Supporting Information

Heteroleptic Platinum(II) NHC Complexes with a C^C* Cyclometalated Ligand – Synthesis, Structure and Photophysics

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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
cd	Candela
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
EQE	External quantum yield
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
LLCT	Ligand-to-ligand charge transfer
LUMO	Lowest unoccupied molecular orbital
MLCT	Metal-to-ligand charge transfer
M.p.	Melting point
NHC	*N*-Heterocyclic carbene
NOESY	Nuclear Overhauser effect spectroscopy
OLED	Organic light-emitting device/diode
PMMA	Poly(methyl methacrylate)
SOC	Spin-orbit coupling
TD-DFT	Time-dependent density functional theory
QY	Quantum yield

2D NMR Spectra

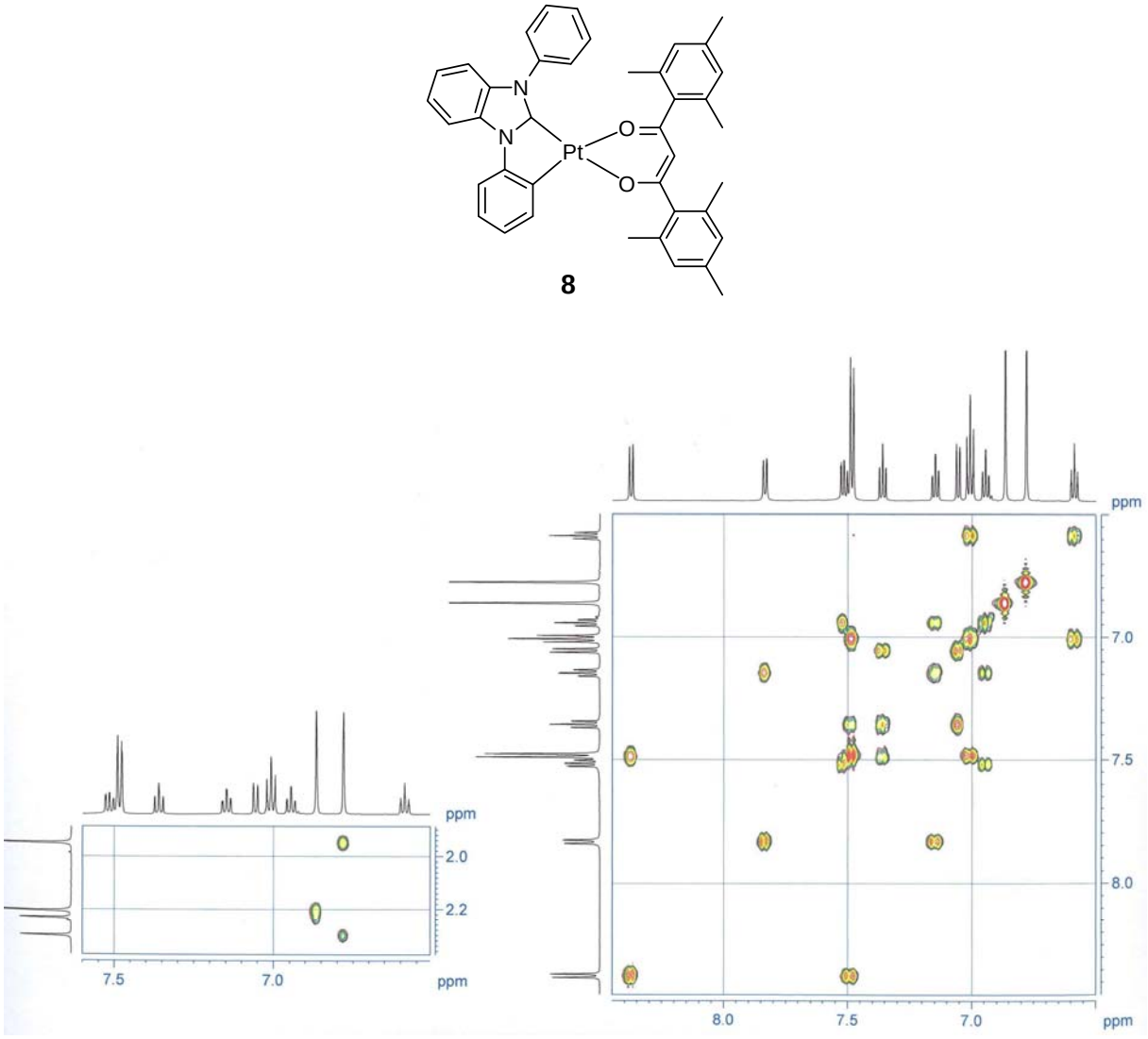

Figure S1. COSY spectrum of complex **8**.

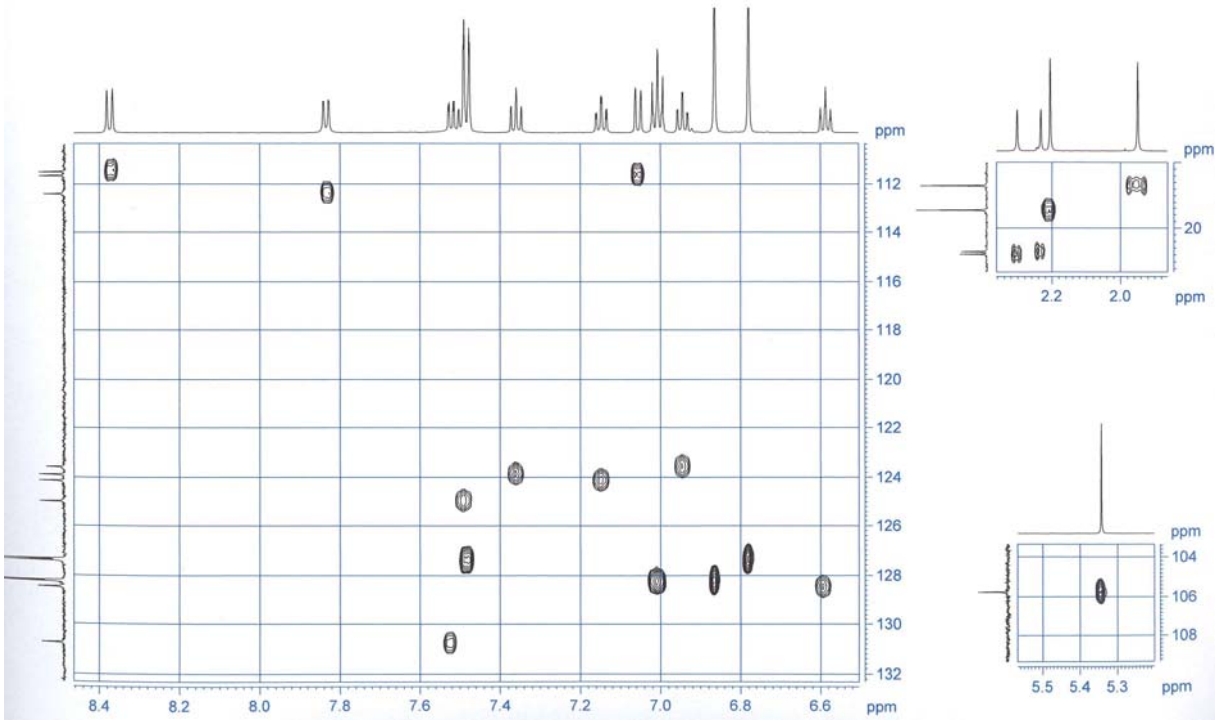

Figure S2. HSQC spectrum of complex **8**.

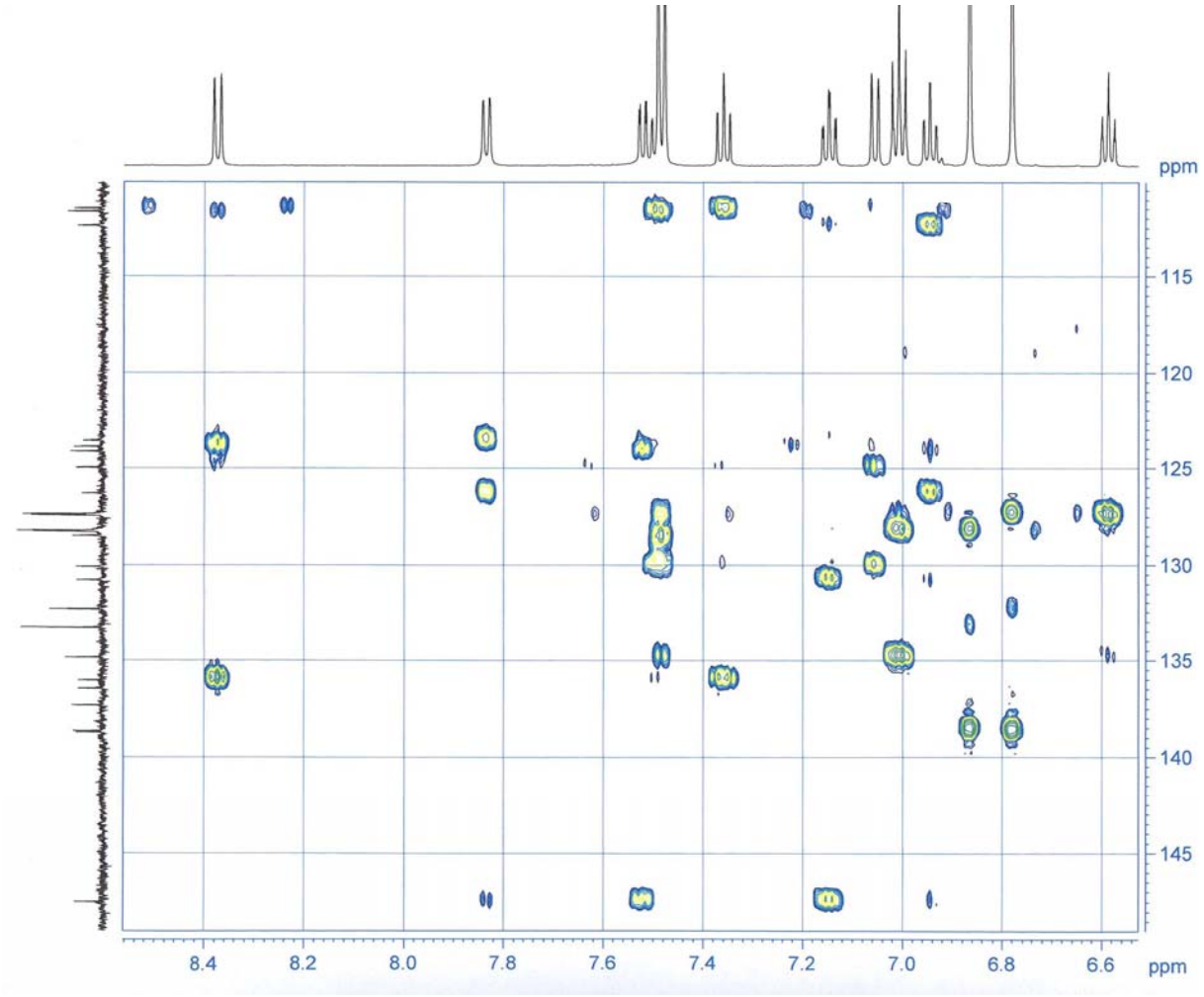

Figure S3. HMBC spectrum of complex **8**.

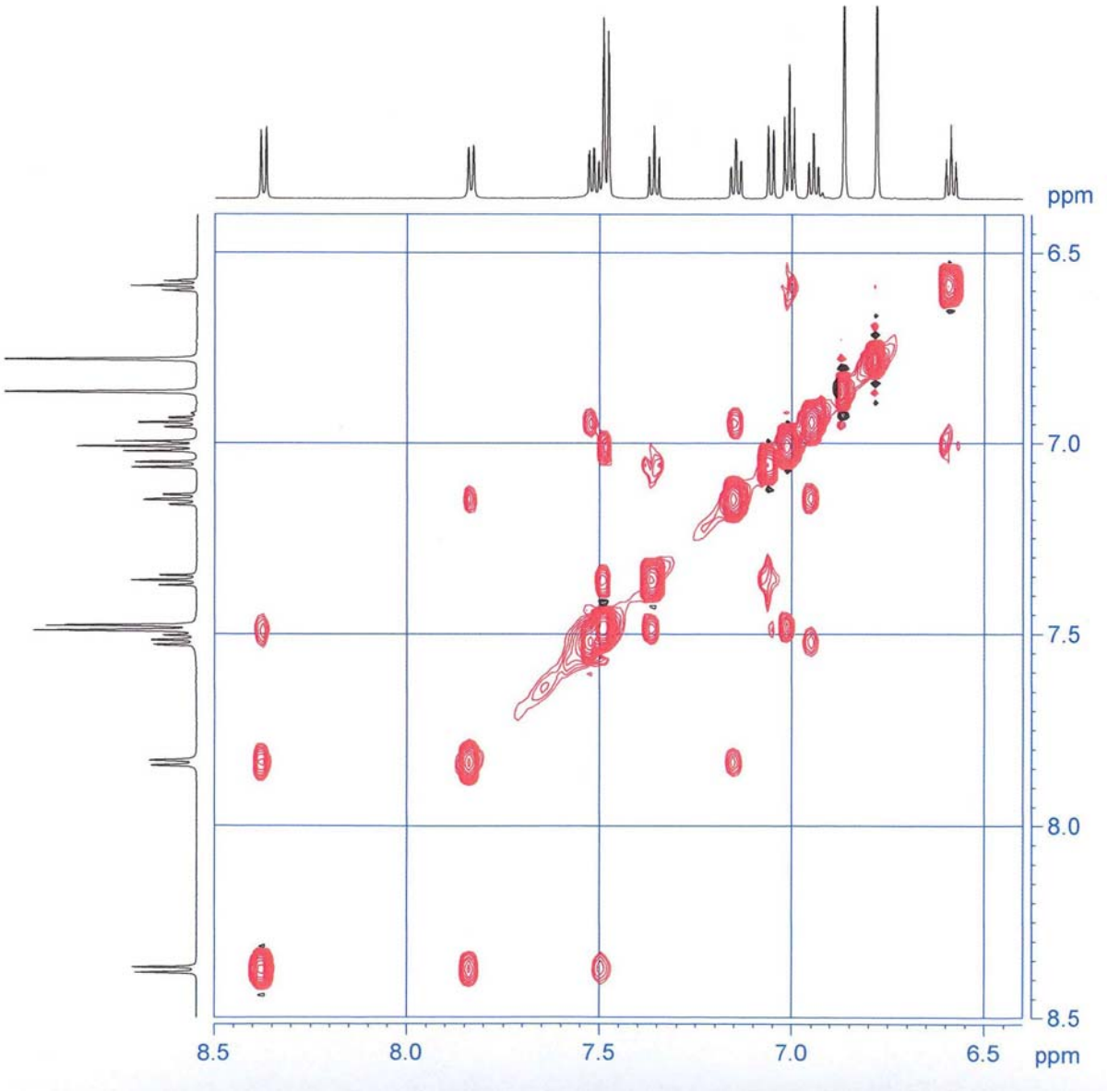

Figure S4. NOESY spectrum of complex **8**.

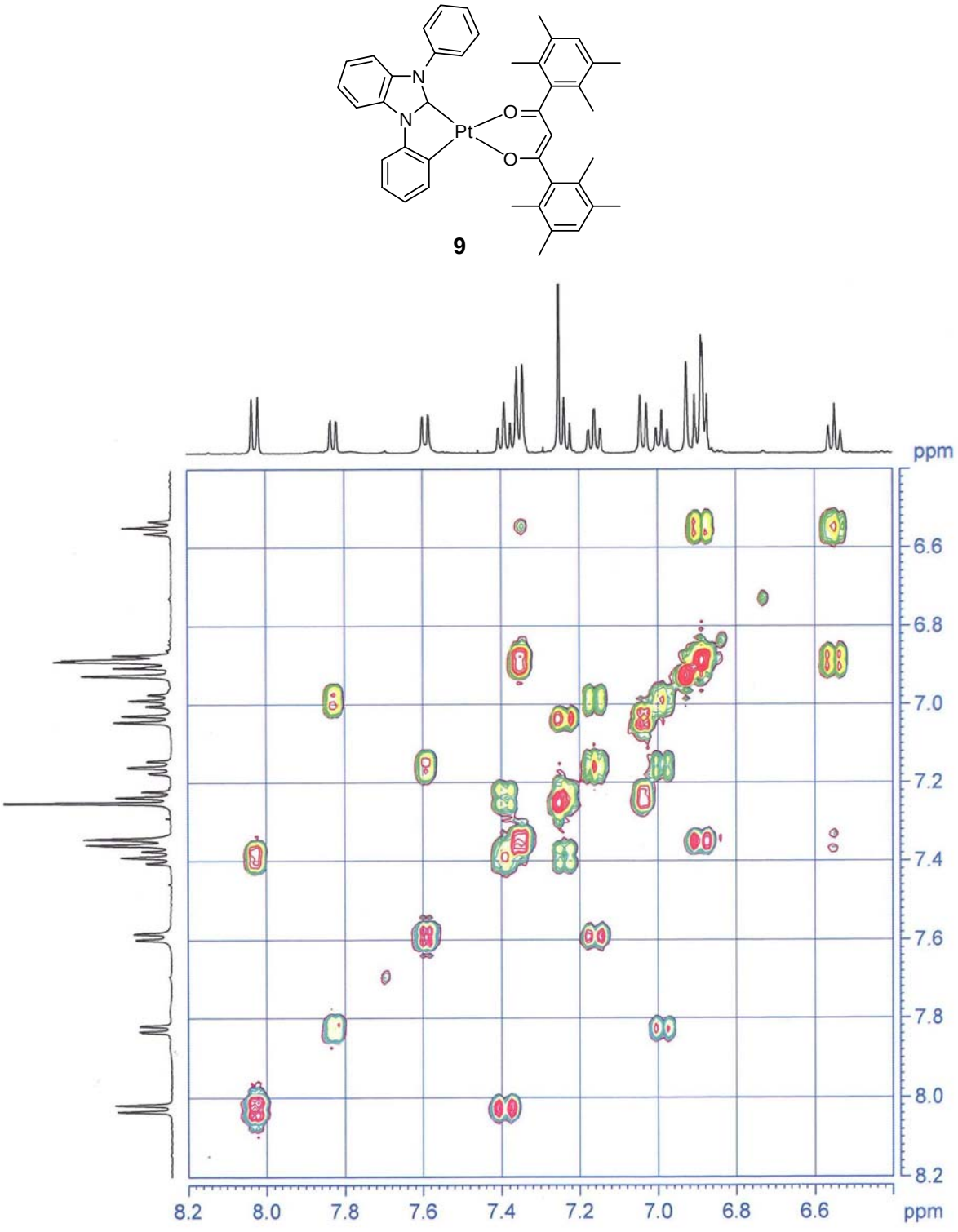

Figure S5. COSY spectrum of complex **9**.

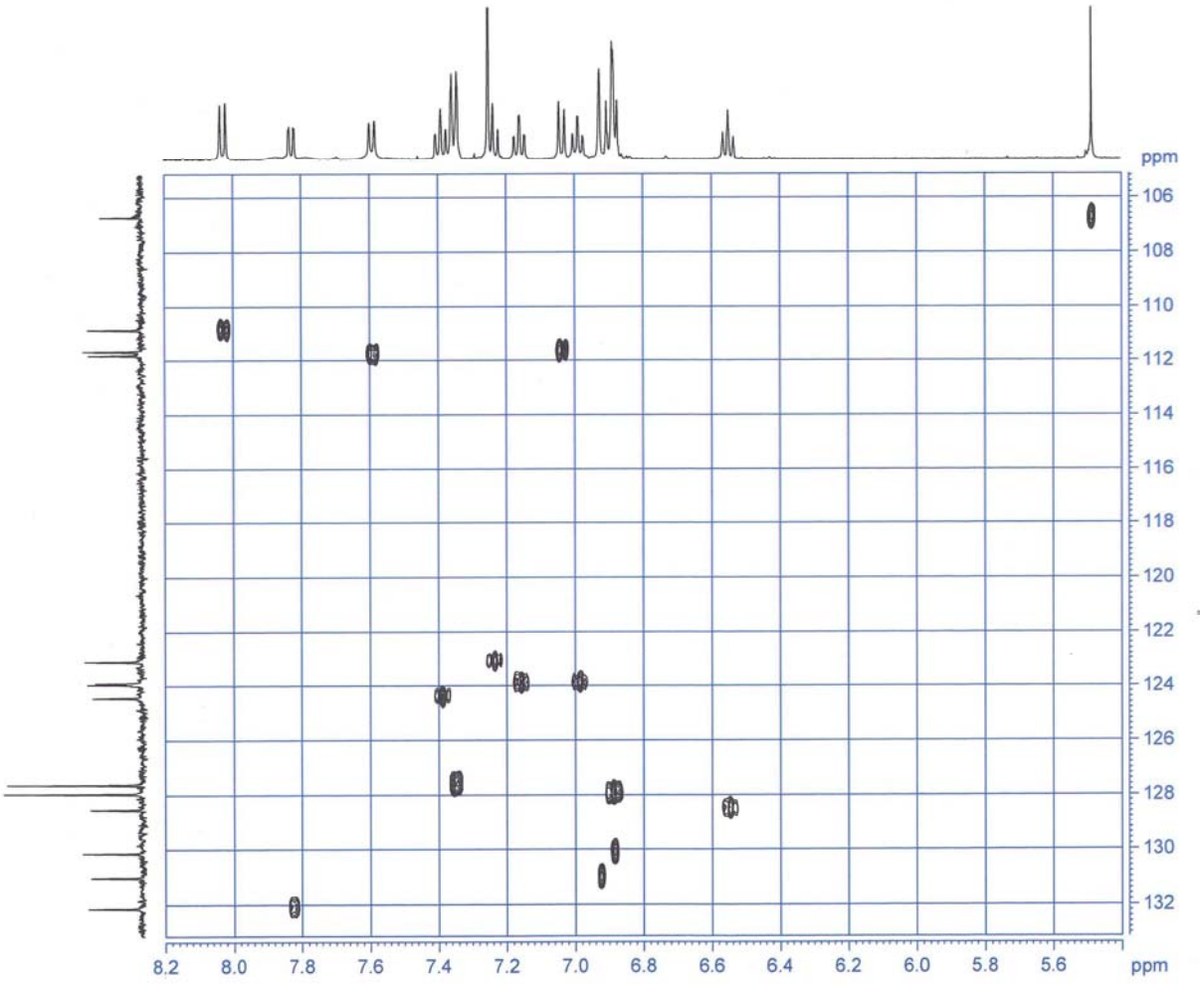

Figure S6. HSQC spectrum of complex **9**.

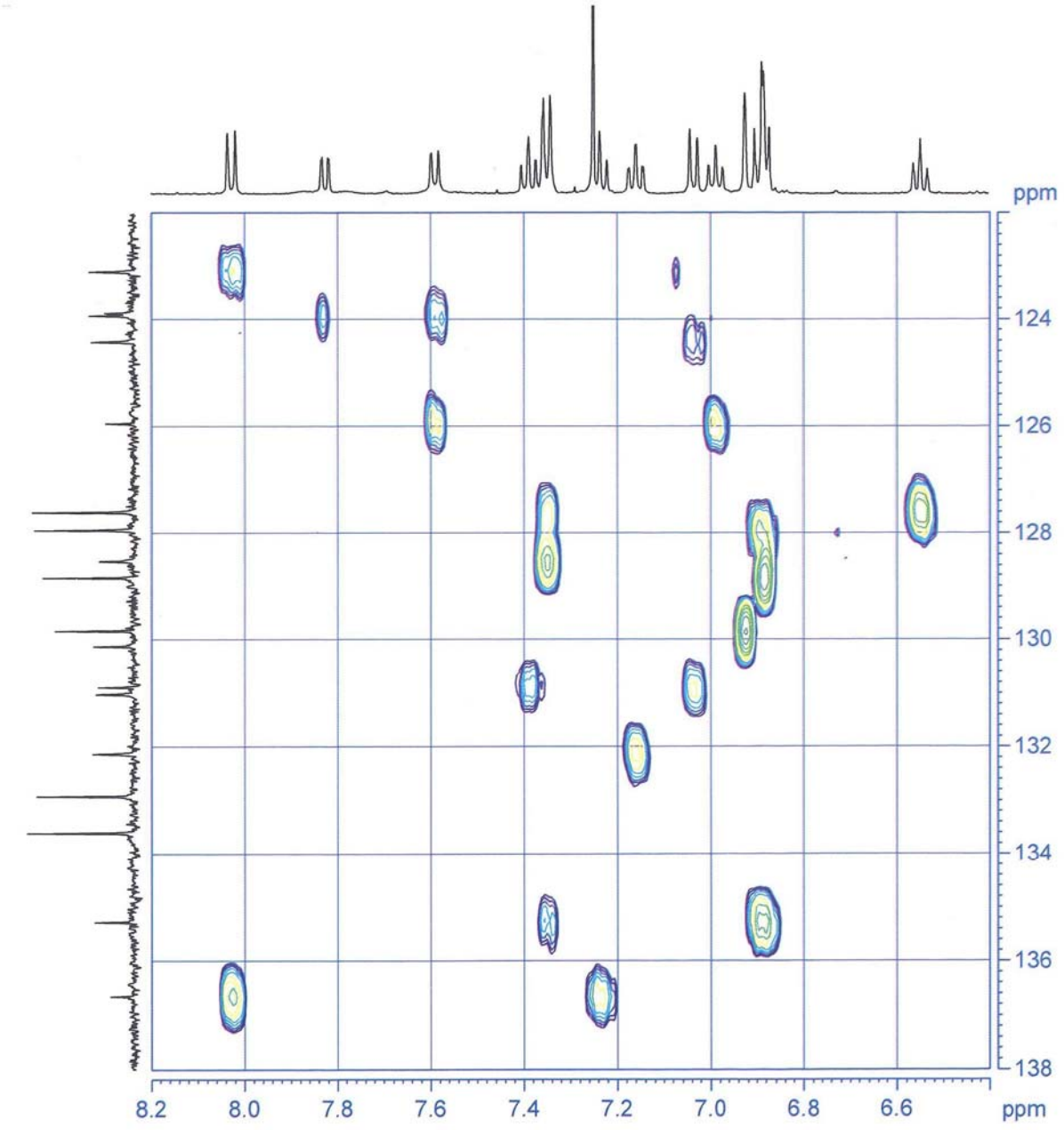

Figure S7. HMBC spectrum of complex **9**.

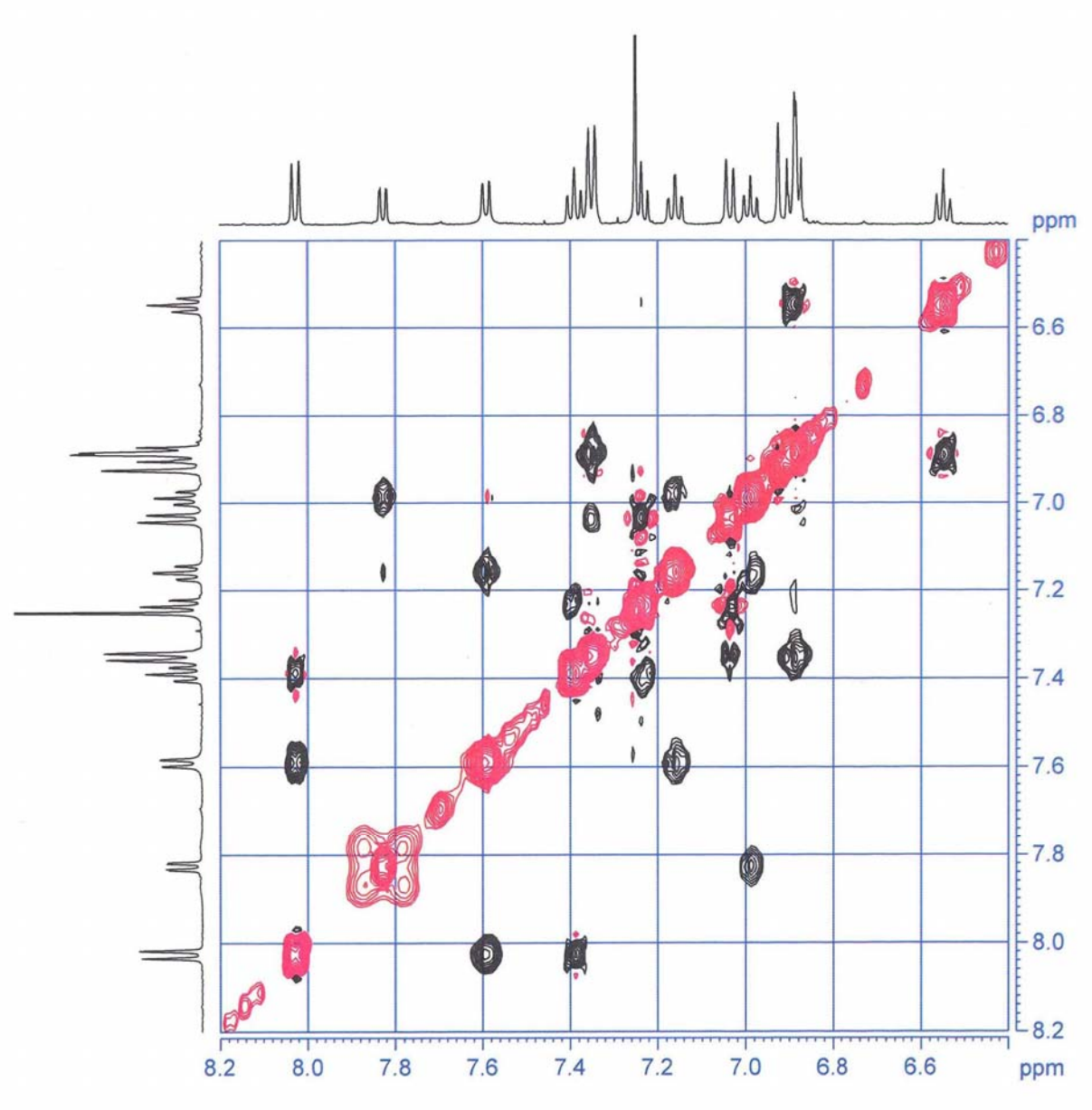

Figure S8. NOESY spectrum of complex **9**.

Solid-State Determination

In the following section the solid-state data for **5**–**8** and **12** are given.

Table S1. Crystal data and crystallographic details for **5**–**7**

Complex	**5**	**6**	**7**
CCDC #	1011748	1011749	1011750
empirical formula	$C_{25}H_{22}N_2O_2Pt$	$C_{30}H_{32}N_2O_2Pt$	$C_{34}H_{24}N_2O_2Pt$
formula weight [g/mol]	577.53	647.67	687.63
T [K]	198(2)	198(2)	198(2)
wavelength [Å]	0.71073	0.71073	0.71073
crystal system	monoclinic	monoclinic	trigonal
space group	*P* $2_1/c$	*P* $2_1/c$	*R* -3
a [Å]	9.9280(16)	12.228(3)	40.894(6)
b [Å]	17.328(4)	13.642(3)	40.894(6)
c [Å]	11.790(3)	16.0740(16)	9.1730(18)
α [°]	90	90	90
β [°]	95.749(16)	98.842(15)	90
γ [°]	90	90	120
U [$Å^3$]	2018.1(8)	2649.5(9)	13285(5)
Z	4	4	18
D_{calc} [Mg/m^3]	1.901	1.624	1.547
μ(MoKα) [mm^{-1}]	6.978	5.325	4.784
crystal size [mm^3]	0.24×0.52×0.83	0.19×0.24×0.40	0.11×0.17×0.62
F(000)	1120	1280	6048
reflections collected	41134	46271	106735
independent reflections	4129 R_{int} = 0.069	5397 R_{int} = 0.051	6028 R_{int} = 0.041
Goodness-of-fit on F^2	1.25	1.11	1.14
R_1 [I>2σ(I)]	0.0442	0.0234	0.0285
wR_2 [I>2σ(I)]	0.1289	0.0427	0.0678
data / restraints / parameters	4129 / 0 / 256	5397 / 0 / 323	6028 / 0 / 352

Table S2. Crystal data and crystallographic details for **8** and **12**

Complex	**8**	**12**
CCDC #	1011751	1011752
empirical formula	$C_{40}H_{36}N_2O_2Pt$	$C_{41}H_{38}N_2O_2Pt$
formula weight [g/mol]	771.80	785.81
T [K]	198(2)	198(2)
wavelength [Å]	0.71073	0.71073
crystal system	triclinic	triclinic
space group	*P* -1	*P* -1
a [Å]	12.0790(15)	10.545(3)
b [Å]	12.265(1)	13.434(2)
c [Å]	13.0310(12)	25.0600(19)
α [°]	71.096(5)	104.184(12)
β [°]	89.240(9)	91.124(11)
γ [°]	66.502(8)	90.253(15)
U [$Å^3$]	1659.9(3)	3441.0(11)
Z	2	4
D_{calc} [Mg/m^3]	1.544	1.517
μ(MoKα) [mm^{-1}]	4.264	4.115
crystal size [mm^3]	0.26×0.44×0.65	0.54×0.54×0.63
F(000)	768	1568
reflections collected	37065	44960
independent reflections	6797 R_{int} = 0.052	11747 R_{int} = 0.054
Goodness-of-fit on F^2	1.03	1.21
R_1 [I>2σ(I)]	0.0266	0.0557
wR_2 [I>2σ(I)]	0.0487	0.1613
data / restraints / parameters	6797 / 0 / 412	11747 / 0 / 829

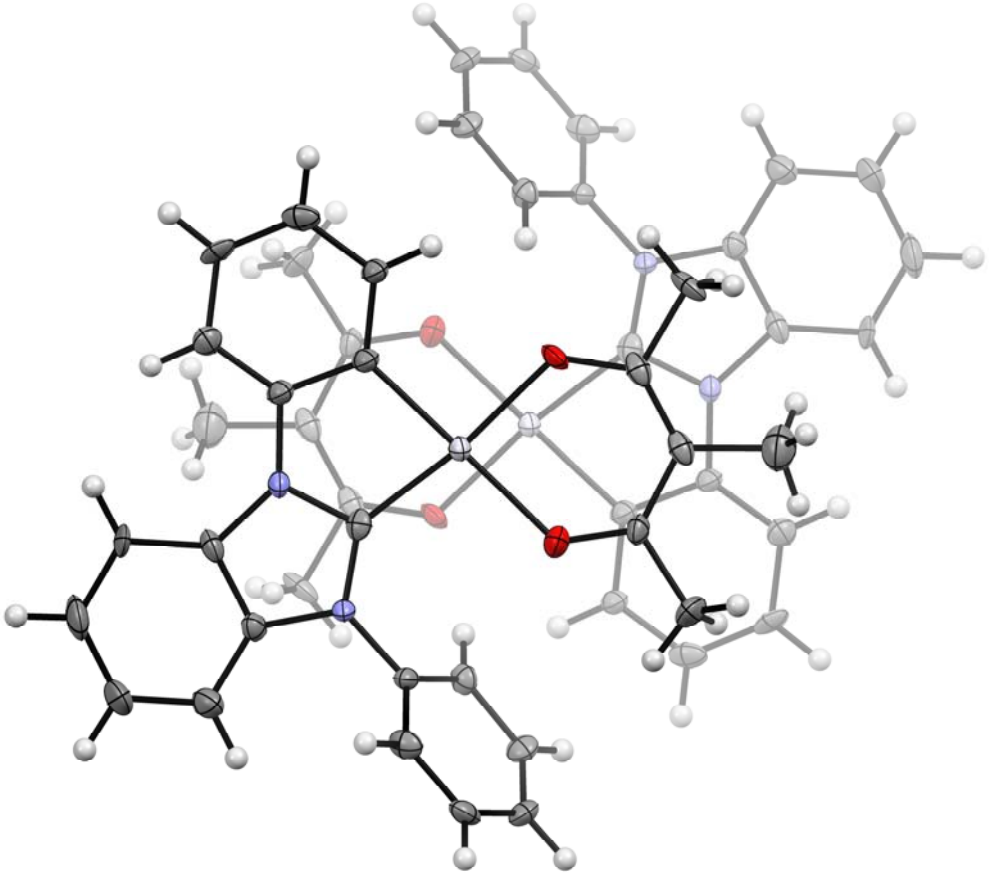

Figure S9. Molecule pair of complex **5** in the solid state.

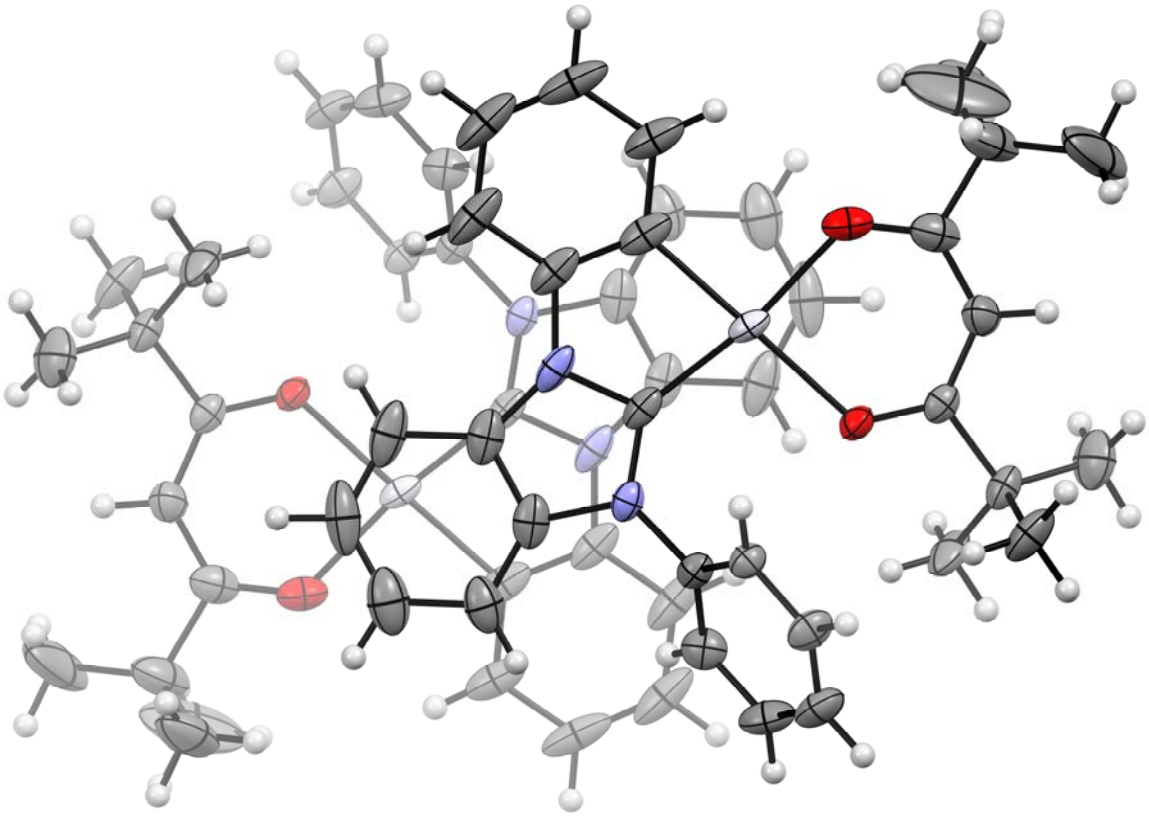

Figure S10. Molecule pair of complex **6** in the solid state.

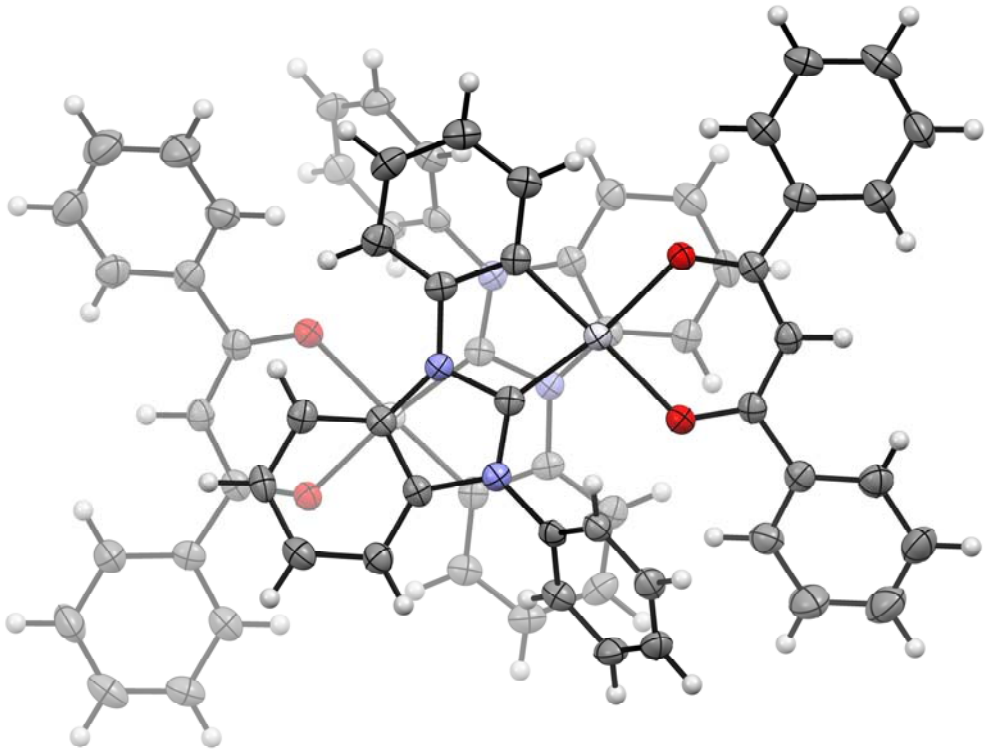

Figure S11. Molecule pair of complex **7** in the solid state.

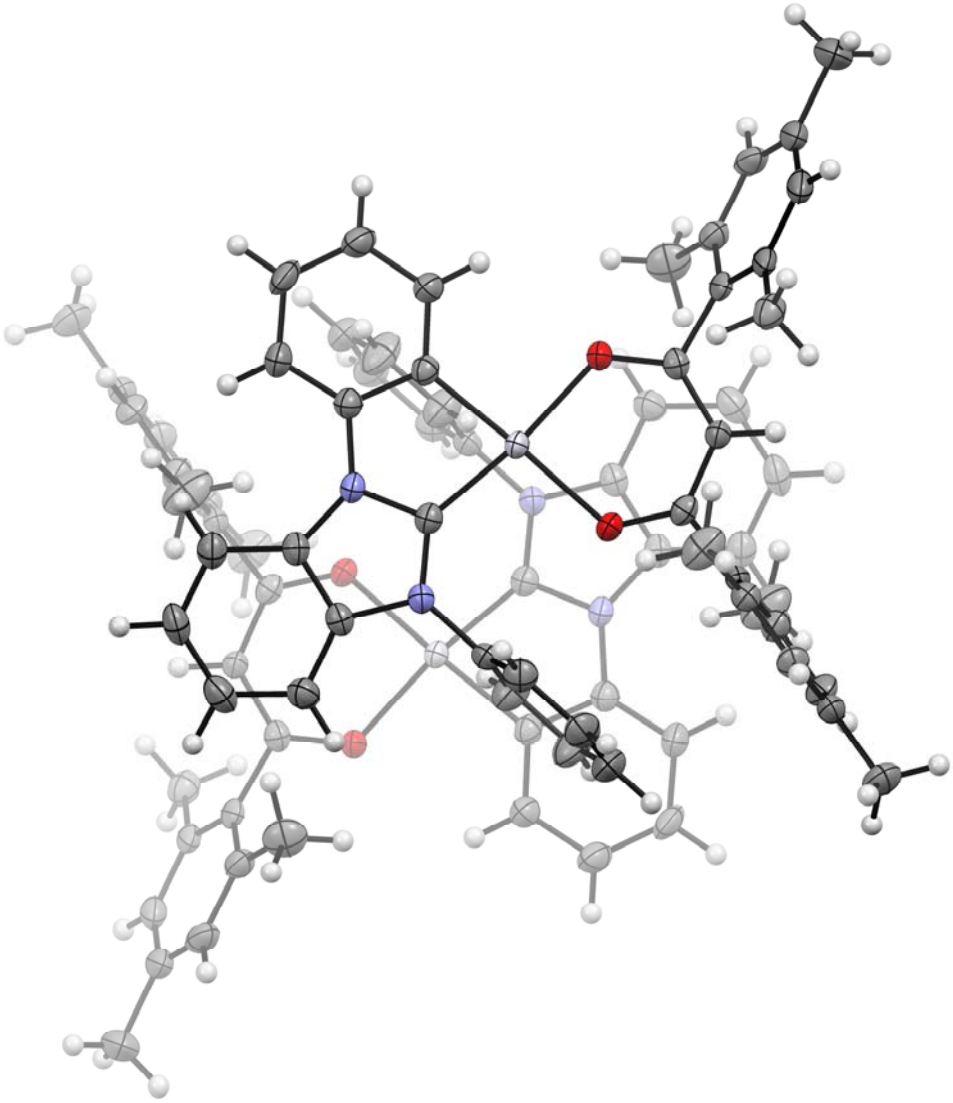

Figure S12. Molecule pair of complex **8** in the solid state.

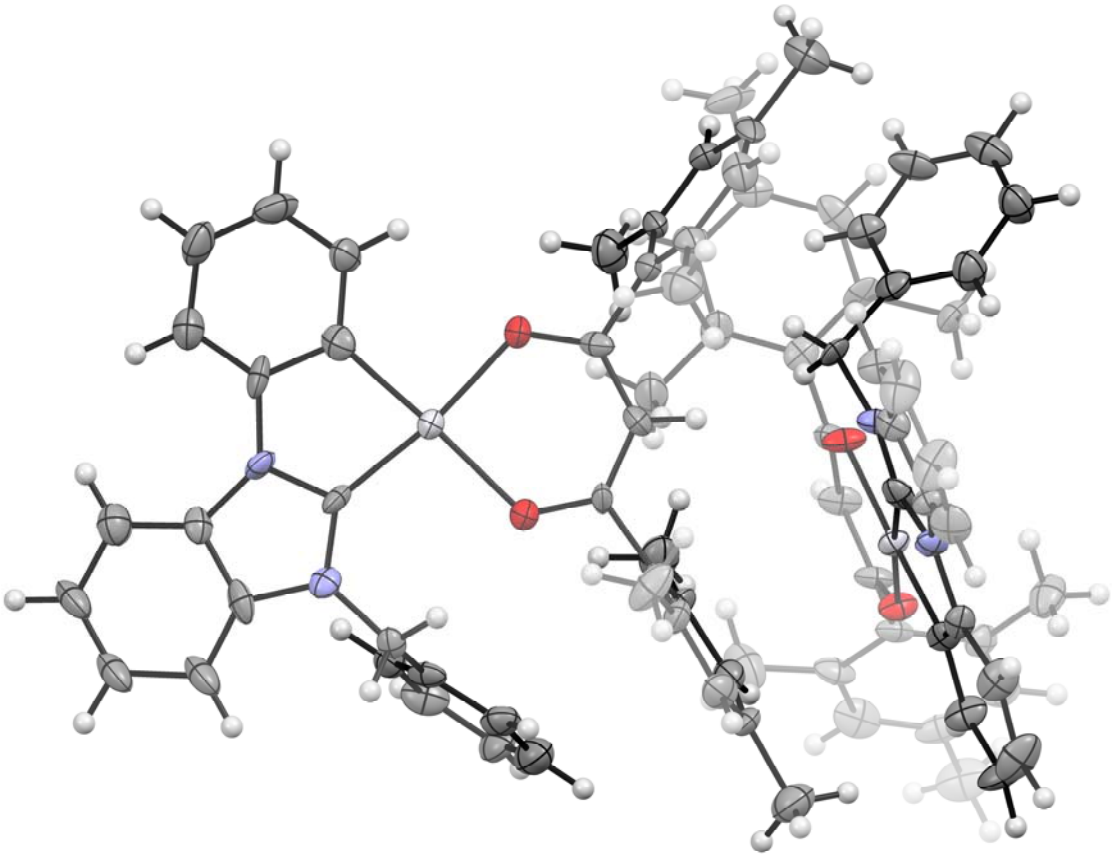

Figure S13. Molecule pair of complex **12** in the solid state.

Photoluminescence Data

In the following section additional photophysical data for the complexes are given.

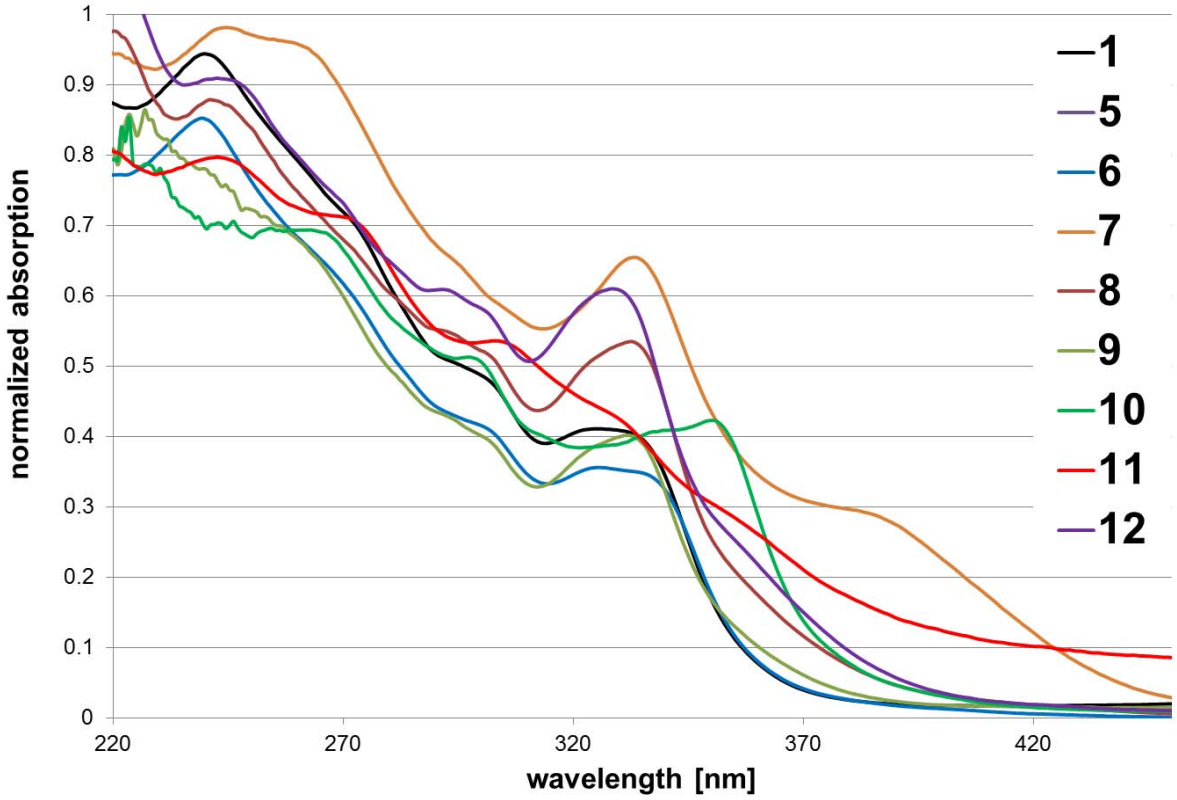

Figure S14. Absorption spectra for **5**–**12** and the reference complex **1** as 100% emitter films.

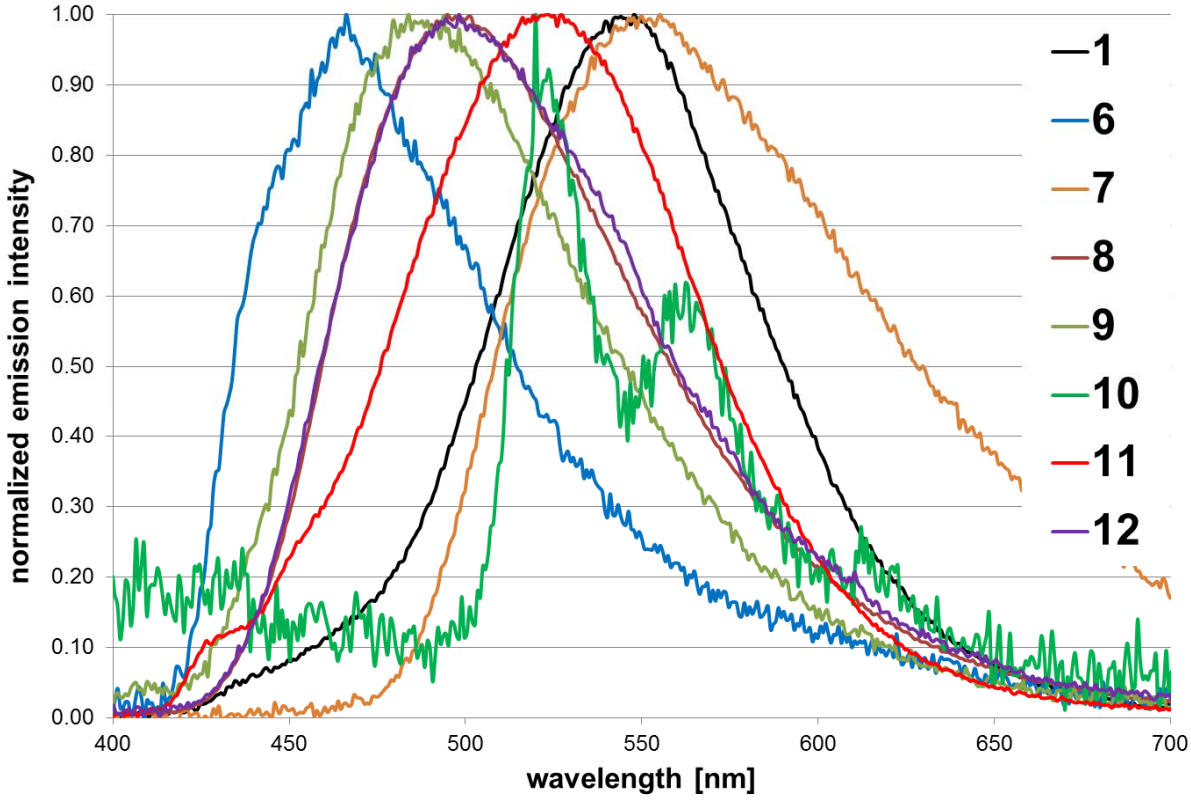

Figure S15. Normalized emission spectra for **6**–**12** and the reference complex **1** as 100% emitter films.

Device Details and Performance

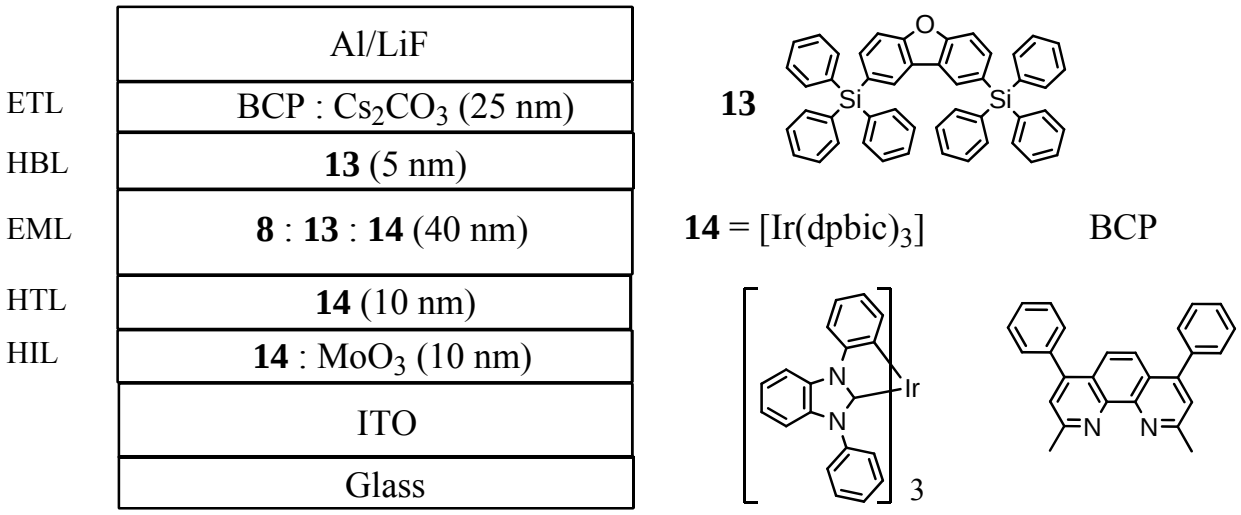

Figure S16. Device layout (left) and structure of **13** and **14** (right). ETL = electron-transport layer, HBL = hole-blocking layer, EML = emission layer, HTL = hole-transport layer, HIL = hole-injection layer. BCP = 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline.

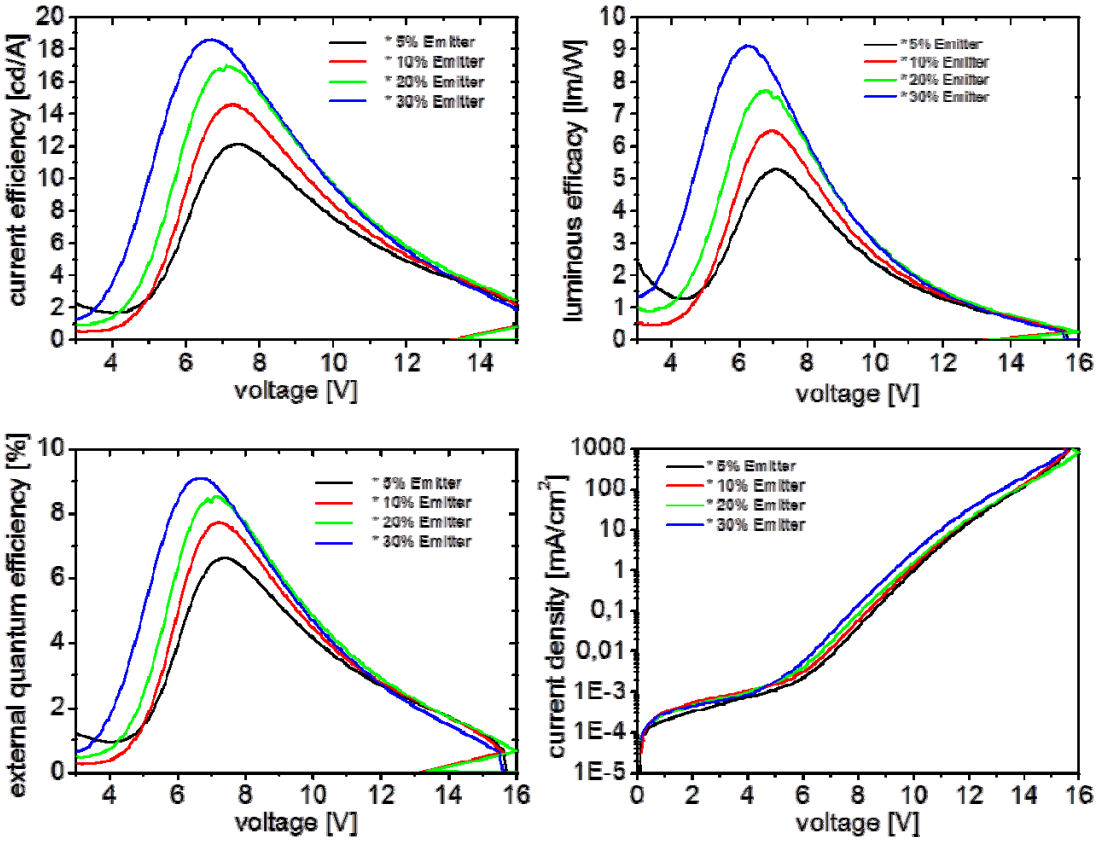

Figure S17. Single-matrix device data at different emitter (**8**) concentrations (5–30%) plotted against the voltage.

Quantum Chemical Calculations

Table S3. Comparison of bond lengths, angles and dihedral angles of **5** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.947(9)	1.951	1.961
Pt(1)-C(9)	1.990(9)	2.002	2.006
Pt(1)-O(1)	2.070(7)	2.132	2.138
Pt(1)-O(2)	2.037(7)	2.074	2.071
O(1)-Pt(1)-O(2)	88.1(3)	86.43	84.94
C(1)-Pt(1)-C(9)	80.6(4)	79.86	79.88
Pt(1)-C(1)-N(1)-C(8)	3.3(1)	2.40	3.02
N(1)-C(1)-Pt(1)-O(1)	175.6(7)	175.63	174.02

Table S4. Comparison of bond lengths, angles and dihedral angles of **6** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.933(4)	1.958	1.967
Pt(1)-C(9)	1.991(3)	2.000	2.004
Pt(1)-O(1)	2.100(2)	2.161	2.137
Pt(1)-O(2)	2.037(3)	2.082	2.072
O(1)-Pt(1)-O(2)	88.79(10)	87.40	86.65
C(1)-Pt(1)-C(9)	79.51(16)	79.99	79.88
Pt(1)-C(1)-N(1)-C(8)	-7.3(4)	-5.01	5.79
N(1)-C(1)-Pt(1)-O(1)	-168.9(2)	-170.02	167.03

Table S5. Comparison of bond lengths, angles and dihedral angles of **7** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.923(4)	1.957	1.969
Pt(1)-C(9)	1.988(5)	1.999	1.946
Pt(1)-O(1)	2.088(4)	2.158	2.134
Pt(1)-O(2)	2.042(3)	2.086	2.131
O(1)-Pt(1)-O(2)	89.35(13)	87.84	87.84
C(1)-Pt(1)-C(9)	79.90(19)	80.05	80.91
Pt(1)-C(1)-N(1)-C(8)	-7.4(4)	-4.05	12.41
N(1)-C(1)-Pt(1)-O(1)	-170.2(3)	-172.81	163.00

Table S6. Comparison of bond lengths, angles and dihedral angles of **8** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.923(3)	1.954	1.966
Pt(1)-C(9)	1.985(3)	2.000	1.946
Pt(1)-O(1)	2.074(2)	2.157	2.137
Pt(1)-O(2)	2.041(2)	2.091	2.131
O(1)-Pt(1)-O(2)	89.68(9)	88.22	88.20
C(1)-Pt(1)-C(9)	79.87(13)	80.07	80.98
Pt(1)-C(1)-N(1)-C(8)	2.8(4)	-1.18	-8.87
N(1)-C(1)-Pt(1)-O(1)	174.7(3)	-177.75	-170.11

Table S7. Comparison of bond lengths, angles and dihedral angles of **12** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**X-ray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.950(12)	1.957	1.956
Pt(1)-C(9)	1.983(12)	2.000	1.946
Pt(1)-O(1)	2.074(8)	2.160	2.148
Pt(1)-O(2)	2.062(8)	2.093	2.120
O(1)-Pt(1)-O(2)	89.9(3)	88.08	88.30
C(1)-Pt(1)-C(9)	79.9(5)	80.04	80.79
Pt(1)-C(1)-N(1)-C(8)	0.3(13)	0.57	2.50
N(1)-C(1)-Pt(1)-O(1)	-177.8(9)	178.06	177.79

Table S8. Data for the wavelength prediction (BP86/6-31G(d)).

Complex	S-T gap [eV]	λ_{max} uncorr. [nm]	S-T gap corr. [eV]	λ_{max} corr. [nm]	λ_{max} exp. [nm]
6	2.20	564	2.59	479	461
7	1.97	630	2.35	527	520
8	2.22	559	2.61	475	473
9	2.22	559	2.61	475	465
10	2.04	607	2.43	510	517
11	2.40	516	2.80	443	454
12	2.23	555	2.63	472	476

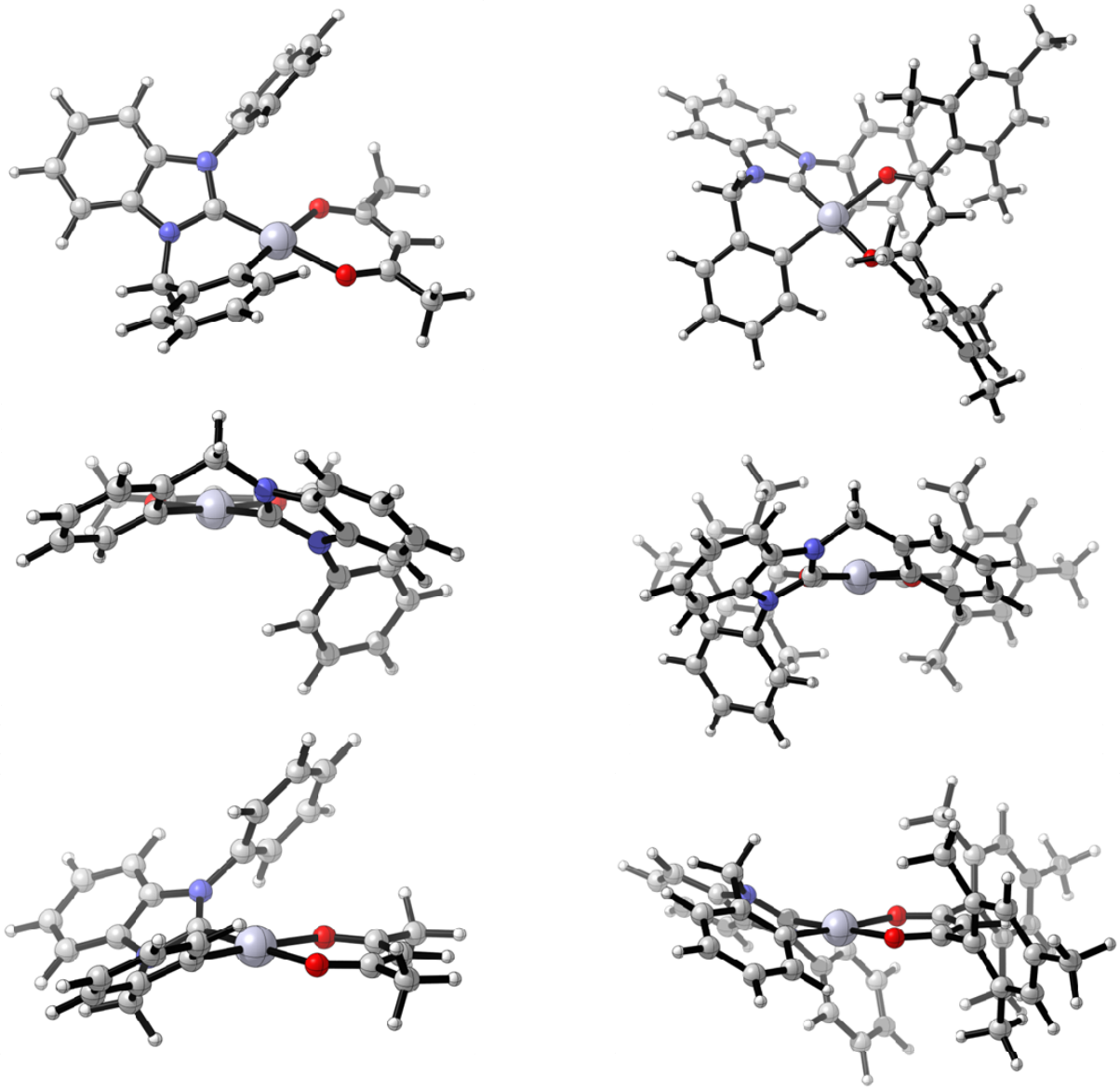

Figure S18. Possible isomers of complex **11** (**11iso**, left) and **12** (**12iso**, right) in the S_0 ground state with cyclometalation to the benzyl ring (B3LYP/6-31G(d)).

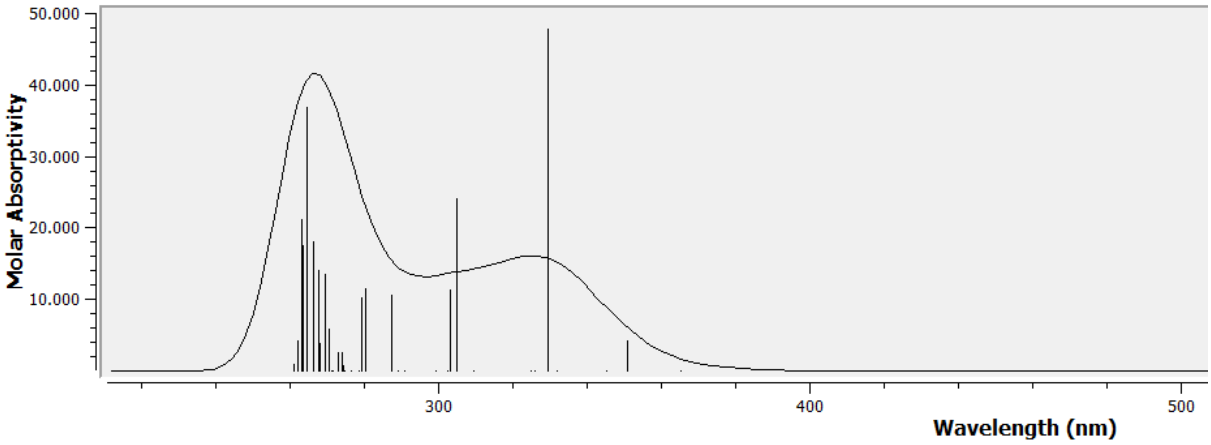

Figure S19. Gaussian shaped absorption spectra and transitions of complex **5** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

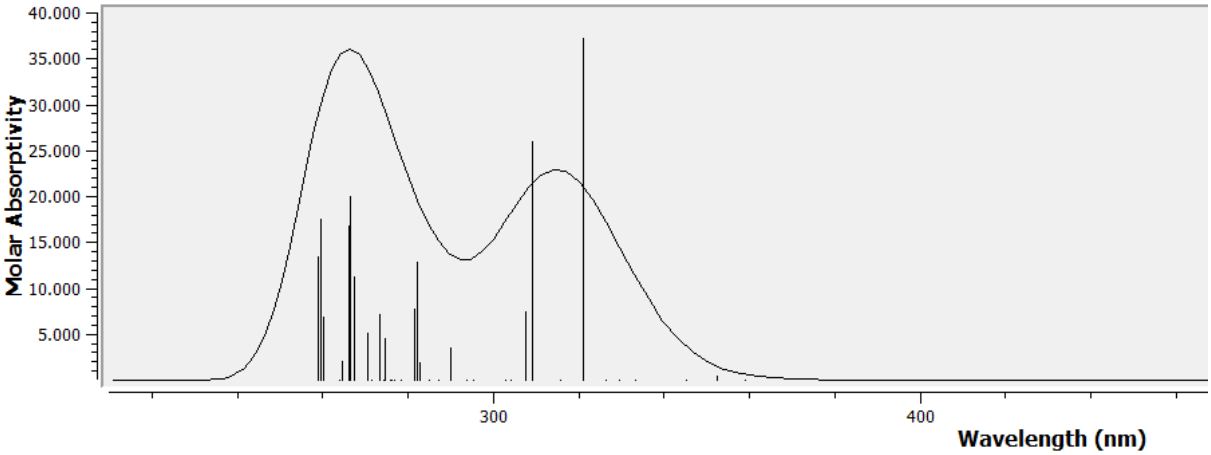

Figure S20. Gaussian shaped absorption spectra and transitions of complex **6** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

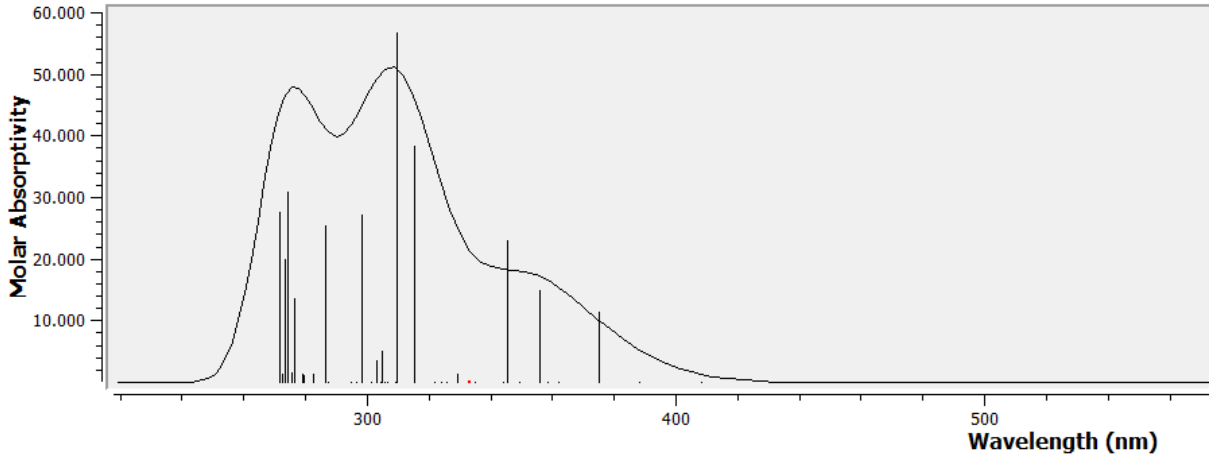

Figure S21. Gaussian shaped absorption spectra and transitions of complex **7** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

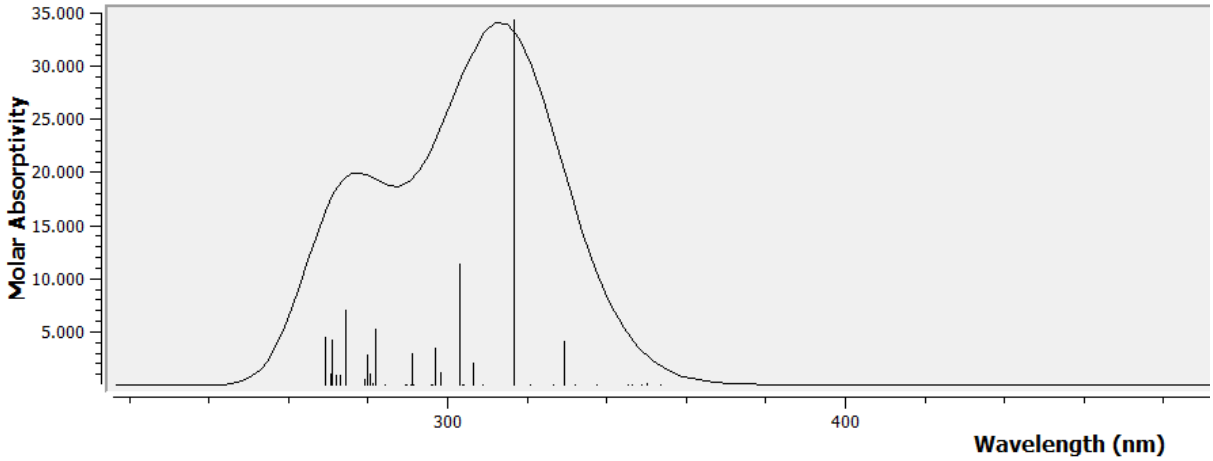

Figure S22. Gaussian shaped absorption spectra and transitions of complex **8** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

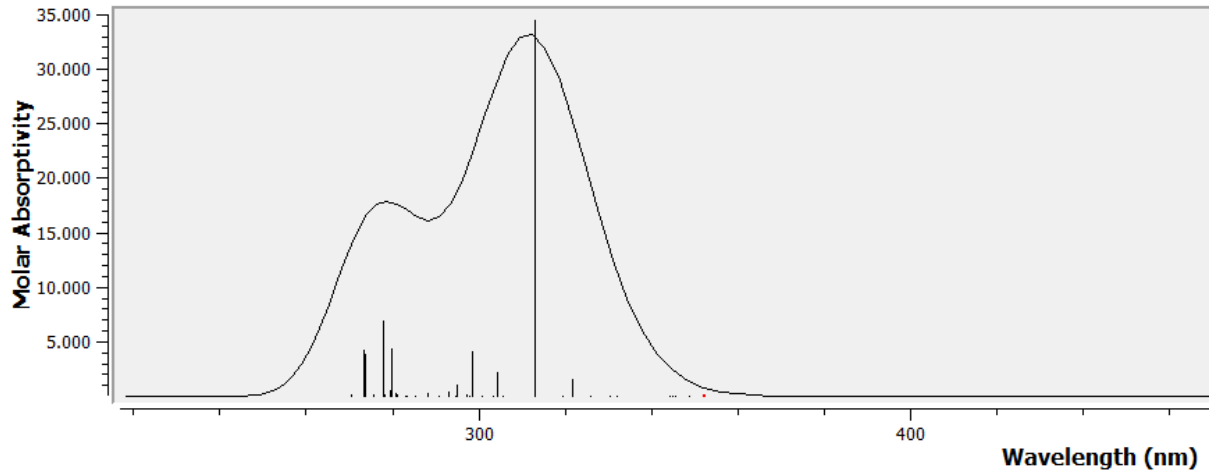

Figure S23. Gaussian shaped absorption spectra and transitions of complex **9** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

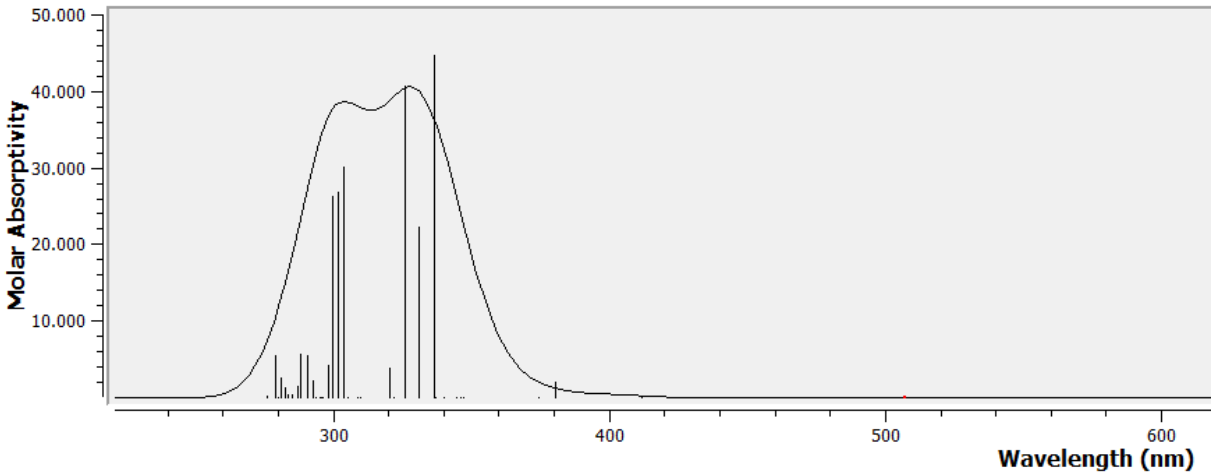

Figure S24. Gaussian shaped absorption spectra and transitions of complex **10** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

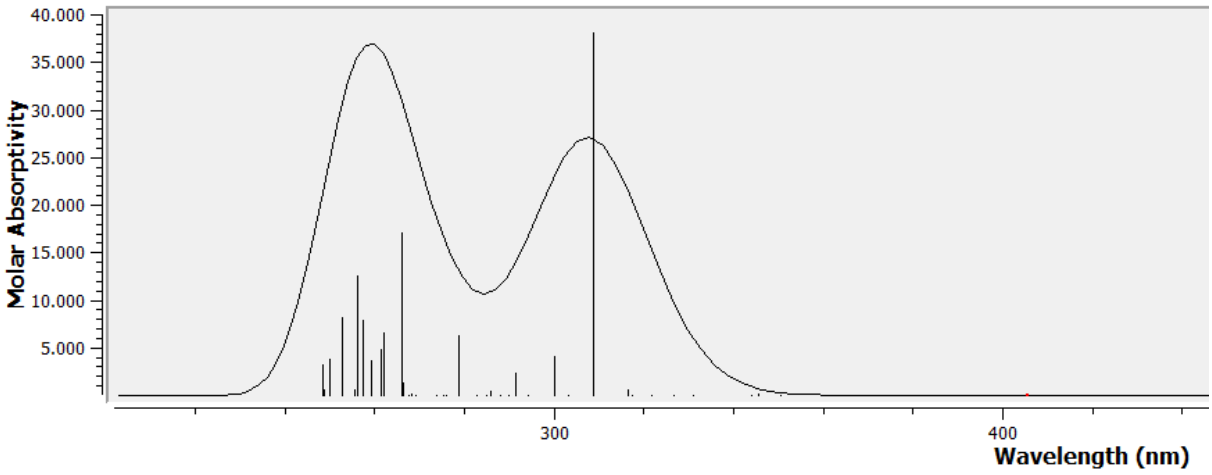

Figure S25. Gaussian shaped absorption spectra and transitions of complex **11** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

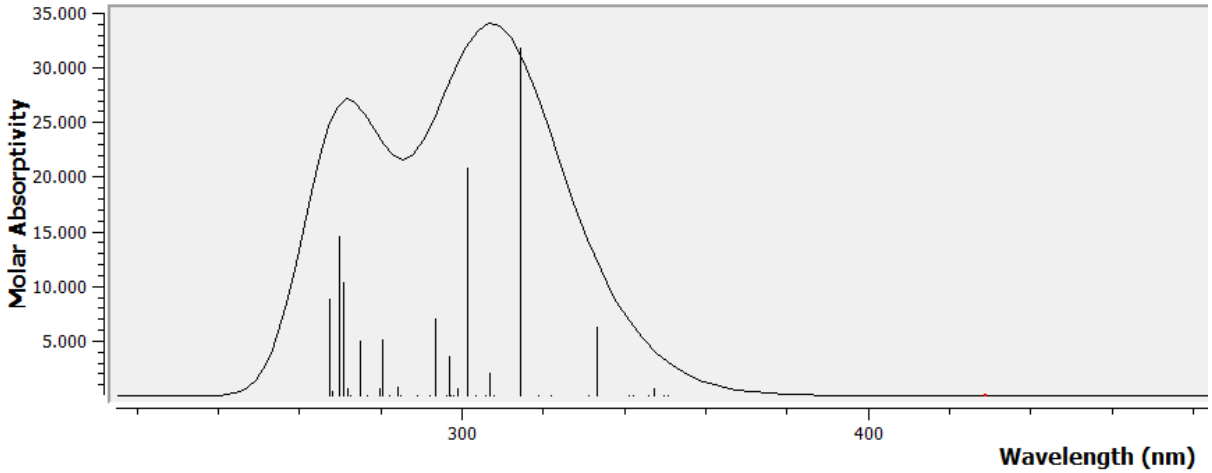

Figure S26. Gaussian shaped absorption spectra and transitions of complex **12** calculated by TD-B3LYP/CPCM (DCM) at the singlet S_0 ground state.

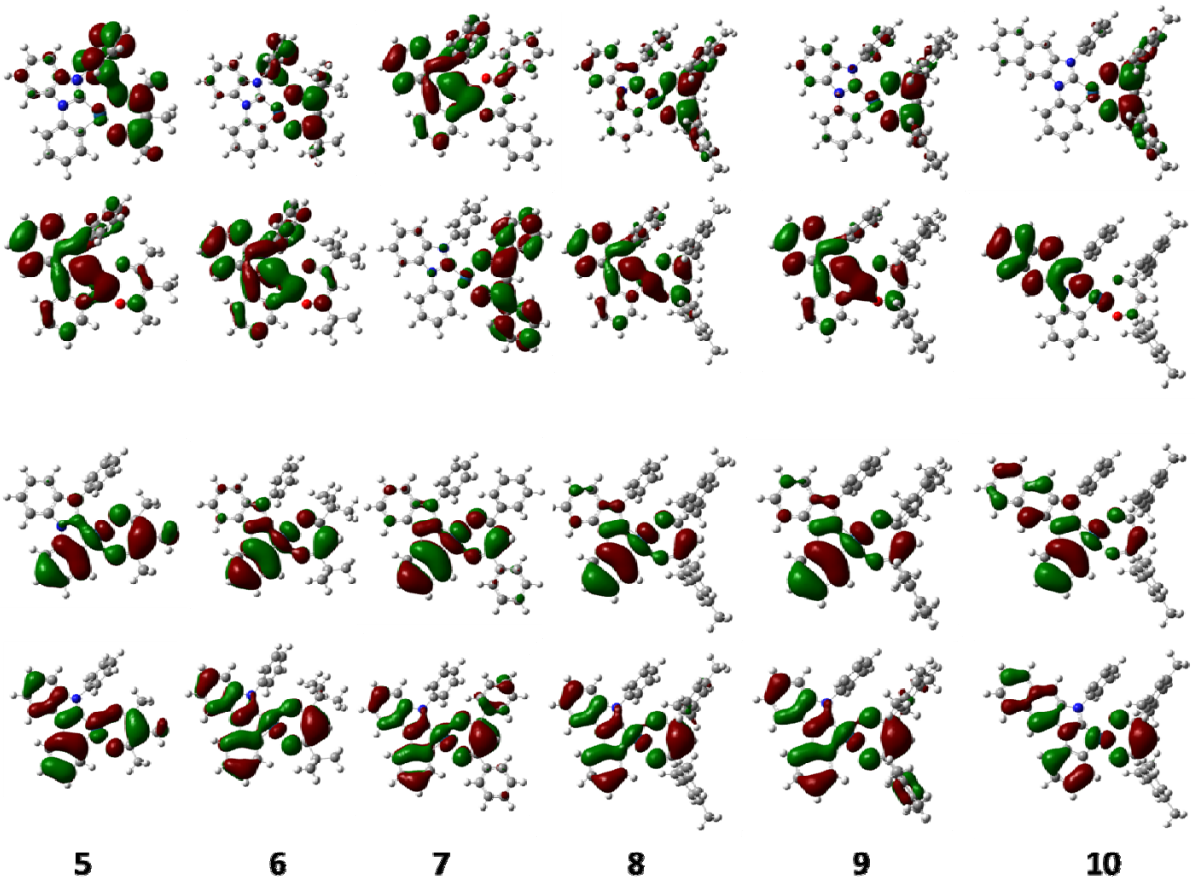

Figure S27. Frontier molecular orbitals (LUMO+1, LUMO, HOMO, HOMO-1 from top to bottom) of the complexes **5**–**10** computed on the singlet S_0 ground state (B3LYP/6-31G(d), isovalue = 0.02).

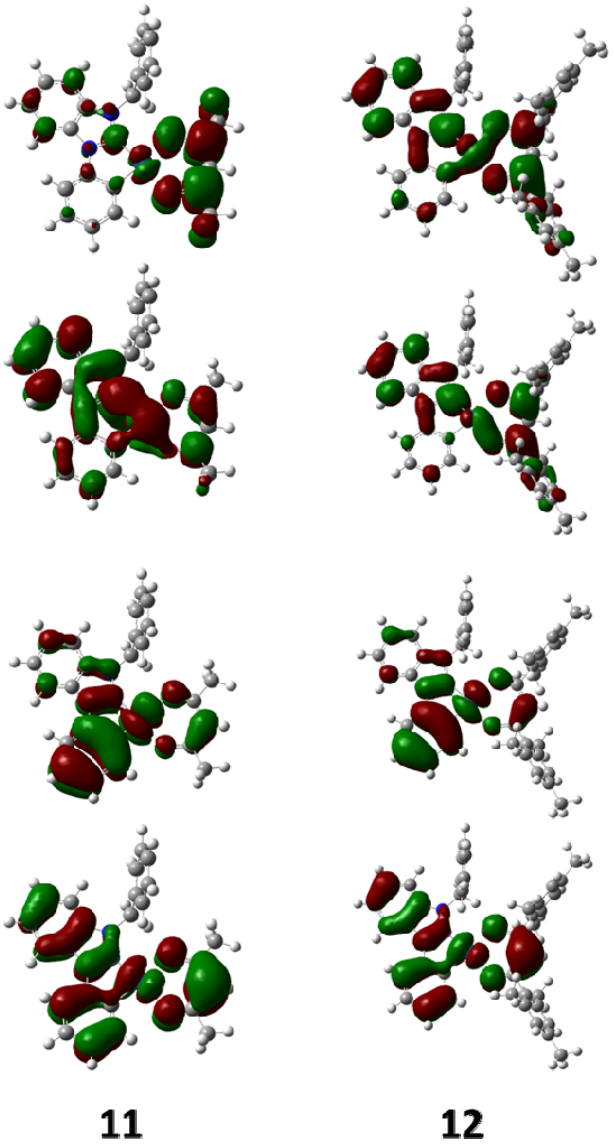

Figure S28. Frontier molecular orbitals (LUMO+1, LUMO, HOMO, HOMO-1 from top to bottom) of the complexes **11** and **12** computed on the singlet S_0 ground state (B3LYP/6-31G(d), isovalue = 0.02).

In the following section the singlet S_0 ground state geometries for **5**–**12** are given (B3LYP/6-31G(d)).

Coordinates for the optimized singlet ground state of **5**.

Pt	0.72873	-0.63530	0.00216
C	-0.20668	-2.40435	0.05362
C	0.39236	-3.66467	0.10331
C	-1.61540	-2.35518	0.01516
C	-0.38621	-4.82846	0.11529
H	1.47560	-3.73075	0.13096
C	-2.40837	-3.49955	0.02590
C	-1.77783	-4.74721	0.07656
H	-3.48975	-3.44873	-0.00079
H	-2.38240	-5.64994	0.08610
C	-1.12948	-0.04154	-0.00280
N	-2.10138	-1.01343	-0.02349
N	-1.77814	1.15864	-0.01564
O	1.73136	1.24222	-0.12391
C	3.76191	-0.92218	-0.04073
C	2.98916	1.44042	-0.16234
C	4.02022	0.46444	-0.09748
C	4.91072	-1.92127	-0.02744
H	5.58377	-1.77969	-0.88017
H	5.51212	-1.82652	0.88481
H	4.49384	-2.92913	-0.06655
C	3.37118	2.90672	-0.29589
H	2.46544	3.49478	-0.45123
H	3.87450	3.26644	0.61064
H	4.06210	3.07015	-1.13077
O	2.61513	-1.49635	-0.00355
H	0.09756	-5.80149	0.15490
C	-1.17951	2.45927	0.08020
C	-0.61982	2.87363	1.28951
C	-1.21934	3.31507	-1.02190
C	-0.09233	4.16003	1.39345
H	-0.59508	2.18766	2.12983
C	-0.69258	4.60262	-0.90896
H	-1.65156	2.96851	-1.95569
C	-0.13119	5.02640	0.29792
H	0.34675	4.48599	2.33197
H	-0.71930	5.27144	-1.76451
H	0.27514	6.03038	0.38458
C	-3.37325	-0.44015	-0.06173
C	-3.16506	0.95264	-0.05358
C	-4.67163	-0.95645	-0.10002
C	-4.21916	1.86165	-0.06792
C	-5.72995	-0.04725	-0.12149
H	-4.86801	-2.01993	-0.11418
C	-5.51167	1.33887	-0.10328
H	-4.03579	2.93052	-0.05343
H	-6.74702	-0.42670	-0.15219
H	-6.36047	2.01593	-0.11707
C	5.45959	0.95699	-0.13302
H	5.76778	1.29614	-1.13340
H	5.61952	1.80056	0.54827
H	6.16510	0.18157	0.16903

Coordinates for the optimized singlet ground state of **6**.

Pt	-0.30551	-0.62914	0.06289
C	0.39470	-2.50273	0.08240
C	-0.35762	-3.67439	0.18635
C	1.78802	-2.63660	-0.07635
C	0.25916	-4.93003	0.13000
H	-1.43299	-3.59986	0.30894
C	2.42099	-3.87547	-0.14058
C	1.63986	-5.03075	-0.03558
H	3.49224	-3.96749	-0.26581
H	2.11950	-6.00446	-0.08283
C	1.61802	-0.27447	-0.01697
N	2.44202	-1.37053	-0.13743
N	2.43462	0.82049	-0.00835
O	-1.10669	1.36931	-0.12433
C	-3.34822	-0.62345	0.01235
C	-2.33790	1.65958	-0.28430
C	-3.41978	0.75668	-0.21468
H	-4.40440	1.17349	-0.34221
C	-4.62724	-1.48779	0.11629
C	-2.60677	3.16511	-0.54285
O	-2.27233	-1.30783	0.14382
H	-0.34303	-5.83148	0.21373
C	2.07208	2.18003	0.26850
C	2.30329	3.16054	-0.69883
C	1.60366	2.52404	1.53793
C	2.07360	4.50158	-0.38578
H	2.66037	2.87076	-1.68239
C	1.37274	3.86586	1.84045
H	1.43226	1.74561	2.27415
C	1.61397	4.85568	0.88413
H	2.25284	5.26654	-1.13579
H	1.01208	4.13803	2.82823
H	1.44043	5.90005	1.12756
C	3.77935	-0.98259	-0.22323
C	3.77549	0.42135	-0.13445
C	4.98557	-1.67587	-0.36185
C	4.95003	1.16914	-0.15541
C	6.16277	-0.92820	-0.39439
H	5.02532	-2.75327	-0.44395
C	6.14962	0.47086	-0.28874
H	4.92765	2.24987	-0.07105
H	7.11081	-1.44666	-0.50274
H	7.08609	1.01993	-0.31161
C	-5.93490	-0.68746	-0.01195
H	-6.02712	0.07470	0.76998

H	-6.02144	-0.19476	-0.98687
H	-6.78861	-1.36793	0.08857
C	-4.57521	-2.54556	-1.01077
H	-3.65774	-3.13666	-0.95204
H	-5.43395	-3.22337	-0.93276
H	-4.60963	-2.06928	-1.99809
C	-4.60798	-2.19420	1.49195
H	-4.66746	-1.46472	2.30884
H	-5.46647	-2.87084	1.58028
H	-3.69086	-2.77401	1.62201
C	-4.05214	3.48193	-0.96948
H	-4.34329	2.92968	-1.87011
H	-4.77729	3.25947	-0.17892
H	-4.13673	4.55183	-1.19445
C	-2.29827	3.91883	0.77118
H	-1.27406	3.72477	1.09702
H	-2.41965	4.99963	0.62562
H	-2.98110	3.60705	1.57104
C	-1.64910	3.64103	-1.65698
H	-1.76308	4.72044	-1.81503
H	-0.61053	3.43185	-1.39514
H	-1.87117	3.13643	-2.60540

Coordinates for the optimized singlet ground state of **7**.

Pt	-0.00411	-0.74811	0.03386
C	0.65120	-2.63712	0.03709
C	-0.13045	-3.79179	0.10992
C	2.04600	-2.79991	-0.07727
C	0.46024	-5.06024	0.05821
H	-1.20633	-3.69387	0.21125
C	2.65261	-4.05202	-0.13665
C	1.84257	-5.19017	-0.06919
H	3.72492	-4.16688	-0.23016
H	2.30144	-6.17398	-0.11319
C	1.92712	-0.43588	0.00083
N	2.73015	-1.54804	-0.10009
N	2.76256	0.64314	0.04108
O	-0.72945	1.28181	-0.06945
C	-3.04276	-0.63655	0.02120
C	-1.95775	1.62649	-0.11155
C	-3.07270	0.76328	-0.06412
H	-4.04484	1.21803	-0.19329
O	-1.99354	-1.37405	0.06325
H	-0.16358	-5.94882	0.11714
C	2.40117	2.01233	0.26782
C	2.75317	2.97706	-0.67950
C	1.78128	2.37772	1.46384
C	2.49481	4.32340	-0.41625
H	3.22374	2.67200	-1.60930
C	1.51414	3.72332	1.71144
H	1.51231	1.61139	2.18301
C	1.87738	4.69761	0.77895
H	2.77271	5.07625	-1.14857
H	1.02506	4.01047	2.63752
H	1.67340	5.74512	0.98089
C	4.07730	-1.18665	-0.13489
C	4.09872	0.21713	-0.03892
C	5.27299	-1.90507	-0.22912
C	5.28938	0.93915	-0.00938
C	6.46603	-1.18268	-0.21192
H	5.29291	-2.98296	-0.31235
C	6.47802	0.21590	-0.09935
H	5.28711	2.01941	0.08210
H	7.40651	-1.72071	-0.28493
H	7.42603	0.74498	-0.08139
C	-4.33383	-1.39517	0.02921
C	-4.36343	-2.69415	-0.50312
C	-5.51480	-0.85763	0.56481
C	-5.54780	-3.42772	-0.51864
H	-3.44975	-3.11077	-0.91317
C	-6.69695	-1.59736	0.56033
H	-5.50277	0.13078	1.01366
C	-6.71888	-2.88213	0.01348
H	-5.55774	-4.42691	-0.94605
H	-7.60007	-1.17187	0.98979
H	-7.64158	-3.45636	0.00667
C	-2.20656	3.09765	-0.26695
C	-1.24934	3.87903	-0.93170
C	-3.36168	3.72263	0.23010
C	-1.45555	5.24426	-1.12052
H	-0.34903	3.39831	-1.29717
C	-3.56007	5.09172	0.05457
H	-4.09663	3.14248	0.77951
C	-2.61172	5.85568	-0.62934
H	-0.71195	5.83297	-1.65153
H	-4.45438	5.56227	0.45450
H	-2.77090	6.92115	-0.77384

Coordinates for the optimized singlet ground state of **8**.

Pt	-0.44798	-0.95775	0.00485
C	-0.99228	-2.88253	0.02991
C	-0.14211	-3.99004	0.04851
C	-2.38097	-3.12436	0.04391
C	-0.66290	-5.28973	0.07851
H	0.93173	-3.83097	0.04284
C	-2.91833	-4.40846	0.07389
C	-2.04152	-5.49824	0.09100
H	-3.98688	-4.58303	0.08311
H	-2.44537	-6.50661	0.11440
C	-2.39190	-0.75851	-0.01708
N	-3.13668	-1.91321	0.02011
N	-3.27801	0.27709	-0.04514
O	0.12482	1.12141	0.01557
C	2.56941	-0.63090	0.04640
C	1.32415	1.55053	0.01772
C	2.49774	0.76979	0.03578
H	3.44073	1.30527	0.04452
O	1.58398	-1.45019	0.03243

H	0.01313	-6.14117	0.09305
C	-2.96560	1.67604	-0.13154
C	-3.21572	2.49891	0.96835
C	-2.46587	2.20271	-1.32254
C	-2.95376	3.86646	0.87323
H	-3.60189	2.06646	1.88656
C	-2.19965	3.56868	-1.40608
H	-2.27805	1.54166	-2.16224
C	-2.44354	4.40088	-0.31156
H	-3.14155	4.51049	1.72758
H	-1.79688	3.98258	-2.32568
H	-2.22934	5.46335	-0.37981
C	-4.50148	-1.62063	0.02389
C	-4.59045	-0.21619	-0.01996
C	-5.66319	-2.39768	0.05588
C	-5.81204	0.45116	-0.04523
C	-6.88873	-1.73114	0.03730
H	-5.63332	-3.47811	0.09338
C	-6.96613	-0.33073	-0.01456
H	-5.85638	1.53403	-0.08598
H	-7.80384	-2.31534	0.06247
H	-7.93832	0.15257	-0.03150
C	1.47659	3.05259	0.02029
C	1.85354	3.73153	-1.15396
C	1.21643	3.76737	1.20590
C	1.97393	5.12563	-1.11735
C	1.36014	5.15818	1.20012
C	1.73550	5.85799	0.04884
H	2.26538	5.65099	-2.02524
H	1.17532	5.70852	2.12107
C	3.92920	-1.28093	0.05351
C	4.67879	-1.34968	1.24263
C	4.42569	-1.84356	-1.13963
C	5.92965	-1.97755	1.21347
C	5.68356	-2.45228	-1.12410
C	6.45097	-2.53371	0.04271
H	6.50875	-2.03480	2.13328
H	6.07221	-2.87651	-2.04823
C	2.12083	2.98926	-2.44644
H	3.04060	2.39476	-2.39207
H	1.30844	2.29396	-2.68666
H	2.22581	3.68951	-3.28133
C	0.79422	3.05263	2.47007
H	-0.18754	2.58333	2.34516
H	1.49717	2.25338	2.73447
H	0.73994	3.74800	3.31363
C	1.85465	7.36515	0.05886
H	0.89715	7.84504	-0.18642
H	2.15882	7.73681	1.04347
H	2.58825	7.71441	-0.67585
C	4.15514	-0.77547	2.54179
H	4.09938	0.31926	2.51016
H	3.14531	-1.13971	2.76311
H	4.80474	-1.05310	3.37783
C	3.62372	-1.78976	-2.42134
H	2.68994	-2.35520	-2.32920
H	3.34556	-0.76014	-2.67835
H	4.19457	-2.20420	-3.25800
C	7.79198	-3.23098	0.04061
H	8.42287	-2.88977	0.86824
H	7.67575	-4.31823	0.14549
H	8.33511	-3.05415	-0.89464

Coordinates for the optimized singlet ground state of **9**.

Pt	-0.57767	-1.02184	-0.01111
C	-1.11335	-2.94941	-0.02710
C	-0.25902	-4.05383	-0.02158
C	-2.50113	-3.19686	-0.05016
C	-0.77488	-5.35574	-0.03962
H	0.81406	-3.89051	-0.00305
C	-3.03353	-4.48314	-0.07036
C	-2.15253	-5.56971	-0.06453
H	-4.10133	-4.66159	-0.09215
H	-2.55232	-6.57988	-0.07984
C	-2.52095	-0.83072	-0.03777
N	-3.26188	-1.98837	-0.05166
N	-3.40971	0.20223	-0.02753
O	-0.02325	1.06153	-0.00568
C	2.43460	-0.67236	0.04489
C	1.17230	1.49869	-0.00278
C	2.35207	0.72777	0.02741
H	3.29022	1.27073	0.03596
O	1.45805	-1.50087	0.03024
H	-0.09567	-6.20478	-0.03470
C	-3.10103	1.60564	-0.01690
C	-3.23675	2.32259	1.17286
C	-2.71943	2.24095	-1.19847
C	-2.97720	3.69369	1.17854
H	-3.53285	1.80521	2.08041
C	-2.45621	3.61014	-1.18257
H	-2.61869	1.66078	-2.11007
C	-2.58387	4.33679	0.00297
H	-3.07862	4.25653	2.10221
H	-2.14610	4.10861	-2.09608
H	-2.36971	5.40147	0.01141
C	-4.62761	-1.69994	-0.04621
C	-4.72020	-0.29497	-0.03161
C	-5.78765	-2.48000	-0.05469
C	-5.94276	0.37068	-0.03239
C	-7.01461	-1.81555	-0.05157
H	-5.75543	-3.56104	-0.06353
C	-7.09519	-0.41433	-0.04185
H	-5.98865	1.45434	-0.02493
H	-7.92851	-2.40218	-0.05764
H	-8.06855	0.06692	-0.04221
C	1.31378	3.00445	-0.02310
C	1.55805	3.66120	-1.24501
C	1.17441	3.71595	1.18457
C	1.67504	5.06501	-1.25209
C	1.29042	5.11899	1.16517

C	1.53907	5.76153	-0.04979
C	3.80477	-1.30657	0.07741
C	4.41607	-1.55997	1.32069
C	4.42776	-1.64639	-1.13928
C	5.69286	-2.15352	1.34089
C	5.70546	-2.23702	-1.10648
C	6.30947	-2.47414	0.12991
C	1.68633	2.90072	-2.54775
H	2.67609	3.04638	-3.00072
H	1.53939	1.82722	-2.41879
H	0.95141	3.25112	-3.28423
C	0.90035	3.00863	2.49394
H	-0.10996	3.23535	2.85954
H	0.97625	1.92375	2.40420
H	1.60134	3.32998	3.27403
C	3.73126	-1.22083	2.62722
H	4.33927	-0.53424	3.23086
H	2.75636	-0.75418	2.47620
H	3.57516	-2.12095	3.23594
C	3.75704	-1.39558	-2.47285
H	3.62040	-2.33249	-3.02837
H	2.77348	-0.93546	-2.36416
H	4.36534	-0.73893	-3.10890
C	1.15288	5.93149	2.43241
H	0.18566	5.76349	2.92401
H	1.92576	5.67521	3.16920
H	1.23865	7.00236	2.22251
C	1.94594	5.81829	-2.53433
H	2.88847	5.50372	-3.00136
H	1.15828	5.65479	-3.28195
H	2.01020	6.89533	-2.35018
C	6.42163	-2.61596	-2.38212
H	5.85318	-3.35123	-2.96679
H	6.57773	-1.74864	-3.03701
H	7.40277	-3.05055	-2.16653
C	6.39538	-2.44740	2.64629
H	6.55796	-1.53701	3.23835
H	5.81389	-3.13167	3.27806
H	7.37254	-2.90778	2.46986
H	1.63197	6.84634	-0.05941
H	7.29761	-2.93071	0.15084

Coordinates for the optimized singlet ground state of **10**.

Pt	0.03915	-0.89872	0.00260
C	-0.66344	-2.77222	0.00125
C	0.09074	-3.94668	0.01116
C	-2.06764	-2.89510	-0.00637
C	-0.53760	-5.19853	0.01116
H	1.17396	-3.87744	0.02156
C	-2.71107	-4.12986	-0.00814
C	-1.92874	-5.28969	0.00075
H	-3.79036	-4.21450	-0.01764
H	-2.41637	-6.26061	-0.00011
C	-1.87649	-0.53616	-0.01756
N	-2.71706	-1.62479	-0.01317
N	-2.66564	0.57473	-0.01725
O	0.77878	1.12751	0.01021
C	3.07246	-0.82361	0.04808
C	2.01002	1.45339	0.00118
C	3.11504	0.57815	0.02752
H	4.09870	1.03497	0.02885
O	2.02366	-1.56037	0.03283
H	0.06415	-6.10403	0.01965
C	-2.23048	1.94372	-0.03822
C	-2.30512	2.69928	1.13302
C	-1.78980	2.51280	-1.23295
C	-1.92175	4.04084	1.10713
H	-2.65182	2.23401	2.05086
C	-1.40256	3.85232	-1.24866
H	-1.74135	1.90423	-2.13026
C	-1.46758	4.61605	-0.08151
H	-1.97191	4.63242	2.01675
H	-1.04456	4.29809	-2.17187
H	-1.15850	5.65700	-0.09724
C	-4.05472	-1.22009	-0.00276
C	-4.01987	0.20331	-0.00701
C	-5.26045	-1.88941	0.00912
C	-5.15821	0.97213	-0.00763
C	-6.46020	-1.13016	0.01345
H	-5.32618	-2.96934	0.01536
C	-6.41267	0.30988	0.00338
H	-5.10664	2.05605	-0.01407
C	2.29024	2.93719	-0.03204
C	2.60565	3.56693	-1.25023
C	2.20947	3.68422	1.15882
C	2.84852	4.94559	-1.25324
C	2.46710	5.05771	1.11155
C	2.78740	5.70903	-0.08432
H	3.09554	5.43284	-2.19487
H	2.41895	5.63291	2.03471
C	4.37564	-1.58052	0.06748
C	5.10215	-1.71102	1.26554
C	4.84238	-2.17566	-1.12177
C	6.30180	-2.43224	1.24910
C	6.05005	-2.87836	-1.09350
C	6.79443	-3.02169	0.08228
H	6.86326	-2.53679	2.17565
H	6.41716	-3.32748	-2.01467
C	2.67848	2.78421	-2.54370
H	3.50143	2.05969	-2.53363
H	1.75794	2.21506	-2.71830
H	2.83111	3.45302	-3.39663
C	1.85073	3.02066	2.46956
H	0.83248	2.61705	2.43851
H	2.51923	2.18018	2.69188
H	1.91346	3.73124	3.29970
C	3.03678	7.19996	-0.11370
H	2.09635	7.76333	-0.18679
H	3.54489	7.53970	0.79573
H	3.65366	7.48597	-0.97225

C	4.60844	-1.10122	2.56017
H	4.64938	-0.00552	2.53544
H	3.56723	-1.37713	2.76272
H	5.21739	-1.43895	3.40463
C	4.06199	-2.05751	-2.41237
H	3.09151	-2.56043	-2.33672
H	3.85617	-1.00960	-2.66337
H	4.61410	-2.50248	-3.24590
C	8.07992	-3.81672	0.09270
H	8.71744	-3.53734	0.93820
H	7.88174	-4.89398	0.17498
H	8.65326	-3.66445	-0.82875
C	-7.63709	1.03519	0.00572
C	-7.73317	-1.76795	0.02677
C	-8.84801	0.38342	0.01829
H	-9.77312	0.95309	0.01996
C	-8.89610	-1.03408	0.02922
H	-9.85787	-1.53936	0.03946
H	-7.59647	2.12179	-0.00265
H	-7.76923	-2.85474	0.03482

Coordinates for the optimized singlet ground state of **11**.

Pt	-1.28704	-0.04460	-0.15150
C	-1.63665	1.86952	0.31077
C	-2.86346	2.42913	0.67185
C	-0.51661	2.72506	0.26214
C	-2.96677	3.79334	0.97165
H	-3.74013	1.79077	0.71802
C	-0.59866	4.08326	0.55662
C	-1.84211	4.61530	0.91435
H	0.26793	4.73133	0.51683
H	-1.92161	5.67358	1.14712
C	0.51411	0.68844	-0.35933
N	0.67207	2.03175	-0.11441
N	1.73653	0.20044	-0.69480
O	-0.88640	-2.10598	-0.65408
C	-3.78987	-1.75334	0.01797
C	-1.74906	-3.04715	-0.66064
C	-3.11414	-2.92881	-0.34989
H	-3.70722	-3.83420	-0.40393
O	-3.28694	-0.58488	0.14330
H	-3.93017	4.21303	1.25083
C	2.03647	-1.19308	-1.04331
C	2.00398	2.40647	-0.29583
C	2.68425	1.22719	-0.66160
C	2.69415	3.61689	-0.19247
C	4.05194	1.21573	-0.92584
C	4.06336	3.60609	-0.46085
H	2.20165	4.53955	0.08332
C	4.73426	2.42754	-0.82078
H	4.56837	0.29893	-1.18662
H	4.62031	4.53535	-0.38571
H	5.80184	2.45668	-1.01680
C	2.81926	-1.92998	0.02903
C	4.02714	-2.56312	-0.28288
C	2.31937	-2.02510	1.33532
C	4.73073	-3.27690	0.69068
H	4.41912	-2.50404	-1.29661
C	3.02369	-2.73146	2.30959
H	1.37591	-1.54649	1.58495
C	4.23135	-3.35934	1.99050
H	5.66805	-3.76270	0.43272
H	2.62691	-2.79627	3.31923
H	4.77770	-3.91013	2.75143
H	1.07616	-1.68318	-1.21539
H	2.59659	-1.18622	-1.98493
C	-1.19940	-4.40504	-1.05256
H	-0.35616	-4.65903	-0.40040
H	-1.95030	-5.19677	-0.99327
H	-0.81293	-4.36015	-2.07786
C	-5.27599	-1.82042	0.30736
H	-5.67995	-2.82991	0.19943
H	-5.46460	-1.46525	1.32689
H	-5.80959	-1.14625	-0.37239

Coordinates for the optimized singlet ground state of **12**.

Pt	-0.15474	-1.03734	-0.23153
C	-0.46010	-3.01182	-0.13102
C	0.51523	-3.99803	0.02711
C	-1.80168	-3.42962	-0.24918
C	0.16090	-5.35248	0.06987
H	1.55607	-3.70190	0.11346
C	-2.17356	-4.77056	-0.20848
C	-1.17438	-5.73625	-0.04602
H	-3.20689	-5.08173	-0.29810
H	-1.44974	-6.78674	-0.01260
C	-2.10227	-1.08864	-0.41682
N	-2.69522	-2.32864	-0.40745
N	-3.09768	-0.17434	-0.54807
O	0.15981	1.09418	-0.38834
C	2.78452	-0.31651	0.02533
C	1.29550	1.67736	-0.33425
C	2.54310	1.05901	-0.13792
H	3.40664	1.71315	-0.09376
O	1.91209	-1.25315	0.01451
H	0.93273	-6.10821	0.19327
C	-2.92843	1.28269	-0.57199
C	-4.07929	-2.20745	-0.54022
C	-4.33327	-0.82352	-0.62286
C	-5.13236	-3.12367	-0.60409
C	-5.62309	-0.31583	-0.76112
C	-6.42388	-2.61554	-0.74718
H	-4.97152	-4.19184	-0.54851
C	-6.66909	-1.23600	-0.82337
H	-5.80761	0.75174	-0.80251
H	-7.25797	-3.30912	-0.79836
H	-7.68861	-0.87761	-0.92872
C	4.19956	-0.77177	0.26936

C	4.55346	-1.23700	1.55281
C	5.14585	-0.76371	-0.77333
C	5.86524	-1.66429	1.77549
C	6.44398	-1.21432	-0.50686
C	6.82752	-1.65939	0.76059
H	6.14085	-2.01514	2.76835
H	7.17232	-1.22157	-1.31572
C	1.25906	3.17725	-0.49356
C	1.02969	3.99405	0.62968
C	1.43006	3.74628	-1.77033
C	0.99151	5.38164	0.45498
C	1.37877	5.13786	-1.89922
C	1.16063	5.97391	-0.79968
H	0.82437	6.01492	1.32434
H	1.51487	5.57885	-2.88510
C	1.66557	2.87965	-2.98841
H	2.61550	2.33553	-2.92057
H	0.87771	2.12607	-3.10274
H	1.69012	3.48503	-3.89980
C	0.81403	3.39640	2.00248
H	-0.15493	2.88610	2.06396
H	1.58344	2.65481	2.24610
H	0.83278	4.17236	2.77410
C	4.78960	-0.30385	-2.17144
H	3.84853	-0.74511	-2.51746
H	4.67106	0.78546	-2.22471
H	5.57431	-0.58504	-2.88089
C	8.24582	-2.10443	1.03364
H	8.73205	-2.47401	0.12447
H	8.85687	-1.27529	1.41567
H	8.27875	-2.90205	1.78401
C	3.54508	-1.27639	2.68004
H	3.03708	-0.31165	2.79908
H	2.76515	-2.02203	2.49137
H	4.03167	-1.52147	3.62914
C	-3.42936	1.96269	0.69031
C	-4.29688	3.05674	0.60747
C	-2.99645	1.53260	1.95247
C	-4.72826	3.71364	1.76270
H	-4.63387	3.40272	-0.36776
C	-3.43105	2.18366	3.10702
H	-2.31934	0.68533	2.02754
C	-4.29832	3.27614	3.01550
H	-5.40239	4.56217	1.68156
H	-3.09064	1.83870	4.07969
H	-4.63578	3.78189	3.91613
H	-1.86229	1.47339	-0.71115
H	-3.46254	1.66730	-1.44781
C	1.08293	7.47405	-0.96853
H	0.05918	7.79649	-1.20262
H	1.38607	7.99660	-0.05484
H	1.72541	7.81996	-1.78568

In the following section the T_1 triplet state geometries for the complexes **5**–**12** are given, which were used for the wavelength prediction (BP86/6-31G(d)).

Coordinates for the optimized triplet state of **5**.

Pt	0.82498	-0.52907	0.24433
C	0.09724	-2.38698	0.12337
C	0.84216	-3.57943	0.17818
C	-1.31653	-2.49122	-0.01156
C	0.20115	-4.82995	0.10256
H	1.92931	-3.51764	0.29474
C	-1.97184	-3.72707	-0.06889
C	-1.19599	-4.90119	-0.01779
H	-3.05979	-3.80181	-0.13435
H	-1.69693	-5.87434	-0.06696
C	-1.08692	-0.13139	0.12218
N	-1.94540	-1.21485	-0.05689
N	-1.87201	0.99824	0.02251
O	1.60850	1.44315	0.14084
C	3.84949	-0.50968	-0.00973
C	2.67095	1.67581	-0.60930
C	3.81169	0.80255	-0.62882
C	5.13068	-1.31414	0.05214
H	5.38410	-1.78449	-0.92213
H	6.00457	-0.70782	0.35324
H	4.99915	-2.12558	0.78607
C	2.65185	3.00260	-1.34753
H	1.65568	3.45196	-1.21168
H	3.40404	3.71934	-0.96119
H	2.83696	2.89232	-2.43399
O	2.79707	-1.11419	0.49106
H	0.79330	-5.75157	0.14290
C	-1.44222	2.34136	0.28285
C	-0.79243	2.64419	1.49172
C	-1.71557	3.35048	-0.65890
C	-0.41688	3.96756	1.75675
H	-0.58086	1.84012	2.20276
C	-1.34206	4.67407	-0.37856
H	-2.19866	3.09314	-1.60710
C	-0.69457	4.98614	0.82856
H	0.09311	4.20359	2.69688
H	-1.55268	5.46083	-1.11136
H	-0.40373	6.02010	1.04393
C	-3.25612	-0.78189	-0.28353
C	-3.21304	0.63623	-0.22086
C	-4.47005	-1.44555	-0.52801
C	-4.36782	1.41818	-0.34751
C	-5.62527	-0.65875	-0.67635
H	-4.53005	-2.53199	-0.60880
C	-5.57992	0.74603	-0.57759
H	-4.32237	2.50766	-0.26719
H	-6.58199	-1.15561	-0.86858
H	-6.50209	1.32681	-0.68299
C	5.08793	1.28744	-1.27419
H	5.55889	0.49377	-1.88278
H	4.92471	2.16317	-1.91925
H	5.83899	1.57734	-0.50996

Coordinates for the optimized triplet state of **6**.

Pt	-0.34511	-0.64206	0.15008
C	0.29684	-2.48683	0.12687
C	-0.50456	-3.65508	0.18624
C	1.75138	-2.66417	0.04052
C	0.07465	-4.92202	0.16282
H	-1.58998	-3.53371	0.25717
C	2.33768	-3.95431	0.04807
C	1.49865	-5.06267	0.10165
H	3.42146	-4.08847	0.04777
H	1.93972	-6.06575	0.11362
C	1.58793	-0.29552	0.18624
N	2.41333	-1.46407	-0.02412
N	2.45328	0.78931	0.00526
O	-1.01435	1.36399	-0.12372
C	-3.40656	-0.50986	-0.03321
C	-2.23009	1.70730	-0.40901
C	-3.36315	0.86597	-0.37604
H	-4.31689	1.33013	-0.61786
C	-4.75578	-1.27496	0.03822
C	-2.37897	3.20913	-0.77381
O	-2.38612	-1.24678	0.23388
H	-0.55184	-5.81971	0.20180
C	2.17657	2.12381	0.42675
C	2.56762	3.21007	-0.38395
C	1.56513	2.35692	1.67528
C	2.37693	4.52303	0.07333
H	2.99955	3.02125	-1.37191
C	1.37807	3.67211	2.11851
H	1.25776	1.50201	2.28531
C	1.78912	4.76100	1.32625
H	2.68220	5.36306	-0.56056
H	0.91750	3.84824	3.09711
H	1.64283	5.78692	1.68083
C	3.72986	-1.08804	-0.32286
C	3.75561	0.33408	-0.28757
C	4.88602	-1.82655	-0.61420
C	4.95589	1.03353	-0.46946
C	6.08637	-1.11728	-0.82742
H	4.87084	-2.91547	-0.68533
C	6.11973	0.28367	-0.73957
H	4.99031	2.12330	-0.39858
H	7.00077	-1.67298	-1.05793
H	7.06684	0.81338	-0.88816
C	-2.10823	4.02625	0.51669
H	-1.11158	3.79190	0.92419
H	-2.15141	5.10884	0.29483
H	-2.86549	3.80527	1.29155
C	-1.30921	3.55514	-1.84039
H	-1.48661	2.99478	-2.77684
H	-1.34865	4.63463	-2.07590
H	-0.29990	3.30890	-1.47588
C	-3.77213	3.58239	-1.32346
H	-4.03538	2.99071	-2.21895

H	-4.56966	3.45000	-0.57002
H	-3.77436	4.64857	-1.61530
C	-4.72343	-2.38714	-1.04296
H	-3.84707	-3.04221	-0.90802
H	-5.63808	-3.00507	-0.97982
H	-4.67343	-1.95377	-2.05854
C	-5.99180	-0.38210	-0.19724
H	-6.06035	0.43261	0.54602
H	-5.99564	0.06562	-1.20742
H	-6.90787	-0.99384	-0.10536
C	-4.86191	-1.92074	1.44432
H	-5.77710	-2.53732	1.51049
H	-3.98854	-2.56035	1.64981
H	-4.91308	-1.14779	2.23288

Coordinates for the optimized triplet state of **7**.

Pt	-0.11054	-0.70704	0.22306
C	0.30832	-2.62591	-0.10726
C	-0.61828	-3.68472	-0.15426
C	1.66606	-2.91860	-0.41593
C	-0.20293	-4.98407	-0.49612
H	-1.66748	-3.47908	0.08005
C	2.09466	-4.20268	-0.76848
C	1.14276	-5.23989	-0.80361
H	3.13458	-4.41782	-1.02298
H	1.46472	-6.25086	-1.07590
C	1.83231	-0.58873	0.01312
N	2.49566	-1.76104	-0.32518
N	2.79994	0.37850	0.14249
O	-0.57832	1.35491	0.25989
C	-3.11494	-0.33971	0.16445
C	-1.74679	1.82932	-0.14921
C	-2.93290	1.03963	-0.19948
O	-2.11295	-1.08993	0.59282
H	-0.93347	-5.80049	-0.52503
C	2.61103	1.72302	0.61502
C	3.14733	2.79185	-0.12575
C	1.95874	1.94925	1.83838
C	3.04379	4.09797	0.37771
H	3.62777	2.59921	-1.09048
C	1.84570	3.26060	2.32091
H	1.54349	1.10374	2.39457
C	2.39493	4.33407	1.60073
H	3.46296	4.93188	-0.19556
H	1.32814	3.44115	3.26875
H	2.30932	5.35484	1.98784
C	3.87599	-1.54658	-0.41711
C	4.07337	-0.17582	-0.11246
C	4.97267	-2.37639	-0.70538
C	5.35083	0.39520	-0.05860
C	6.25154	-1.79966	-0.66909
H	4.85442	-3.43451	-0.94275
C	6.44093	-0.43981	-0.34648
H	5.48900	1.44714	0.20485
H	7.12080	-2.42706	-0.89163
H	7.45420	-0.02658	-0.31606
C	-1.77389	3.24075	-0.57457
C	-2.97195	3.99581	-0.72096
C	-0.54407	3.90032	-0.84530
C	-2.93735	5.33122	-1.13649
C	-0.51700	5.23370	-1.26208
C	-1.71186	5.96253	-1.41622
H	-3.87667	5.88792	-1.23444
H	0.44695	5.71174	-1.47374
C	-4.44699	-0.94845	0.17455
C	-4.62021	-2.22654	0.78482
C	-5.60074	-0.33469	-0.39918
C	-5.86984	-2.84661	0.82108
C	-6.84701	-0.96640	-0.36388
C	-6.99785	-2.22517	0.24745
H	-5.97184	-3.82586	1.30377
H	-7.71169	-0.47275	-0.82257
H	-3.94249	3.54959	-0.47892
H	0.38396	3.33543	-0.72652
H	-1.68861	7.00764	-1.74421
H	-3.74923	-2.70307	1.24313
H	-7.97726	-2.71489	0.27531
H	-5.52213	0.63342	-0.90452
H	-3.83429	1.56766	-0.51641

Coordinates for the optimized triplet state of **8**.

Pt	0.43340	-0.94222	0.01357
C	0.96732	-2.82052	-0.36499
C	0.09632	-3.90851	-0.56365
C	2.36640	-3.05183	-0.49562
C	0.60431	-5.18223	-0.87718
H	-0.98175	-3.74180	-0.46953
C	2.88747	-4.31222	-0.80731
C	1.98893	-5.38074	-0.99759
H	3.96069	-4.48794	-0.90686
H	2.38504	-6.37256	-1.24162
C	2.37649	-0.73501	0.03144
N	3.12759	-1.86849	-0.26817
N	3.28168	0.26959	0.28572
O	-0.09434	1.10025	0.18098
C	-2.61188	-0.65300	-0.03066
C	-1.30988	1.57861	-0.05461
C	-2.48019	0.77712	-0.12986
H	-3.41529	1.32971	-0.25458
O	-1.56951	-1.45709	0.09488
H	-0.08251	-6.02279	-1.02839
C	2.97930	1.58480	0.77936
C	3.50256	2.70682	0.11177
C	2.21632	1.73362	1.94977
C	3.26128	3.98909	0.62776
H	4.07659	2.57226	-0.81090
C	1.97645	3.02068	2.45074
H	1.81789	0.84702	2.45155

C	2.50025	4.14790	1.79749
H	3.66062	4.86510	0.10561
H	1.37604	3.14081	3.35865
H	2.30864	5.15040	2.19446
C	4.49759	-1.58733	-0.21822
C	4.59776	-0.21871	0.14236
C	5.65665	-2.35321	-0.42804
C	5.83439	0.40979	0.33319
C	6.89708	-1.71771	-0.25465
H	5.61480	-3.40533	-0.71327
C	6.98785	-0.36318	0.12492
H	5.89275	1.45840	0.63681
H	7.81338	-2.29532	-0.41497
H	7.97205	0.09614	0.26241
C	-1.41622	3.04163	-0.32412
C	-2.29708	3.87377	0.42995
C	-0.62067	3.62361	-1.35963
C	-2.37235	5.24566	0.12799
C	-0.73983	4.99568	-1.62537
C	-1.60694	5.83192	-0.89418
H	-3.04456	5.87933	0.72227
H	-0.14428	5.42688	-2.44161
C	-3.95267	-1.26378	0.08998
C	-5.00992	-0.93846	-0.82321
C	-4.20875	-2.21770	1.13454
C	-6.26816	-1.54021	-0.66167
C	-5.48625	-2.78203	1.24795
C	-6.53780	-2.46365	0.36474
H	-7.06192	-1.29585	-1.38057
H	-5.67551	-3.48750	2.06838
C	-3.13534	3.33757	1.57566
H	-4.08467	2.88207	1.23159
H	-2.60014	2.56024	2.14819
H	-3.40844	4.15219	2.26946
C	0.30890	2.78330	-2.21046
H	1.19481	2.45865	-1.63881
H	-0.18738	1.86118	-2.56491
H	0.65041	3.35257	-3.09262
C	-1.68680	7.31559	-1.18482
H	-0.85108	7.86812	-0.71170
H	-1.63192	7.51976	-2.26954
H	-2.62537	7.75415	-0.80310
C	-4.80812	-0.01289	-2.00890
H	-4.96082	1.05413	-1.75196
H	-3.79171	-0.09987	-2.43002
H	-5.53240	-0.24985	-2.80801
C	-3.15973	-2.58777	2.16355
H	-2.37969	-3.24628	1.74402
H	-2.63110	-1.69610	2.54555
H	-3.62834	-3.10562	3.01872
C	-7.89449	-3.11961	0.49717
H	-8.68574	-2.51719	0.01747
H	-7.90963	-4.11933	0.01939
H	-8.17183	-3.26702	1.55669

Coordinates for the optimized triplet state of **9**.

Pt	0.51540	-1.00466	0.14606
C	0.97079	-2.88849	-0.31475
C	0.05780	-3.94499	-0.49370
C	2.35295	-3.15654	-0.52491
C	0.50902	-5.22191	-0.87382
H	-1.00703	-3.75288	-0.32531
C	2.81800	-4.42095	-0.90288
C	1.87832	-5.45590	-1.07776
H	3.87855	-4.62526	-1.06424
H	2.23020	-6.45027	-1.37375
C	2.46651	-0.86084	0.08296
N	3.16224	-2.00422	-0.30009
N	3.41613	0.10746	0.31478
O	0.05116	1.04386	0.40465
C	-2.50479	-0.62135	0.06080
C	-1.12228	1.55921	0.05156
C	-2.31673	0.79933	-0.07075
H	-3.22500	1.38075	-0.26238
O	-1.50078	-1.44900	0.30765
H	-0.21005	-6.03769	-1.01069
C	3.18288	1.41136	0.87100
C	3.73190	2.53942	0.23420
C	2.46199	1.54148	2.06970
C	3.56141	3.80703	0.81120
H	4.27263	2.42150	-0.71060
C	2.29103	2.81444	2.63081
H	2.03917	0.65140	2.54457
C	2.84301	3.94665	2.00989
H	3.98387	4.68745	0.31516
H	1.72324	2.91922	3.56135
H	2.70721	4.93805	2.45495
C	4.54114	-1.76629	-0.32080
C	4.70610	-0.41508	0.07969
C	5.66082	-2.56008	-0.62171
C	5.97228	0.16557	0.22425
C	6.92952	-1.97140	-0.49558
H	5.56779	-3.59912	-0.94053
C	7.08600	-0.63550	-0.07373
H	6.08386	1.19915	0.56236
H	7.81578	-2.57152	-0.72657
H	8.09105	-0.21313	0.02650
C	-1.14693	3.01734	-0.27430
C	-1.99234	3.90866	0.45006
C	-0.31078	3.49772	-1.32771
C	-2.01721	5.27944	0.09675
C	-0.32999	4.87441	-1.65230
C	-1.18520	5.73338	-0.94042
C	-3.87700	-1.19037	0.05812
C	-4.77264	-0.89967	-1.01961
C	-4.29314	-2.03140	1.14048
C	-6.08818	-1.41751	-0.98769
C	-5.60318	-2.56470	1.13738
C	-6.47565	-2.23970	0.08456

C	-2.83921	3.43633	1.61678
H	-3.91530	3.37571	1.35728
H	-2.53015	2.44061	1.97201
H	-2.76557	4.13598	2.47005
C	0.56537	2.55434	-2.12718
H	1.59956	2.53300	-1.73429
H	0.19415	1.51740	-2.09282
H	0.62221	2.86312	-3.18592
C	-4.33223	-0.10331	-2.23421
H	-4.71985	0.93551	-2.22492
H	-3.23489	-0.04499	-2.31215
H	-4.70796	-0.56520	-3.16566
C	-3.38500	-2.32903	2.31731
H	-2.91643	-3.32843	2.22807
H	-2.56047	-1.60642	2.40087
H	-3.95327	-2.32381	3.26480
C	0.53840	5.43778	-2.76024
H	1.60754	5.19690	-2.61083
H	0.26020	5.03560	-3.75388
H	0.44467	6.53631	-2.81224
C	-2.90600	6.26285	0.83055
H	-3.97030	5.96109	0.80287
H	-2.63366	6.35088	1.90075
H	-2.83084	7.27022	0.38614
C	-6.08981	-3.46346	2.25700
H	-5.42191	-4.33182	2.40928
H	-6.14009	-2.93089	3.22678
H	-7.10071	-3.84918	2.03968
C	-7.07358	-1.13142	-2.10284
H	-7.20167	-0.04638	-2.27644
H	-6.74798	-1.56798	-3.06750
H	-8.06566	-1.55422	-1.86852
H	-1.20156	6.79993	-1.20262
H	-7.49460	-2.64933	0.09535

Coordinates for the optimized triplet state of **10**.

Pt	0.06085	-0.86948	-0.04963
C	-0.64211	-2.72134	-0.03737
C	0.12872	-3.90199	-0.02083
C	-2.06580	-2.86171	-0.03474
C	-0.49035	-5.15977	-0.01268
H	1.21971	-3.81673	-0.01149
C	-2.69697	-4.11845	-0.03371
C	-1.89730	-5.26787	-0.02288
H	-3.78405	-4.21505	-0.05099
H	-2.37354	-6.25426	-0.02324
C	-1.85981	-0.49544	-0.08625
N	-2.72337	-1.61432	-0.04016
N	-2.70937	0.59498	-0.07261
O	0.79617	1.14653	-0.02531
C	3.09649	-0.84083	0.07429
C	2.04799	1.46121	0.00893
C	3.14476	0.56984	0.07252
H	4.13983	1.02229	0.12141
O	2.03315	-1.57638	0.00770
H	0.12243	-6.06870	-0.00066
C	-2.31326	1.97317	-0.14901
C	-2.70990	2.85621	0.87124
C	-1.58072	2.43030	-1.25589
C	-2.36902	4.21395	0.77538
H	-3.26924	2.47417	1.73133
C	-1.24181	3.78780	-1.33807
H	-1.28033	1.72044	-2.03153
C	-1.63592	4.68075	-0.32808
H	-2.67166	4.90471	1.56983
H	-0.66118	4.14822	-2.19328
H	-1.36464	5.73938	-0.39758
C	-4.05586	-1.22033	0.01588
C	-4.04867	0.19048	-0.01343
C	-5.28572	-1.93322	0.07637
C	-5.23915	0.95079	-0.02951
C	-6.51512	-1.19493	0.08166
H	-5.32670	-3.02211	0.12562
C	-6.49536	0.25708	0.02184
H	-5.21271	2.04205	-0.08601
C	2.34034	2.94336	0.00524
C	2.95458	3.55277	-1.11970
C	1.97942	3.72137	1.13475
C	3.20269	4.93734	-1.08805
C	2.26397	5.09921	1.12674
C	2.87096	5.72946	0.02621
H	3.67325	5.40881	-1.96130
H	2.00326	5.69681	2.01034
C	4.39310	-1.61020	0.12757
C	5.13596	-1.68072	1.33247
C	4.84696	-2.27877	-1.03892
C	6.33401	-2.41984	1.34440
C	6.05530	-2.99427	-0.98138
C	6.81327	-3.08250	0.20119
H	6.90729	-2.48028	2.27892
H	6.41408	-3.49800	-1.88881
C	3.33673	2.75497	-2.35309
H	4.22976	2.12686	-2.17838
H	2.52734	2.07320	-2.66850
H	3.56533	3.42907	-3.19672
C	1.31154	3.09196	2.34030
H	0.27592	2.78999	2.10574
H	1.84131	2.17937	2.66862
H	1.28398	3.79731	3.18848
C	3.14225	7.22012	0.02781
H	2.39760	7.76774	-0.58191
H	3.10173	7.63716	1.04893
H	4.13622	7.45227	-0.39545
C	4.65979	-0.99643	2.59983
H	4.71090	0.10497	2.51873
H	3.60882	-1.24975	2.82778
H	5.27802	-1.29831	3.46258
C	4.06013	-2.21593	-2.33306
H	3.09283	-2.74098	-2.24225
H	3.82604	-1.17246	-2.61397

H	4.62544	-2.67473	-3.16201
C	8.09352	-3.89109	0.24460
H	8.74729	-3.57117	1.07463
H	7.88391	-4.96877	0.38884
H	8.66451	-3.79656	-0.69630
C	-7.72903	0.94639	0.01881
C	-7.76610	-1.85606	0.13992
C	-8.97200	0.25376	0.07730
H	-9.90662	0.82508	0.07365
C	-8.99190	-1.13524	0.13904
H	-9.94052	-1.68033	0.18562
H	-7.72063	2.04174	-0.02823
H	-7.78030	-2.95176	0.18352

Coordinates for the optimized triplet state of **11**.

Pt	-1.31648	-0.03786	-0.14358
C	-1.61725	1.83312	0.32063
C	-2.85040	2.41323	0.70451
C	-0.43469	2.72058	0.25365
C	-2.93899	3.76977	1.00918
H	-3.73179	1.76651	0.75643
C	-0.53434	4.10256	0.56788
C	-1.77064	4.60949	0.93931
H	0.33602	4.76024	0.52633
H	-1.86056	5.67311	1.18645
C	0.49915	0.63056	-0.37753
N	0.69059	2.04348	-0.12724
N	1.75658	0.15236	-0.71948
O	-0.92840	-2.07852	-0.68181
C	-3.86221	-1.70365	0.02960
C	-1.82299	-3.01553	-0.69584
C	-3.18624	-2.88455	-0.37082
H	-3.79292	-3.79191	-0.43861
C	-5.34938	-1.76940	0.33270
H	-5.76139	-2.78194	0.19748
H	-5.53226	-1.44390	1.37285
H	-5.89514	-1.06930	-0.32546
C	-1.28891	-4.37490	-1.11536
H	-0.86530	-4.30833	-2.13398
H	-0.46518	-4.67322	-0.44217
H	-2.06470	-5.15689	-1.10255
O	-3.34400	-0.53348	0.17219
H	-3.89666	4.21004	1.30657
C	2.03811	2.38732	-0.33452
C	2.69938	1.17571	-0.69459
C	2.74040	3.59692	-0.25672
C	4.07652	1.15612	-0.96872
C	4.12393	3.57652	-0.53935
H	2.25094	4.53576	0.00825
C	4.77291	2.37781	-0.88535
H	4.59149	0.22449	-1.21623
H	4.69337	4.50937	-0.48371
H	5.84863	2.38849	-1.09245
C	2.06047	-1.24533	-1.03757
H	1.08889	-1.74692	-1.18852
H	2.61477	-1.26862	-1.99518
C	2.85897	-1.95194	0.04985
C	2.40926	-1.94143	1.38624
C	4.03446	-2.65727	-0.26989
C	3.12690	-2.62189	2.38037
H	1.49329	-1.39468	1.64102
C	4.75071	-3.34477	0.72437
H	4.38930	-2.67414	-1.30876
C	4.29886	-3.32692	2.05271
H	2.76823	-2.60516	3.41586
H	5.66456	-3.88905	0.45983
H	4.85726	-3.85867	2.83139

Coordinates for the optimized triplet state of **12**.

Pt	-0.02146	-1.02012	0.21092
C	-0.15399	-3.00273	0.32562
C	0.87274	-3.88563	0.70874
C	-1.43284	-3.55625	0.03511
C	0.63501	-5.27113	0.78355
H	1.85342	-3.47092	0.96417
C	-1.68824	-4.92887	0.11143
C	-0.63459	-5.78789	0.48421
H	-2.67752	-5.34490	-0.09275
H	-0.82138	-6.86553	0.54607
C	-1.91698	-1.24598	-0.23046
N	-2.38721	-2.55142	-0.30679
N	-2.95870	-0.43592	-0.59030
O	0.06220	1.10548	0.16451
C	2.87285	-0.08762	0.31477
C	1.16077	1.80975	-0.09786
C	2.47034	1.25441	0.00879
H	3.29126	1.96037	-0.15070
O	2.02148	-1.05964	0.60935
H	1.44329	-5.94829	1.08250
C	-2.91174	1.03333	-0.65186
C	-3.72067	-2.57074	-0.73221
C	-4.08671	-1.20924	-0.90407
C	-4.64275	-3.59463	-1.00466
C	-5.36647	-0.83129	-1.32914
C	-5.92428	-3.21513	-1.43560
H	-4.38685	-4.65043	-0.90159
C	-6.28389	-1.86014	-1.59276
H	-5.64040	0.22159	-1.43580
H	-6.66059	-3.99569	-1.65373
H	-7.29532	-1.60440	-1.92459
C	4.30418	-0.45848	0.20942
C	5.31015	0.24156	0.94954
C	4.69252	-1.54609	-0.64004
C	6.65259	-0.14943	0.82122
C	6.04869	-1.88923	-0.73458
C	7.05091	-1.21211	-0.01130
H	7.41372	0.38137	1.40885
H	6.33770	-2.70502	-1.41108

C	0.99413	3.26389	-0.36311
C	0.23748	4.07223	0.54195
C	1.58374	3.86975	-1.51399
C	0.10020	5.44461	0.28190
C	1.41034	5.24877	-1.72907
C	0.67298	6.05896	-0.84883
H	-0.46193	6.06028	0.99721
H	1.85552	5.70106	-2.62561
C	2.35822	3.06686	-2.54287
H	3.41114	2.89516	-2.24572
H	1.90936	2.07186	-2.70873
H	2.38374	3.59985	-3.50965
C	-0.37084	3.50046	1.80688
H	-1.30636	2.94845	1.60771
H	0.31269	2.78703	2.30043
H	-0.60385	4.30908	2.52159
C	3.68703	-2.28928	-1.49484
H	3.11313	-3.03334	-0.91510
H	2.94025	-1.60422	-1.93477
H	4.19828	-2.82025	-2.31682
C	8.50077	-1.63424	-0.10530
H	8.72120	-2.47714	0.57930
H	8.75921	-1.97323	-1.12469
H	9.18290	-0.80888	0.16413
C	4.96766	1.36054	1.91494
H	4.84811	2.33960	1.41067
H	4.02434	1.16110	2.45250
H	5.77082	1.48597	2.66218
C	-3.84293	1.70156	0.34893
C	-4.67561	2.76190	-0.05731
C	-3.85160	1.30431	1.70166
C	-5.50357	3.41632	0.86935
H	-4.67018	3.08221	-1.10700
C	-4.68419	1.95236	2.62603
H	-3.20232	0.48345	2.02831
C	-5.51269	3.00982	2.21275
H	-6.14525	4.24068	0.53838
H	-4.68309	1.63258	3.67406
H	-6.16193	3.51529	2.93628
H	-1.85864	1.31431	-0.46361
H	-3.16920	1.34051	-1.68224
C	0.47798	7.53647	-1.11556
H	-0.51425	7.74033	-1.56401
H	0.53578	8.12768	-0.18362
H	1.23896	7.92649	-1.81385

In the following section the triplet state geometries for the complexes **5**–**12** are given, which were used for the spin density calculations (B3LYP/6-31G(d)).

Coordinates for the optimized triplet state of **5**.

Pt	0.80706	-0.54557	0.25260
C	0.03521	-2.39395	0.14646
C	0.73774	-3.59798	0.22911
C	-1.36002	-2.46449	-0.04480
C	0.07153	-4.82545	0.12003
H	1.81193	-3.56956	0.38417
C	-2.04186	-3.67292	-0.15306
C	-1.30882	-4.86254	-0.07064
H	-3.11467	-3.71749	-0.29258
H	-1.82734	-5.81371	-0.15408
C	-1.09642	-0.11386	0.06716
N	-1.96172	-1.16899	-0.09755
N	-1.84966	1.02144	0.00806
O	1.66311	1.41335	0.25358
C	3.80220	-0.64675	-0.09922
C	2.74678	1.67582	-0.42993
C	3.82871	0.73038	-0.54879
C	5.03120	-1.52263	-0.17879
H	5.47285	-1.55588	-1.18412
H	5.83132	-1.20552	0.50870
H	4.74154	-2.53904	0.09826
C	2.83524	3.07636	-0.99918
H	1.84787	3.53566	-0.91164
H	3.54915	3.71856	-0.46028
H	3.12637	3.09140	-2.05819
O	2.75986	-1.19972	0.47031
H	0.63389	-5.75375	0.18558
C	-1.38673	2.36290	0.21605
C	-0.84778	2.72733	1.45049
C	-1.53003	3.30180	-0.80827
C	-0.44497	4.04558	1.65757
H	-0.73672	1.97888	2.22774
C	-1.13137	4.62141	-0.58954
H	-1.93955	2.99554	-1.76613
C	-0.58951	4.99451	0.64280
H	-0.01763	4.33035	2.61454
H	-1.24035	5.35419	-1.38410
H	-0.27905	6.02201	0.81083
C	-3.26900	-0.71362	-0.27214
C	-3.19800	0.69127	-0.19925
C	-4.49876	-1.34604	-0.47739
C	-4.32896	1.49714	-0.30251
C	-5.63131	-0.53955	-0.59209
H	-4.58867	-2.42146	-0.54765
C	-5.55246	0.85860	-0.50216
H	-4.25532	2.57658	-0.22965
H	-6.59664	-1.01046	-0.75261
H	-6.45641	1.45386	-0.58899
C	5.12207	1.19956	-1.15964
H	5.29599	0.69571	-2.12221
H	5.14253	2.27449	-1.33617
H	5.97615	0.94034	-0.52263

Coordinates for the optimized triplet state of **6**.

Pt	0.37645	-0.57472	0.26288
C	-0.18161	-2.49436	0.11568
C	0.64038	-3.61655	0.24044
C	-1.53921	-2.71108	-0.19839
C	0.12912	-4.90552	0.04358
H	1.68437	-3.47604	0.50077
C	-2.06566	-3.98237	-0.40529
C	-1.21367	-5.08644	-0.28301
H	-3.10745	-4.14015	-0.65329
H	-1.61163	-6.08489	-0.44136
C	-1.56382	-0.35369	0.02840
N	-2.28303	-1.49167	-0.24650
N	-2.45745	0.67557	0.06297
O	0.99824	1.46849	0.18163
C	3.39414	-0.38257	0.10013
C	2.12280	1.80172	-0.42189
C	3.26519	0.95347	-0.39048
H	4.18213	1.39903	-0.75440
C	4.72342	-1.14704	0.12780
C	2.14368	3.19927	-1.05481
O	2.36778	-1.04104	0.59235
H	0.78307	-5.76809	0.14463
C	-2.19790	2.02233	0.48209
C	-1.66102	2.26192	1.74847
C	-2.56171	3.08225	-0.35277
C	-1.49215	3.57662	2.18080
H	-1.37943	1.42505	2.37861
C	-2.39770	4.39459	0.09297
H	-2.96104	2.87771	-1.34142
C	-1.86688	4.64353	1.36012
H	-1.07190	3.76582	3.16424
H	-2.67876	5.22009	-0.55458
H	-1.74016	5.66570	1.70522
C	-3.63767	-1.19509	-0.40363
C	-3.75175	0.19295	-0.19819
C	-4.77148	-1.96149	-0.68951
C	-4.98086	0.84736	-0.23827
C	-6.00059	-1.30474	-0.74468
H	-4.71800	-3.02721	-0.86449
C	-6.10793	0.07564	-0.51735
H	-5.05496	1.91338	-0.05609
H	-6.89417	-1.88072	-0.96601
H	-7.08251	0.55247	-0.55880
C	1.00012	3.27512	-2.09488
H	0.04481	3.01505	-1.63216
H	0.92156	4.28776	-2.51126
H	1.17891	2.57940	-2.92384
C	1.89765	4.25376	0.05069
H	2.71858	4.25278	0.77837
H	1.82861	5.26063	-0.38143
H	0.96879	4.04125	0.58554
C	3.47143	3.52394	-1.76384
H	4.31492	3.56405	-1.06392

H	3.70717	2.79252	-2.54637
H	3.40120	4.50747	-2.24305
C	5.92187	-0.29270	-0.32472
H	5.82048	0.04304	-1.36387
H	6.05804	0.58977	0.31190
H	6.84063	-0.88739	-0.26370
C	4.98259	-1.63941	1.57194
H	4.13633	-2.22670	1.93814
H	5.88453	-2.26306	1.61105
H	5.12505	-0.79184	2.25319
C	4.60818	-2.37239	-0.81310
H	5.51663	-2.98639	-0.76434
H	3.75505	-2.99792	-0.53541
H	4.46780	-2.05567	-1.85373

Coordinates for the optimized triplet state of **7**.

Pt	0.08149	-0.75652	0.09989
C	-0.46132	-2.62078	-0.03514
C	0.39865	-3.74391	-0.07150
C	-1.90178	-2.86869	-0.12216
C	-0.10956	-5.02301	-0.17843
H	1.46842	-3.57137	-0.01820
C	-2.41360	-4.18586	-0.19928
C	-1.52171	-5.23621	-0.23039
H	-3.47848	-4.37824	-0.20097
H	-1.90180	-6.25296	-0.28341
C	-1.87203	-0.51799	0.17573
N	-2.62444	-1.71951	-0.10833
N	-2.79594	0.52219	0.03354
O	0.66390	1.29142	-0.04324
C	3.13031	-0.44875	0.01956
C	1.85977	1.71325	-0.23085
C	3.03663	0.94179	-0.18419
H	3.97006	1.48377	-0.23603
O	2.15136	-1.25710	0.16563
H	0.55684	-5.87991	-0.21624
C	-2.60981	1.83697	0.54853
C	-2.08570	2.02144	1.83468
C	-3.00521	2.94428	-0.21203
C	-1.98748	3.30722	2.36249
H	-1.77102	1.15539	2.40717
C	-2.91318	4.22737	0.32955
H	-3.36925	2.79729	-1.22395
C	-2.41129	4.41414	1.61910
H	-1.58897	3.44409	3.36410
H	-3.22631	5.08175	-0.26429
H	-2.34343	5.41328	2.04053
C	-3.95782	-1.40067	-0.38759
C	-4.06006	0.00551	-0.28197
C	-5.06417	-2.17991	-0.72096
C	-5.28831	0.64165	-0.44702
C	-6.29291	-1.53338	-0.91056
H	-4.99268	-3.25278	-0.84094
C	-6.40132	-0.14920	-0.76199
H	-5.38134	1.71493	-0.33297
H	-7.16704	-2.12170	-1.17168
H	-7.36607	0.33150	-0.89682
C	1.97584	3.18487	-0.49065
C	3.05134	3.74259	-1.20177
C	0.95883	4.03501	-0.02969
C	3.11482	5.11631	-1.43135
H	3.82676	3.09980	-1.60603
C	1.02956	5.40893	-0.24927
H	0.12075	3.60434	0.50419
C	2.10768	5.95555	-0.94941
H	3.94805	5.53032	-1.99304
H	0.23774	6.05243	0.12497
H	2.15998	7.02690	-1.12540
C	4.48453	-1.08448	0.10228
C	4.63513	-2.25914	0.85733
C	5.60590	-0.56057	-0.56054
C	5.87708	-2.88116	0.96356
H	3.76755	-2.66573	1.36593
C	6.84603	-1.19109	-0.46440
H	5.50425	0.32546	-1.17922
C	6.98740	-2.34945	0.30251
H	5.97998	-3.78202	1.56281
H	7.70130	-0.77979	-0.99389
H	7.95548	-2.83711	0.38084

Coordinates for the optimized triplet state of **8**.

Pt	-0.41179	-0.97533	-0.08516
C	-0.91926	-2.85226	-0.01572
C	-0.03790	-3.95774	0.02762
C	-2.36142	-3.13364	-0.02631
C	-0.52210	-5.24992	0.05948
H	1.02938	-3.76178	0.03691
C	-2.84530	-4.46564	-0.02380
C	-1.93308	-5.49531	0.02312
H	-3.90356	-4.68203	-0.08608
H	-2.29094	-6.52144	0.02055
C	-2.36321	-0.77195	-0.21003
N	-3.10648	-2.00115	-0.05015
N	-3.31456	0.23924	-0.06963
O	0.11565	1.09510	-0.02077
C	2.61910	-0.59140	0.05113
C	1.30524	1.55638	0.05647
C	2.49661	0.80992	0.10382
H	3.42042	1.37143	0.18562
O	1.66807	-1.43728	-0.04591
H	0.16026	-6.09376	0.10351
C	-3.07997	1.61993	-0.33087
C	-3.51250	2.58210	0.58976
C	-2.44080	2.01325	-1.51144
C	-3.31760	3.93706	0.31761
H	-3.98302	2.26587	1.51583
C	-2.24207	3.36753	-1.76886
H	-2.10225	1.25458	-2.20887

C	-2.68198	4.33379	-0.86016
H	-3.65270	4.68085	1.03540
H	-1.74242	3.66999	-2.68490
H	-2.52184	5.38833	-1.06521
C	-4.46784	-1.71981	0.12959
C	-4.58617	-0.31067	0.10557
C	-5.58560	-2.53124	0.31176
C	-5.83456	0.30112	0.20917
C	-6.83691	-1.91224	0.43837
H	-5.50949	-3.60930	0.36054
C	-6.95531	-0.52168	0.37638
H	-5.93254	1.37914	0.15989
H	-7.72031	-2.52664	0.58106
H	-7.93622	-0.06266	0.46150
C	1.40802	3.05855	0.12946
C	1.95079	3.79505	-0.94082
C	0.93553	3.71907	1.28325
C	2.02059	5.18958	-0.83237
C	1.04167	5.11027	1.35370
C	1.57726	5.86649	0.30561
C	4.00261	-1.18927	0.08787
C	4.70543	-1.28175	1.30401
C	4.56842	-1.68007	-1.10579
C	5.97864	-1.86322	1.30169
C	5.84622	-2.24490	-1.06217
C	6.56739	-2.35019	0.13167
C	2.44664	3.12694	-2.20669
H	3.41427	2.63296	-2.05682
H	1.75032	2.36006	-2.56261
H	2.57421	3.86495	-3.00534
C	0.32975	2.95107	2.43711
H	-0.64223	2.52943	2.16021
H	0.96485	2.11123	2.74314
H	0.18863	3.60244	3.30549
C	4.10904	-0.77978	2.60179
H	4.73403	-1.06842	3.45271
H	4.01476	0.31262	2.61061
H	3.10450	-1.18628	2.76687
C	3.82117	-1.59069	-2.41833
H	2.88362	-2.15578	-2.38180
H	3.55531	-0.55361	-2.65840
H	4.42707	-1.98211	-3.24126
H	6.28855	-2.61368	-1.98593
H	6.52183	-1.93858	2.24194
H	0.69481	5.61729	2.25251
H	2.43458	5.75934	-1.66238
C	1.64775	7.37374	0.39530
H	0.67744	7.83387	0.16385
H	1.92676	7.70289	1.40277
H	2.37926	7.78381	-0.30896
C	7.93188	-2.99974	0.15911
H	8.53932	-2.62229	0.98869
H	7.85251	-4.08838	0.28295
H	8.48083	-2.82013	-0.77193

Coordinates for the optimized triplet state of **9**.

Pt	-0.53101	-1.03791	-0.11148
C	-1.01994	-2.92011	-0.06269
C	-0.12739	-4.01673	-0.02116
C	-2.45883	-3.21608	-0.09352
C	-0.59839	-5.31408	-0.00763
H	0.93760	-3.80965	0.00037
C	-2.92862	-4.55305	-0.10934
C	-2.00619	-5.57359	-0.06189
H	-3.98366	-4.78019	-0.18565
H	-2.35338	-6.60328	-0.07829
C	-2.48349	-0.85206	-0.25346
N	-3.21545	-2.09128	-0.11609
N	-3.44696	0.14687	-0.10531
O	-0.02388	1.03622	-0.04461
C	2.49243	-0.62533	0.07157
C	1.15838	1.50918	0.06172
C	2.35597	0.77451	0.13413
H	3.27186	1.34522	0.23530
O	1.55237	-1.47992	-0.04354
H	0.09224	-6.15126	0.03485
C	-3.22537	1.53558	-0.33329
C	-3.68073	2.47179	0.60300
C	-2.57799	1.96272	-1.49726
C	-3.49989	3.83480	0.36322
H	-4.15856	2.12919	1.51582
C	-2.39244	3.32471	-1.72187
H	-2.22229	1.22394	-2.20730
C	-2.85451	4.26534	-0.79755
H	-3.85515	4.55861	1.09184
H	-1.88575	3.65320	-2.62498
H	-2.70435	5.32596	-0.97715
C	-4.58176	-1.82683	0.05139
C	-4.71443	-0.41884	0.04736
C	-5.69331	-2.65224	0.20678
C	-5.97034	0.17851	0.14520
C	-6.95247	-2.04810	0.32765
H	-5.60706	-3.73013	0.23880
C	-7.08448	-0.65805	0.28604
H	-6.07887	1.25608	0.11095
H	-7.83115	-2.67368	0.44943
H	-8.07106	-0.21037	0.36603
C	1.23987	3.01490	0.14258
C	1.75484	3.75553	-0.94060
C	0.76504	3.64565	1.31187
C	1.80648	5.16019	-0.84032
C	0.81719	5.04921	1.39639
C	1.33874	5.77384	0.32209
C	3.88557	-1.20671	0.12563
C	4.48974	-1.44476	1.37541
C	4.53719	-1.51415	-1.08501
C	5.78655	-1.99314	1.40876
C	5.83575	-2.05585	-1.03888
C	6.43075	-2.28158	0.20417

C	2.22507	3.09583	-2.22015
H	3.29555	3.27165	-2.39258
H	2.06788	2.01651	-2.21579
H	1.69779	3.50783	-3.09027
C	0.20186	2.84838	2.46900
H	-0.89480	2.89872	2.48199
H	0.47186	1.79217	2.41843
H	0.55637	3.23948	3.42930
C	3.77569	-1.14153	2.67517
H	4.35014	-0.43839	3.29231
H	2.78735	-0.70738	2.51473
H	3.64457	-2.05152	3.27532
C	3.87905	-1.26988	-2.42609
H	3.81540	-2.19729	-3.00972
H	2.86507	-0.87841	-2.32849
H	4.45723	-0.55818	-3.03043
C	0.31641	5.78106	2.62102
H	-0.72884	5.53273	2.84484
H	0.89836	5.52953	3.51767
H	0.37978	6.86488	2.48099
C	2.35221	6.00361	-1.96976
H	3.38728	5.73508	-2.21844
H	1.76845	5.88291	-2.89217
H	2.33892	7.06593	-1.70641
C	6.58471	-2.39385	-2.30724
H	6.05535	-3.14645	-2.90643
H	6.71414	-1.51502	-2.95247
H	7.57974	-2.78973	-2.08116
C	6.48119	-2.27312	2.72139
H	6.60122	-1.36316	3.32412
H	5.91706	-2.98473	3.33861
H	7.47730	-2.69493	2.55477
H	1.37869	6.85956	0.39325
H	7.43468	-2.70168	0.23532

Coordinates for the optimized triplet state of **10**.

Pt	0.05376	-0.88077	-0.02047
C	-0.66287	-2.74212	-0.02035
C	0.08930	-3.92108	-0.01415
C	-2.07044	-2.86707	-0.02021
C	-0.53923	-5.16985	-0.01309
H	1.17237	-3.85221	-0.00791
C	-2.71383	-4.10528	-0.02451
C	-1.93384	-5.26243	-0.02039
H	-3.79285	-4.18923	-0.03798
H	-2.41981	-6.23403	-0.02386
C	-1.87043	-0.50764	-0.05388
N	-2.72202	-1.60366	-0.02428
N	-2.69148	0.58480	-0.05785
O	0.81138	1.13414	0.00360
C	3.08831	-0.83469	0.06618
C	2.04577	1.45135	0.01675
C	3.14246	0.56745	0.05726
H	4.12973	1.01538	0.08282
O	2.03485	-1.56217	0.02898
H	0.06133	-6.07619	-0.00816
C	-2.27571	1.95782	-0.11315
C	-2.55559	2.79772	0.96716
C	-1.63935	2.44444	-1.25483
C	-2.18747	4.14229	0.90090
H	-3.04616	2.39557	1.84837
C	-1.27024	3.78750	-1.30915
H	-1.42787	1.77048	-2.07794
C	-1.54320	4.63694	-0.23498
H	-2.39807	4.79866	1.74044
H	-0.76102	4.16911	-2.18890
H	-1.24695	5.68074	-0.28052
C	-4.04456	-1.19765	0.00531
C	-4.02714	0.19078	-0.02108
C	-5.29076	-1.90483	0.04808
C	-5.21366	0.97008	-0.03882
C	-6.50467	-1.15736	0.04473
H	-5.33871	-2.98368	0.09099
C	-6.47135	0.29285	-0.00289
H	-5.17150	2.05194	-0.08245
C	2.33436	2.93291	0.00500
C	2.81861	3.55402	-1.16234
C	2.08040	3.69224	1.16447
C	3.04999	4.93459	-1.14476
C	2.33945	5.06594	1.14124
C	2.82741	5.70742	-0.00186
H	3.41544	5.41648	-2.04999
H	2.15305	5.65012	2.04076
C	4.38606	-1.60081	0.09895
C	5.09112	-1.75097	1.30766
C	4.87038	-2.18231	-1.08970
C	6.28725	-2.47788	1.30232
C	6.07376	-2.89222	-1.05000
C	6.79691	-3.05479	0.13625
H	6.83259	-2.59680	2.23680
H	6.45470	-3.33084	-1.97062
C	3.07913	2.76976	-2.43152
H	3.97255	2.13982	-2.34375
H	2.24494	2.10286	-2.67590
H	3.23263	3.44572	-3.27895
C	1.53596	3.04385	2.41771
H	0.51787	2.67368	2.25743
H	2.14324	2.18234	2.72076
H	1.51839	3.75464	3.24992
C	3.12935	7.18857	0.00608
H	2.47203	7.72959	0.69571
H	4.16247	7.38279	0.32494
H	3.01123	7.62818	-0.99043
C	4.57651	-1.15578	2.60088
H	4.60200	-0.05966	2.58299
H	3.53678	-1.44682	2.79012
H	5.18077	-1.49099	3.44970
C	4.11317	-2.04189	-2.39189
H	3.13835	-2.53942	-2.33958
H	3.91787	-0.98946	-2.63190

H	4.67669	-2.47921	-3.22185
C	8.07781	-3.85701	0.15901
H	8.72042	-3.56324	0.99586
H	7.87381	-4.93106	0.26615
H	8.64814	-3.72821	-0.76772
C	-7.68637	0.98853	-0.01006
C	-7.75348	-1.79852	0.08524
C	-8.94156	0.30818	0.03101
H	-9.86018	0.88757	0.02421
C	-8.97477	-1.06311	0.07903
H	-9.91931	-1.59793	0.11161
H	-7.66949	2.07476	-0.04638
H	-7.78408	-2.88463	0.12007

Coordinates for the optimized triplet state of **11**.

Pt	-1.30878	-0.04439	-0.15806
C	-1.66218	1.81578	0.28834
C	-2.90952	2.37348	0.64550
C	-0.49967	2.73063	0.23112
C	-3.03351	3.71841	0.93050
H	-3.77013	1.71415	0.69050
C	-0.64342	4.11314	0.51802
C	-1.88609	4.58653	0.86119
H	0.19861	4.79065	0.46543
H	-2.01027	5.64297	1.08309
C	0.49091	0.68239	-0.39622
N	0.63828	2.08437	-0.11648
N	1.76797	0.22996	-0.68027
O	-0.86384	-2.09121	-0.61843
C	-3.79176	-1.80594	0.03495
C	-1.70317	-3.05632	-0.59364
C	-3.07041	-2.97155	-0.29137
H	-3.63299	-3.89728	-0.32013
O	-3.33002	-0.62248	0.12950
H	-3.99576	4.13786	1.20877
C	2.09798	-1.13530	-1.07771
C	1.98722	2.45423	-0.25988
C	2.68011	1.26896	-0.60730
C	2.65982	3.66534	-0.12823
C	4.05843	1.28301	-0.82887
C	4.04417	3.67784	-0.35357
H	2.14910	4.58105	0.13910
C	4.72521	2.50608	-0.69759
H	4.59631	0.37454	-1.07374
H	4.58843	4.61179	-0.25533
H	5.79850	2.54062	-0.86245
C	2.87578	-1.90828	-0.02606
C	4.06302	-2.56725	-0.36291
C	2.39324	-2.00730	1.28670
C	4.76096	-3.31354	0.59042
H	4.44361	-2.50084	-1.38056
C	3.09160	-2.74671	2.24052
H	1.46907	-1.50263	1.55598
C	4.27715	-3.40301	1.89559
H	5.68250	-3.81858	0.31274
H	2.70811	-2.81444	3.25526
H	4.81896	-3.97929	2.64086
H	1.14890	-1.63489	-1.28418
H	2.67149	-1.09233	-2.01235
C	-1.10928	-4.40724	-0.94018
H	-0.25415	-4.60638	-0.28465
H	-1.83171	-5.22200	-0.84879
H	-0.72881	-4.38458	-1.96847
C	-5.27858	-1.91931	0.30929
H	-5.64237	-2.94722	0.23888
H	-5.49467	-1.52980	1.31065
H	-5.82865	-1.29599	-0.40520

Coordinates for the optimized triplet state of **12**.

Pt	-0.09315	-1.05940	-0.11205
C	-0.34671	-2.97948	0.07701
C	0.65830	-3.94137	0.31933
C	-1.73956	-3.46627	-0.04472
C	0.34734	-5.28145	0.43666
H	1.68376	-3.59890	0.41363
C	-2.04553	-4.84629	0.08684
C	-1.01818	-5.72646	0.32125
H	-3.06319	-5.20725	0.01724
H	-1.23819	-6.78522	0.42745
C	-2.03673	-1.14008	-0.31762
N	-2.61188	-2.45714	-0.27471
N	-3.09944	-0.28534	-0.55360
O	0.14808	1.06277	-0.33883
C	2.83930	-0.24220	0.08655
C	1.26795	1.68365	-0.32248
C	2.53799	1.11884	-0.12506
H	3.37912	1.80292	-0.13908
O	2.00802	-1.20901	0.12846
H	1.12676	-6.01461	0.62165
C	-2.99808	1.16657	-0.65922
C	-3.99806	-2.37386	-0.49556
C	-4.28304	-0.99650	-0.65776
C	-5.00598	-3.32964	-0.58295
C	-5.58707	-0.55631	-0.89189
C	-6.31430	-2.88622	-0.82512
H	-4.80639	-4.38790	-0.47722
C	-6.59414	-1.52402	-0.97299
H	-5.81348	0.49896	-0.99144
H	-7.11586	-3.61465	-0.89577
H	-7.61695	-1.20521	-1.15322
C	4.28428	-0.63319	0.25773
C	4.96219	-0.35222	1.45883
C	4.93758	-1.31207	-0.79185
C	6.29835	-0.75084	1.58536
C	6.27472	-1.68095	-0.62454
C	6.97540	-1.40789	0.55549
H	6.82035	-0.54370	2.51761
H	6.78139	-2.19833	-1.43734

C	1.17501	3.17530	-0.52162
C	0.74673	3.98570	0.54873
C	1.48886	3.74502	-1.77027
C	0.65866	5.36716	0.35225
C	1.37562	5.13133	-1.92386
C	0.96448	5.96032	-0.87657
H	0.34103	5.99548	1.18242
H	1.61587	5.57316	-2.88922
C	1.93288	2.89228	-2.93980
H	2.92584	2.45775	-2.77311
H	1.24528	2.05644	-3.11233
H	1.97852	3.48689	-3.85762
C	0.38666	3.38640	1.89015
H	-0.54569	2.81336	1.83146
H	1.16232	2.69824	2.24657
H	0.25413	4.16875	2.64386
C	4.21836	-1.63272	-2.08390
H	3.38775	-2.32697	-1.91754
H	3.78819	-0.73125	-2.53772
H	4.90246	-2.08208	-2.81026
C	8.42842	-1.79769	0.70100
H	8.62601	-2.78284	0.26319
H	9.08640	-1.08103	0.19115
H	8.73159	-1.82802	1.75278
C	4.27673	0.34512	2.61486
H	4.06557	1.39719	2.38908
H	3.31841	-0.12643	2.86040
H	4.90553	0.31653	3.51033
C	-3.62515	1.90470	0.51267
C	-4.44844	3.01378	0.28973
C	-3.35910	1.51172	1.83189
C	-4.99495	3.72369	1.36180
H	-4.66127	3.32767	-0.73035
C	-3.90806	2.21662	2.90318
H	-2.72320	0.64916	2.01486
C	-4.72690	3.32563	2.67173
H	-5.63344	4.58243	1.17133
H	-3.69551	1.90004	3.92096
H	-5.15422	3.87308	3.50760
H	-1.93377	1.40333	-0.73234
H	-3.47524	1.47923	-1.59661
C	0.82642	7.45263	-1.07377
H	-0.19812	7.72346	-1.36317
H	1.05777	8.00180	-0.15441
H	1.49336	7.81642	-1.86280