- Supporting Information -

Photoluminescence of a New Material: Cyclometalated C^C* Thiazole-2-ylidene Platinum(II) Complexes

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Table of Contents:

List of Abbreviations

2D NMR	One-/two-dimensional Nuclear Magnetic Resonance Spectroscopy
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
Mp	Melting point
NHC	N-Heterocyclic carbene
NOESY	Nuclear Overhauser effect spectroscopy
OLED	Organic light-emitting device/diode
PMMA	Poly(methyl methacrylate)
QY	Quantum yield

Solid-State Structure Determination (Details)

The following section contains the solid-state data for **8, 9**,**18** and **25**–**27**.

Table S1. Crystal data and crystallographic details for **8, 9 and 18**

structure	**8**	**9**	**18**
empirical formula	C11 H11 N S2	C11 H10 Br N S2	C11 H11 Br F6 N P S
formula weight [g/mol]	221.35	300.24	414.15
T [K]	198 K	198 K	198 K
wavelength [Å]	0.71073	0.71073	0.71073
crystal system	monoclinic	orthorhombic	monoclinic
space group	P 21/c	P 21 21 21	P 21/c
a [Å]	8.887(3)	6.2980(12)	11.871(2)
b [Å]	14.837(3)	8.2180(11)	9.4960(4)
c [Å]	16.891(8)	23.779(5)	14.914(4)
α [°]	90	90	90
β [°]	100.92(3)	90	117.62(2)
γ [°]	90	90	90
U [$Å^3$]	2186.9(14)	1230.7(4)	1489.6(5)
Z	8	4	4
D_{calc} [Mg/m^3]	1.345	1.620	1.847
μ(MoKα) [mm^{-1}]	0.445	3.464	3.062
crystal size [mm^3]	0.750 x 0.460 x 0.280	0.607 x 0.600 x 0.586	0.448 x 0.270 x 0.234
F(000)	928	600	816
reflections collected	33618	14543	25967
independent reflections	4047	2324	2775
Goodness-of-fit on F^2	1.079	1.369	1.048
R_1 [I>2σ(I)]	0.0634	0.0464	0.0521
wR_2 [I>2σ(I)]	0.1538	0.1383	0.0893
data / restraints / parameters	4047 / 0 / 257	2324 / 0 / 138	2775 / 0 / 192

Table S2. Crystal data and crystallographic details for complexes **25**–**27**

complex	**25**	**26**	**27**
empirical formula	C16 H17 N O2 Pt S	C16 H16 Br N O2 Pt S	C17 H19 N O3 Pt S
formula weight [g/mol]	482.46	561.35	512.48
T [K]	198 K	198 K	198 K
wavelength [Å]	0.71073	0.71073	0.71073
crystal system	monoclinic	monoclinic	monoclinic
space group	C 2/c	P 21/c	P 21/c
a [Å]	18.113(4)	11.518(3)	9.5740(19)
b [Å]	7.7290(15)	7.5600(11)	7.2950(2)
c [Å]	22.149(4)	21.820(3)	24.7060(19)
α [°]	90	90	90
β [°]	100.57(3)	121.46(3)	105.09(1)
γ [°]	90	90	90
U [$Å^3$]	3048.1(11)	1620.7(7)	1666.0(4)
Z	8	4	4
D_{calc} [Mg/m^3]	2.103	2.301	2.043
μ(MoKα) [mm^{-1}]	9.346	11.257	8.561
crystal size [mm^3]	0.520 x 0.330 x 0.210	0.590 x 0.410 x 0.220	0.351 x 0.217 x 0.142
F(000)	1840	1056	984
reflections collected	37053	28118	27579
independent reflections	3137	3013	3099
Goodness-of-fit on F^2	1.303	1.211	1.257
R_1 [I>2σ(I)]	0.0217	0.0411	0.0405
wR_2 [I>2σ(I)]	0.0601	0.1018	0.1010
data / restraints / parameters	3137 / 0 / 195	3013 / 0 / 185	3099 / 0 / 213

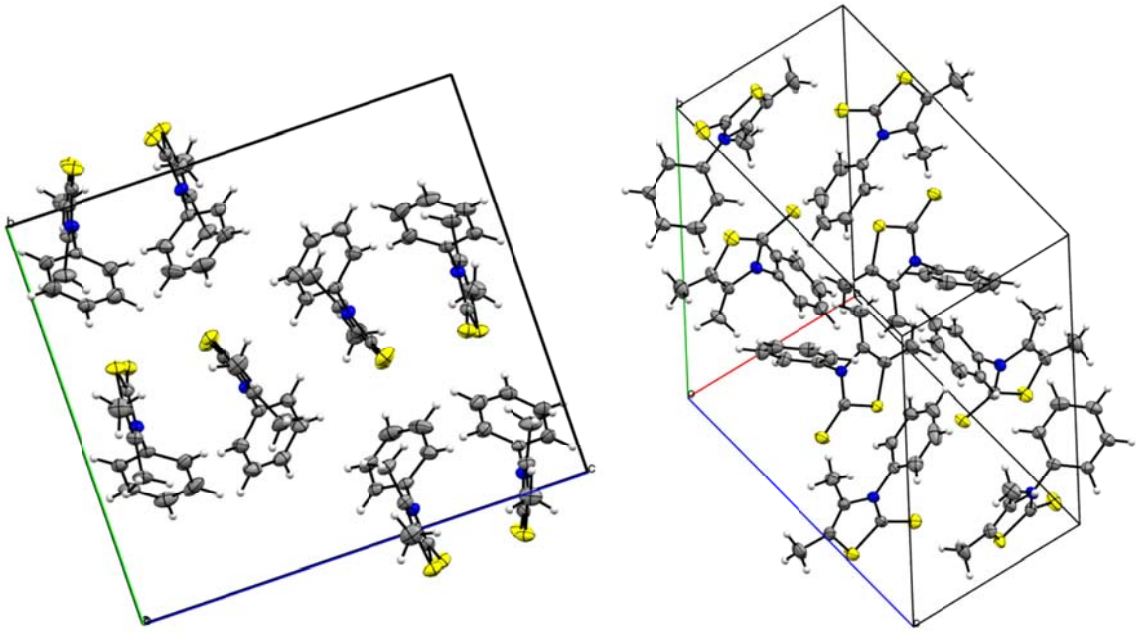


Figure S1. Orientation of **8** in the solid state.

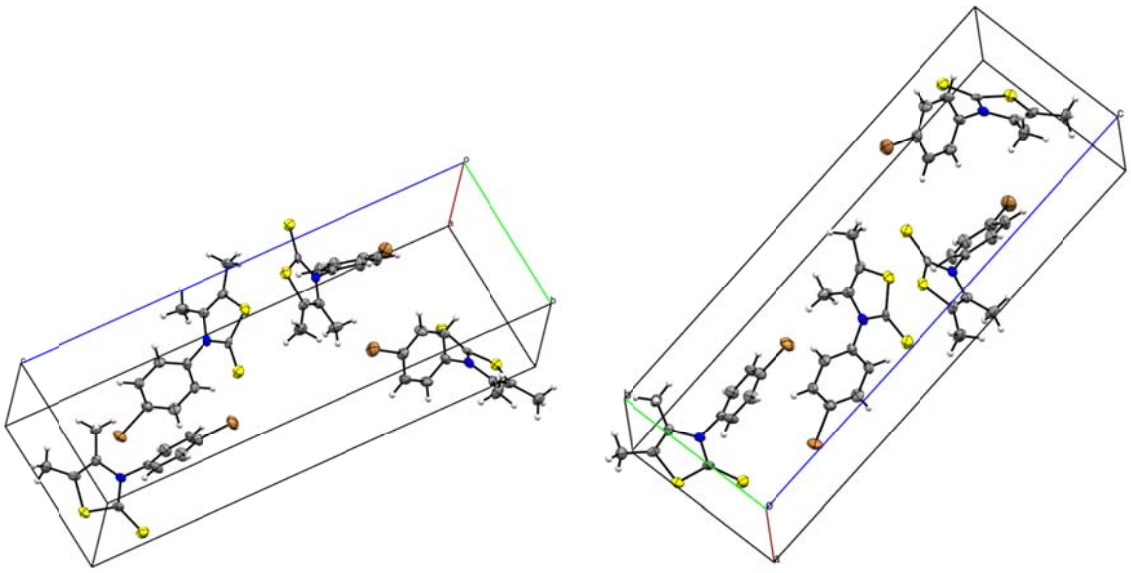


Figure S2. Orientation of **9** in the solid state.

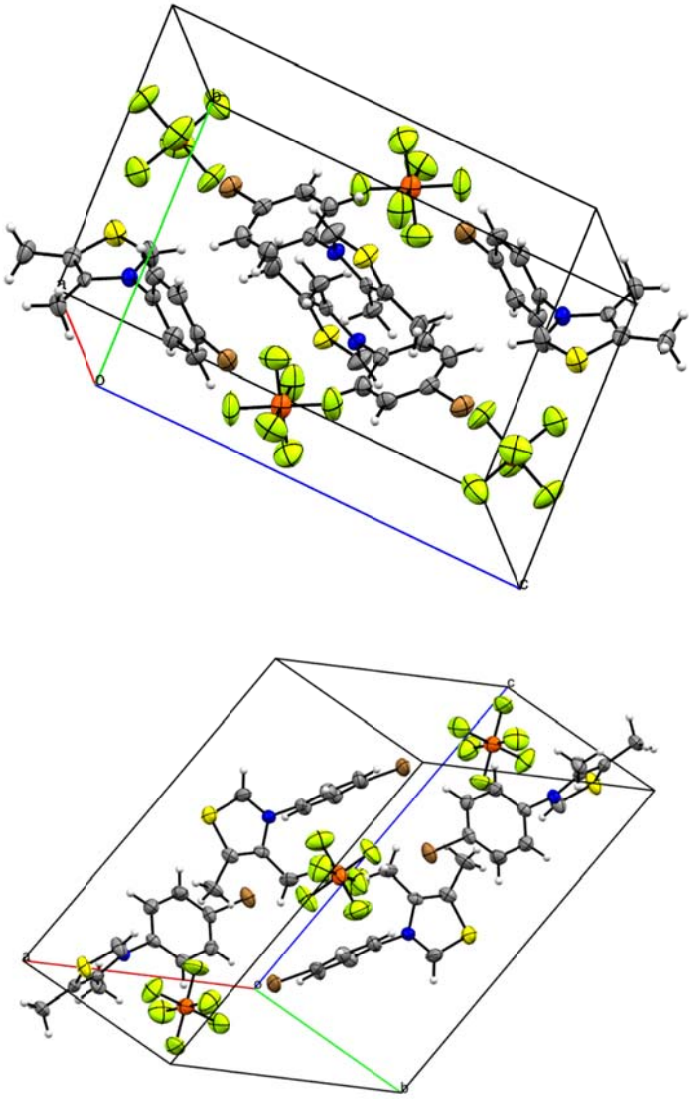


Figure S3. Orientation of **18** in the solid state.

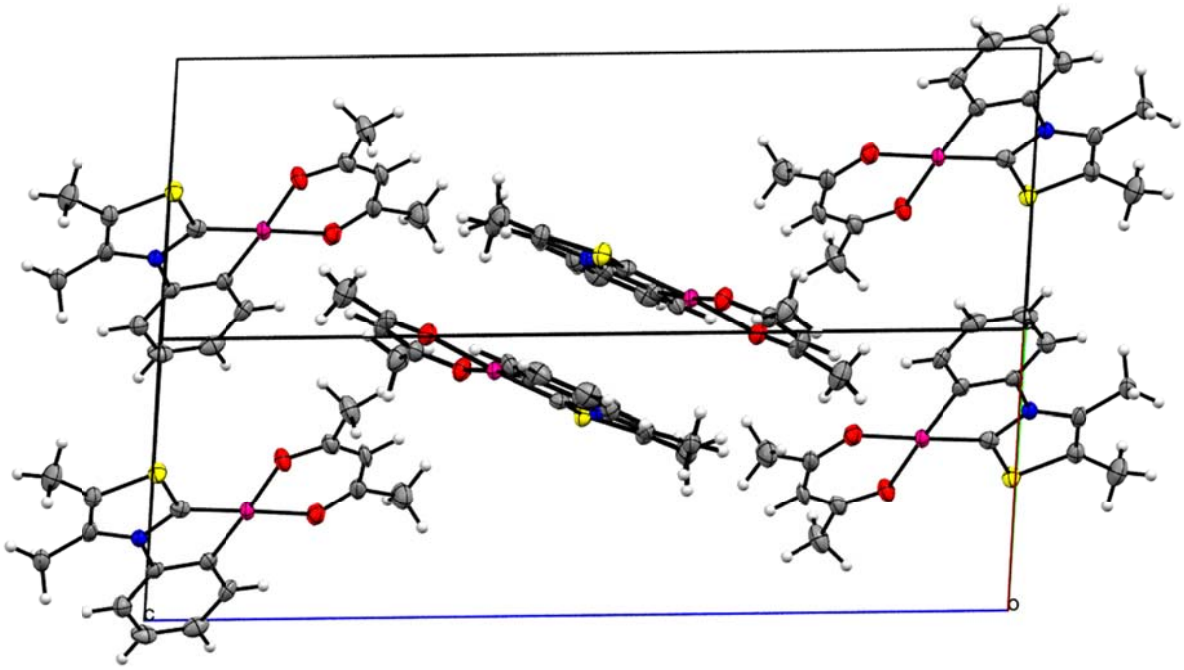


Figure S4. Orientation of **25** in the solid state.

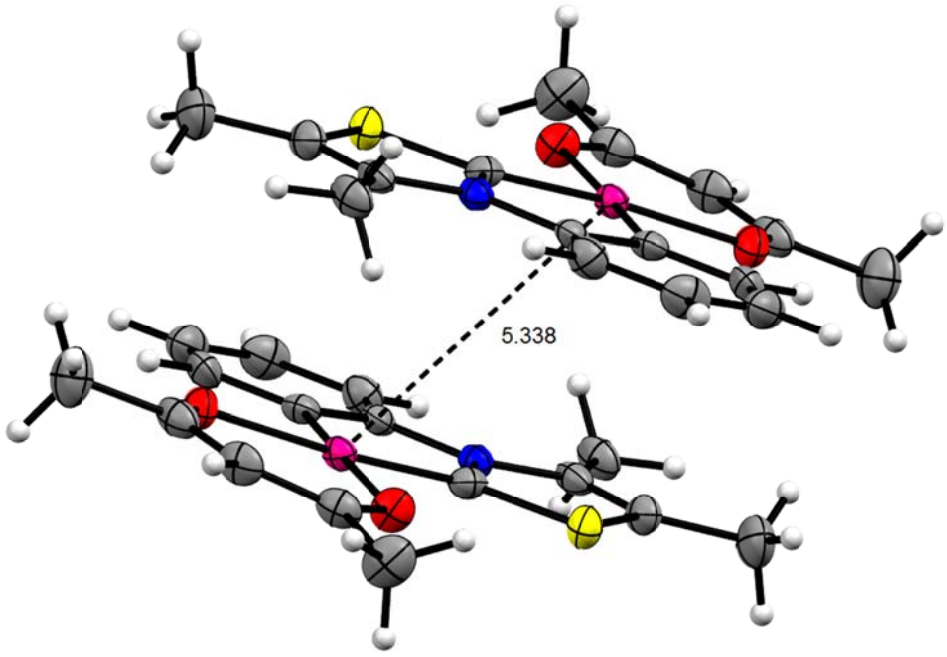


Figure S5. Orientation of **25** in the solid state with highlighted Pt…Pt-distances (in Å).

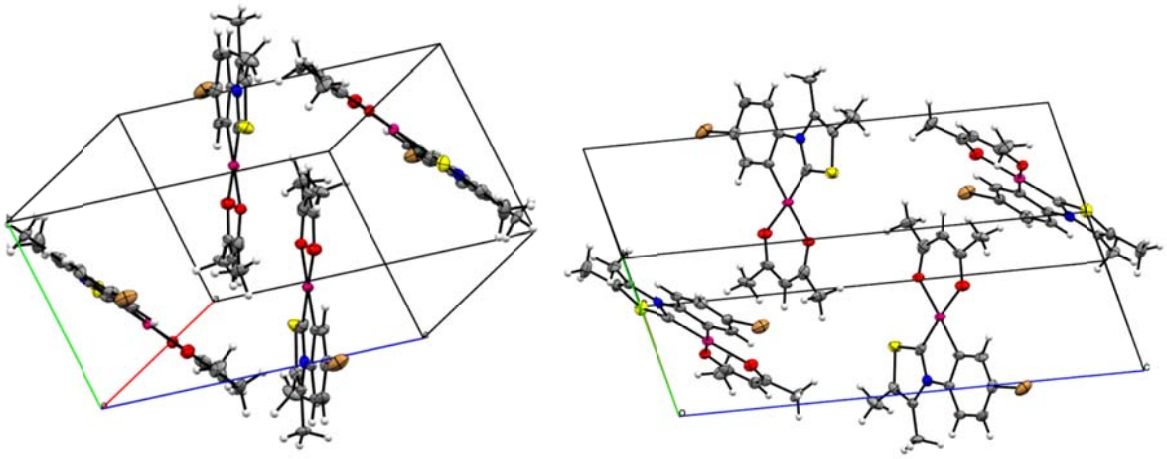


Figure S6. Orientation of **26** in the solid state.

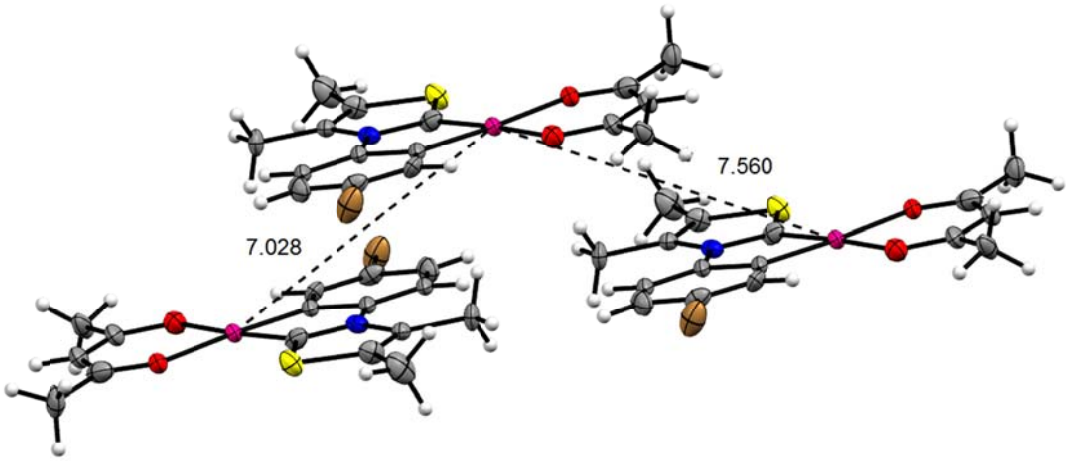


Figure S7. Orientation of **26** in the solid state with highlighted Pt…Pt-distances (in Å).

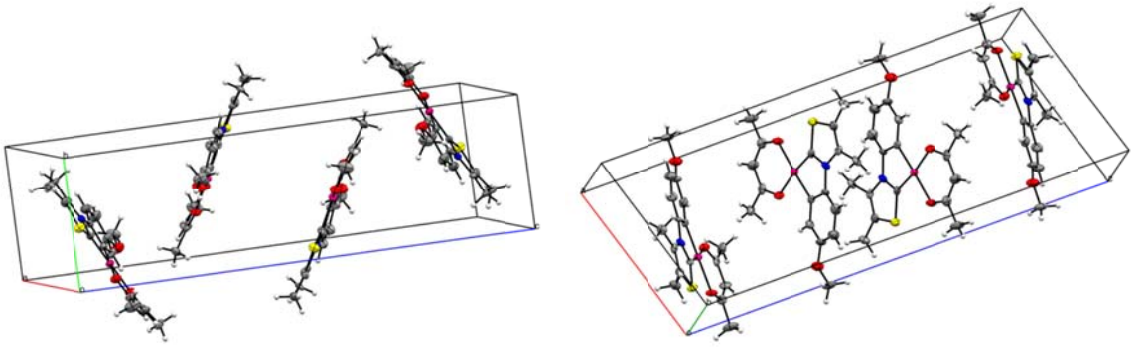


Figure S8. Orientation of **27** in the solid state.

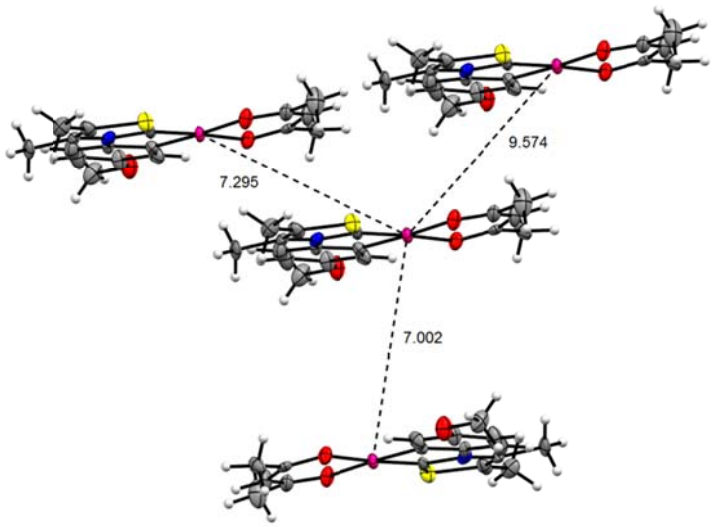


Figure S9. Orientation of **27** in the solid state with highlighted Pt…Pt-distances (in Å).

Photoluminescence Data

In the following section additional photophysical data for the complexes **25**–**31** are given.

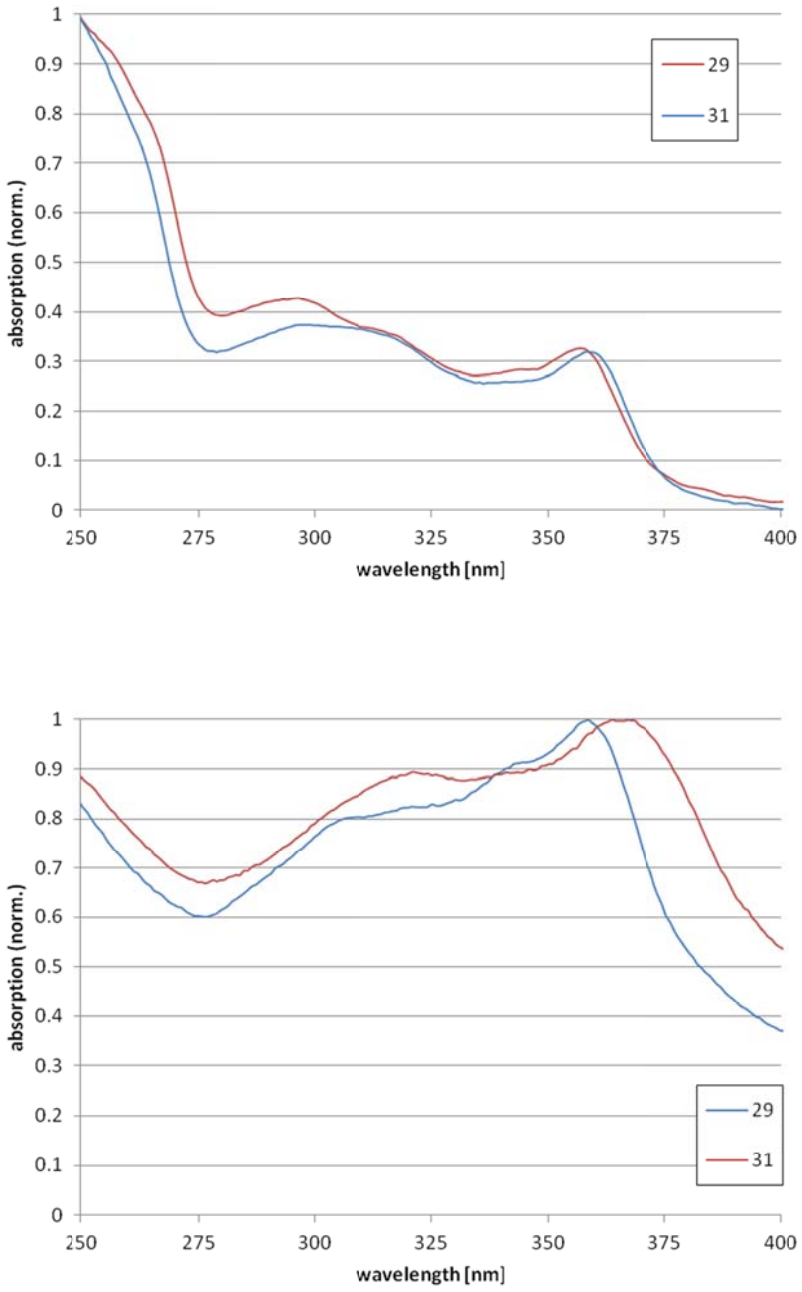


Figure S10. Comparison of absorption spectra of complexes **29** and **31** at room temperature (top: 2 wt % in PMMA; bottom: 100 % film).

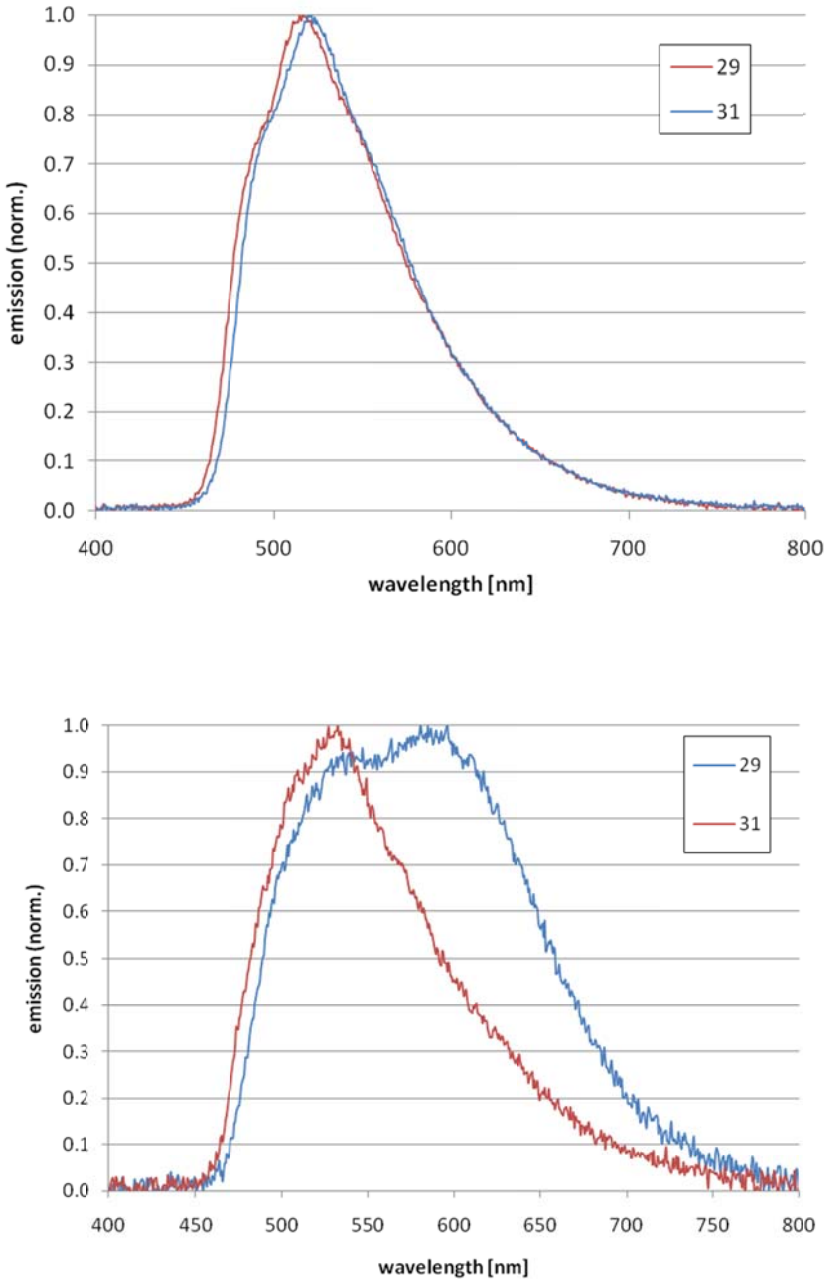


Figure S11. Comparison of emission spectra of complexes **29** and **31** at room temperature (top: 2 wt % in PMMA; bottom: 100 % film).

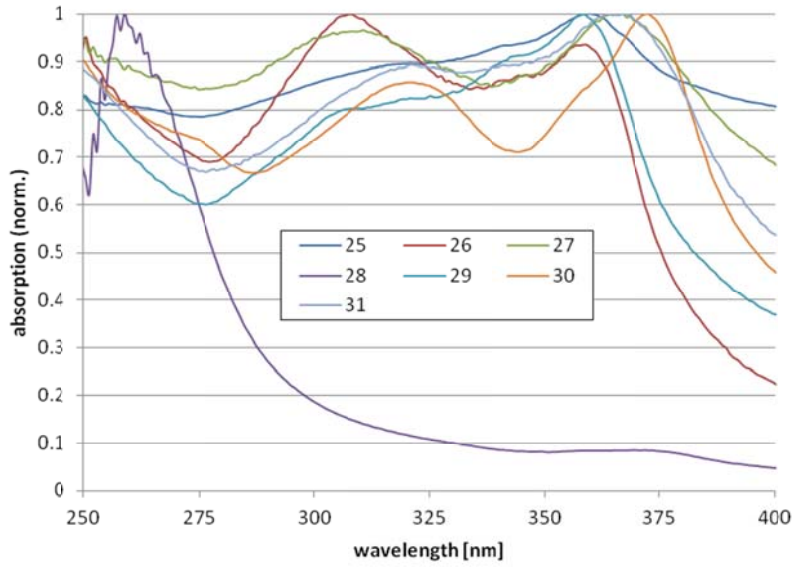


Figure S12. Absorption spectra for **25**–**31** as 100 % emitter films.

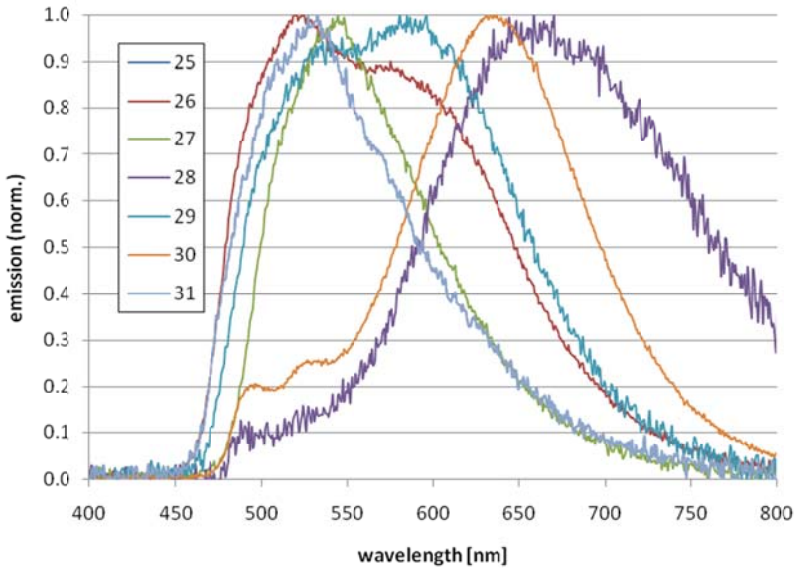


Figure S13. Emission spectra for **25**–**31** as 100 % emitter films.

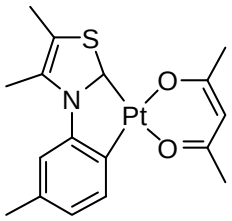
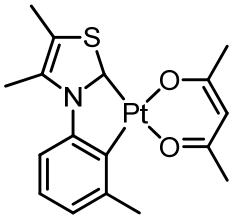
Table S3. Photoluminescence Data (100 % film, room temperature) of the complexes **25**–**31**.

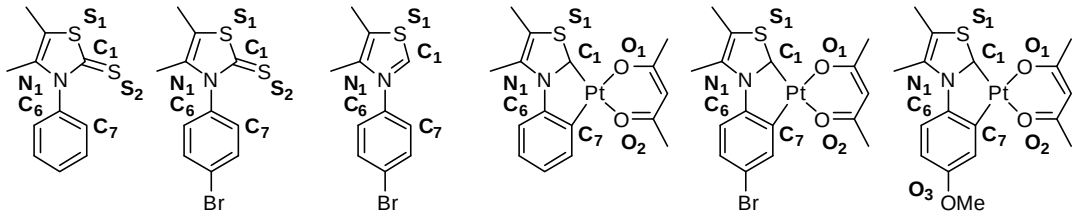
	λ_{exc} (nm)[a]	CIE x;y[b]	λ_{em} (nm)[c]	ϕ[d]	τ_0(μs)[e]	k_r (10^3 s^{-1})[f]	k_{nr} (10^3 s^{-1})[g]
25	370	0.35;0.54	531	0.14	7.93	123.9	971.8
26	360	0.40;0.51	523	0.40	7.13	140.8	1704.0
27	360	0.39;0.56	544	0.17	19.99	49.7	2838.6
28	370	0.58;0.42	666	0.25	6.45	157.2	1192.5
29	360	0.43;0.51	583	0.26	8.04	125.0	1539.2
30	370	0.54;0.43	634	0.68	3.58	277.6	784.0
31	360	0.35;0.56	534	0.29	10.35	97.0	2122.9

[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 $\tau_0 = \tau_v/\varphi$. [f]$k_r = \varphi/\tau_v$. [g]$k_{nr} = (1 - \varphi)/\tau_v$.

Quantum Chemical Calculations

Table S4. Calculated free energy differences (B3LYP/6-31G(d)) for the two possible isomers of complex **31**.

Compound **31**	**structure a** **5-Me**	**structure b** **3-Me**	Free energy difference (**a**-**b**)
	Free energy: -1381.591005 Hartree 	Free energy: -1381.584590 Hartree 	$-6.415 \cdot 10^{-3}$ Hartree - 4.0 kcal/mol



8 **9** **18** **25** **26** **27**

Table S5. Comparison of bond lengths, angles and dihedral angles of **8** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and B3LYP/6-311++G(d,p)).

		DFT	
Bond [Å]/Angles [°]	**X-ray**	**B3LYP/6-31G(d)**	**B3LYP/6-311++G(d,p)**
S(1)-C(1)	1.718(6)	1.766	1.764
C(1)-S(2)	1.662(6)	1.661	1.659
C(1)-N(1)	1.357(7)	1.379	1.377
N(1)-C(6)	1.434(7)	1.441	1.441
S(1)-C(1)-S(2)	124.2(4)	124.8	124.7
S(1)-C(1)-N(1)	108.5(4)	107.4	107.4
N(1)-C(1)-S(2)	127.3(4)	127.9	127.9
C(7)-C(6)-N(1)-C(1)	-74.1(7)	-90.4	-90.1
C(6)-N(1)-C(1)-S(2)	-1.9(8)	0.0	0.0

Table S6. Comparison of bond lengths, angles and dihedral angles of **9** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and B3LYP/6-311++G(d,p)).

		DFT	
Bond [Å]/Angles [°]	**X-ray**	**B3LYP/6-31G(d)**	**B3LYP/6-311++G(d,p)**
S(1)-C(1)	1.726(10)	1.765	1.763
C(1)-S(2)	1.663(9)	1.660	1.659
C(1)-N(1)	1.363(12)	1.380	1.378
N(1)-C(6)	1.458(12)	1.439	1.439
S(1)-C(1)-S(2)	124.4(6)	124.9	124.8
S(1)-C(1)-N(1)	107.9(6)	107.3	107.4
N(1)-C(1)-S(2)	127.7(7)	127.7	127.7
C(7)-C(6)-N(1)-C(1)	-79.3(12)	-90.4	-90.1
C(6)-N(1)-C(1)-S(2)	6.0(13)	0.0	0.0

Table S7. Comparison of bond lengths, angles and dihedral angles of **18** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and B3LYP/6-311++G(d,p)).

		DFT	
Bond [Å]/Angles [°]	**X-ray**	**B3LYP/6-31G(d)**	**B3LYP/6-311++G(d,p)**
S(1)-C(1)	1.657(8)	1.692	1.670
C(1)-N(1)	1.320(9)	1.330	1.327
N(1)-C(6)	1.446(9)	1.456	1.457
S(1)-C(1)-N(1)	112.2(5)	112.4	112.4
C(7)-C(6)-N(1)-C(1)	-95.6(7)	-89.8	-90.3
C(6)-N(1)-C(1)-S(1)	178.3(4)	180.0	179.8

Table S8. Comparison of bond lengths, angles and dihedral angles of **25** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and BP86/6-31G(d)).

		DFT			
		B3LYP/6-31G(d)		**BP86/6-31G(d)**	
Bond [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.690(5)	1.721	1.750	1.733	1.762
C(1)-N(1)	1.352(6)	1.360	1.458	1.358	1.456
N(1)-C(6)	1.442(5)	1.449	1.367	1.448	1.379
Pt(1)-C(1)	1.907(5)	1.928	1.932	1.920	1.923
Pt(1)-C(7)	1.967(4)	1.994	1.947	1.992	1.980
Pt(1)-O(1)	2.082(3)	2.140	2.131	2.134	2.133
Pt(1)-O(2)	2.052(3)	2.092	2.132	2.091	2.126
S(1)-C(1)-N(1)	109.2(3)	109.9	109.3	109.6	109.6
O(1)-Pt(1)-O(2)	90.61(13)	89.1	88.9	90.3	90.2
C(1)-Pt(1)-C(7)	79.4(2)	79.5	80.7	79.8	80.9
Pt(1)-C(1)-N(1)-C(6)	-2.8(5)	0.0	-5.8	0.0	0.0
N(1)-C(1)-Pt(1)-O(1)	179.4(4)	180.0	-175.0	180.0	180.0

Table S9. Comparison of bond lengths, angles and dihedral angles of **26** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and BP86/6-31G(d)).

		DFT			
		B3LYP/6-31G(d)		**BP86/6-31G(d)**	
Bond [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.696(15)	1.720	1.756	1.732	1.761
C(1)-N(1)	1.343(16)	1.361	1.456	1.378	1.457
N(1)-C(6)	1.429(17)	1.446	1.364	1.446	1.376
Pt(1)-C(1)	1.907(11)	1.930	1.930	1.922	1.921
Pt(1)-C(7)	1.957(13)	1.992	1.949	1.989	1.954
Pt(1)-O(1)	2.076(8)	2.134	2.128	2.131	2.133
Pt(1)-O(2)	2.041(8)	2.090	2.124	2.087	2.118
S(1)-C(1)-N(1)	108.5(8)	109.9	109.5	109.6	109.6
O(1)-Pt(1)-O(2)	90.7(3)	89.4	89.2	90.7	90.6
C(1)-Pt(1)-C(7)	79.9(5)	79.5	80.6	79.8	80.9
Pt(1)-C(1)-N(1)-C(6)	0.3(14)	0.0	0.0	0.0	0.0
N(1)-C(1)-Pt(1)-O(1)	179.9(9)	180.0	180.0	180.0	180.0

Table S10. Comparison of bond lengths, angles and dihedral angles of **27** from the solid-state determination and DFT calculations (B3LYP/6-31G(d) and BP86/6-31G(d)).

		DFT			
		B3LYP/6-31G(d)		**BP86/6-31G(d)**	
Bond [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**	**Singlet**	**Triplet**
S(1)-C(1)	1.724(11)	1.721	1.775	1.734	1.782
C(1)-N(1)	1.363(15)	1.360	1.477	1.376	1.474
N(1)-C(6)	1.460(14)	1.447	1.370	1.446	1.381
Pt(1)-C(1)	1.905(11)	1.929	1.927	1.922	1.920
Pt(1)-C(7)	2.002(11)	1.994	1.964	1.991	1.967
Pt(1)-O(1)	2.090(8)	2.138	2.138	2.136	2.145
Pt(1)-O(2)	2.044(7)	2.091	2.127	2.089	2.116
S(1)-C(1)-N(1)	108.4(8)	109.9	108.4	109.6	108.6
O(1)-Pt(1)-O(2)	91.4(3)	89.2	89.0	90.5	90.4
C(1)-Pt(1)-C(7)	79.9(5)	79.6	80.9	79.9	81.0
Pt(1)-C(1)-N(1)-C(6)	-1.6(12)	0.0	-11.1	0.0	-11.0
N(1)-C(1)-Pt(1)-O(1)	178.3(8)	180.0	-171.1	180.0	-171.3

Table S11. Comparison of bond lengths, angles and dihedral angles of **25–27** from the solid-state determination and DFT calculations (B3LYP/6-311++G(d,p)).

	complex 25		**complex 26**		**complex 27**	
Bond [Å]/Angles [°]	**X-ray**	**DFT**	**X-ray**	**DFT**	**X-ray**	**DFT**
S(1)-C(1)	1.690(5)	1.719	1.696(15)	1.718	1.724(11)	1.720
C(1)-N(1)	1.352(6)	1.358	1.343(16)	1.359	1.363(15)	1.357
N(1)-C(6)	1.442(5)	1.448	1.429(17)	1.445	1.460(14)	1.446
Pt(1)-C(1)	1.907(5)	1.925	1.907(11)	1.927	1.905(11)	1.927
Pt(1)-C(7)	1.967(4)	1.992	1.957(13)	1.990	2.002(11)	1.992
Pt(1)-O(1)	2.082(3)	2.147	2.076(8)	2.140	2.090(8)	2.144
Pt(1)-O(2)	2.052(3)	2.105	2.041(8)	2.102	2.044(7)	2.103
S(1)-C(1)-N(1)	109.2(3)	110.0	108.5(8)	109.9	108.4(8)	110.0
O(1)-Pt(1)-O(2)	90.61(13)	88.2	90.7(3)	88.6	91.4(3)	88.4
C(1)-Pt(1)-C(7)	79.4(2)	79.5	79.9(5)	79.5	79.9(5)	79.6
Pt(1)-C(1)-N(1)-C(6)	-2.8(5)	0.0	0.3(14)	0.0	-1.6(12)	0.0
N(1)-C(1)-Pt(1)-O(1)	179.4(4)	180.0	179.9(9)	180.0	178.3(8)	180.0

Table S12. Summary of the prediction of wavelength maxima using the procedure described by Unger and Straßner (BP86/6-31G(d)).[1]

complex	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]
25	2.177	569.4	2.568	482.8	510	26.7
26	2.168	572.0	2.558	484.6	508	23.3
27	2.055	603.4	2.443	507.5	526	18.5
28	2.122	584.3	2.511	493.7	515	21.3
29	2.138	579.9	2.528	490.5	516	25.5
30	2.098	591.1	2.487	498.6	520	21.4
31	2.504	586.4	2.504	495.2	521	26.2
					average	**23.3**

[a] $\Delta\lambda_{max}$= (λ_{max} exp. – λ_{max} corr.)

Table S13. Summary of the prediction of wavelength maxima using the procedure described by Unger and Straßner (B3LYP/6-31G(d)).[1]

complex	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]
25	2.184	567.7	2.478	500.3	510	9.2
26	2.235	554.8	2.527	490.6	508	17.3
27	2.071	598.7	2.369	523.4	526	2.6
28	2.240	553.5	2.532	489.6	515	25.4
29	2.160	574.1	2.455	505.1	516	10.9
30	2.212	560.5	2.505	494.9	520	25.1
31	2.162	573.6	2.456	504.7	521	16.7
					average	**15.3**

[a] $\Delta\lambda_{max}$= (λ_{max} exp. – λ_{max} corr.)

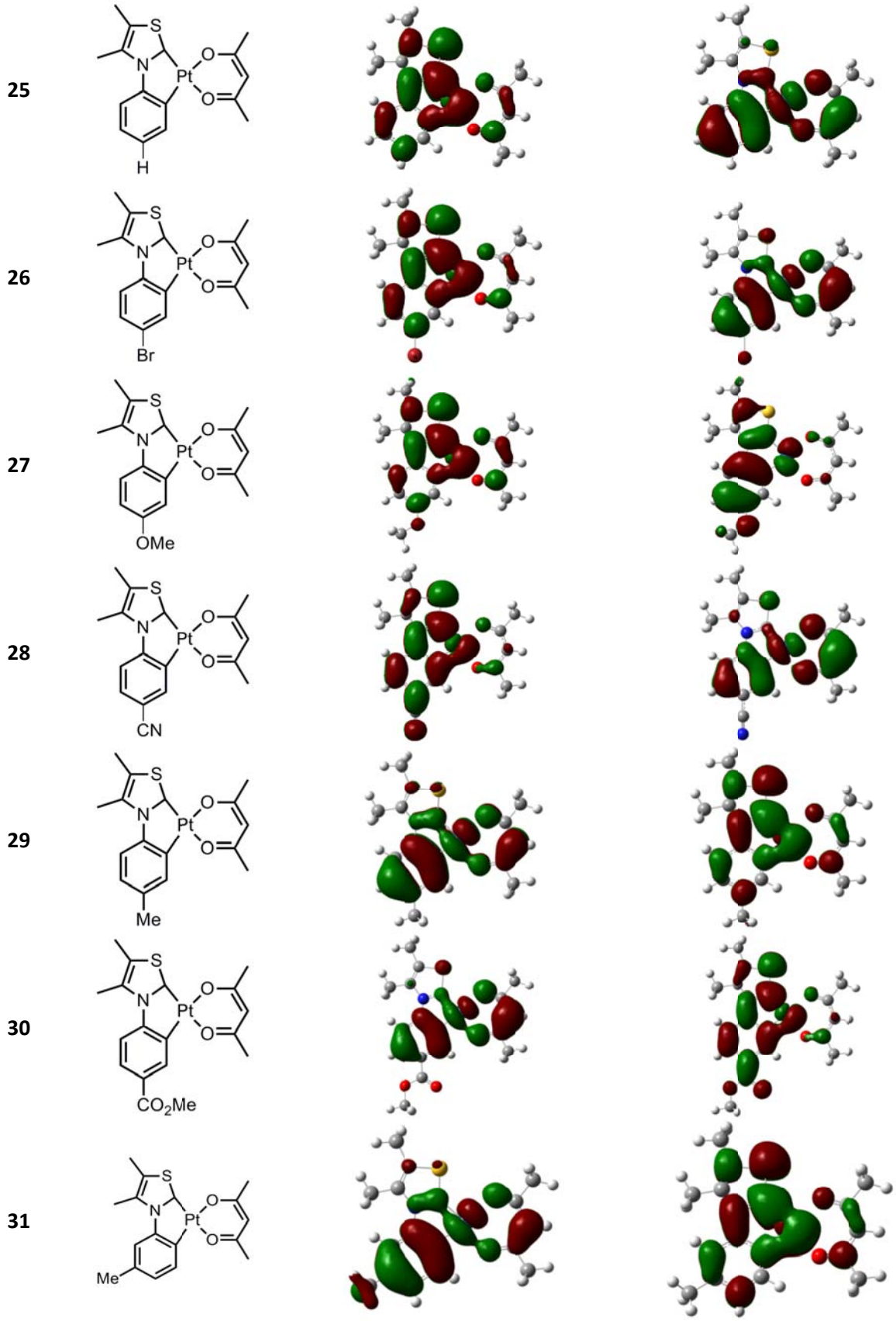


Figure S14. FMOs (left: LUMO; right HOMO) of the calculated singlet ground state structures (isovalue=0.02, B3LYP/6-31G(d)).

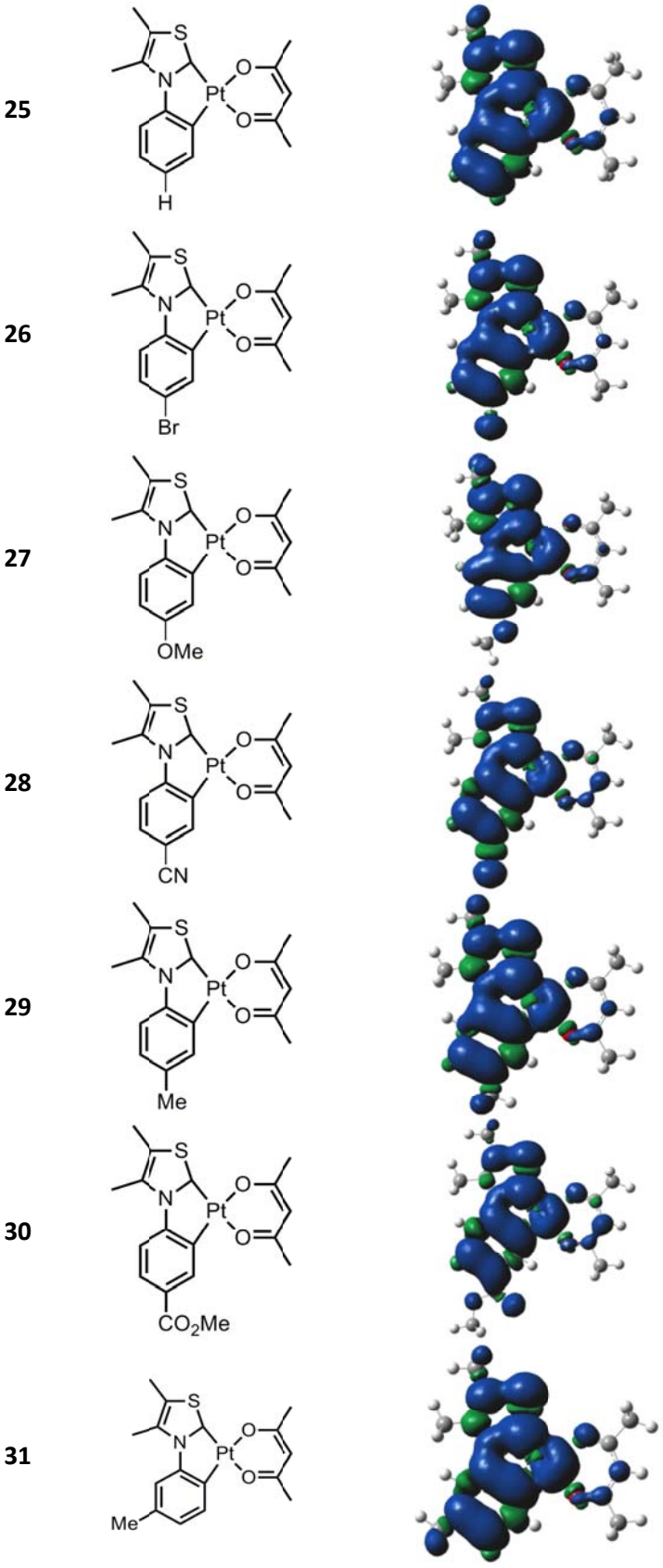


Figure S15. Spin densities of the calculated triplet ground state structures (isovalue=0.02, B3LYP/ 6-31G(d)).

In the following section the coordinates of the singlet ground state structure geometries for **25**–**31** are given (B3LYP/6-31G(d)).

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

C	0.10732	3.01851	0.00016
C	1.03519	4.06485	0.00032
C	2.40119	3.78802	0.00035
C	2.85587	2.46534	0.00028
C	1.91861	1.43168	0.00020
C	0.52797	1.68663	0.00006
H	-0.95779	3.22994	0.00010
H	0.69042	5.09605	0.00039
C	1.08931	-0.75868	-0.00037
C	3.43231	-0.69643	0.00045
C	3.23900	-2.04462	0.00014
N	2.20989	0.01249	0.00010
Pt	-0.64802	0.07649	-0.00044
C	-3.04914	-1.80961	0.00014
C	-3.61710	0.64052	0.00034
O	-1.77689	-1.74207	-0.00017
O	-2.44275	1.15177	-0.00000
C	-3.60593	-3.22054	0.00022
H	-4.69857	-3.24357	0.00074
H	-3.23673	-3.75689	-0.88147
H	-3.23585	-3.75715	0.88137
C	-4.73291	1.66623	0.00074
H	-4.63500	2.31047	-0.88063
H	-5.72546	1.20910	0.00096
H	-4.63452	2.31029	0.88219
C	-3.94657	-0.72365	0.00040
H	-5.00272	-0.96660	0.00070
H	3.12715	4.59638	0.00042
H	3.92034	2.28505	0.00024
S	1.52297	-2.42397	-0.00018
C	4.76472	-0.00994	0.00109
H	4.89985	0.61817	-0.88598
H	4.89890	0.61830	0.88821
H	5.56318	-0.75380	0.00157
C	4.24231	-3.15965	0.00025
H	5.26663	-2.77898	0.00021
H	4.12642	-3.79829	0.88435
H	4.12643	-3.79846	-0.88372

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

C	2.22153	-0.36319	0.00003
C	3.40619	0.37299	-0.00010
C	3.40014	1.76423	-0.00022
C	2.17889	2.44496	-0.00020
C	0.99138	1.71396	-0.00006
C	0.99272	0.29990	0.00004
H	2.24343	-1.44690	0.00011
C	-1.31160	1.29136	0.00001
C	-0.82493	3.58564	-0.00004

C	-2.18564	3.63910	-0.00005
N	-0.34978	2.25458	-0.00003
Pt	-0.79942	-0.56898	0.00018
C	-3.07191	-2.59656	-0.00026
C	-0.75930	-3.58691	-0.00001
O	-2.78310	-1.35455	0.00020
O	-0.05022	-2.51955	0.00034
C	-4.55821	-2.89640	-0.00079
H	-4.77241	-3.96794	-0.00065
H	-5.02184	-2.43820	0.88035
H	-5.02110	-2.43862	-0.88253
C	0.05451	-4.86455	0.00016
H	0.70427	-4.88182	0.88267
H	-0.57010	-5.76109	-0.00190
H	0.70767	-4.87993	-0.87983
C	-2.16033	-3.67006	-0.00035
H	-2.58517	-4.66695	-0.00072
H	4.33084	2.31951	-0.00032
H	2.20083	3.52427	-0.00029
S	-2.86944	2.01990	0.00003
C	0.09326	4.77035	-0.00005
H	0.73519	4.78854	0.88741
H	0.73516	4.78858	-0.88753
H	-0.49233	5.69106	-0.00001
C	-3.09964	4.82834	-0.00003
H	-2.53846	5.76598	-0.00084
H	-3.74918	4.83013	-0.88368
H	-3.74811	4.83097	0.88441
Br	5.08629	-0.54810	-0.00011

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

C	-1.30940	-2.26702	0.00014
C	-2.63351	-2.73713	-0.00027
C	-3.69688	-1.83025	-0.00072
C	-3.43832	-0.45297	-0.00067
C	-2.12410	0.00161	-0.00011
C	-1.03428	-0.90583	0.00017
H	-0.49897	-2.98860	0.00036
C	-0.33037	1.50658	-0.00026
C	-2.40518	2.59398	0.00046
C	-1.57981	3.67776	0.00040
N	-1.68427	1.37986	-0.00006
Pt	0.77729	-0.07319	-0.00006
C	3.79093	0.39781	-0.00083
C	3.08780	-2.01760	0.00105
O	2.64841	0.96218	-0.00108
O	1.81383	-1.88912	0.00107
C	4.96664	1.35620	-0.00176
H	5.93105	0.84218	-0.00150
H	4.90654	2.00432	-0.88364
H	4.90680	2.00570	0.87913
C	3.55928	-3.45794	0.00212
H	3.15800	-3.97235	-0.87860
H	4.64860	-3.54500	0.00199

H	3.15832	-3.97094	0.88380
C	4.04229	-0.98813	0.00018
H	5.08237	-1.29285	0.00028
H	-4.72650	-2.16755	-0.00113
H	-4.28615	0.21603	-0.00117
S	0.10277	3.17296	-0.00010
C	-3.90321	2.63971	0.00119
H	-4.32515	2.15529	-0.88609
H	-4.32422	2.15348	0.88791
H	-4.24210	3.67699	0.00240
C	-1.91629	5.13950	0.00073
H	-2.99690	5.30208	0.00111
H	-1.50543	5.64240	0.88460
H	-1.50606	5.64264	-0.88330
O	-2.77741	-4.09594	-0.00024
C	-4.08776	-4.63265	-0.00090
H	-3.96886	-5.71805	-0.00086
H	-4.65052	-4.33098	0.89326
H	-4.64962	-4.33095	-0.89560

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

C	0.33436	2.68272	0.00019
C	1.36088	3.64502	0.00026
C	2.70330	3.23897	0.00021
C	3.02525	1.88266	0.00012
C	1.99581	0.93911	0.00011
C	0.63354	1.32212	0.00009
H	-0.70364	2.99842	0.00019
C	0.96549	-1.16263	-0.00009
C	3.30885	-1.31390	0.00013
C	2.99085	-2.63747	0.00001
N	2.15455	-0.49561	0.00004
Pt	-0.68677	-0.16811	-0.00016
C	-3.25582	-1.80017	-0.00027
C	-3.57855	0.69388	0.00019
O	-1.98143	-1.85968	-0.00034
O	-2.35692	1.08312	0.00022
C	-3.94730	-3.14902	-0.00045
H	-5.03667	-3.06441	-0.00046
H	-3.63216	-3.71903	-0.88196
H	-3.63221	-3.71922	0.88096
C	-4.58331	1.82672	0.00045
H	-4.42019	2.45784	-0.88061
H	-5.61677	1.47219	0.00041
H	-4.42015	2.45750	0.88175
C	-4.04058	-0.63108	-0.00004
H	-5.11544	-0.76837	-0.00001
H	3.49380	3.98186	0.00023
H	4.06822	1.60605	0.00005
S	1.24640	-2.85794	-0.00019
C	4.69919	-0.75325	0.00042
H	4.89307	-0.14170	-0.88742
H	4.89262	-0.14155	0.88826
H	5.42480	-1.56812	0.00068

C	3.88653	-3.84052	0.00007
H	4.94144	-3.55596	-0.00035
H	3.71174	-4.46492	0.88443
H	3.71119	-4.46538	-0.88385
C	1.03914	5.04258	0.00038
N	0.78079	6.17732	0.00048

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

C	-0.23669	2.81440	-0.00007
C	-1.20291	3.83462	-0.00232
C	-2.55156	3.47113	-0.00600
C	-2.94548	2.12850	-0.00518
C	-1.96517	1.13893	-0.00120
C	-0.58909	1.46631	0.00051
H	0.81912	3.07355	0.00050
C	-1.02592	-1.00581	-0.00019
C	-3.36908	-1.06029	0.00042
C	-3.10947	-2.39734	0.00111
N	-2.18379	-0.29204	-0.00069
Pt	0.66703	-0.08299	0.00040
C	3.16478	-1.84287	-0.00118
C	3.60503	0.63353	0.00038
O	1.89101	-1.84171	-0.00070
O	2.40611	1.08370	0.00107
C	3.79468	-3.22282	-0.00255
H	4.88701	-3.18852	-0.00258
H	3.45373	-3.77886	0.87830
H	3.45367	-3.77709	-0.88449
C	4.66690	1.71522	0.00050
H	4.53521	2.35405	0.88136
H	5.68159	1.30949	0.00151
H	4.53664	2.35278	-0.88153
C	4.00478	-0.71172	-0.00063
H	5.07214	-0.89944	-0.00114
H	-3.31839	4.24194	-0.00982
H	-4.00153	1.90321	-0.00908
S	-1.37682	-2.69109	0.00069
C	-4.73266	-0.43810	0.00142
H	-4.89434	0.18613	0.88680
H	-4.89829	0.18083	-0.88697
H	-5.49513	-1.21884	0.00536
C	-4.05755	-3.55966	0.00172
H	-5.09898	-3.22851	0.00776
H	-3.91536	-4.18927	-0.88503
H	-3.90699	-4.19495	0.88297
C	-0.78355	5.28664	0.00502
H	-0.10332	5.50969	-0.82615
H	-1.64672	5.95518	-0.07909
H	-0.25198	5.54351	0.93038

Optimized singlet ground state structure of **30**.

C	-2.20701	-0.47713	-0.00002
C	-3.44331	0.18729	0.00002
C	-3.48032	1.58645	0.00001
C	-2.29641	2.32400	-0.00002
C	-1.07515	1.64595	-0.00009
C	-1.00819	0.23305	-0.00005
H	-2.19172	-1.56163	0.00001
C	1.24466	1.33431	0.00010
C	0.64789	3.60457	-0.00029
C	2.00417	3.72263	-0.00022
N	0.23644	2.25156	-0.00006
Pt	0.82575	-0.54647	0.00007
C	3.19462	-2.46718	0.00028
C	0.93136	-3.56424	-0.00047
O	2.84752	-1.24009	0.00048
O	0.17468	-2.53068	-0.00017
C	4.69374	-2.69582	0.00059
H	4.95965	-3.75582	0.00043
H	5.13474	-2.21591	-0.88062
H	5.13430	-2.21630	0.88224
C	0.17594	-4.87702	-0.00100
H	-0.47488	-4.92126	-0.88164
H	0.84005	-5.74479	-0.00135
H	-0.47489	-4.92200	0.87961
C	2.33511	-3.58242	-0.00021
H	2.80619	-4.55835	-0.00041
H	-4.43349	2.10197	0.00004
H	-2.36338	3.40121	0.00008
S	2.76538	2.13747	-0.00001
C	-0.32437	4.74555	-0.00044
H	-0.96668	4.73365	-0.88763
H	-0.96648	4.73402	0.88691
H	0.21790	5.69245	-0.00067
C	2.86205	4.95288	-0.00001
H	2.25868	5.86380	-0.00349
H	3.50784	4.98637	0.88579
H	3.51283	4.98304	-0.88224
C	-4.68256	-0.63779	0.00009
O	-4.70927	-1.85317	0.00032
O	-5.80978	0.11877	-0.00003
C	-7.03737	-0.62084	0.00036
H	-7.10639	-1.25441	0.88910
H	-7.83088	0.12773	0.00104
H	-7.10740	-1.25376	-0.88878

Optimized singlet ground state structure of **31**.

C	-0.66762	2.76856	-0.00443
C	-1.81885	3.56025	-0.01200
C	-3.09281	2.98350	-0.01202
C	-3.19776	1.58451	-0.01030
C	-2.04297	0.80189	-0.00100

C	-0.75260	1.37512	0.00131
H	0.31375	3.23354	-0.00790
H	-1.72519	4.64454	-0.02003
C	-0.72169	-1.13193	-0.00160
C	-3.01361	-1.62351	0.00096
C	-2.50821	-2.88827	0.00050
N	-1.99277	-0.64642	-0.00154
Pt	0.77088	0.08857	0.00036
C	3.54781	-1.17552	-0.00060
C	3.52013	1.33996	0.00298
O	2.29582	-1.41140	-0.00116
O	2.25830	1.55948	0.00291
C	4.42334	-2.41416	-0.00244
H	5.49021	-2.17725	-0.00072
H	4.19067	-3.02508	0.87731
H	4.19272	-3.02097	-0.88559
C	4.36260	2.59989	0.00502
H	4.11555	3.20128	0.88748
H	5.43493	2.38956	0.00462
H	4.11545	3.20421	-0.87539
C	4.16259	0.09216	0.00141
H	-4.18695	1.15044	-0.01763
S	-0.75126	-2.85280	-0.00138
C	-4.47067	-1.27120	0.00557
H	-4.74483	-0.68552	0.88952
H	-4.75445	-0.69885	-0.88416
H	-5.07062	-2.18270	0.01558
C	-3.22132	-4.20779	0.00162
H	-4.30638	-4.07830	0.00439
H	-2.96114	-4.80104	-0.88345
H	-2.95653	-4.80220	0.88452
H	5.24625	0.10591	0.00169
C	-4.33835	3.84104	0.01336
H	-5.19376	3.32507	-0.43719
H	-4.62412	4.10800	1.04022
H	-4.18800	4.77872	-0.53283

In the following section the coordinates of the triplet state structure geometries for **25**–**31** are given (B3LYP/6-31G(d)).

Optimized triplet state structure of **25**.

C	0.03760	2.98152	0.03447
C	0.92841	4.03834	0.03486
C	2.32882	3.78636	-0.01333
C	2.83621	2.50602	-0.05021
C	1.93607	1.40546	-0.03264
C	0.49064	1.64589	-0.00094
H	-1.03360	3.15457	0.05998
H	0.57110	5.06369	0.06578
C	1.08033	-0.79128	-0.14378
C	3.46215	-0.62416	0.01537
C	3.28538	-1.97879	0.04821
N	2.25011	0.07499	-0.05551
Pt	-0.64748	0.06666	-0.03474
C	-3.04503	-1.81854	-0.00438
C	-3.64233	0.62734	0.06928
O	-1.77088	-1.74515	-0.04488
O	-2.48051	1.15329	0.04133
C	-3.58633	-3.23488	-0.01820
H	-4.67800	-3.27162	0.01699
H	-3.23841	-3.74643	-0.92292
H	-3.18024	-3.78592	0.83778
C	-4.77756	1.63111	0.13180
H	-4.71789	2.30208	-0.73289
H	-5.76137	1.15583	0.14794
H	-4.66498	2.25115	1.02875
C	-3.95221	-0.74572	0.04938
H	-5.00446	-1.00328	0.07883
H	3.01953	4.62543	-0.02700
H	3.90548	2.36740	-0.10045
S	1.58854	-2.47012	-0.00313
C	4.78653	0.07685	0.07409
H	4.97297	0.67190	-0.82752
H	4.85268	0.74411	0.94107
H	5.59492	-0.65063	0.15810
C	4.32247	-3.05479	0.13553
H	5.33645	-2.65400	0.20165
H	4.15040	-3.68542	1.01704
H	4.27547	-3.71088	-0.74303

Optimized triplet state structure of **26**.

C	2.19363	-0.35086	0.00002
C	3.36500	0.38227	-0.00006
C	3.34757	1.80713	-0.00021
C	2.15843	2.49599	-0.00021
C	0.93061	1.77290	-0.00004
C	0.95083	0.30532	0.00001
H	2.21037	-1.43474	0.00007

C	-1.36972	1.26072	0.00001
C	-0.83889	3.59316	0.00013
C	-2.20458	3.62668	-0.00003
N	-0.33390	2.28385	0.00005
Pt	-0.78658	-0.57859	0.00001
C	-3.00700	-2.65950	-0.00006
C	-0.67681	-3.61699	0.00004
O	-2.74586	-1.40923	-0.00002
O	0.01645	-2.54507	0.00005
C	-4.48786	-2.98427	-0.00001
H	-4.68480	-4.05910	-0.00100
H	-4.95762	-2.53355	0.88174
H	-4.95809	-2.53175	-0.88056
C	0.14740	-4.88927	0.00015
H	0.79879	-4.90044	0.88164
H	-0.46950	-5.79116	0.00020
H	0.79883	-4.90056	-0.88130
C	-2.08054	-3.71719	-0.00004
H	-2.49177	-4.71976	-0.00006
H	4.28720	2.34830	-0.00035
H	2.18789	3.57474	-0.00040
S	-2.94904	2.02518	-0.00024
C	0.05721	4.79531	0.00044
H	0.70016	4.82301	0.88790
H	0.69989	4.82374	-0.88719
H	-0.53895	5.70867	0.00091
C	-3.10897	4.81975	-0.00000
H	-2.55714	5.76236	-0.00004
H	-3.76122	4.80997	-0.88239
H	-3.76118	4.80998	0.88242
Br	5.05572	-0.49319	-0.00001

Optimized triplet state structure of **27**.

C	1.16590	2.30729	0.01053
C	2.45349	2.85259	0.00072
C	3.58864	2.00078	-0.07682
C	3.43541	0.63000	-0.12066
C	2.13349	0.06294	-0.07858
C	0.96380	0.93156	-0.03227
H	0.31192	2.97537	0.05178
C	0.36600	-1.51079	-0.25477
C	2.56645	-2.42911	0.04587
C	1.79221	-3.56175	0.08800
N	1.81433	-1.26919	-0.09867
Pt	-0.77992	0.02671	-0.06172
C	-3.77207	-0.56304	0.00364
C	-3.18571	1.88396	0.12958
O	-2.60921	-1.07948	-0.06968
O	-1.91134	1.82291	0.07847
C	-4.90441	-1.57278	-0.01596
H	-5.89011	-1.10547	0.05128
H	-4.84852	-2.16164	-0.93872
H	-4.78071	-2.27224	0.81874

C	-3.73542	3.29356	0.24017
H	-3.38105	3.88999	-0.60837
H	-4.82771	3.32045	0.26491
H	-3.34550	3.76520	1.14978
C	-4.08788	0.80598	0.09689
H	-5.14107	1.05613	0.15060
H	4.58875	2.41677	-0.11388
H	4.31999	0.01709	-0.20718
S	0.06092	-3.24597	-0.04128
C	4.05870	-2.40037	0.19293
H	4.55291	-2.03238	-0.71429
H	4.36533	-1.76044	1.02839
H	4.44093	-3.40292	0.38884
C	2.23327	-4.98131	0.26010
H	3.31563	-5.07579	0.37397
H	1.75860	-5.42666	1.14400
H	1.93113	-5.58687	-0.60409
O	2.53401	4.20637	0.05890
C	3.80999	4.83066	0.05046
H	3.61560	5.90255	0.11325
H	4.41590	4.52169	0.91186
H	4.35785	4.61653	-0.87621

Optimized triplet state structure of **28**.

C	0.17830	2.67051	0.00025
C	1.14048	3.68342	0.00042
C	2.54493	3.32436	0.00046
C	2.96034	2.01973	0.00035
C	1.98912	0.97682	0.00018
C	0.54770	1.32095	0.00011
H	-0.87765	2.91921	0.00021
C	1.00590	-1.14756	-0.00013
C	3.38564	-1.15194	0.00008
C	3.12139	-2.48667	-0.00009
N	2.20228	-0.37245	0.00005
Pt	-0.67543	-0.18906	-0.00018
C	-3.17205	-1.92808	-0.00009
C	-3.62432	0.54890	-0.00004
O	-1.89225	-1.92650	-0.00014
O	-2.43091	1.00105	-0.00008
C	-3.79042	-3.31107	-0.00009
H	-4.88272	-3.28505	-0.00008
H	-3.44395	-3.86306	-0.88128
H	-3.44394	-3.86306	0.88110
C	-4.69493	1.62059	0.00004
H	-4.56896	2.25997	-0.88117
H	-5.70578	1.20601	0.00007
H	-4.56888	2.25991	0.88128
C	-4.01453	-0.80471	-0.00005
H	-5.08051	-0.99870	-0.00001
H	3.28111	4.12192	0.00059
H	4.01970	1.81466	0.00038
S	1.39349	-2.84217	-0.00028

C	4.74999	-0.53146	0.00030
H	4.91675	0.08911	-0.88753
H	4.91654	0.08895	0.88828
H	5.51297	-1.31113	0.00032
C	4.08226	-3.63641	-0.00009
H	5.12280	-3.30419	-0.00028
H	3.93137	-4.26907	0.88313
H	3.93111	-4.26928	-0.88311
C	0.77295	5.05438	0.00056
N	0.48574	6.18647	0.00067

Optimized triplet state structure of **29**.

C	-0.13560	2.78651	0.01454
C	-1.05142	3.82732	0.01615
C	-2.44671	3.50153	-0.01331
C	-2.90730	2.20641	-0.03578
C	-1.96877	1.13705	-0.02536
C	-0.53378	1.43650	-0.00619
H	0.92981	2.99762	0.02974
C	-1.02970	-1.02348	-0.09762
C	-3.42021	-0.94713	0.00550
C	-3.19347	-2.29304	0.03651
N	-2.23230	-0.20236	-0.04003
Pt	0.66448	-0.10003	-0.02616
C	3.13530	-1.89098	0.00240
C	3.63634	0.57712	0.03991
O	1.85967	-1.86864	-0.02539
O	2.45463	1.05712	0.01844
C	3.73325	-3.28476	-0.00005
H	4.82584	-3.27688	0.02334
H	3.35909	-3.84078	0.86720
H	3.39670	-3.82150	-0.89443
C	4.73221	1.62534	0.07668
H	4.60298	2.25513	0.96455
H	5.73388	1.18871	0.09177
H	4.63982	2.27918	-0.79826
C	4.00025	-0.78236	0.03361
H	5.06215	-0.99770	0.05491
H	-3.17095	4.31334	-0.02171
H	-3.97200	2.03105	-0.06624
S	-1.47740	-2.71960	0.01279
C	-4.77047	-0.29533	0.03089
H	-4.89173	0.35403	0.90565
H	-4.94827	0.30767	-0.86715
H	-5.55346	-1.05353	0.07525
C	-4.19041	-3.40831	0.09565
H	-5.22011	-3.04655	0.14286
H	-4.10016	-4.05641	-0.78547
H	-4.01330	-4.03765	0.97706
C	-0.62436	5.27095	0.04527
H	0.46571	5.36249	0.05067
H	-1.00540	5.82002	-0.82669
H	-1.01053	5.78585	0.93584

Optimized triplet state structure of **30**.

C	-2.18548	-0.45117	-0.00006
C	-3.40429	0.21788	-0.00002
C	-3.40661	1.66198	0.00007
C	-2.24716	2.39833	0.00009
C	-0.99553	1.72652	0.00000
C	-0.96640	0.24521	-0.00005
H	-2.17313	-1.53579	-0.00011
C	1.30713	1.30911	0.00002
C	0.71758	3.61276	-0.00001
C	2.07504	3.69310	-0.00006
N	0.25984	2.27166	-0.00000
Pt	0.79815	-0.56068	-0.00006
C	3.10708	-2.54799	0.00006
C	0.82112	-3.60324	0.00006
O	2.78589	-1.30886	0.00004
O	0.08740	-2.56089	0.00003
C	4.60115	-2.80045	0.00010
H	4.85033	-3.86441	0.00012
H	5.04877	-2.32660	-0.88104
H	5.04872	-2.32659	0.88126
C	0.04937	-4.90699	0.00011
H	-0.60196	-4.94287	-0.88051
H	0.70222	-5.78315	0.00006
H	-0.60183	-4.94288	0.88083
C	2.23044	-3.64408	0.00007
H	2.68420	-4.62807	0.00009
H	-4.36183	2.17456	0.00014
H	-2.31825	3.47534	0.00017
S	2.85160	2.10776	-0.00007
C	-0.22724	4.77629	0.00007
H	-0.87055	4.77936	-0.88723
H	-0.87035	4.77939	0.88751
H	0.33388	5.71195	0.00002
C	2.94755	4.91133	0.00013
H	2.36436	5.83501	-0.00215
H	3.59648	4.92598	0.88447
H	3.59981	4.92379	-0.88177
C	-4.64905	-0.56922	-0.00004
O	-4.71174	-1.78710	-0.00009
O	-5.75965	0.22264	0.00005
C	-7.00509	-0.48386	0.00007
H	-7.09202	-1.11593	0.88855
H	-7.77958	0.28466	0.00030
H	-7.09223	-1.11560	-0.88863

Optimized triplet state structure of **31**.

C	0.54525	2.75715	0.00001
C	1.64664	3.58498	0.00005
C	2.97606	3.03885	0.00008

C	3.16608	1.67096	0.00002
C	2.04789	0.79621	-0.00003
C	0.68483	1.35152	0.00000
H	-0.45954	3.16787	-0.00001
H	1.52530	4.66535	0.00002
C	0.73377	-1.15318	-0.00020
C	3.09353	-1.52467	-0.00002
C	2.62522	-2.80326	0.00007
N	2.05617	-0.56995	-0.00011
Pt	-0.76939	0.06574	-0.00005
C	-3.52223	-1.24126	0.00002
C	-3.56379	1.27710	-0.00001
O	-2.26252	-1.45171	-0.00004
O	-2.31422	1.53127	0.00000
C	-4.36340	-2.50277	0.00021
H	-5.43649	-2.29587	-0.00034
H	-4.11298	-3.10522	-0.88049
H	-4.11377	-3.10442	0.88169
C	-4.44942	2.50841	0.00001
H	-4.22273	3.11936	-0.88140
H	-5.51413	2.26254	-0.00049
H	-4.22347	3.11880	0.88200
C	-4.17021	0.00622	0.00001
H	4.17798	1.29410	0.00002
S	0.85856	-2.89938	0.00002
C	4.54063	-1.13113	-0.00019
H	4.80291	-0.54329	-0.88737
H	4.80321	-0.54337	0.88696
H	5.17097	-2.02155	-0.00033
C	3.39721	-4.08655	0.00020
H	4.47726	-3.92206	0.00061
H	3.14833	-4.68950	0.88269
H	3.14896	-4.68935	-0.88257
H	-5.25380	-0.01142	0.00003
C	4.14924	3.98260	0.00021
H	5.10445	3.44909	0.00020
H	4.12496	4.63863	-0.88015
H	4.12487	4.63846	0.88070

In the following section the coordinates of the singlet ground state structure geometries for **25**–**31** are given (BP86/6-31G(d)).

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

C	0.08564	3.02503	-0.00028
C	1.01374	4.08165	-0.00086
C	2.38987	3.81122	-0.00135
C	2.85524	2.48402	-0.00113
C	1.91806	1.43914	-0.00036
C	0.51616	1.68774	-0.00010
H	-0.99000	3.23084	0.00001
H	0.66033	5.11959	-0.00101
C	1.08022	-0.75743	-0.00027
C	3.43971	-0.68705	0.00050
C	3.24560	-2.04796	0.00064
N	2.21449	0.02137	-0.00011
Pt	-0.65038	0.07353	-0.00007
C	-3.03988	-1.82417	-0.00086
C	-3.61794	0.64030	0.00119
O	-1.75442	-1.75590	-0.00112
O	-2.43421	1.16428	0.00115
C	-3.59453	-3.24045	-0.00194
H	-4.69600	-3.26449	-0.00136
H	-3.22363	-3.78224	-0.89050
H	-3.22263	-3.78398	0.88513
C	-4.73951	1.66574	0.00238
H	-4.64621	2.31749	-0.88492
H	-5.73793	1.20031	0.00227
H	-4.64570	2.31596	0.89075
C	-3.94120	-0.73251	0.00026
H	-5.00643	-0.98028	0.00038
H	3.11715	4.63048	-0.00193
H	3.93018	2.30577	-0.00168
S	1.52426	-2.43230	-0.00007
C	4.77381	0.00178	0.00126
H	4.91178	0.63472	-0.89344
H	4.91005	0.63582	0.89542
H	5.57955	-0.74806	0.00251
C	4.25444	-3.16106	0.00120
H	5.28507	-2.77061	0.00105
H	4.14331	-3.80593	0.89248
H	4.14342	-3.80669	-0.88953

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

C	2.22781	-0.34214	-0.00002
C	3.40869	0.41484	-0.00002
C	3.38747	1.81506	0.00000
C	2.15118	2.48446	0.00003
C	0.96575	1.73444	0.00001
C	0.98415	0.31050	-0.00002
H	2.26244	-1.43489	-0.00003
C	-1.33697	1.26294	0.00009
C	-0.88048	3.58049	-0.00002

C	-2.25458	3.61102	-0.00005
N	-0.38274	2.25536	0.00007
Pt	-0.79369	-0.58077	0.00004
C	-3.03816	-2.63672	-0.00013
C	-0.69430	-3.59539	-0.00009
O	-2.77102	-1.37641	0.00010
O	0.00881	-2.50771	-0.00005
C	-4.52326	-2.96279	-0.00011
H	-4.71814	-4.04696	-0.00181
H	-5.00100	-2.51292	0.88872
H	-5.00167	-2.50991	-0.88703
C	0.14184	-4.86340	0.00018
H	0.79813	-4.87407	0.88890
H	-0.47546	-5.77566	-0.00142
H	0.80088	-4.87267	-0.88650
C	-2.10108	-3.69733	-0.00025
H	-2.51300	-4.71034	-0.00039
H	4.31999	2.38480	0.00002
H	2.15793	3.57395	0.00009
S	-2.91531	1.97551	0.00001
C	0.01911	4.78261	0.00003
H	0.66619	4.81376	0.89488
H	0.66618	4.81387	-0.89483
H	-0.58771	5.70081	0.00010
C	-3.18631	4.78932	-0.00012
H	-2.63057	5.74109	-0.00050
H	-3.84109	4.78592	-0.89101
H	-3.84070	4.78639	0.89106
Br	5.10406	-0.48609	-0.00005

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

C	-1.32716	-2.26148	0.00014
C	-2.66373	-2.72050	-0.00050
C	-3.72674	-1.79841	-0.00114
C	-3.45445	-0.41655	-0.00103
C	-2.12741	0.02860	-0.00017
C	-1.03850	-0.89469	0.00022
H	-0.51526	-2.99538	0.00047
C	-0.30114	1.50822	-0.00054
C	-2.37817	2.62689	0.00085
C	-1.53001	3.70914	0.00082
N	-1.67264	1.40106	-0.00011
Pt	0.77907	-0.08114	-0.00019
C	3.79489	0.35994	-0.00147
C	3.05563	-2.06205	0.00202
O	2.64988	0.94866	-0.00198
O	1.76917	-1.92072	0.00196
C	4.98675	1.30505	-0.00317
H	5.95087	0.77198	-0.00260
H	4.93856	1.95963	-0.89195
H	4.93898	1.96231	0.88365
C	3.51069	-3.51203	0.00408
H	3.10222	-4.02937	-0.88260

H	4.60787	-3.61078	0.00375
H	3.10304	-4.02658	0.89277
C	4.02477	-1.03681	0.00043
H	5.07024	-1.35815	0.00067
H	-4.76803	-2.13004	-0.00180
H	-4.30266	0.26790	-0.00179
S	0.15208	3.18147	-0.00020
C	-3.87796	2.69355	0.00210
H	-4.31203	2.21239	-0.89263
H	-4.31047	2.20957	0.89604
H	-4.20491	3.74453	0.00400
C	-1.85115	5.17670	0.00152
H	-2.93969	5.34927	0.00268
H	-1.43352	5.68171	0.89215
H	-1.43537	5.68220	-0.88970
O	-2.81831	-4.08629	-0.00053
C	-4.14941	-4.59735	-0.00161
H	-4.04972	-5.69356	-0.00163
H	-4.71059	-4.28117	0.90027
H	-4.70917	-4.28099	-0.90430

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

C	0.28639	2.69055	0.00019
C	1.30381	3.67634	0.00024
C	2.66254	3.28915	0.00017
C	3.00834	1.93112	0.00008
C	1.98863	0.96506	0.00008
C	0.61033	1.32778	0.00009
H	-0.76562	2.99126	0.00022
C	0.97116	-1.15287	-0.00010
C	3.33345	-1.27221	0.00009
C	3.02798	-2.61168	-0.00002
N	2.16748	-0.46688	0.00001
Pt	-0.68512	-0.18020	-0.00012
C	-3.23194	-1.84757	-0.00021
C	-3.58453	0.65848	0.00014
O	-1.94406	-1.89671	-0.00028
O	-2.35562	1.06896	0.00015
C	-3.91025	-3.20777	-0.00033
H	-5.00912	-3.13232	-0.00034
H	-3.58915	-3.78141	-0.88821
H	-3.58919	-3.78154	0.88749
C	-4.60402	1.78345	0.00031
H	-4.44988	2.42304	-0.88717
H	-5.64111	1.41266	0.00030
H	-4.44982	2.42282	0.88794
C	-4.03037	-0.67932	-0.00003
H	-5.11344	-0.82955	-0.00001
H	3.44622	4.05206	0.00018
H	4.06478	1.66674	-0.00000
S	1.28014	-2.85567	-0.00020
C	4.71923	-0.69383	0.00033
H	4.90915	-0.07513	-0.89487

H	4.90878	-0.07505	0.89554
H	5.46056	-1.50716	0.00052
C	3.94226	-3.80348	0.00003
H	5.00115	-3.49849	-0.00037
H	3.77832	-4.43656	0.89133
H	3.77780	-4.43700	-0.89086
C	0.95857	5.06912	0.00036
N	0.67619	6.21261	0.00046

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

C	-0.20793	2.82124	-0.00011
C	-1.17137	3.85527	-0.00238
C	-2.53200	3.50103	-0.00642
C	-2.94044	2.15507	-0.00563
C	-1.96249	1.15113	-0.00141
C	-0.57418	1.46840	0.00042
H	0.85944	3.07224	0.00054
C	-1.02098	-1.00239	-0.00010
C	-3.38135	-1.04191	0.00029
C	-3.12475	-2.39245	0.00128
N	-2.19070	-0.27784	-0.00084
Pt	0.66818	-0.08910	0.00040
C	3.15132	-1.86664	-0.00134
C	3.60607	0.62365	0.00035
O	1.86435	-1.86300	-0.00081
O	2.39814	1.08864	0.00112
C	3.77677	-3.25324	-0.00282
H	4.87801	-3.22137	-0.00285
H	3.43339	-3.81499	0.88438
H	3.43332	-3.81308	-0.89120
C	4.67612	1.70299	0.00055
H	4.55060	2.34867	0.88827
H	5.69610	1.28678	0.00091
H	4.55121	2.34835	-0.88750
C	3.99726	-0.73135	-0.00076
H	5.07354	-0.92555	-0.00135
H	-3.29762	4.28598	-0.01050
H	-4.00761	1.93452	-0.00996
S	-1.38755	-2.69665	0.00109
C	-4.74473	-0.41315	0.00098
H	-4.90728	0.21688	0.89358
H	-4.91092	0.21141	-0.89483
H	-5.51656	-1.19787	0.00485
C	-4.08230	-3.54993	0.00212
H	-5.12937	-3.20582	0.00701
H	-3.94603	-4.18750	-0.89092
H	-3.93914	-4.19168	0.89104
C	-0.73953	5.30726	0.00575
H	-0.05006	5.52765	-0.83019
H	-1.60364	5.98868	-0.08023
H	-0.20269	5.56266	0.93898

Optimized singlet ground state structure of **30**.

C	-2.21390	-0.44948	-0.00008
C	-3.44803	0.23649	-0.00005
C	-3.46583	1.64545	0.00002
C	-2.26559	2.37081	0.00003
C	-1.04647	1.67179	-0.00003
C	-0.99896	0.24786	-0.00006
H	-2.21528	-1.54364	-0.00012
C	1.27492	1.30648	0.00003
C	0.71158	3.60282	-0.00002
C	2.08243	3.69604	-0.00002
N	0.27459	2.25564	0.00001
Pt	0.82043	-0.55832	-0.00006
C	3.15530	-2.51794	-0.00005
C	0.85524	-3.57619	0.00013
O	2.83376	-1.27043	-0.00009
O	0.10723	-2.51936	0.00012
C	4.65347	-2.77855	-0.00010
H	4.89703	-3.85293	-0.00008
H	5.11106	-2.30641	-0.88796
H	5.11114	-2.30635	0.88769
C	0.07221	-4.87738	0.00026
H	-0.58542	-4.91325	-0.88664
H	0.72623	-5.76371	0.00020
H	-0.58520	-4.91321	0.88732
C	2.26529	-3.61813	0.00005
H	2.72044	-4.61249	0.00008
H	-4.42059	2.17729	0.00006
H	-2.31575	3.45897	0.00010
S	2.81834	2.09209	0.00007
C	-0.24061	4.76385	-0.00003
H	-0.88875	4.76589	-0.89455
H	-0.88855	4.76606	0.89463
H	0.32459	5.70821	-0.00015
C	2.96095	4.91442	0.00020
H	2.36445	5.84099	-0.00255
H	3.61315	4.94102	0.89258
H	3.61710	4.93838	-0.88934
C	-4.69886	-0.57761	-0.00007
O	-4.74413	-1.80397	-0.00007
O	-5.82523	0.20635	0.00002
C	-7.06103	-0.53805	0.00008
H	-7.13106	-1.17785	0.89576
H	-7.85828	0.21940	0.00045
H	-7.13144	-1.17733	-0.89596

Optimized singlet ground state structure of **31**.

C	0.65857	2.77608	-0.00447
C	1.81528	3.57333	-0.01218
C	3.09903	2.99597	-0.01235
C	3.20749	1.58915	-0.01062
C	2.04726	0.80006	-0.00093
C	0.74663	1.37459	0.00143

H	-0.33264	3.24189	-0.00829
H	1.71963	4.66680	-0.02034
C	0.70899	-1.13300	-0.00179
C	3.01715	-1.62874	0.00107
C	2.50347	-2.90391	0.00082
N	1.99686	-0.64789	-0.00171
Pt	-0.77348	0.08772	0.00020
C	-3.54651	-1.17912	-0.00070
C	-3.51479	1.35264	0.00342
O	-2.28251	-1.42293	-0.00150
O	-2.23991	1.57719	0.00312
C	-4.42669	-2.41963	-0.00279
H	-5.50126	-2.17665	-0.00038
H	-4.19907	-3.03333	-0.89287
H	-4.19609	-3.03847	0.88293
C	-4.35798	2.61704	0.00585
H	-4.11148	3.22830	-0.88092
H	-5.43878	2.40401	0.00554
H	-4.11136	3.22496	0.89490
C	-4.15839	0.09761	0.00171
H	4.20618	1.15143	-0.01827
S	0.74027	-2.86580	-0.00128
C	4.47762	-1.27964	0.00587
H	4.76734	-0.70428	-0.89149
H	4.75706	-0.68956	0.89680
H	5.07982	-2.20094	0.01675
C	3.21787	-4.22532	0.00206
H	4.31185	-4.09143	0.00700
H	2.95259	-4.82711	0.89094
H	2.96052	-4.82441	-0.89101
H	-5.25196	0.11344	0.00218
C	4.34524	3.85845	0.01337
H	4.62103	4.14594	1.04695
H	5.21445	3.33337	-0.42138
H	4.19898	4.79474	-0.55381

In the following section the coordinates of the triplet state structure geometries for **25**–**31** are given (BP86/6-31G(d)).

Optimized triplet state structure of **25**.

C	0.02132	2.99607	0.00008
C	0.91637	4.06448	0.00004
C	2.32585	3.81275	-0.00014
C	2.84086	2.52308	-0.00021
C	1.93895	1.41952	-0.00008
C	0.48113	1.65814	-0.00003
H	-1.06020	3.16692	0.00017
H	0.55249	5.09751	0.00011
C	1.07435	-0.78355	-0.00032
C	3.46456	-0.62746	0.00025
C	3.28196	-1.99496	0.00026
N	2.24969	0.07638	-0.00008
Pt	-0.64932	0.06939	-0.00019
C	-3.02934	-1.83749	-0.00021
C	-3.64200	0.62393	0.00038
O	-1.74036	-1.76438	-0.00037
O	-2.47215	1.16344	0.00028
C	-3.56718	-3.25973	-0.00041
H	-4.66819	-3.29854	-0.00009
H	-3.18728	-3.79671	-0.88810
H	-3.18674	-3.79718	0.88675
C	-4.78617	1.62516	0.00097
H	-4.70717	2.27837	-0.88680
H	-5.77457	1.13891	0.00099
H	-4.70682	2.27773	0.88917
C	-3.94221	-0.76039	0.00017
H	-5.00349	-1.02445	0.00034
H	3.02226	4.65907	-0.00025
H	3.92164	2.38518	-0.00041
S	1.57626	-2.47243	-0.00016
C	4.79429	0.07011	0.00070
H	4.92393	0.70631	-0.89374
H	4.92302	0.70679	0.89492
H	5.61043	-0.66782	0.00131
C	4.31946	-3.07735	0.00062
H	5.34441	-2.67349	0.00067
H	4.21082	-3.72644	0.89004
H	4.21106	-3.72679	-0.88857

Optimized triplet state structure of **26**.

C	2.20503	-0.34273	0.00006
C	3.37985	0.40821	0.00003
C	3.35262	1.84018	-0.00007
C	2.14690	2.52286	-0.00010
C	0.92481	1.78421	0.00000
C	0.95570	0.30779	0.00002
H	2.23108	-1.43598	0.00011
C	-1.37857	1.24094	-0.00013

C	-0.88100	3.58557	0.00002
C	-2.26095	3.59950	-0.00018
N	-0.35863	2.28170	-0.00006
Pt	-0.78157	-0.58559	0.00001
C	-2.99947	-2.67034	-0.00003
C	-0.64626	-3.61831	-0.00026
O	-2.75128	-1.40355	-0.00006
O	0.05111	-2.53344	0.00009
C	-4.48166	-3.00898	0.00120
H	-4.66891	-4.09445	-0.00602
H	-4.96003	-2.56631	0.89337
H	-4.96461	-2.55307	-0.88167
C	0.18715	-4.88914	-0.00067
H	0.84489	-4.90107	0.88709
H	-0.43174	-5.80036	-0.00081
H	0.84464	-4.90066	-0.88863
C	-2.05771	-3.72303	-0.00046
H	-2.46565	-4.73764	-0.00072
H	4.29554	2.39379	-0.00015
H	2.16564	3.61202	-0.00023
S	-2.97653	1.98141	-0.00043
C	0.00002	4.80143	0.00045
H	0.64808	4.83818	0.89521
H	0.64819	4.83885	-0.89421
H	-0.61366	5.71457	0.00076
C	-3.18154	4.78304	-0.00017
H	-2.63303	5.73839	-0.00124
H	-3.84019	4.76882	-0.88891
H	-3.83881	4.76996	0.88962
Br	5.08138	-0.45471	0.00013

Optimized triplet state structure of **27**.

C	-1.23275	-2.28395	0.01431
C	-2.54677	-2.79183	-0.00230
C	-3.66155	-1.90351	-0.09528
C	-3.46448	-0.52790	-0.14320
C	-2.14043	-0.00223	-0.08351
C	-0.99005	-0.90903	-0.02767
H	-0.39155	-2.98267	0.06080
C	-0.31564	1.51509	-0.25267
C	-2.48360	2.51431	0.05132
C	-1.66284	3.63025	0.08676
N	-1.76992	1.32792	-0.10413
Pt	0.77953	-0.05042	-0.05832
C	3.78726	0.46027	0.00280
C	3.11580	-1.98324	0.12656
O	2.63385	1.02752	-0.06894
O	1.82931	-1.88303	0.07418
C	4.95829	1.43189	-0.01209
H	5.93403	0.92397	0.04919
H	4.92360	2.03593	-0.93656
H	4.86414	2.13545	0.83461
C	3.61876	-3.41343	0.24525

H	3.23057	-4.01453	-0.59653
H	4.71871	-3.47627	0.25449
H	3.22677	-3.86804	1.17336
C	4.05367	-0.92711	0.09163
H	5.10757	-1.21478	0.14519
H	-4.68193	-2.29295	-0.14491
H	-4.33575	0.11818	-0.24962
S	0.05544	3.24833	-0.06718
C	-3.97540	2.53243	0.22304
H	-4.29161	1.87326	1.05194
H	-4.32266	3.55017	0.45564
H	-4.50259	2.20437	-0.69208
C	-2.05666	5.06492	0.27017
H	-3.14393	5.19041	0.39700
H	-1.55684	5.49725	1.15784
H	-1.74583	5.67227	-0.60109
O	-2.66394	-4.15356	0.06409
C	-3.97347	-4.72719	0.05248
H	-3.82030	-5.81411	0.12635
H	-4.57661	-4.38274	0.91455
H	-4.51113	-4.49702	-0.88764

Optimized triplet state structure of **28**.

C	-0.17724	2.67956	-0.00024
C	-1.14900	3.70489	-0.00033
C	-2.55816	3.34287	-0.00027
C	-2.97199	2.02513	-0.00015
C	-1.99514	0.98476	-0.00008
C	-0.55129	1.32875	-0.00011
H	0.88755	2.93124	-0.00026
C	-0.99471	-1.14811	0.00012
C	-3.38293	-1.16348	0.00004
C	-3.10781	-2.51140	0.00016
N	-2.20589	-0.37865	0.00002
Pt	0.67511	-0.18819	0.00006
C	3.16841	-1.93672	0.00012
C	3.62234	0.55853	0.00002
O	1.87536	-1.94083	0.00014
O	2.41934	1.01920	0.00001
C	3.79064	-3.32262	0.00016
H	4.89166	-3.29305	0.00017
H	3.44452	-3.88201	0.88776
H	3.44453	-3.88206	-0.88741
C	4.69735	1.63132	-0.00002
H	4.57431	2.27769	0.88746
H	5.71497	1.21012	-0.00005
H	4.57426	2.27767	-0.88752
C	4.01055	-0.80479	0.00006
H	5.08640	-0.99981	0.00006
H	-3.30262	4.14492	-0.00031
H	-4.04058	1.81416	-0.00009
S	-1.37240	-2.85383	0.00025
C	-4.75347	-0.55128	-0.00010
H	-4.92533	0.07386	0.89490

H	-4.92517	0.07378	-0.89518
H	-5.51846	-1.34215	-0.00014
C	-4.06541	-3.66632	0.00018
H	-5.11508	-3.33210	0.00050
H	-3.91430	-4.30495	-0.88992
H	-3.91387	-4.30527	0.88997
C	-0.77962	5.07474	-0.00048
N	-0.48486	6.22094	-0.00060

Optimized triplet state structure of **29**.

C	-0.12688	2.80045	-0.00005
C	-1.04950	3.85132	-0.00008
C	-2.45269	3.52295	-0.00019
C	-2.91664	2.21674	-0.00020
C	-1.97413	1.14748	-0.00009
C	-0.52862	1.44739	-0.00006
H	0.94831	3.01298	-0.00002
C	-1.02248	-1.01743	-0.00001
C	-3.41899	-0.95641	0.00009
C	-3.18272	-2.31499	0.00010
N	-2.23212	-0.20551	-0.00001
Pt	0.66509	-0.09722	-0.00002
C	3.12267	-1.90660	-0.00013
C	3.63308	0.57786	0.00013
O	1.83266	-1.88807	0.00002
O	2.44207	1.06978	-0.00002
C	3.72101	-3.30490	-0.00037
H	4.82268	-3.29623	-0.00063
H	3.36455	-3.85804	0.88712
H	3.36411	-3.85791	-0.88776
C	4.73561	1.62521	0.00054
H	4.63043	2.27358	0.88916
H	5.74299	1.17933	-0.00008
H	4.62987	2.27492	-0.88703
C	3.99041	-0.79206	-0.00003
H	5.06177	-1.01172	-0.00005
H	-3.18407	4.34076	-0.00031
H	-3.99164	2.03857	-0.00034
S	-1.45883	-2.72472	0.00003
C	-4.77461	-0.31041	0.00018
H	-4.92837	0.32081	0.89444
H	-4.92861	0.32058	-0.89419
H	-5.56134	-1.07968	0.00038
C	-4.17699	-3.43731	0.00020
H	-5.21704	-3.07377	0.00026
H	-4.04331	-4.08185	-0.88912
H	-4.04319	-4.08180	0.88953
C	-0.61946	5.29732	-0.00001
H	0.47961	5.38908	-0.00002
H	-1.00483	5.83715	-0.88762
H	-1.00479	5.83703	0.88770

Optimized triplet state structure of **30**.

C	-2.19660	-0.43333	-0.00002
C	-3.42195	0.25314	0.00000
C	-3.40987	1.70188	0.00004
C	-2.23130	2.43012	0.00004
C	-0.98651	1.74027	-0.00001
C	-0.97100	0.25597	-0.00001
H	-2.19783	-1.52762	-0.00002
C	1.32454	1.28634	0.00003
C	0.76509	3.60649	-0.00007
C	2.13859	3.66660	-0.00010
N	0.28808	2.27447	-0.00002
Pt	0.79367	-0.56763	0.00003
C	3.09257	-2.57048	-0.00001
C	0.77871	-3.60974	-0.00002
O	2.78591	-1.31404	0.00003
O	0.04442	-2.55307	0.00000
C	4.58782	-2.84096	-0.00002
H	4.82503	-3.91666	-0.00006
H	5.04742	-2.37010	-0.88754
H	5.04741	-2.37017	0.88755
C	-0.00541	-4.91057	-0.00003
H	-0.66321	-4.94470	-0.88687
H	0.64711	-5.79790	-0.00015
H	-0.66303	-4.94482	0.88694
C	2.19663	-3.65964	-0.00003
H	2.64428	-4.65730	-0.00006
H	-4.36754	2.22932	0.00008
H	-2.28887	3.51817	0.00009
S	2.88918	2.06345	-0.00005
C	-0.16206	4.78711	-0.00007
H	-0.81108	4.80032	-0.89449
H	-0.81087	4.80047	0.89451
H	0.41861	5.72187	-0.00018
C	3.02833	4.87468	0.00008
H	2.44950	5.81206	-0.00218
H	3.68331	4.88451	0.89123
H	3.68656	4.88229	-0.88867
C	-4.67221	-0.52820	-0.00001
O	-4.74970	-1.75813	-0.00004
O	-5.78738	0.28767	0.00001
C	-7.03567	-0.43024	-0.00000
H	-7.12065	-1.06985	0.89515
H	-7.81913	0.34207	0.00021
H	-7.12083	-1.06952	-0.89538

Optimized triplet state structure of **31**.

C	0.56143	2.76751	0.00021
C	1.67841	3.59557	0.00017
C	3.00952	3.03755	0.00000
C	3.18911	1.65603	-0.00012
C	2.06002	0.79131	0.00000

C	0.69380	1.35816	0.00016
H	-0.44951	3.18826	0.00025
H	1.56270	4.68581	0.00023
C	0.71660	-1.15221	-0.00017
C	3.07677	-1.55445	0.00009
C	2.58629	-2.84060	-0.00001
N	2.05138	-0.58802	-0.00005
Pt	-0.76918	0.07413	-0.00004
C	-3.52224	-1.23245	0.00000
C	-3.55092	1.30401	0.00005
O	-2.25091	-1.45816	-0.00007
O	-2.28840	1.55840	-0.00002
C	-4.37378	-2.49217	0.00007
H	-5.45389	-2.27522	0.00018
H	-4.12829	-3.10269	-0.88745
H	-4.12812	-3.10272	0.88752
C	-4.43404	2.54178	0.00010
H	-4.20728	3.15883	-0.88806
H	-5.50772	2.29543	0.00018
H	-4.20715	3.15886	0.88821
C	-4.16237	0.02589	0.00008
H	4.20775	1.26733	-0.00038
S	0.81480	-2.90731	-0.00013
C	4.53091	-1.17880	0.00042
H	4.80330	-0.58921	-0.89392
H	4.80272	-0.58872	0.89461
H	5.15544	-2.08483	0.00086
C	3.34518	-4.13415	0.00005
H	4.43565	-3.97623	0.00013
H	3.09143	-4.74121	0.88954
H	3.09158	-4.74119	-0.88950
H	-5.25597	0.01358	0.00015
C	4.19430	3.97156	-0.00027
H	4.17735	4.63517	0.88613
H	5.15290	3.42580	-0.00030
H	4.17717	4.63492	-0.88686

The following paragraph contains the singlet ground state structure geometries for the 3-methyl regioisomer of complex **31** (B3LYP/6-31G(d)).

C	0.19664	3.02741	0.00007
C	1.19463	4.01654	0.00004
C	2.54658	3.69713	-0.00002
C	2.94183	2.36112	-0.00003
C	1.95618	1.37429	0.00001
C	0.56607	1.66458	0.00004
H	0.89296	5.06152	0.00006
C	1.11630	-0.80271	-0.00001
C	3.45389	-0.77485	0.00000
C	3.23784	-2.11970	-0.00001
N	2.23902	-0.04738	-0.00001
Pt	-0.61779	0.01641	0.00004
C	-2.84806	-2.09533	-0.00022
C	-3.64869	0.27920	0.00007
O	-1.59061	-1.88790	-0.00018
O	-2.52944	0.89899	0.00014
C	-3.24884	-3.55760	-0.00042
H	-4.33285	-3.69627	-0.00030
H	-2.82471	-4.05155	-0.88216
H	-2.82447	-4.05186	0.88103
C	-4.85833	1.19392	0.00019
H	-4.82295	1.84485	-0.88091
H	-5.80260	0.64388	0.00009
H	-4.82299	1.84459	0.88148
C	-3.85069	-1.10959	-0.00010
H	3.99487	2.12994	-0.00009
S	1.51848	-2.47731	-0.00007
C	4.80366	-0.12224	0.00006
H	4.95728	0.50099	-0.88723
H	4.95715	0.50106	0.88733
H	5.58054	-0.88851	0.00015
C	4.22201	-3.25209	0.00002
H	5.25334	-2.89134	-0.00018
H	4.09424	-3.88853	0.88407
H	4.09399	-3.88878	-0.88380
H	-4.87796	-1.45486	-0.00014
C	-1.24299	3.48632	0.00012
H	-1.78477	3.11255	-0.87328
H	-1.78472	3.11251	0.87355
H	-1.29436	4.58045	0.00015
H	3.29916	4.48067	-0.00004

In the following section the singlet ground state structure geometries for **8**, **9** and **18** are given (B3LYP/6-31G(d)), which were used for comparison reasons with the corresponding solid-state structures.

Optimized singlet ground state structure of **8**.

C	3.96796	-0.47175	0.00005
C	3.27453	-0.39377	1.20984
C	1.88763	-0.24113	1.21338
C	1.20126	-0.17014	-0.00000
C	1.88768	-0.24106	-1.21337
C	3.27456	-0.39370	-1.20977
H	5.04810	-0.58835	0.00005
H	3.81231	-0.44659	2.15213
H	1.33655	-0.16483	2.14563
H	1.33662	-0.16468	-2.14563
H	3.81240	-0.44651	-2.15203
C	-1.09562	-1.15932	-0.00002
C	-2.40668	-0.81836	-0.00004
N	-0.23422	-0.03948	-0.00002
C	-0.83734	1.20067	0.00003
S	-2.58363	0.93709	0.00001
C	-0.49994	-2.53505	-0.00014
H	0.13050	-2.69926	-0.88164
H	0.13013	-2.69955	0.88157
H	-1.28715	-3.29137	-0.00040
C	-3.62350	-1.69320	0.00008
H	-3.35028	-2.75185	0.00004
H	-4.24710	-1.50999	0.88395
H	-4.24724	-1.50998	-0.88369
S	-0.10503	2.69104	-0.00002

Optimized singlet ground state structure of **9**.

C	-2.63487	-0.09294	-0.00001
C	-1.95259	-0.07196	-1.21438
C	-0.55847	-0.03472	-1.21091
C	0.13497	-0.02221	0.00004
C	-0.55853	-0.03358	1.21097
C	-1.95264	-0.07081	1.21437
H	-2.49850	-0.08095	-2.15113
H	-0.00942	-0.00529	-2.14673
H	-0.00952	-0.00328	2.14678
H	-2.49864	-0.07894	2.15109
C	2.33838	-1.20401	0.00017
C	3.67289	-0.97281	0.00008
N	1.57395	-0.01469	0.00005
C	2.27919	1.17169	-0.00013
S	3.99631	0.76195	-0.00010
C	1.62926	-2.52473	0.00032
H	0.98796	-2.63721	0.88221
H	0.98816	-2.63750	-0.88168
H	2.35064	-3.34386	0.00052
C	4.81330	-1.94525	0.00014

H	4.45419	-2.97794	-0.00010
H	5.44985	-1.81347	-0.88355
H	5.44948	-1.81377	0.88414
S	1.67057	2.71592	-0.00025
Br	-4.56050	-0.15265	-0.00000

Optimized singlet ground state structure of **18**.

C	2.47414	-0.05765	0.00002
C	1.78658	-0.10262	-1.21504
C	0.39531	-0.19097	-1.21868
C	-0.28236	-0.23310	0.00008
C	0.39532	-0.19035	1.21879
C	1.78659	-0.10201	1.21509
H	2.33051	-0.07237	-2.15242
H	-0.14869	-0.23013	-2.15759
H	-0.14866	-0.22905	2.15773
H	2.33051	-0.07128	2.15247
C	-2.59912	0.77592	-0.00008
C	-3.91331	0.38898	-0.00002
N	-1.73499	-0.33255	0.00008
C	-2.35001	-1.51127	0.00016
S	-4.03502	-1.35856	0.00014
C	-2.03074	2.16117	-0.00025
H	-1.40843	2.33391	0.88409
H	-1.40797	2.33346	-0.88435
H	-2.83210	2.90091	-0.00065
C	-5.15713	1.22640	-0.00019
H	-4.90504	2.28873	0.00005
H	-5.76937	1.02684	-0.88633
H	-5.76977	1.02660	0.88562
H	-1.81012	-2.44867	0.00033
Br	4.37751	0.06339	-0.00003

In the following section the singlet ground state structure geometries for **8**, **9** and **18** as well as **25**–**27** are given (B3LYP/6-31++G(d,p)), which were used for comparison reasons with the corresponding solid-state structures.

Optimized singlet ground state structure of **8**.

C	3.96280	-0.47531	0.00001
C	3.27024	-0.39893	1.20739
C	1.88549	-0.24894	1.21019
C	1.20016	-0.18114	0.00003
C	1.88550	-0.24873	-1.21015
C	3.27025	-0.39872	-1.20736
H	5.04090	-0.58799	0.00000
H	3.80734	-0.44799	2.14750
H	1.33666	-0.16999	2.14106
H	1.33667	-0.16961	-2.14100
H	3.80736	-0.44762	-2.14747
C	-1.10497	-1.15778	0.00004
C	-2.41050	-0.80810	0.00001
N	-0.23483	-0.04451	0.00004
C	-0.82805	1.19769	0.00009
S	-2.57403	0.94962	-0.00007
C	-0.52355	-2.53737	0.00003
H	0.10284	-2.70679	-0.88016
H	0.10260	-2.70690	0.88038
H	-1.31687	-3.28320	-0.00012
C	-3.63355	-1.67101	-0.00000
H	-3.37015	-2.72922	-0.00004
H	-4.25309	-1.48215	0.88225
H	-4.25313	-1.48209	-0.88221
S	-0.08474	2.68132	-0.00007

Optimized singlet ground state structure of **9**.

C	-2.63386	-0.09895	0.00003
C	-1.95255	-0.07917	-1.21343
C	-0.56068	-0.04366	-1.20784
C	0.13126	-0.03411	-0.00003
C	-0.56065	-0.04276	1.20781
C	-1.95252	-0.07826	1.21345
H	-2.49680	-0.08461	-2.14859
H	-0.01281	-0.01109	-2.14186
H	-0.01276	-0.00951	2.14179
H	-2.49675	-0.08302	2.14863
C	2.34455	-1.20262	0.00012
C	3.67421	-0.96220	0.00007
N	1.57042	-0.01953	-0.00005
C	2.26570	1.16974	-0.00030
S	3.98401	0.77595	-0.00007
C	1.64969	-2.52848	0.00037
H	1.01192	-2.64618	0.88089
H	1.01208	-2.64660	-0.88021
H	2.37821	-3.33754	0.00063
C	4.82194	-1.92312	0.00024

H	4.47278	-2.95622	0.00007
H	5.45491	-1.78541	-0.88184
H	5.45454	-1.78555	0.88260
S	1.64591	2.70841	-0.00038
Br	-4.54856	-0.15217	0.00007

Optimized singlet ground state structure of **18**.

C	2.47278	-0.05763	0.00069
C	1.78718	-0.12394	-1.21297
C	0.39844	-0.21466	-1.21301
C	-0.27846	-0.23828	0.00297
C	0.39779	-0.17417	1.21780
C	1.78654	-0.08374	1.21554
H	2.32995	-0.10854	-2.14895
H	-0.14389	-0.26909	-2.14978
H	-0.14495	-0.19809	2.15558
H	2.32883	-0.03757	2.15078
C	-2.59374	0.77221	-0.01071
C	-3.90582	0.38991	-0.01173
N	-1.73192	-0.33629	0.00421
C	-2.34779	-1.51175	0.01606
S	-4.02985	-1.35603	0.00838
C	-2.03297	2.15739	-0.01705
H	-1.44738	2.34945	0.88542
H	-1.37982	2.31670	-0.87811
H	-2.83695	2.88949	-0.05824
C	-5.14349	1.23279	-0.00496
H	-4.92187	2.24253	-0.34965
H	-5.91013	0.81893	-0.66282
H	-5.56556	1.30278	1.00154
H	-1.81457	-2.45051	0.02537
Br	4.36756	0.06588	-0.00087

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

C	-0.11570	3.01509	0.00002
C	-1.04307	4.05893	0.00005
C	-2.40668	3.78176	0.00004
C	-2.85749	2.45979	-0.00003
C	-1.92103	1.42927	-0.00009
C	-0.53332	1.68476	-0.00003
H	0.94671	3.22839	0.00005
H	-0.69928	5.08789	0.00010
C	-1.09134	-0.75840	0.00008
C	-3.43303	-0.69939	-0.00011
C	-3.23999	-2.04385	0.00013
N	-2.21074	0.01073	-0.00011
Pt	0.64319	0.07709	-0.00005
C	3.06052	-1.80615	0.00014
C	3.62633	0.64493	0.00012
O	1.79268	-1.73630	0.00006

O	2.45451	1.14888	0.00007
C	3.61865	-3.21324	0.00021
H	4.70859	-3.23276	0.00009
H	3.24867	-3.74608	0.88047
H	3.24844	-3.74627	-0.87984
C	4.74076	1.66777	0.00016
H	4.63996	2.30887	0.88027
H	5.72978	1.20962	0.00026
H	4.64011	2.30877	-0.88004
C	3.95591	-0.71941	0.00016
H	5.01003	-0.96100	0.00021
H	-3.13161	4.58762	0.00009
H	-3.91934	2.27770	-0.00001
S	-1.52257	-2.42235	-0.00033
C	-4.76480	-0.01602	-0.00019
H	-4.89956	0.60939	0.88560
H	-4.89950	0.60931	-0.88605
H	-5.55848	-0.76106	-0.00019
C	-4.24004	-3.15923	0.00040
H	-5.26211	-2.78022	0.00082
H	-4.12359	-3.79528	-0.88220
H	-4.12296	-3.79546	0.88280

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

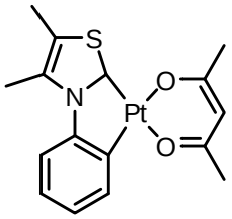
C	2.21856	-0.37002	-0.00017
C	3.40424	0.35983	-0.00021
C	3.40669	1.74828	-0.00016
C	2.18903	2.43215	-0.00008
C	1.00068	1.70889	-0.00005
C	0.99438	0.29786	-0.00008
H	2.23330	-1.45194	-0.00020
C	-1.30241	1.30023	0.00011
C	-0.80547	3.59037	0.00006
C	-2.16216	3.65167	0.00019
N	-0.33699	2.25644	0.00004
Pt	-0.80099	-0.56058	0.00004
C	-3.08892	-2.58704	0.00022
C	-0.78278	-3.59321	-0.00000
O	-2.78930	-1.35189	0.00021
O	-0.07275	-2.53268	-0.00006
C	-4.57392	-2.87746	0.00035
H	-4.79250	-3.94530	0.00041
H	-5.03002	-2.41615	0.88055
H	-5.03016	-2.41621	-0.87981
C	0.01833	-4.87538	-0.00009
H	0.66714	-4.89404	0.87983
H	-0.61380	-5.76324	-0.00005
H	0.66697	-4.89402	-0.88014
C	-2.18451	-3.66556	0.00013
H	-2.61529	-4.65736	0.00016
H	4.33647	2.30086	-0.00019
H	2.21521	3.50909	-0.00003
S	-2.85511	2.03522	0.00026

C	0.11620	4.76975	-0.00009
H	0.75554	4.78491	0.88605
H	0.75545	4.78473	-0.88630
H	-0.46614	5.68935	-0.00016
C	-3.06982	4.84328	0.00022
H	-2.50499	5.77555	0.00074
H	-3.71615	4.84847	-0.88250
H	-3.71679	4.84790	0.88246
Br	5.08575	-0.57318	-0.00034

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

C	1.29563	-2.27203	-0.00008
C	2.61361	-2.75040	0.00002
C	3.68211	-1.85406	0.00016
C	3.43235	-0.47623	0.00016
C	2.12485	-0.01375	0.00001
C	1.03033	-0.91139	-0.00007
H	0.48134	-2.98610	-0.00014
C	0.34449	1.50354	0.00007
C	2.42503	2.57619	-0.00004
C	1.61046	3.66358	0.00005
N	1.69495	1.36704	0.00002
Pt	-0.77351	-0.06611	-0.00004
C	-3.79471	0.42257	0.00004
C	-3.11193	-1.99914	-0.00006
O	-2.64973	0.97241	0.00003
O	-1.84252	-1.87762	-0.00008
C	-4.96087	1.38781	0.00013
H	-5.92590	0.88084	0.00011
H	-4.89288	2.03310	0.88032
H	-4.89291	2.03322	-0.87999
C	-3.59703	-3.43185	-0.00012
H	-3.19983	-3.94544	0.87974
H	-4.68456	-3.50612	-0.00000
H	-3.20003	-3.94529	-0.88015
C	-4.05688	-0.96059	0.00000
H	-5.09736	-1.25565	0.00002
H	4.70753	-2.19640	0.00028
H	4.28249	0.18611	0.00032
S	-0.07691	3.17097	0.00010
C	3.92133	2.61253	-0.00026
H	4.33788	2.12671	0.88562
H	4.33760	2.12624	-0.88601
H	4.26348	3.64595	-0.00058
C	1.95554	5.12141	0.00008
H	3.03467	5.27569	-0.00006
H	1.54933	5.62502	-0.88228
H	1.54957	5.62491	0.88261
O	2.74985	-4.11046	-0.00001
C	4.05710	-4.66275	0.00018
H	3.92456	-5.74375	0.00017
H	4.61801	-4.36742	-0.89387
H	4.61775	-4.36742	0.89440

2D-NMR Spectra of Complex 25



25

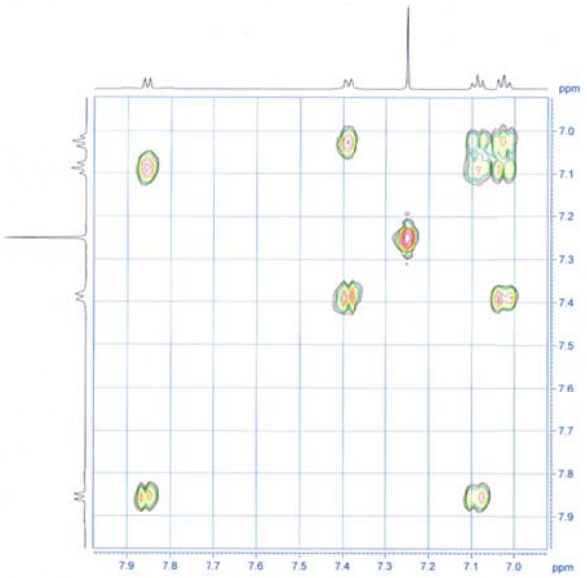


Figure S16. COSY spectrum of complex **25**.

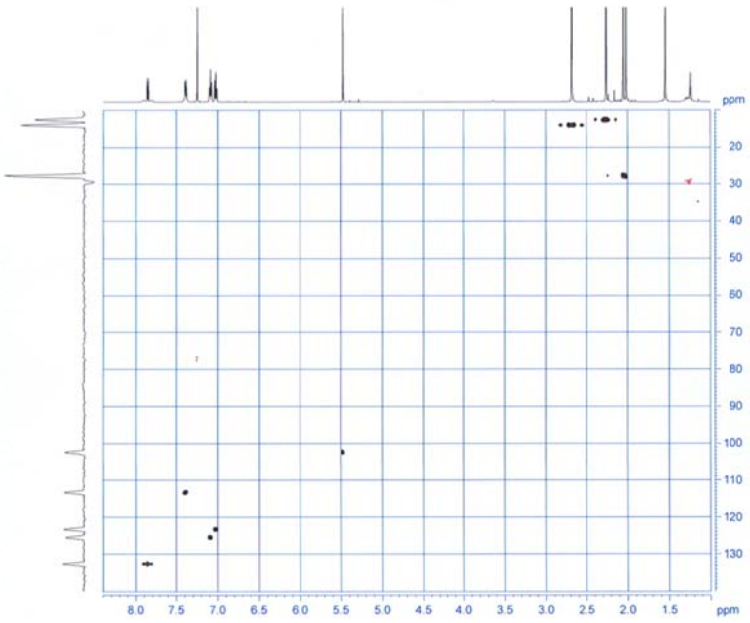


Figure S17. HSQC spectrum of complex **25**.

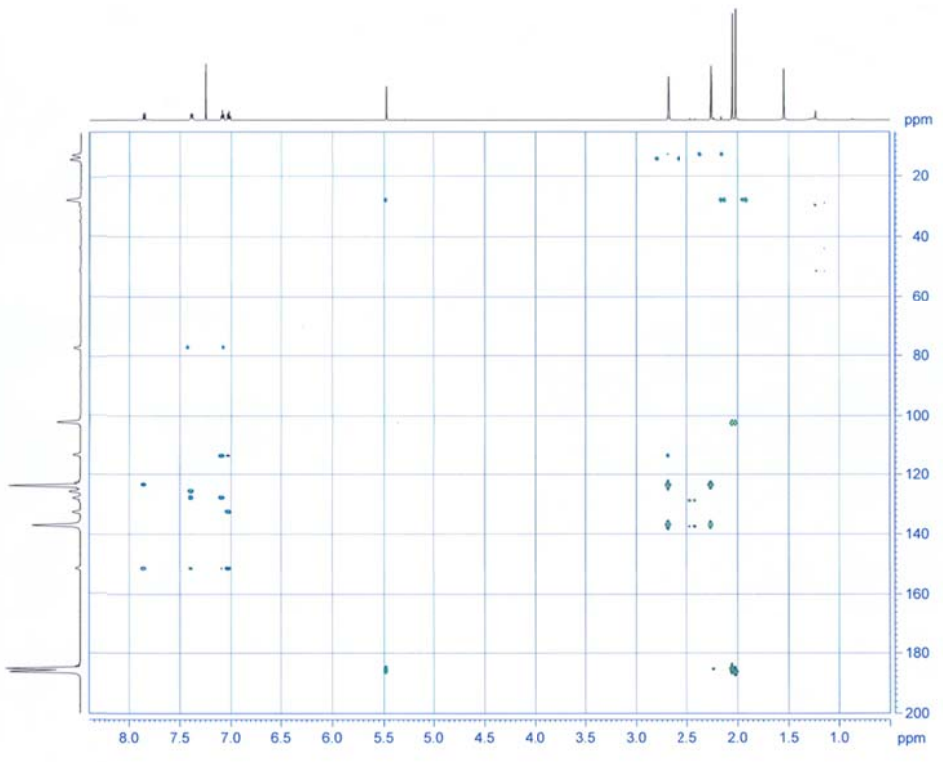


Figure S18. HMBC spectrum of complex **25**.

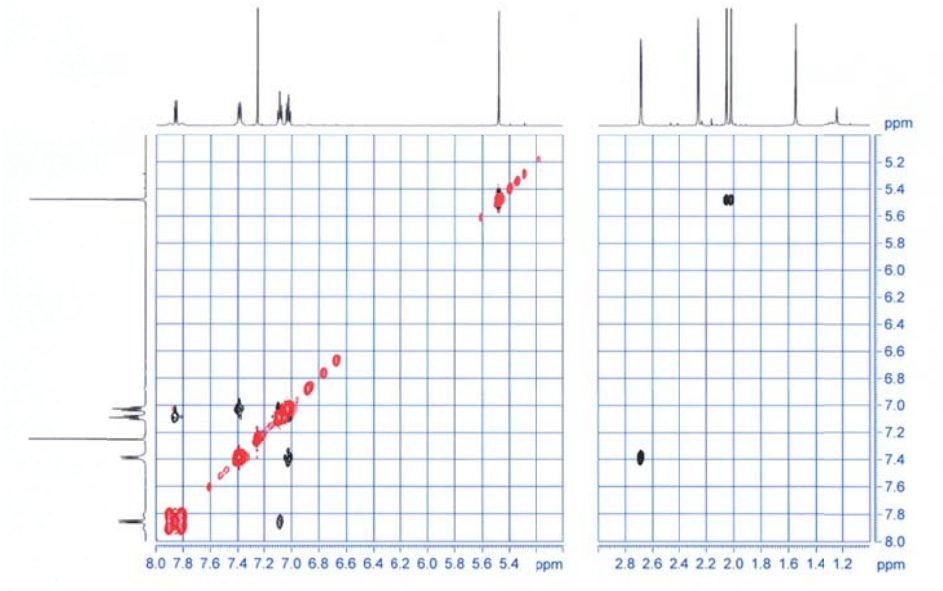


Figure S19. NOESY spectrum of complex **25**.

References

(1) Unger, Y.; Strassner, T.; Lennartz, C. *J. Organomet. Chem.* **2013**, *748*, 63-67.