13624
C	-1.22749	1.25085	-0.06570
C	0.14822	1.60923	-0.04125
H	1.52117	3.27345	-0.04655
H	-0.28085	5.01430	-0.14198
C	-0.22207	-0.87745	-0.03225
C	-2.57749	-0.98055	-0.03630
C	-2.29020	-2.32472	-0.05357
N	-1.40928	-0.18446	-0.03620
Pt	1.43787	0.08987	-0.00640
C	3.98084	-1.59827	0.04342
C	4.34560	0.90729	0.05068
O	2.69479	-1.64219	0.01891
O	3.12195	1.32901	0.02772
C	4.65667	-2.96101	0.05666
H	5.75584	-2.88880	0.07611
H	4.31845	-3.53320	0.93920
H	4.34990	-3.53497	-0.83616
C	5.37574	2.02456	0.07057
H	5.21056	2.66450	0.95597
H	6.40993	1.64553	0.08955
H	5.24364	2.66569	-0.81950
C	4.78484	-0.43286	0.05883
H	5.86725	-0.58811	0.07971
H	-2.68685	4.32342	-0.21558
H	-3.30340	1.92129	-0.17601
S	-0.54615	-2.58426	-0.05358
C	-3.95840	-0.42498	0.02964
C	-4.50448	-0.01927	1.26765
C	-4.75413	-0.34670	-1.13336
C	-5.81642	0.47194	1.33523
H	-3.89092	-0.08404	2.17273
C	-6.06743	0.14429	-1.06167
H	-4.33276	-0.66265	-2.09385
C	-6.59918	0.55658	0.17099
H	-6.22921	0.78722	2.29982
H	-6.67487	0.20548	-1.97138
H	-7.62372	0.94097	0.22559
C	-3.25034	-3.47855	-0.03793
H	-3.09623	-4.12191	0.84794
H	-4.28773	-3.10703	-0.01540
H	-3.13375	-4.11630	-0.93352

Optimized singlet ground-state structure of **28**.

C	1.98948	3.04575	-0.18003
C	1.33668	4.28415	-0.31446
C	-0.06350	4.34142	-0.38968
C	-0.83120	3.16594	-0.31089
C	-0.16464	1.94255	-0.14672
C	1.25386	1.85117	-0.10274
H	3.08275	2.99378	-0.14344
H	1.92528	5.20747	-0.37353
C	0.12424	-0.39176	-0.04458
C	-2.14623	0.24954	-0.03551
C	-2.29423	-1.12531	-0.04866
N	-0.79010	0.63833	-0.05876
Pt	2.00172	0.00721	-0.00405
C	3.87859	-2.39715	0.13614
C	5.01771	-0.13563	0.11765
O	2.64552	-2.03283	0.07750
O	3.99159	0.65143	0.05655
C	4.08706	-3.90300	0.18618
H	5.15157	-4.18308	0.23330
H	3.56652	-4.31919	1.06736
H	3.63218	-4.36906	-0.70629
C	6.34809	0.59840	0.14734
H	6.37565	1.27980	1.01659
H	7.20826	-0.08759	0.20142
H	6.44473	1.22582	-0.75698
C	5.00937	-1.54525	0.15727
H	5.98608	-2.03448	0.20999
H	-0.57344	5.30287	-0.51513
H	-1.91698	3.22461	-0.38848
S	-0.70789	-1.91037	-0.05056
C	-3.27065	1.22095	0.03872
C	-3.50507	1.95325	1.22500
C	-4.14686	1.38065	-1.05518
C	-4.59189	2.83554	1.30701
H	-2.82707	1.83151	2.07686
C	-5.23352	2.26473	-0.96824
H	-3.96866	0.80986	-1.97243
C	-5.45756	2.99403	0.21067
H	-4.76358	3.40006	2.23012
H	-5.90536	2.38386	-1.82532
H	-6.30582	3.68424	0.27694
C	-3.51543	-1.95228	-0.02350
C	-3.56872	-3.14939	-0.77813
C	-4.63731	-1.60301	0.76607
C	-4.70742	-3.96549	-0.75020
H	-2.71429	-3.42971	-1.40509
C	-5.77573	-2.41991	0.78548
H	-4.60719	-0.69559	1.37566
C	-5.81783	-3.60313	0.02939
H	-4.72782	-4.88517	-1.34537
H	-6.63198	-2.13359	1.40642
H	-6.70864	-4.24047	0.05090

Optimized singlet ground-state structure of **29**.

C	-0.51893	3.07387	0.00664
C	0.28786	4.22403	-0.06485
C	1.68237	4.10476	-0.15931
C	2.28977	2.83641	-0.15671
C	1.47473	1.70041	-0.04485
C	0.05647	1.79287	0.00760
H	-1.60954	3.16221	0.05137
C	0.89222	-0.57792	-0.06200
C	3.22043	-0.23431	0.02971
C	3.16413	-1.65254	-0.03754
N	1.92792	0.32904	-0.02886
Pt	-0.91526	0.05228	-0.00510
C	-3.06829	-2.10594	-0.03070
C	-3.92056	0.27458	0.10715
O	-1.79921	-1.89121	-0.06075
O	-2.80357	0.93128	0.10152
C	-3.46029	-3.57380	-0.08924
H	-4.55056	-3.72264	-0.03837
H	-3.08041	-4.02112	-1.02546
H	-2.98271	-4.11800	0.74503
C	-5.14963	1.16367	0.18836
H	-5.15839	1.86193	-0.66783
H	-6.08836	0.58746	0.19122
H	-5.10175	1.77855	1.10506
C	-4.08582	-1.12436	0.04751
H	-5.11579	-1.49168	0.06368
H	2.31165	4.99733	-0.24348
H	3.37142	2.76926	-0.27944
S	1.49284	-2.21390	-0.11048
C	4.47082	0.39758	0.18239
H	4.55351	1.47660	0.30662
C	4.32522	-2.43779	-0.00640
H	4.25829	-3.52889	-0.06327
C	5.62785	-0.39253	0.21738
H	6.59854	0.09971	0.33747
C	5.56470	-1.79530	0.11210
H	6.48399	-2.38922	0.13836
H	-0.17627	5.21728	-0.06323

In the following section the coordinates of the triplet-state structure geometries for **23**–**29** are given (BP86/6-31G(d)).

Optimized triplet-state structure of **23**.

C	1.17838	2.67703	0.00008
C	2.35816	3.42084	0.00017
C	3.63507	2.75989	0.00020
C	3.73794	1.37578	0.00017
C	2.53886	0.61516	0.00010
C	1.21178	1.26156	0.00000
H	0.20197	3.17248	0.00003
H	2.32439	4.51538	0.00019
C	1.10839	-1.27494	0.00008
C	3.44682	-1.72730	0.00007
C	2.94449	-2.99440	0.00004
H	4.49861	-1.44073	0.00005
H	3.52922	-3.91457	-0.00001
N	2.45667	-0.75127	0.00011
Pt	-0.31090	0.03846	-0.00017
C	-3.11910	-1.12314	0.00020
C	-3.01764	1.41291	0.00001
O	-1.85970	-1.41457	0.00003
O	-1.74428	1.60353	-0.00021
C	-4.03229	-2.33794	0.00030
H	-5.10001	-2.06711	0.00102
H	-3.81798	-2.95948	-0.88756
H	-3.81689	-2.96015	0.88742
C	-3.83721	2.69289	0.00014
H	-3.57863	3.29830	-0.88728
H	-4.92175	2.50056	-0.00086
H	-3.58018	3.29713	0.88883
C	-3.69274	0.16607	0.00023
H	-4.78541	0.21012	0.00041
H	4.54918	3.36429	0.00026
H	4.71978	0.89053	0.00022
S	1.18109	-3.04410	0.00005

Optimized triplet-state structure of **24**.

C	-0.72287	2.79738	-0.00017
C	-1.80664	3.67304	-0.00008
C	-3.14339	3.15443	0.00014
C	-3.40242	1.78997	0.00023
C	-2.30491	0.88291	0.00009
C	-0.91746	1.39541	-0.00010
H	0.30558	3.17314	-0.00031
H	-1.64935	4.75676	-0.00015
C	-1.04179	-1.12009	0.00027
C	-3.41627	-1.41310	0.00010
C	-2.96419	-2.70626	0.00001

N	-2.35525	-0.49284	0.00017
Pt	0.48999	0.04709	-0.00014
C	3.18699	-1.36982	0.00004
C	3.31906	1.16373	0.00020
O	1.90707	-1.54284	-0.00007
O	2.06825	1.47042	0.00018
C	3.98509	-2.66350	0.00013
H	5.07323	-2.49179	-0.00023
H	3.71449	-3.26304	0.88779
H	3.71394	-3.26350	-0.88705
C	4.25210	2.36407	0.00019
H	4.04946	2.99018	0.88775
H	5.31477	2.07443	0.00112
H	4.05080	2.98912	-0.88843
C	3.87755	-0.13871	0.00015
H	4.96962	-0.19568	0.00022
H	-3.98830	3.85251	0.00024
H	-4.43580	1.44235	0.00044
S	-1.21867	-2.87819	0.00000
C	-4.86578	-1.02205	0.00005
H	-3.60795	-3.58684	-0.00007
H	-5.13547	-0.43089	-0.89420
H	-5.48591	-1.93284	-0.00007
H	-5.13559	-0.43105	0.89438

Optimized triplet-state structure of **25**.

C	-1.53651	2.97809	0.10754
C	-1.05385	4.28288	0.08094
C	0.34613	4.51996	-0.05409
C	1.26316	3.47144	-0.13950
C	0.78717	2.14096	-0.07660
C	-0.65080	1.87157	0.01801
H	-2.60914	2.77279	0.18518
H	-1.74128	5.13300	0.14862
C	0.72593	-0.22080	-0.24837
C	2.90364	0.73353	-0.01789
C	3.19121	-0.63105	-0.03866
N	1.54052	0.96550	-0.12935
Pt	-1.18795	0.00315	-0.06451
C	-2.76864	-2.59887	0.00167
C	-4.18897	-0.50270	0.17952
O	-1.59068	-2.07391	-0.10754
O	-3.28006	0.40361	0.10540
C	-2.77139	-4.11723	-0.02375
H	-3.78364	-4.54160	0.06878
H	-2.31513	-4.47054	-0.96574
H	-2.14172	-4.49945	0.79960
C	-5.60190	0.03594	0.33094
H	-5.83597	0.70519	-0.51639
H	-6.35751	-0.76418	0.37559
H	-5.66906	0.64454	1.25088
C	-3.99104	-1.90881	0.13565
H	-4.89046	-2.52575	0.21512

H	0.71634	5.55009	-0.10230
H	2.31989	3.70148	-0.26971
S	1.74554	-1.66158	-0.19286
C	3.89856	1.84498	0.15041
H	3.97503	2.46353	-0.76326
H	3.61548	2.50614	0.98892
H	4.88800	1.41683	0.35324
C	4.45114	-1.37551	0.07512
O	4.48855	-2.60785	0.09024
O	5.57925	-0.59388	0.15006
C	6.80584	-1.35079	0.26424
H	7.60628	-0.59808	0.30327
H	6.80106	-1.96382	1.18075
H	6.93487	-2.01440	-0.60654

Optimized triplet-state structure of **26**.

C	0.34714	2.87127	-0.21387
C	-0.65944	3.81725	-0.39777
C	-2.02371	3.39616	-0.51971
C	-2.39262	2.05919	-0.43205
C	-1.37612	1.08802	-0.21613
C	0.04097	1.49082	-0.13726
H	1.39750	3.17138	-0.13962
H	-0.41666	4.88300	-0.46686
C	-0.29055	-1.00853	-0.00401
C	-2.68145	-1.10533	-0.15185
C	-2.32812	-2.42435	-0.30554
N	-1.54271	-0.27310	-0.09513
Pt	1.33047	0.03855	0.01667
C	3.91126	-1.58103	0.15296
C	4.24124	0.93424	0.14069
O	2.62263	-1.65309	0.09961
O	3.01970	1.33665	0.08832
C	4.60373	-2.93328	0.20145
H	5.70122	-2.84768	0.24220
H	4.25255	-3.49487	1.08572
H	4.32012	-3.52467	-0.68757
C	5.26506	2.05772	0.17319
H	5.07525	2.70610	1.04742
H	6.30073	1.68560	0.22071
H	5.15052	2.68815	-0.72700
C	4.69597	-0.40798	0.17075
H	5.77936	-0.54959	0.21666
H	-2.80192	4.14831	-0.69324
H	-3.43838	1.76907	-0.54180
S	-0.60393	-2.72199	-0.32499
C	-4.07360	-0.65379	0.06073
C	-4.41892	0.14440	1.17875
C	-5.10045	-1.09833	-0.80355
C	-5.75575	0.48786	1.41740
H	-3.63371	0.48300	1.86329
C	-6.43776	-0.75547	-0.55621
H	-4.83733	-1.70168	-1.67946

C	-6.77043	0.04025	0.55244
H	-6.00804	1.10163	2.28931
H	-7.22101	-1.10355	-1.23880
H	-7.81453	0.31227	0.74197
H	-3.03755	-3.25230	-0.33327

Optimized triplet-state structure of **27**.

C	0.52873	2.94419	-0.19702
C	-0.45301	3.92205	-0.34725
C	-1.83252	3.54572	-0.42974
C	-2.23784	2.22001	-0.34385
C	-1.24476	1.21481	-0.17312
C	0.18357	1.57357	-0.11944
H	1.58915	3.21207	-0.14611
H	-0.17845	4.98037	-0.41441
C	-0.21558	-0.91176	0.03007
C	-2.60918	-0.93740	-0.09465
C	-2.32345	-2.28426	-0.19663
N	-1.44815	-0.14292	-0.06584
Pt	1.43482	0.08475	0.02159
C	3.97094	-1.60881	0.12873
C	4.37147	0.89559	0.08458
O	2.68082	-1.64683	0.10280
O	3.16078	1.33310	0.05229
C	4.62848	-2.97907	0.17651
H	5.72854	-2.92245	0.19293
H	4.28174	-3.52259	1.07374
H	4.31016	-3.57119	-0.70021
C	5.42720	1.98997	0.08574
H	5.27710	2.64861	0.96012
H	6.45281	1.58868	0.11127
H	5.30927	2.61843	-0.81541
C	4.78867	-0.45783	0.11856
H	5.86841	-0.62957	0.14384
H	-2.59261	4.32321	-0.56806
H	-3.29518	1.96431	-0.41841
S	-0.58633	-2.62196	-0.22651
C	-3.97636	-0.38331	0.07938
C	-4.34177	0.24672	1.29258
C	-4.94588	-0.52093	-0.93896
C	-5.64401	0.73046	1.47567
H	-3.59702	0.35269	2.08902
C	-6.25093	-0.03869	-0.74933
H	-4.66399	-0.99349	-1.88628
C	-6.60283	0.58915	0.45609
H	-5.91405	1.21449	2.42080
H	-6.99125	-0.14834	-1.54962
H	-7.62023	0.96826	0.60240
C	-3.29658	-3.42403	-0.21621
H	-3.10274	-4.12069	0.62091
H	-4.33290	-3.05944	-0.13523
H	-3.20495	-4.00886	-1.15096

Optimized triplet-state structure of **28**.

C	2.01212	3.06213	0.06510
C	1.39153	4.31229	-0.08523
C	0.00206	4.39274	-0.28733
C	-0.78830	3.23278	-0.29824
C	-0.16298	1.99092	-0.09405
C	1.25219	1.87905	0.03975
H	3.09835	2.98717	0.18008
H	1.99435	5.22788	-0.06679
C	0.11344	-0.33799	-0.18462
C	-2.15113	0.33436	-0.14513
C	-2.28490	-1.13299	-0.22090
N	-0.81585	0.70031	-0.09476
Pt	1.97654	0.03170	0.01629
C	3.83146	-2.39892	-0.06327
C	4.98763	-0.16808	0.24868
O	2.60483	-2.01542	-0.10907
O	3.96582	0.63043	0.25256
C	4.02614	-3.90037	-0.19977
H	5.08607	-4.19727	-0.15535
H	3.47252	-4.41859	0.60354
H	3.59619	-4.24174	-1.15847
C	6.31745	0.54310	0.42818
H	6.31668	1.09301	1.38654
H	7.17287	-0.15059	0.41357
H	6.44769	1.29263	-0.37307
C	4.96885	-1.56892	0.10138
H	5.93934	-2.07244	0.12277
H	-0.47866	5.36479	-0.44174
H	-1.85985	3.31328	-0.47810
S	-0.67305	-1.87360	-0.48974
C	-3.28793	1.24809	-0.11398
C	-3.44542	2.23673	0.90111
C	-4.33840	1.08967	-1.06414
C	-4.58580	3.04540	0.93662
H	-2.67410	2.34501	1.67057
C	-5.46809	1.91311	-1.02634
H	-4.24101	0.32486	-1.84133
C	-5.60143	2.89670	-0.02874
H	-4.69114	3.79042	1.73341
H	-6.25194	1.78645	-1.78148
H	-6.49194	3.53335	0.00511
C	-3.40957	-1.95890	0.03988
C	-3.36409	-3.36172	-0.30562
C	-4.62169	-1.48816	0.67316
C	-4.43976	-4.20546	-0.06257
H	-2.47238	-3.76187	-0.80174
C	-5.68563	-2.35270	0.91202
H	-4.68452	-0.45475	1.01562
C	-5.62017	-3.71431	0.54338
H	-4.37205	-5.26042	-0.35165
H	-6.58163	-1.96646	1.41143
H	-6.46630	-4.38303	0.73195

Optimized triplet-state structure of **29**.

C	0.55688	3.03086	-0.01304
C	-0.22920	4.17669	-0.09882
C	-1.65192	4.06083	-0.20386
C	-2.29122	2.82562	-0.18016
C	-1.50410	1.65168	-0.04661
C	-0.03358	1.74149	-0.00328
H	1.64867	3.09787	0.03446
C	-0.89027	-0.63008	0.01542
C	-3.24826	-0.20312	0.06204
C	-3.21165	-1.61979	-0.08146
N	-1.95592	0.35146	0.01421
Pt	0.92251	0.04765	0.02096
C	3.08530	-2.09468	-0.00951
C	3.95839	0.28635	0.07086
O	1.81037	-1.87612	-0.01135
O	2.85174	0.94137	0.08246
C	3.46015	-3.56637	-0.04927
H	4.54988	-3.72678	-0.04037
H	3.01123	-4.08433	0.81711
H	3.03411	-4.03068	-0.95677
C	5.20285	1.15772	0.11308
H	5.18733	1.78222	1.02447
H	6.13283	0.56765	0.09931
H	5.20173	1.84695	-0.75054
C	4.10863	-1.12478	0.02505
H	5.13539	-1.50126	0.02047
H	-2.25661	4.96757	-0.31863
H	-3.37280	2.77875	-0.31163
S	-1.55665	-2.24098	-0.21314
C	-4.48378	0.44211	0.27114
H	-4.53707	1.51151	0.47691
C	-4.39075	-2.37357	-0.08429
H	-4.35032	-3.46109	-0.20164
C	-5.66370	-0.32282	0.26927
H	-6.62238	0.18075	0.43053
C	-5.62341	-1.71289	0.07977
H	-6.55157	-2.29399	0.07714
H	0.23224	5.16987	-0.11141

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