Electronic Supplementary Information

Blue Phosphorescent Nitrile Containing C^C* cyclometalated NHC Platinum(II) complexes

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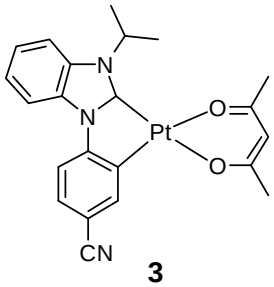
List of Abbreviations

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
KO^{t}Bu	Potassium *tert*-butanolate
LLCT	Ligand-to-ligand charge transfer
LUMO	Lowest unoccupied molecular orbital
Mesacac	Dimesitoylmethanate
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
PhOLED	Phosphorescent organic light-emitting devices
PMMA	Poly(methyl methacrylate)
SOC	Spin-orbit coupling

2D NMR Spectra



3

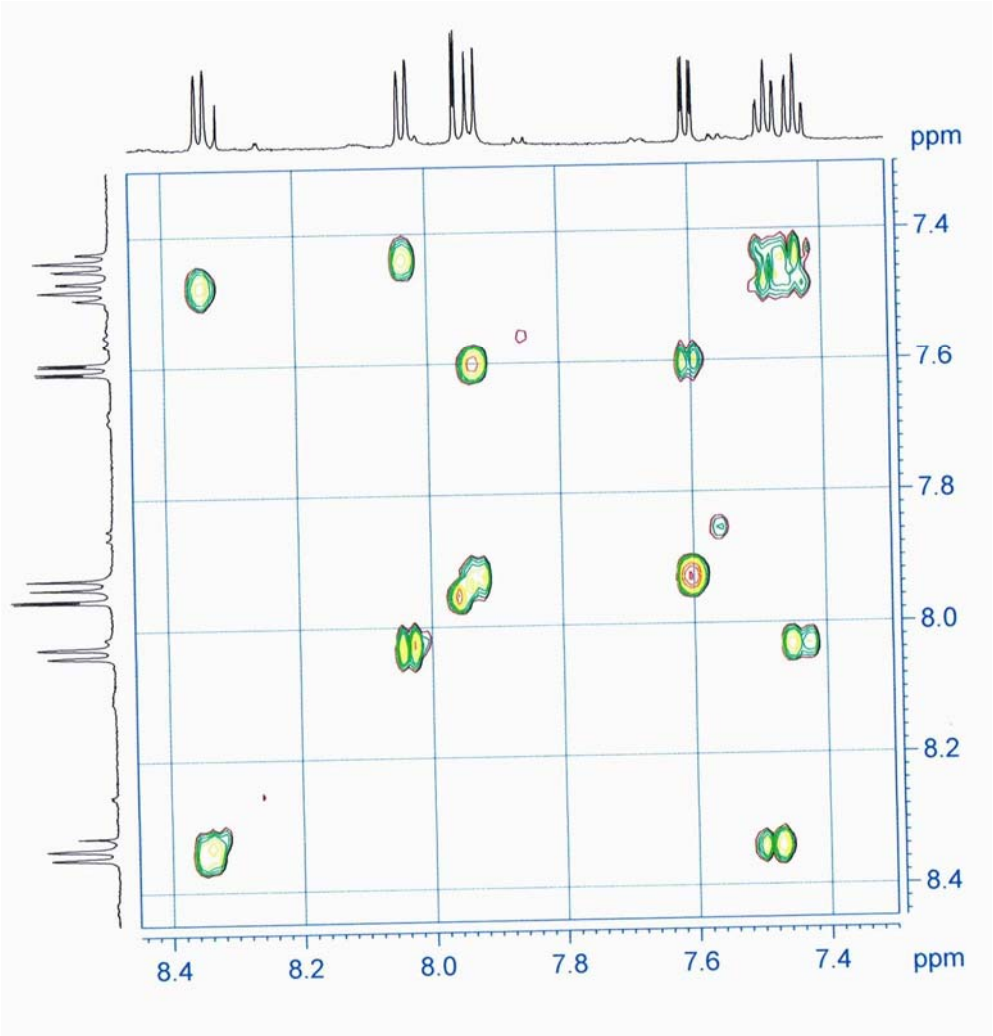


Figure S1. COSY spectrum of complex **3**.

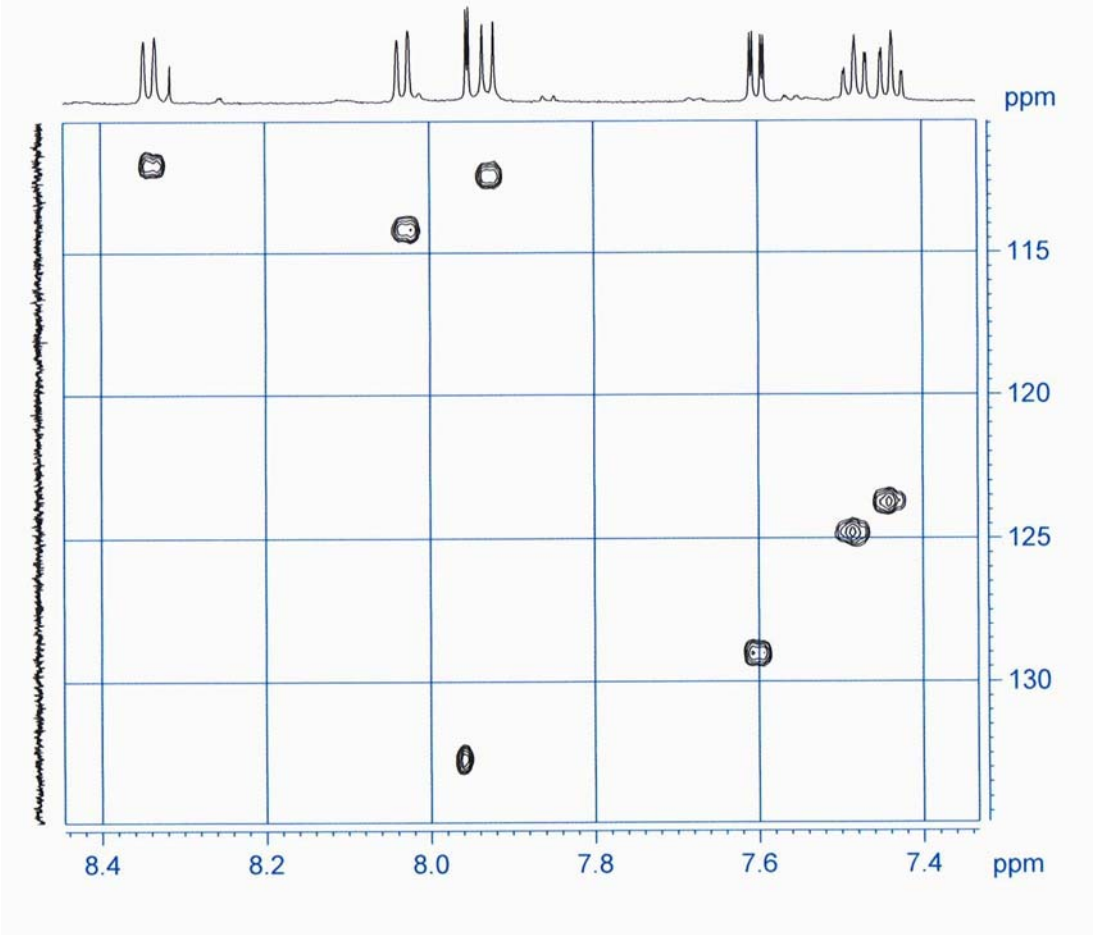


Figure S2. HSQC spectrum of complex **3**.

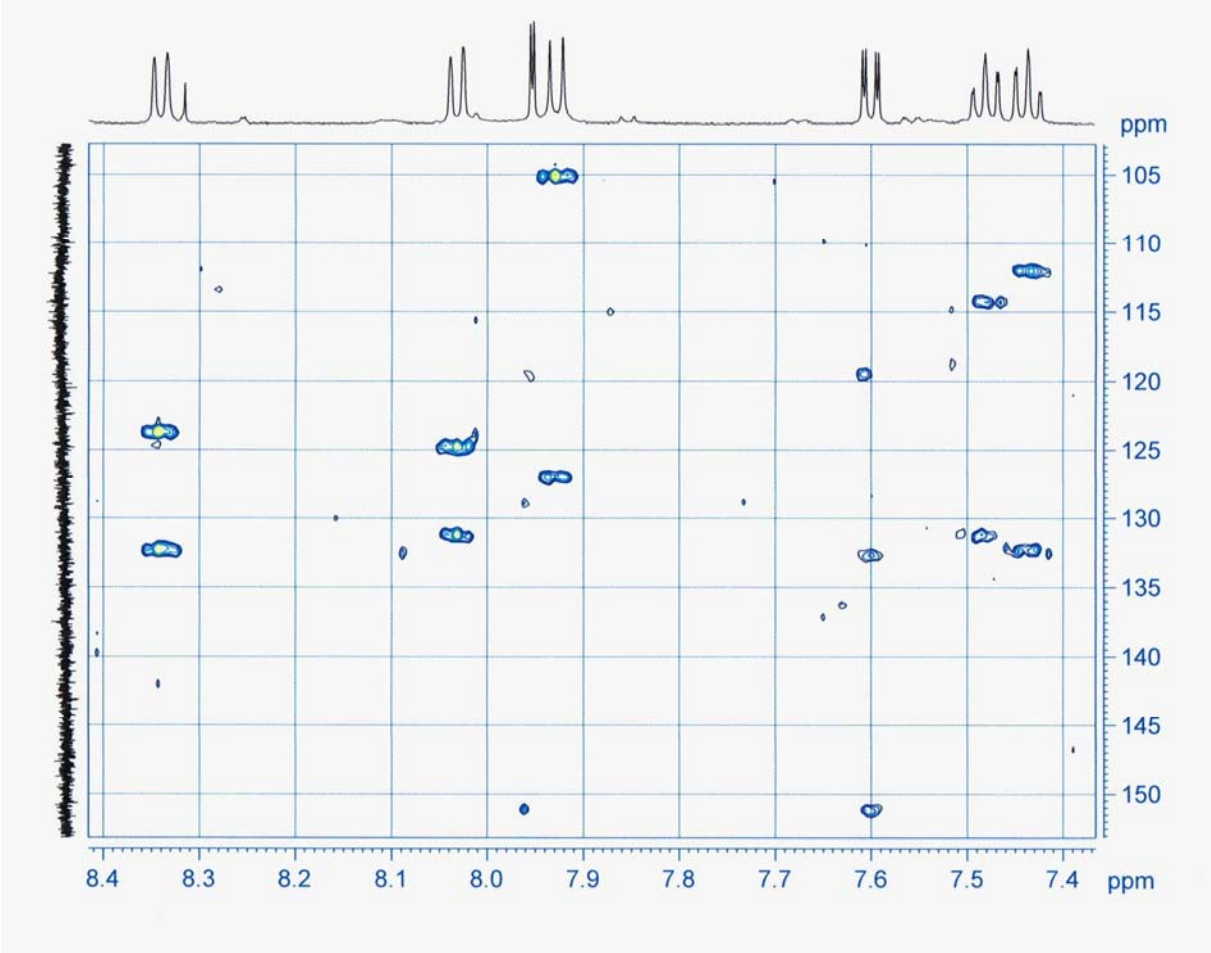


Figure S3. HMBC spectrum of complex **3**.

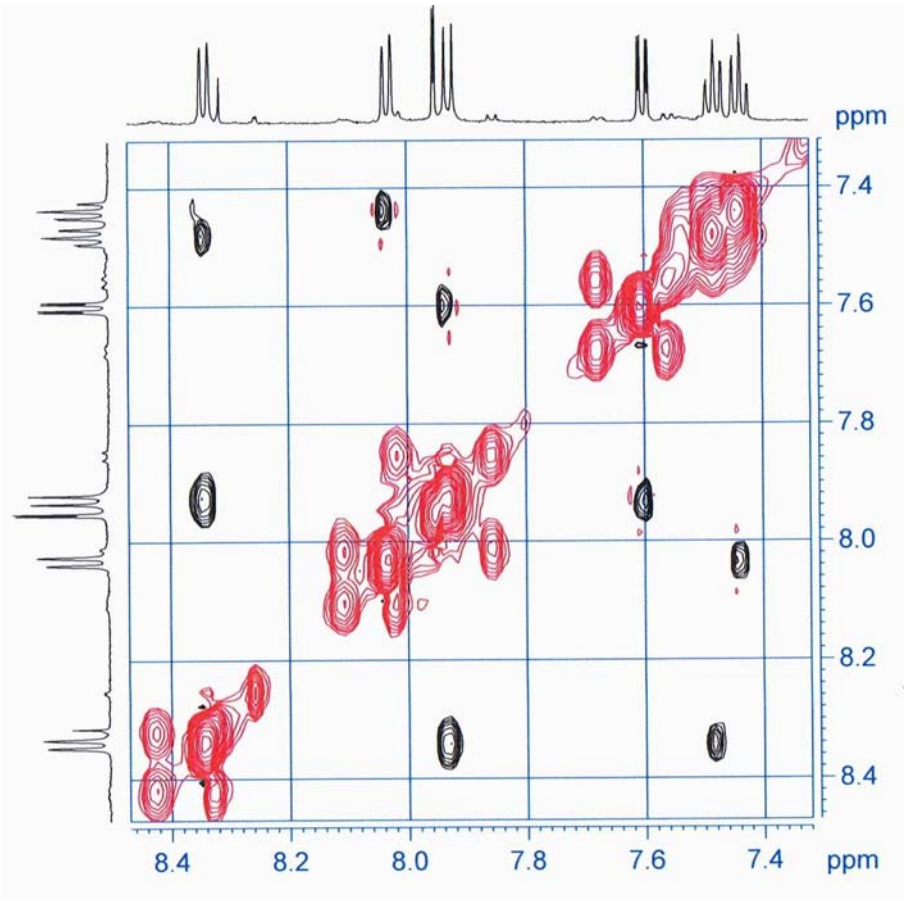
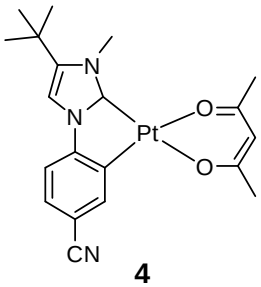


Figure S4. NOESY spectrum of complex **3**.



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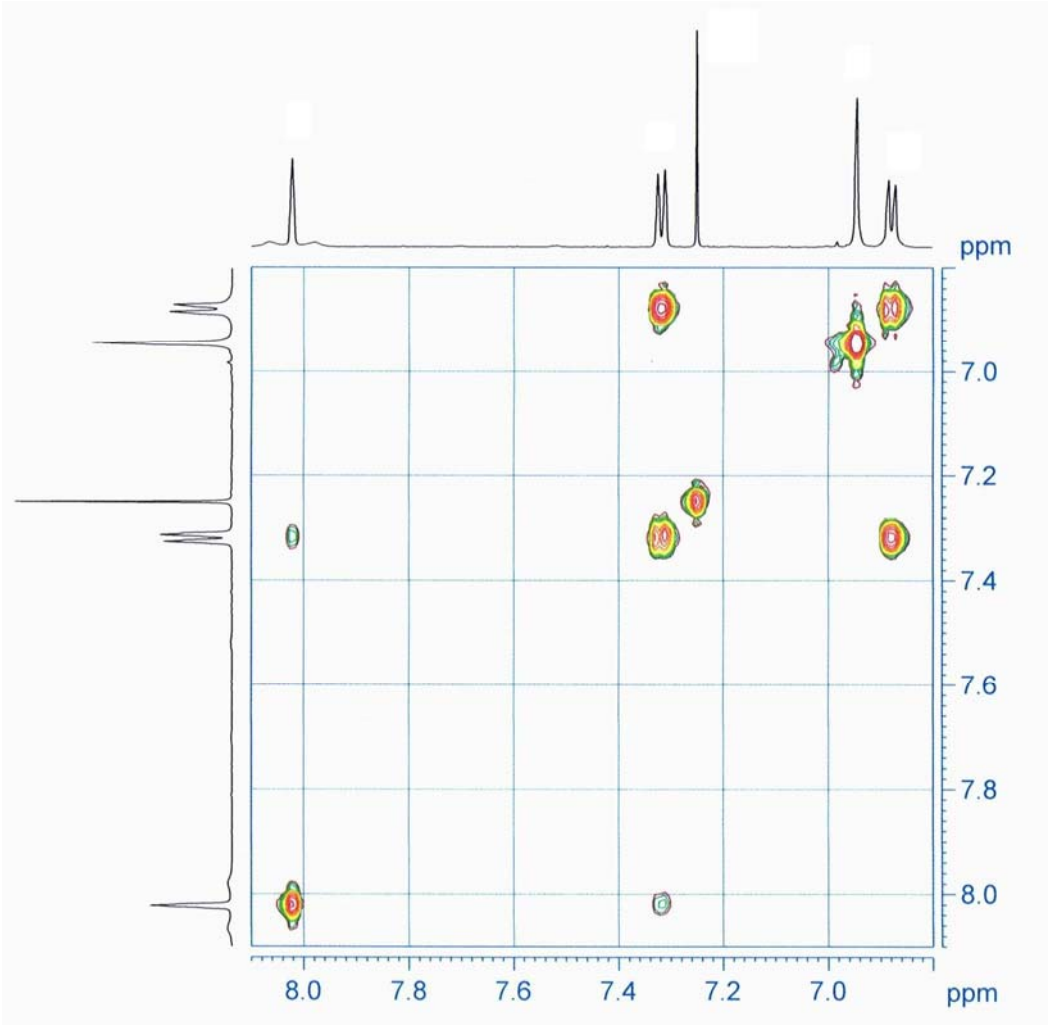


Figure S5. COSY spectrum of complex **4**.

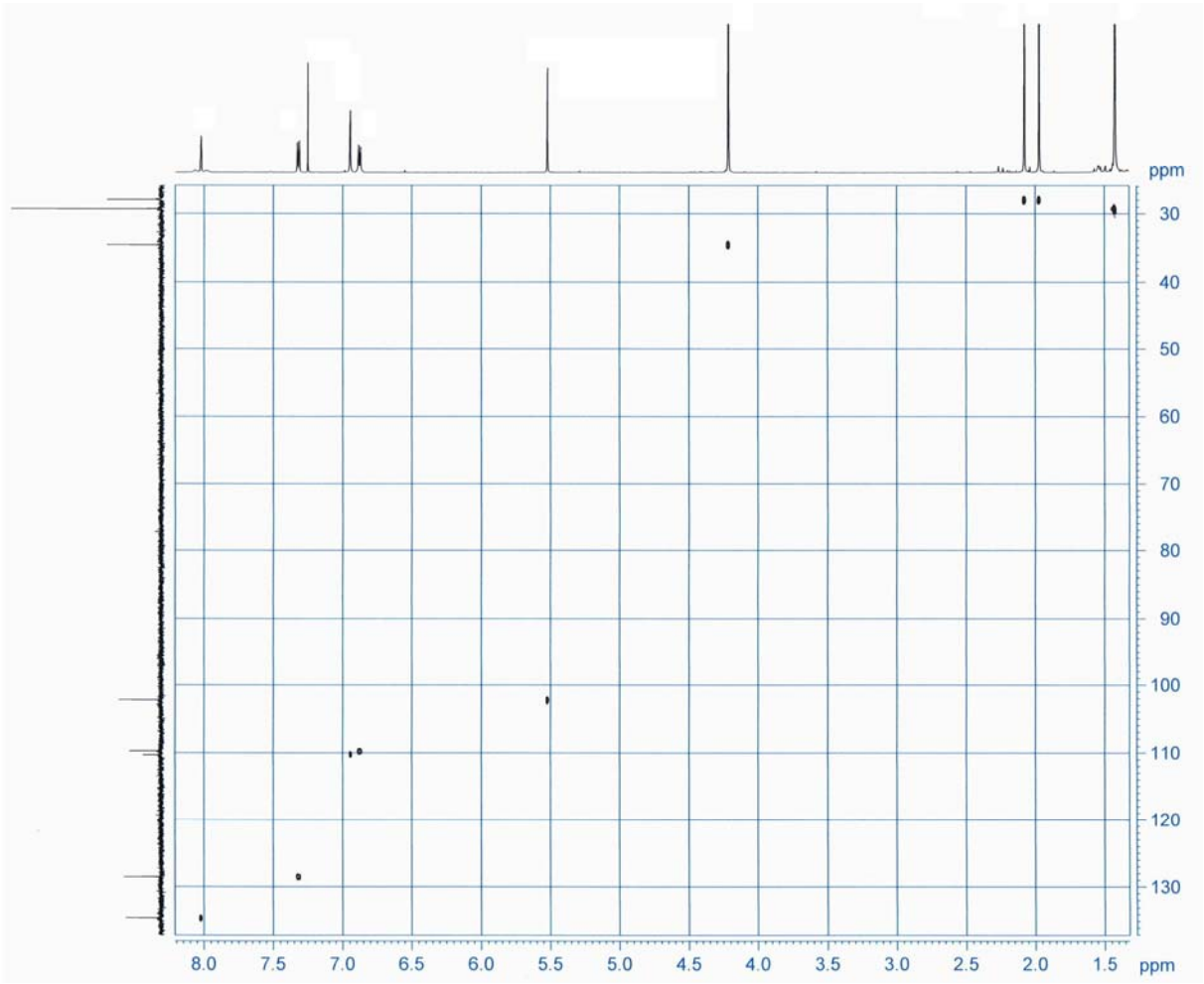


Figure S6. HSQC spectrum of complex **4**.

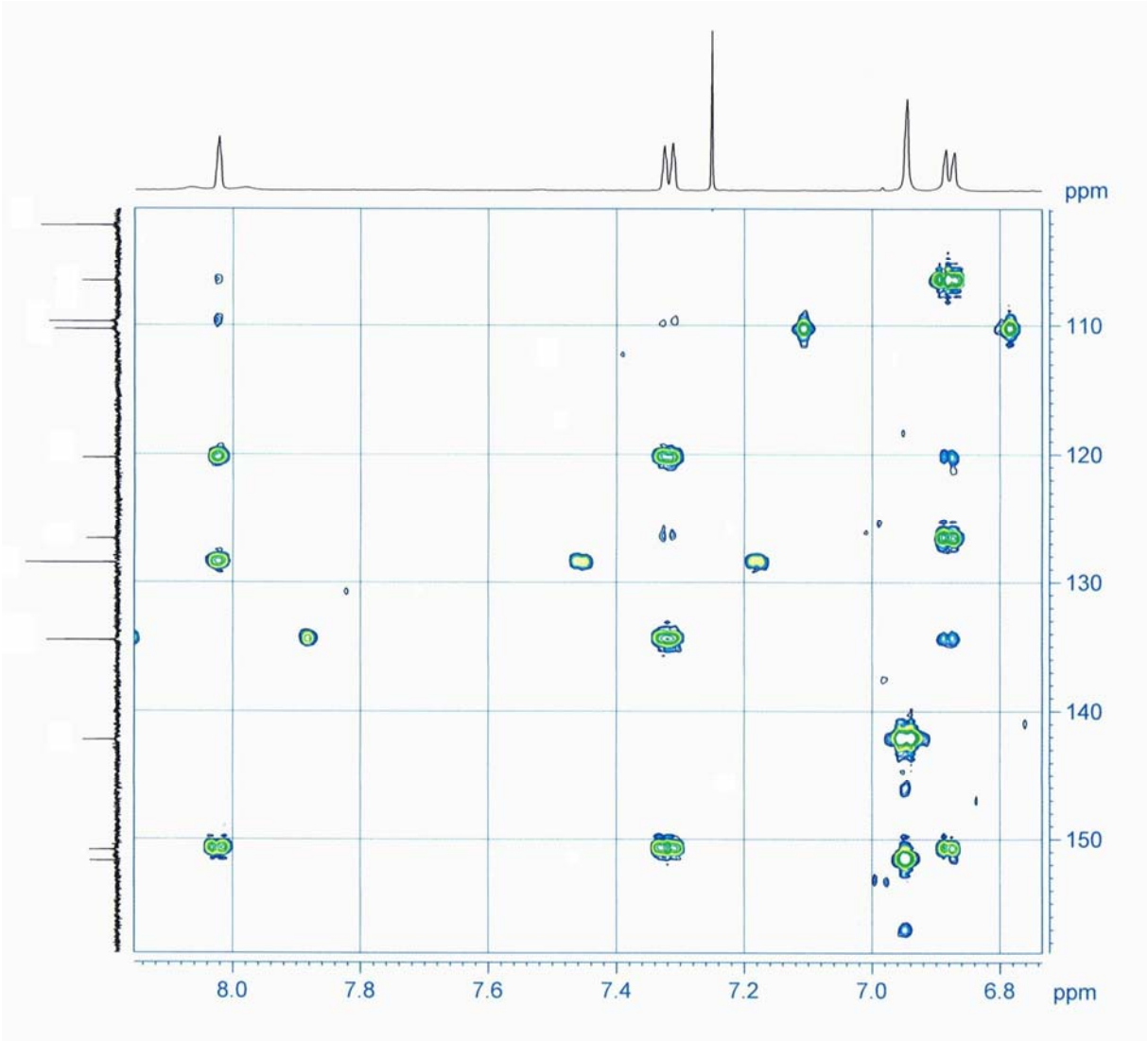


Figure S7. HMBC spectrum of complex **4**.

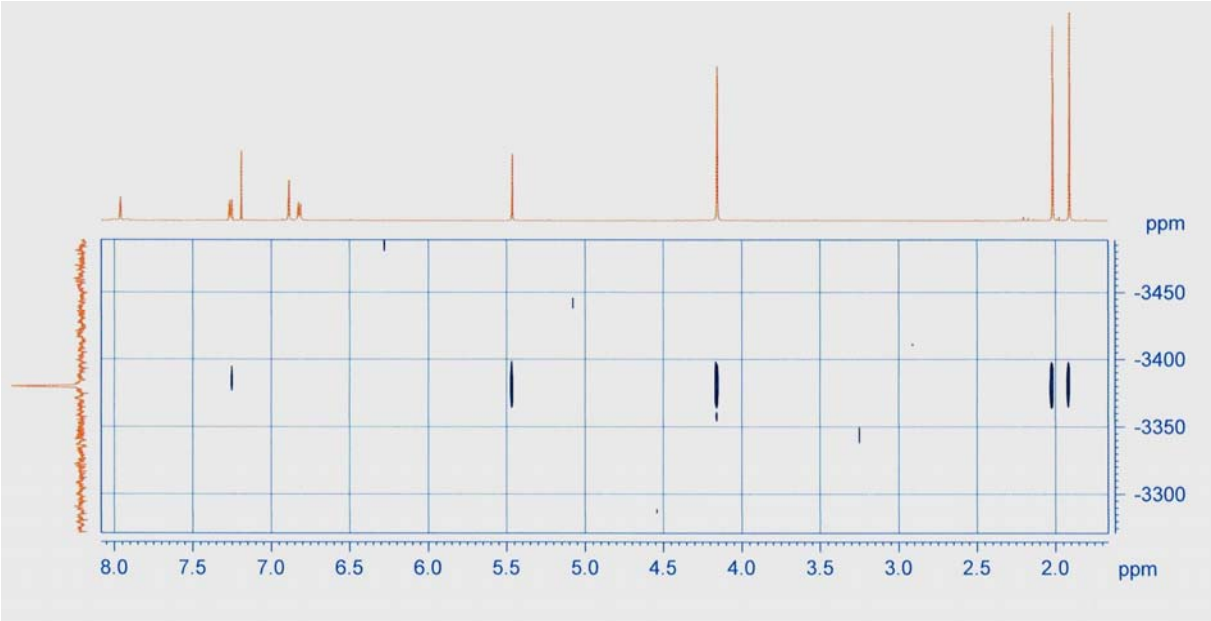
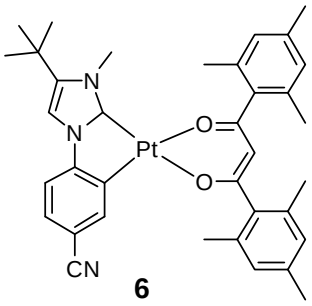


Figure S8. $^{1}H/^{195}Pt$ HMBC spectrum of complex **4**.



6

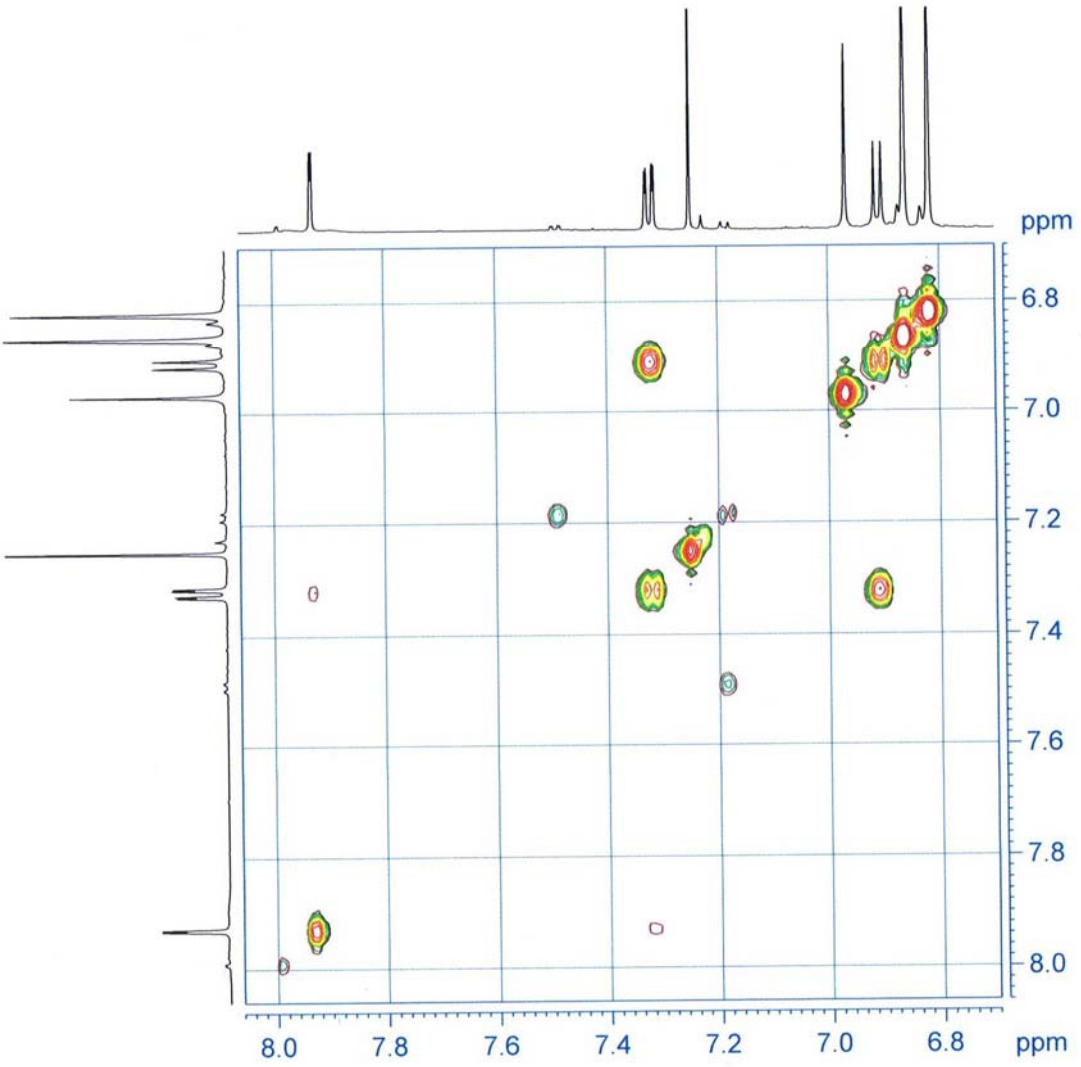


Figure S9. COSY spectrum of complex **6**.

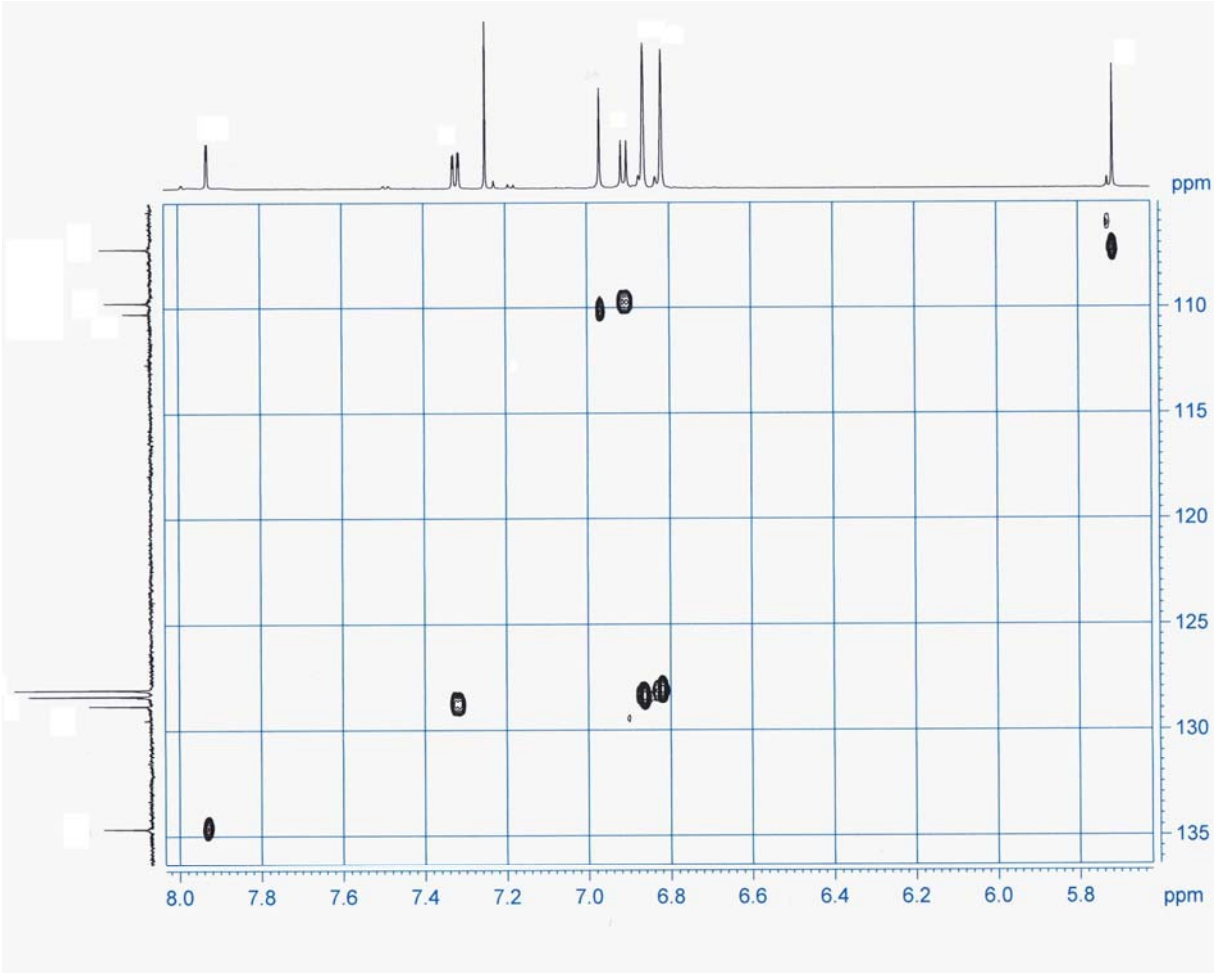


Figure S10. HSQC spectrum of complex **6**.

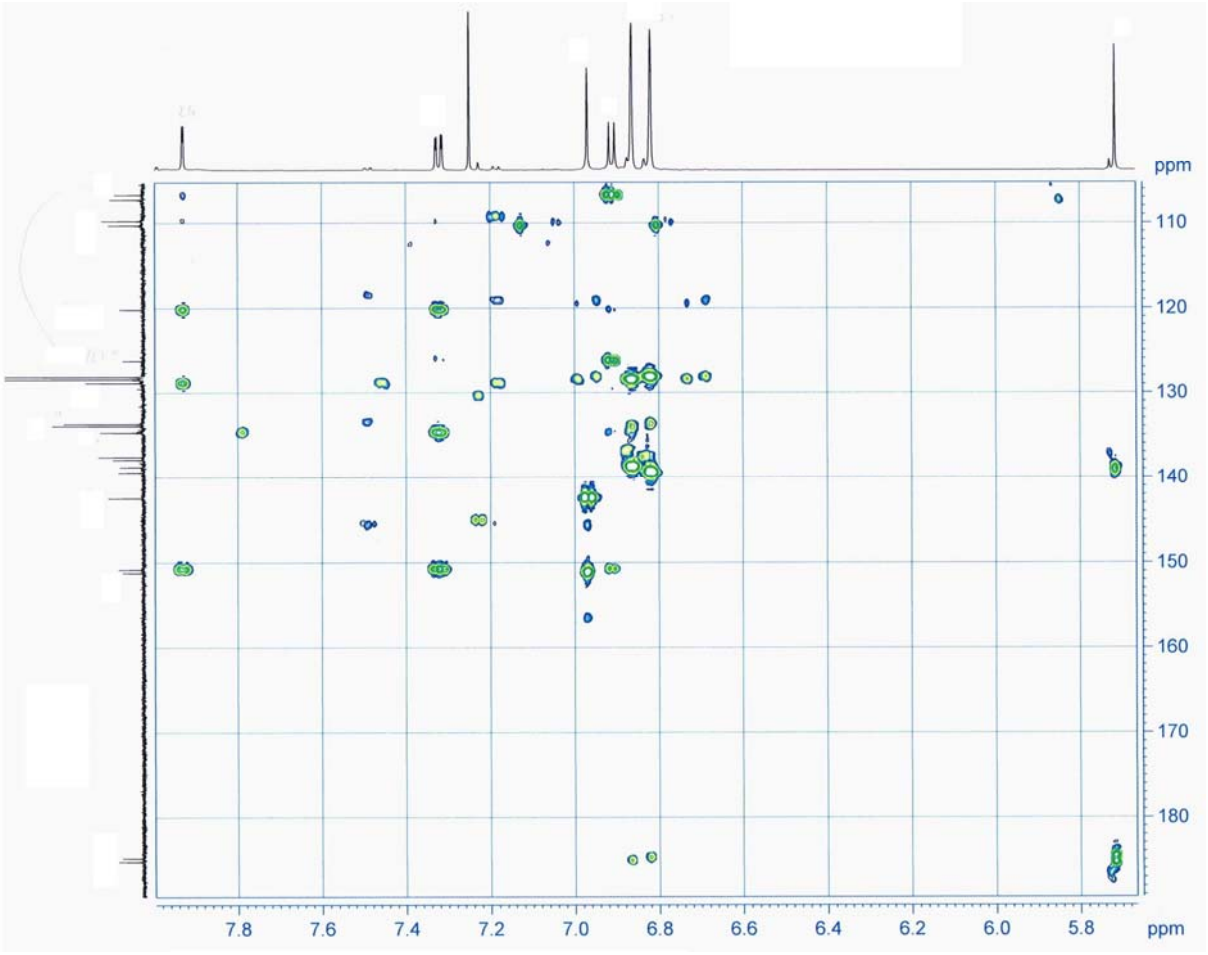


Figure S11. HMBC spectrum of complex **6**.

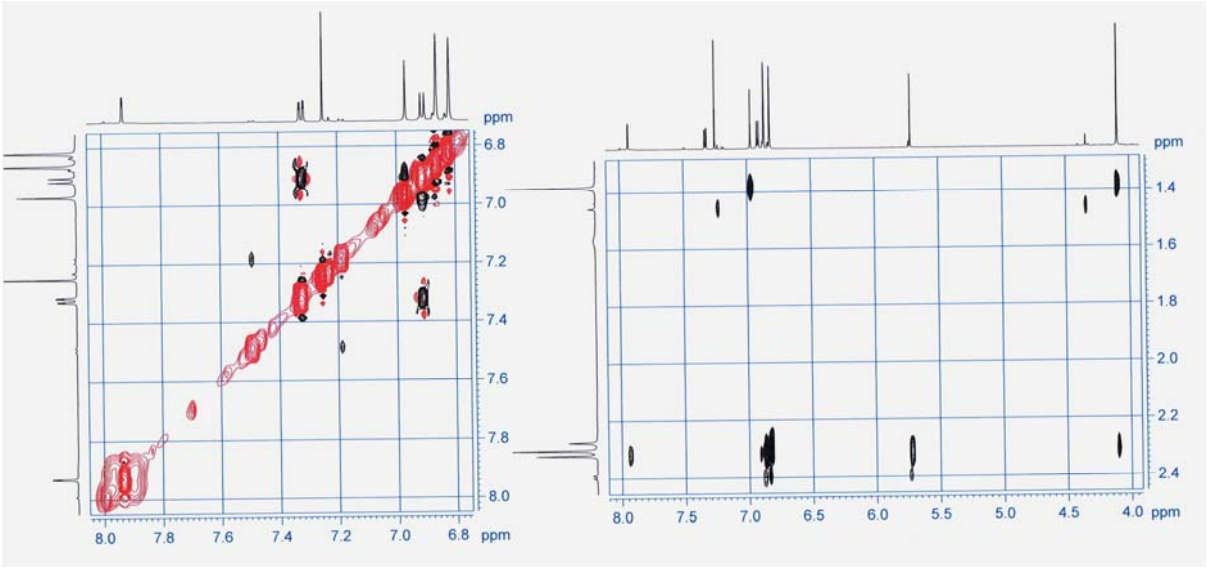


Figure S12. NOESY spectrum of complex **6**.

Solid-State Structure Determination

In the following section the solid-state data for **3**, **4** and **5** is given.

Table S1. Crystal data and crystallographic details for **3**, **4** and **5**.

Complex	**3**	**4**	**5**
CCDC #	972158	972159	972160
empirical formula	$C_{22}H_{21}N_3O_2Pt$	$C_{20}H_{23}N_3O_2Pt$	$C_{38}H_{37}N_3O_2Pt$
formula weight [g/mol]	554.1	532.5	762.8
T [K]	198(2)	198(2)	198(2)
wavelength [Å]	0.71073	0.71073	0.71073
crystal system	monoclinic	monoclinic	orthorhombic
space group	*C* 2/*c*	*P* $2_1/c$	*P* $2_12_12_1$
a [Å]	25.953(5)	12.4720(19)	10.251(2)
b [Å]	11.773(2)	9.6470(9)	13.9000(6)
c [Å]	14.429(3)	16.8840(18)	22.872(3)
α [°]	90	90	90
β [°]	103.65(3)	110.760(7)	90
γ [°]	90	90	90
U [$Å^3$]	4284.2(15)	1899.5(4)	3259.0(8)
Z	8	4	4
D_{calc} [Mg/m^3]	1.719	1.862	1.555
μ(MoKα) [mm^{-1}]	6.571	7.406	4.343
crystal size [mm^3]	0.34×0.39×0.39	0.84×0.48×0.37	0.34×0.31×0.30
F(000)	2144	1032	1520
reflections collected	84091	36075	70606
independent reflections	3917 R_{int} = 0.032	3814 R_{int} = 0.039	6671 R_{int} = 0.061
Goodness-of-fit on F^2	1.140	1.148	1.215
R_1 [I>2σ(I)]	0.0207	0.0227	0.0359
wR_2 [I>2σ(I)]	0.0567	0.0456	0.0836
data / restraints / parameters	3917/ 0 / 245	3814 / 0 / 241	6671 / 0 / 405

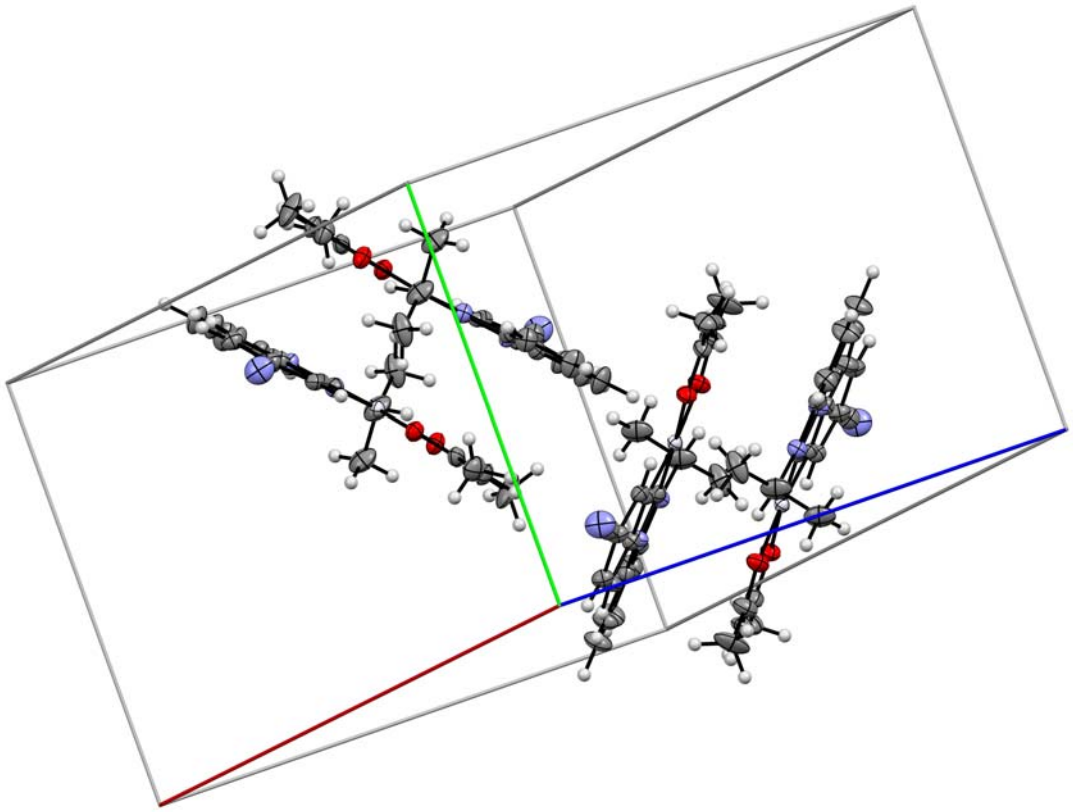


Figure S13. Representation of complex **3** in the solid state. The shortest Pt–Pt distance is found to be 3.26 Å. The molecules form two planes with an angle of 86 °.

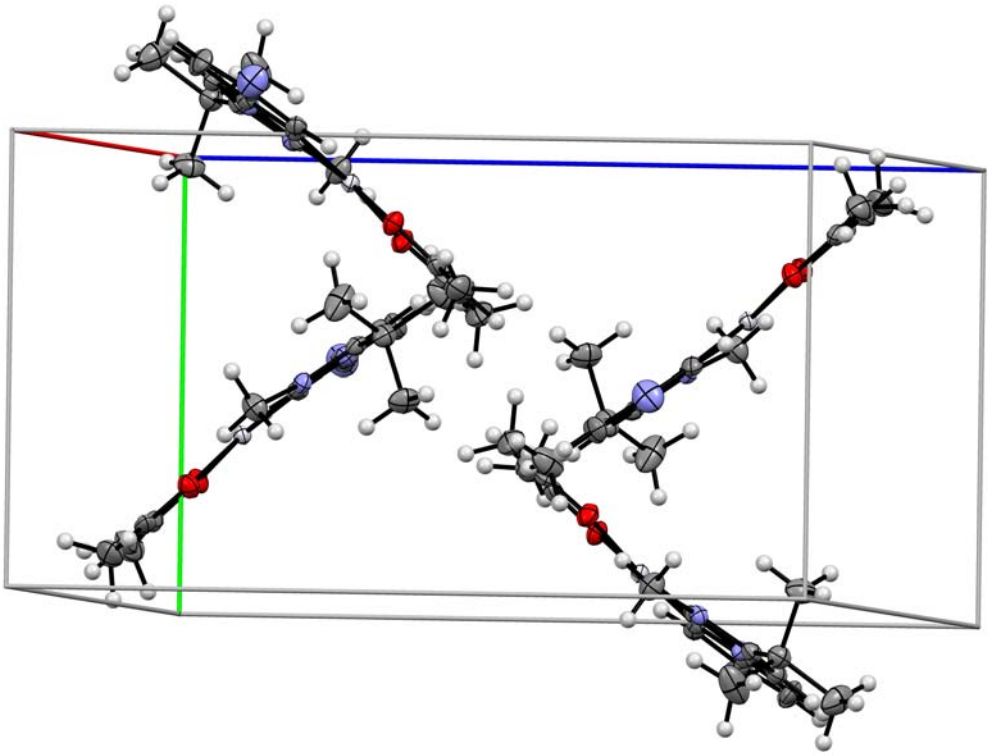


Figure S14. Representation of complex **4** in the solid state. The shortest Pt–Pt distance is found to be 3.28 Å. The molecules form two planes with an angle of 81 °.

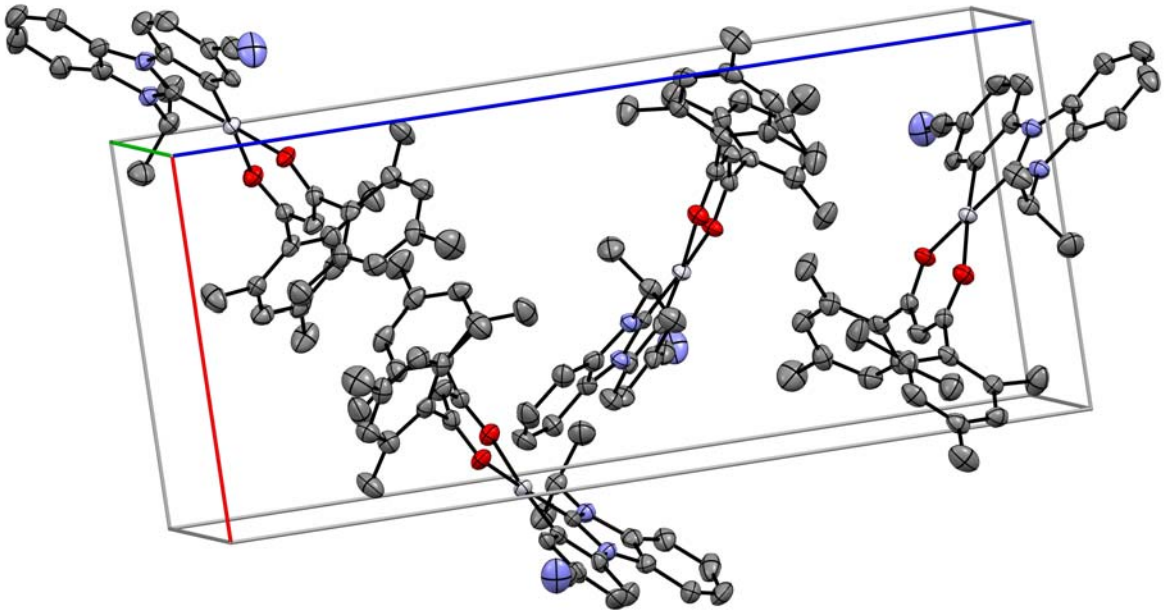


Figure S15. Representation of complex **5** in the solid state (hydrogen atoms omitted for clarity). The shortest Pt–Pt distance is found to be 7.88 Å.

Photoluminescence Data

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

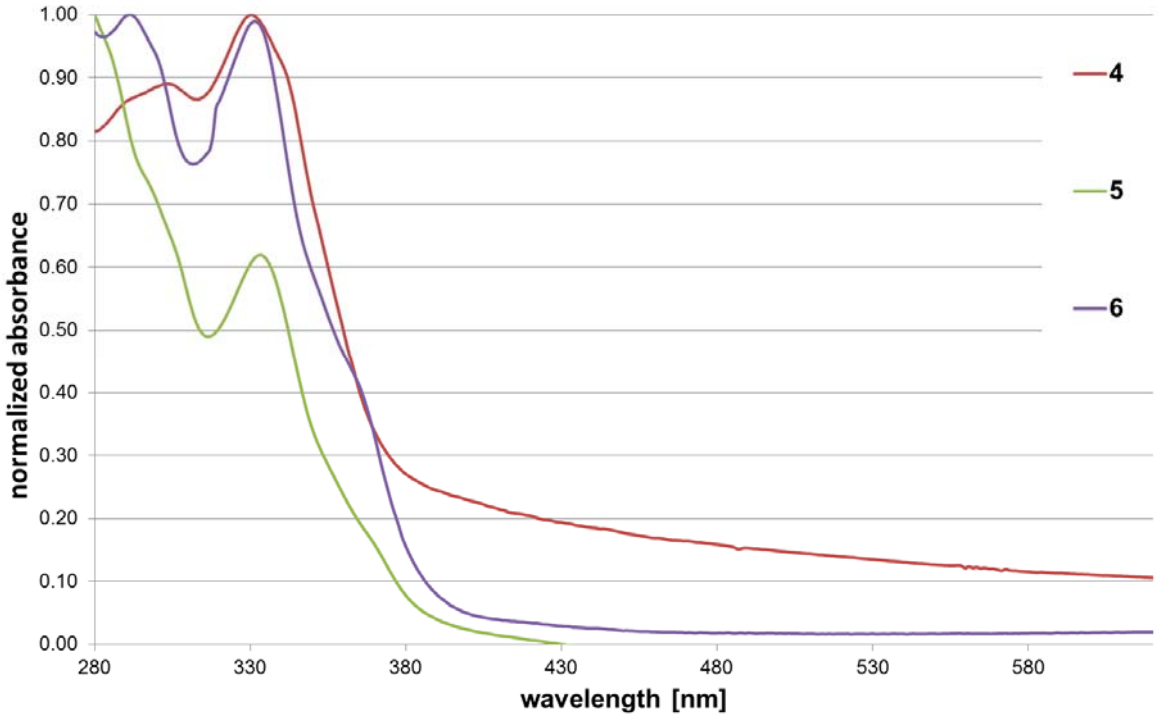


Figure S16. Absorption spectra for the complexes **4-6** as 100% emitter films.

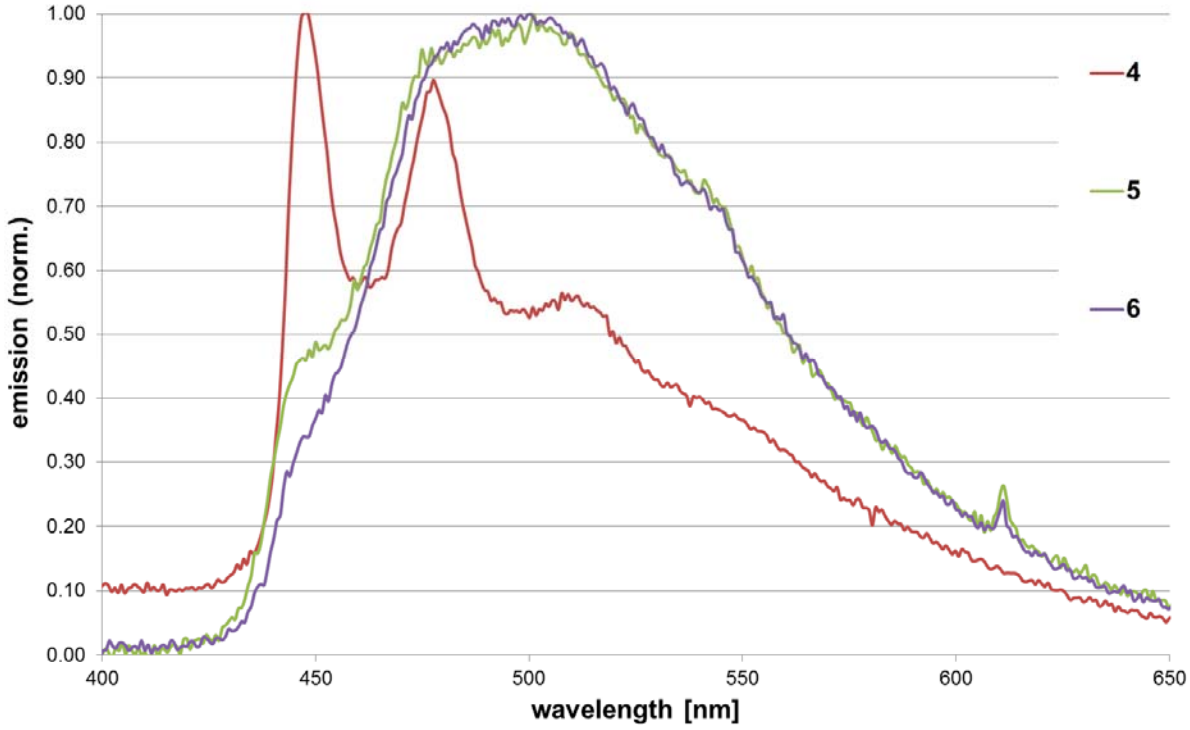


Figure S17. Emission spectra for the complexes **4-6** as 100% emitter films.

Quantum Chemical Calculations

Table S2. Comparison of bond lengths, angles and dihedral angles of **3** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**Xray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.940(4)	1.964	1.966
Pt(1)-C(9)	1.969(4)	1.995	1.952
Pt(1)-O(1)	2.087(3)	2.154	2.151
Pt(1)-O(2)	2.059(3)	2.089	2.106
O(1)-Pt(1)-O(2)	89.35(13)	87.75	87.60
C(1)-Pt(1)-C(9)	80.46(18)	80.08	81.05
Pt(1)-C(1)-N(1)-C(8)	-1.5(5)	0.01	0.00
N(1)-C(1)-Pt(1)-O(1)	177.1(3)	179.99	180.00

Table S3. Comparison of bond lengths, angles and dihedral angles of **4** from the solid-state determination and DFT calculations (B3LYP/6-31G(d)).

		DFT	
Bonds [Å]/Angles [°]	**Xray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.954(4)	1.972	1.967
Pt(1)-C(9)	1.986(4)	2.001	1.962
Pt(1)-O(1)	2.083(3)	2.148	2.151
Pt(1)-O(2)	2.047(3)	2.086	2.100
O(1)-Pt(1)-O(2)	90.22(11)	88.43	88.21
C(1)-Pt(1)-C(9)	80.26(15)	80.05	81.19
Pt(1)-C(1)-N(1)-C(8)	3.5(4)	-0.42	-0.31
N(1)-C(1)-Pt(1)-O(1)	171.1(3)	-178.98	178.78

Table S4. 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 [°]	**Xray**	**Singlet**	**Triplet**
Pt(1)-C(1)	1.957(7)	1.965	1.972
Pt(1)-C(9)	1.999(7)	1.996	1.998
Pt(1)-O(1)	2.082(5)	2.150	2.141
Pt(1)-O(2)	2.030(4)	2.090	2.083
O(1)-Pt(1)-O(2)	89.26(17)	87.95	87.19
C(1)-Pt(1)-C(9)	80.4(3)	80.12	80.05
Pt(1)-C(1)-N(1)-C(8)	4.2(8)	-0.32	-2.25
N(1)-C(1)-Pt(1)-O(1)	171.2(5)	-179.62	178.04

Table S5. Data for the wavelength prediction (BP86/6-31G(d)).

Complex	S-T gap [eV][a]	λ_{max} uncorr. [nm]	S-T gap corr. [eV][b]	λ_{max} corr. [nm][b]	λ_{max} exp. [nm]
3	2.304	538	2.698	460	444, 473
4	2.332	534	2.715	457	443, 474
5	2.309	537	2.703	459	442, 471
6	2.162	573	2.552	486	443, 471

[a] Singlet ground state not optimized but geometry taken from the optimized triplet ground state. [b] Correction method taken from ref.[1]

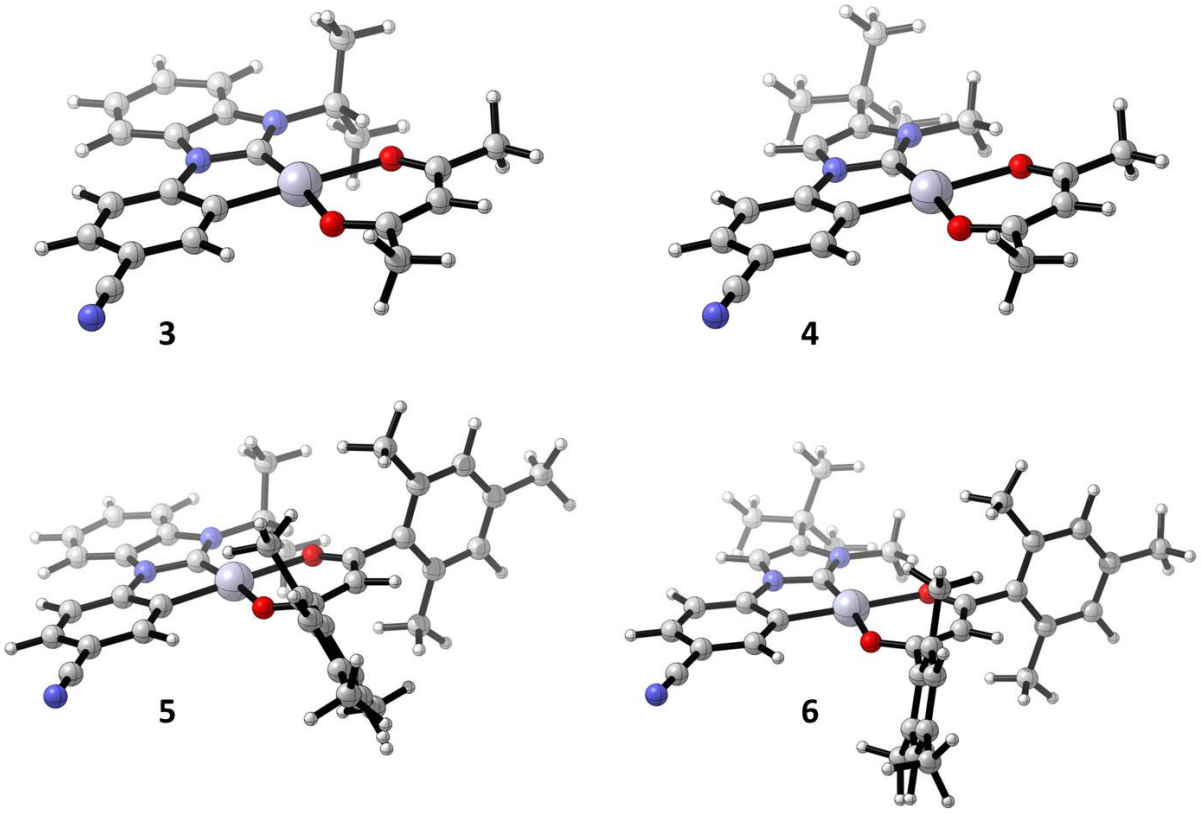


Figure S18. CYLview plot of the optimised singlet ground state structures (B3LYP/6-31G(d)).

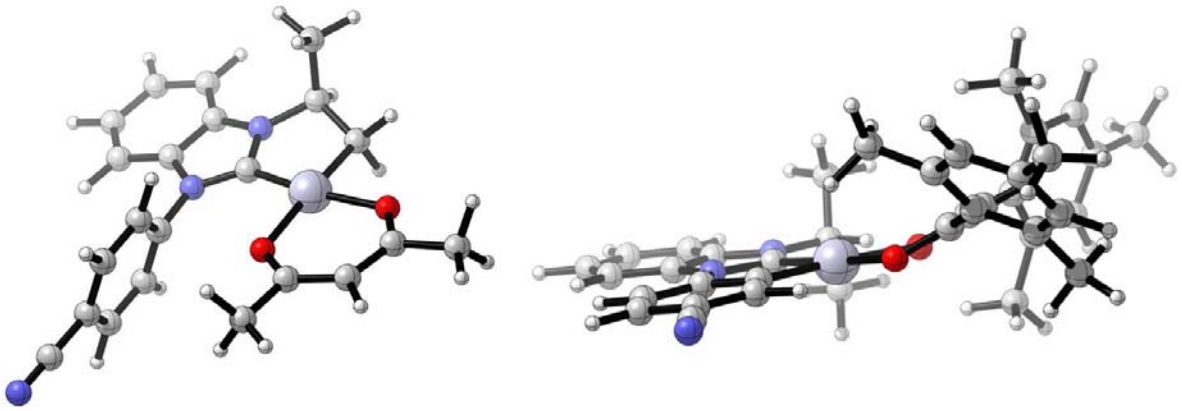


Figure S19. Possible isomer of complex **3** (left) and **5** in the triplet state (right, B3LYP/6-31G(d)).

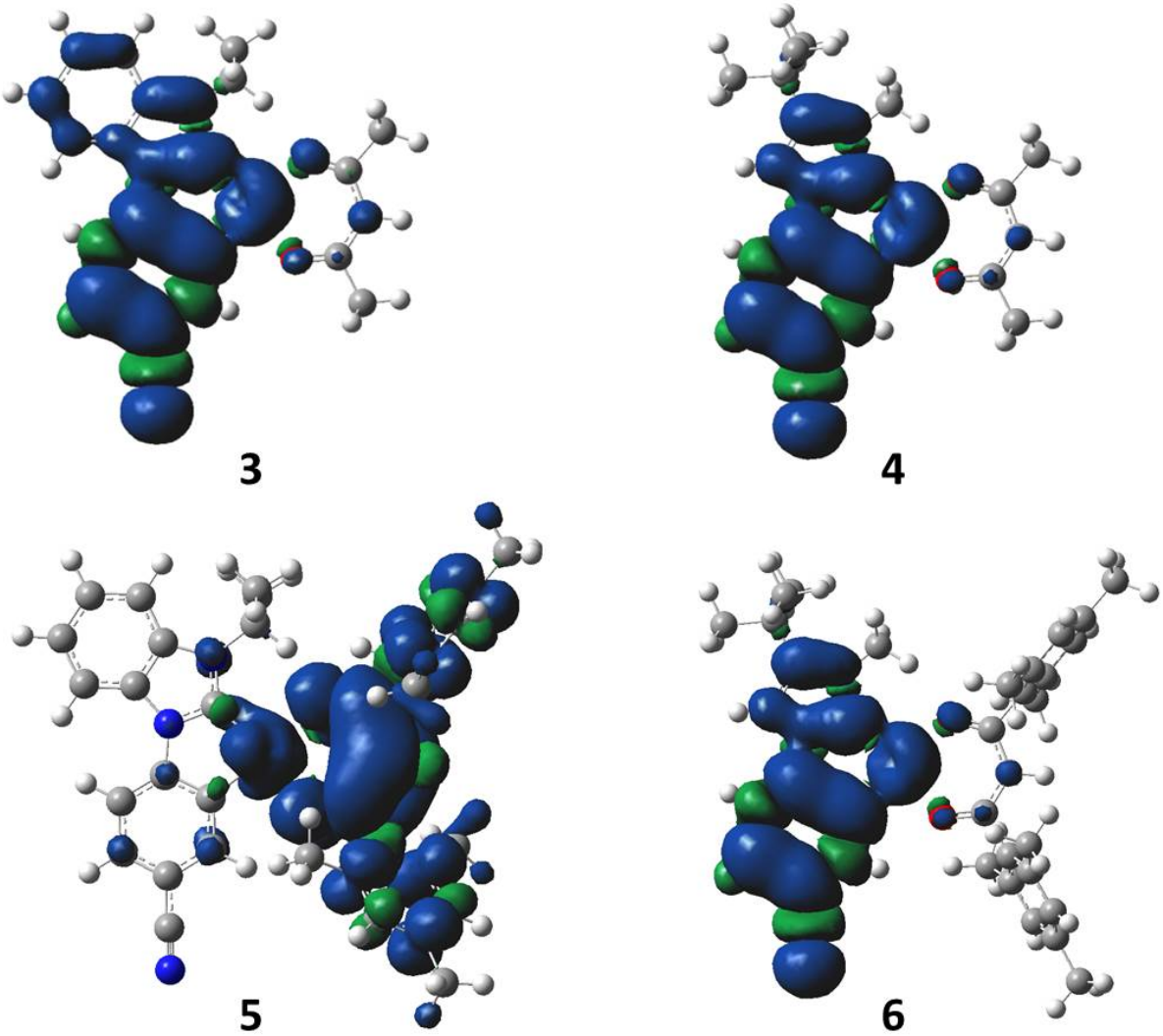


Figure S20. Spin densities computed on the optimized geometries of the first triplet state (B3LYP/6-31G(d), isovalue = 0.02).

In the following section the singlet ground state geometries for **3**-**6** are given (B3LYP/6-31G(d)).

Coordinates for the optimized singlet ground state of **3**.

Pt	-1.07036	-0.46615	-0.04719
C	-0.42402	-2.35297	-0.00975
C	-1.21909	-3.49560	-0.01540
C	0.97633	-2.52421	0.02564
C	-0.63257	-4.77674	0.01347
H	-2.29855	-3.39595	-0.04228
C	1.57556	-3.78263	0.05447
C	0.76309	-4.91528	0.04828
H	2.64968	-3.90749	0.08137
H	1.20821	-5.90429	0.07033
C	0.86911	-0.15858	-0.00465
N	1.66666	-1.28291	0.02765
N	1.69643	0.91657	0.00241
O	-1.78299	1.56648	-0.08790
C	-4.10393	-0.33250	-0.12027
C	-3.00969	1.92276	-0.12109
C	-4.12595	1.07161	-0.13721
H	-5.10090	1.54351	-0.16564
C	-5.41278	-1.09341	-0.14194
H	-6.28245	-0.43265	-0.17010
H	-5.43521	-1.75401	-1.01614
H	-5.47646	-1.73322	0.74559
C	-3.22964	3.42274	-0.14457
H	-2.76854	3.87359	0.74191
H	-2.73225	3.85122	-1.02253
H	-4.28813	3.69252	-0.16991
O	-3.06663	-1.07993	-0.08722
C	1.22594	2.32207	-0.02557
C	1.67765	3.03059	-1.30918
C	1.61618	3.06134	1.26084
H	1.34641	2.47408	-2.19179
H	1.24324	2.52565	2.13968
C	3.01443	-0.92217	0.05569
C	3.03224	0.48822	0.03950
C	4.20451	-1.65333	0.09295
C	4.23683	1.19404	0.06013
C	5.40350	-0.94246	0.11337
H	4.21703	-2.73446	0.10613
C	5.42086	0.45926	0.09724
H	4.26365	2.27624	0.04807
H	6.34056	-1.49015	0.14239
H	6.37071	0.98496	0.11387
C	-1.46360	-5.94504	0.00728
N	-2.13742	-6.89415	0.00230
H	2.76325	3.15489	-1.36920
H	1.22492	4.02719	-1.34685
H	1.16217	4.05806	1.25315
H	2.69768	3.18839	1.36945
H	0.13956	2.24636	-0.05059

Coordinates for the optimized singlet ground state of **4**.

Pt	-1.12297	-1.07347	-0.02409
C	-0.57314	0.82008	-0.01343
N	0.77145	1.05202	0.00987
N	-1.15131	2.04936	-0.02233
O	-3.25556	-0.82451	-0.09847
C	-2.54585	-3.74519	-0.06543
C	-4.10503	-1.77915	-0.13018
C	-3.81967	-3.15379	-0.11405
H	-4.66742	-3.82811	-0.14270
C	-2.43258	-5.25538	-0.05364
H	-3.40609	-5.75030	-0.08841
H	-1.83281	-5.58223	-0.91067
H	-1.90067	-5.57325	0.85035
C	-5.55222	-1.33055	-0.19051
H	-5.77574	-0.69969	0.67768
H	-5.70700	-0.71646	-1.08539
H	-6.25259	-2.16893	-0.21019
O	-1.42153	-3.13806	-0.02886
C	-2.60382	2.21972	0.02204
C	1.03323	2.40814	0.01619
C	-0.16399	3.06229	-0.00358
C	1.60669	-0.09112	0.03286
C	2.99715	-0.04614	0.06041
C	0.86542	-1.29115	0.02663
C	3.69981	-1.24973	0.08379
C	1.58690	-2.48248	0.05026
C	2.99713	-2.46624	0.07894
H	1.05939	-3.43026	0.04626
H	2.03708	2.79704	0.02910
H	-2.92932	2.91815	-0.75051
H	-3.06480	1.24700	-0.14591
H	-2.91221	2.59354	1.00207
C	3.72402	-3.70202	0.10331
N	4.31523	-4.70454	0.12319
H	3.53504	0.89761	0.06401
H	4.78432	-1.25208	0.10572
C	-0.39778	4.56539	-0.04464
C	0.96757	5.27448	0.09825
H	1.64624	5.01383	-0.72123
H	0.82056	6.35921	0.07278
H	1.45440	5.02396	1.04721
C	-1.01019	4.99125	-1.40202
H	-2.00274	4.56323	-1.57037
H	-1.11486	6.08209	-1.43599
H	-0.36584	4.68444	-2.23280
C	-1.29938	5.04314	1.11892
H	-2.32789	4.68515	1.02952
H	-0.90372	4.71185	2.08540
H	-1.33671	6.13847	1.12639

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

Pt	-0.61282	-0.45870	-0.02899
C	-1.39864	-2.29334	-0.05270
C	-0.69140	-3.49241	-0.07691
C	-2.80835	-2.35835	-0.04399
C	-1.37355	-4.72577	-0.08813
H	0.39293	-3.47473	-0.08956
C	-3.50099	-3.56808	-0.05551
C	-2.77604	-4.75843	-0.07685
H	-4.58175	-3.61230	-0.04863
H	-3.29494	-5.71103	-0.08554
C	-2.52526	-0.00659	-0.01868
N	-3.40409	-1.06882	-0.02432
N	-3.26965	1.12702	-0.00273
O	0.24204	1.51409	-0.00196
C	2.42482	-0.55077	-0.02457
C	1.49375	1.78060	0.01335
C	2.54505	0.85038	-0.00061
H	3.55173	1.25241	0.01979
O	1.33323	-1.22049	-0.03348
C	-2.69590	2.49506	0.00729
C	-3.05312	3.23638	1.30185
C	-3.06921	3.26145	-1.26799
H	-2.74794	2.65212	2.17595
H	-2.77268	2.69568	-2.15719
C	-4.72160	-0.60884	-0.01097
C	-4.63395	0.79892	0.00279
C	-5.96334	-1.24946	-0.00912
C	-5.78260	1.59276	0.01819
C	-7.10590	-0.45109	0.00638
H	-6.05700	-2.32662	-0.01896
C	-7.01852	0.94814	0.01978
H	-5.72765	2.67380	0.02869
H	-8.08162	-0.92741	0.00816
H	-7.92676	1.54295	0.03172
C	-0.63559	-5.95488	-0.10991
N	-0.04105	-6.95540	-0.12597
H	-4.12232	3.45288	1.38992
H	-2.51475	4.18958	1.32642
H	-2.53368	4.21653	-1.27920
H	-4.13984	3.47685	-1.33978
H	-1.61799	2.34064	-0.00048
C	1.83171	3.24999	0.04951
C	1.91148	3.97398	-1.15510
C	2.02734	3.89272	1.28672
C	2.19941	5.34182	-1.09981
C	2.31156	5.26233	1.29483
C	2.40142	6.00587	0.11391
H	2.26761	5.90153	-2.03084
H	2.46654	5.75997	2.25044
C	3.67873	-1.38261	-0.00908
C	4.50198	-1.45535	-1.14895
C	4.00298	-2.10776	1.15682
C	5.65050	-2.25380	-1.09778
C	5.16686	-2.88039	1.16518
C	6.00247	-2.97229	0.04708
H	6.28309	-2.31824	-1.98100
H	5.42488	-3.42915	2.06899
C	1.69776	3.29380	-2.48971
H	2.45103	2.51722	-2.67117
H	0.71974	2.80124	-2.53543
H	1.75457	4.01483	-3.31085
C	1.93525	3.12735	2.58892
H	0.97796	2.60048	2.67664
H	2.72309	2.36841	2.66706
H	2.03159	3.80063	3.44615
C	2.68151	7.49076	0.15124
H	3.16969	7.82988	-0.76866
H	1.75398	8.06933	0.25954
H	3.32775	7.75571	0.99517
C	4.16880	-0.71211	-2.42572
H	3.11945	-0.84561	-2.71107
H	4.33994	0.36711	-2.32794
H	4.78981	-1.07094	-3.25245
C	3.12575	-2.05227	2.38835
H	2.90719	-1.01844	2.68252
H	2.16164	-2.54177	2.21351
H	3.61139	-2.54857	3.23396
C	7.23313	-3.84898	0.07016
H	6.97583	-4.89830	-0.12681
H	7.95861	-3.54221	-0.69057
H	7.73033	-3.81679	1.04612

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

Pt	0.56173	-0.58383	-0.00003
C	2.53109	-0.46564	0.01774
N	3.19954	-1.65433	-0.02432
N	3.49499	0.49048	0.06168
O	0.08988	1.51066	0.02085
C	-2.43279	-0.13617	-0.01419
C	-1.09564	1.99339	0.01830
C	-2.29561	1.26382	0.00287
H	-3.21382	1.84045	0.00969
O	-1.48453	-0.99588	-0.01723
C	3.17053	1.91217	0.19065
C	4.56484	-1.44718	-0.00867
C	4.77999	-0.10085	0.04513
C	2.40300	-2.82461	-0.06287
C	2.91383	-4.11817	-0.10550
C	1.02354	-2.53098	-0.05129
C	2.01709	-5.18466	-0.13766
C	0.14402	-3.61104	-0.08588
C	0.63502	-4.93302	-0.12787
H	-0.92650	-3.43500	-0.08274
H	5.26835	-2.26156	-0.04274
H	3.71387	2.49632	-0.55358
H	2.09876	2.03308	0.03828

H	3.42826	2.27031	1.19087
C	-0.28158	-6.03539	-0.16007
N	-1.02143	-6.93365	-0.18493
H	3.98363	-4.30629	-0.11372
H	2.37993	-6.20640	-0.17040
C	6.11869	0.62276	0.03909
C	7.24338	-0.43508	0.10127
H	7.21579	-1.10661	-0.76386
H	8.21677	0.06631	0.10002
H	7.17814	-1.03880	1.01317
C	6.30404	1.43037	-1.26945
H	5.57753	2.24153	-1.37192
H	7.30265	1.88244	-1.28716
H	6.20891	0.77998	-2.14555
C	6.28005	1.55213	1.26565
H	5.59156	2.40036	1.24506
H	6.11916	1.00252	2.19969
H	7.29734	1.95971	1.28432
C	-1.17608	3.49923	0.02356
C	-1.03024	4.20197	-1.18798
C	-1.36093	4.19094	1.23560
C	-1.09047	5.59904	-1.16660
C	-1.40904	5.58892	1.21066
C	-1.28394	6.31204	0.02061
H	-0.98179	6.14354	-2.10285
H	-1.54659	6.12560	2.14763
C	-3.81966	-0.72190	-0.00428
C	-4.30087	-1.31778	1.17963
C	-4.61226	-0.69774	-1.16722
C	-5.58644	-1.86480	1.18152
C	-5.88910	-1.26954	-1.12147
C	-6.39591	-1.85620	0.04055
H	-5.96314	-2.31447	2.09836
H	-6.50030	-1.25854	-2.02186
C	-1.49581	3.45120	2.54913
H	-2.41585	2.85551	2.58503
H	-0.66230	2.75686	2.70698
H	-1.51711	4.15105	3.39023
C	-1.37891	7.82050	0.01525
H	-2.42009	8.15295	-0.09442
H	-0.99940	8.25005	0.94884
H	-0.81086	8.25587	-0.81397
C	-0.81252	3.46830	-2.49320
H	0.11236	2.88055	-2.47188
H	-1.62772	2.76369	-2.69849
H	-0.75268	4.16866	-3.33181
C	-3.45563	-1.36592	2.43358
H	-2.58791	-2.02175	2.30290
H	-3.06657	-0.37459	2.69667
H	-4.03808	-1.73673	3.28245
C	-4.11116	-0.08708	-2.45896
H	-4.05586	1.00683	-2.39901
H	-3.10682	-0.44487	-2.71213
H	-4.77764	-0.34024	-3.28937
C	-7.76649	-2.49245	0.05915
H	-8.40106	-2.10177	-0.74327
H	-7.70038	-3.58037	-0.07577
H	-8.27798	-2.31668	1.01228

In the following section the triplet state geometries for the complexes **3-6** are given, which were used for the wavelength prediction (BP86/6-31G(d)).

Coordinates for the optimized triplet state of **3**.

Pt	-0.83420	-0.34626	0.00002
C	-0.71187	1.60392	-0.00006
C	-1.78987	2.49367	-0.00013
C	0.66465	2.16266	-0.00005
C	-1.57753	3.89494	-0.00016
H	-2.80837	2.09570	-0.00016
C	0.88395	3.56943	-0.00001
C	-0.20431	4.41573	-0.00006
H	1.89004	3.99261	0.00009
H	-0.05946	5.50001	-0.00002
C	1.11603	-0.16806	0.00005
N	1.61321	1.17229	-0.00005
N	2.22824	-0.98689	0.00005
O	-0.96275	-2.49008	0.00008
C	-3.74213	-1.27858	-0.00026
C	-2.06516	-3.16780	-0.00004
C	-3.37265	-2.64599	-0.00028
H	-4.19032	-3.37173	-0.00041
C	-5.21422	-0.90716	-0.00046
H	-5.87213	-1.79038	-0.00052
H	-5.44002	-0.28924	0.88703
H	-5.43979	-0.28929	-0.88804
C	-1.86980	-4.67480	0.00031
H	-1.28325	-4.97310	-0.88733
H	-1.28679	-4.97312	0.89028
H	-2.82422	-5.22445	-0.00150
O	-2.94431	-0.26824	-0.00010
C	2.14832	-2.46821	0.00018
C	2.74852	-3.05502	1.29056
C	2.74894	-3.05532	-1.28986
H	2.25641	-2.62129	2.17774
H	2.25705	-2.62189	-2.17730
C	3.02081	1.15517	-0.00012
C	3.39704	-0.21984	-0.00003
C	3.98264	2.17421	-0.00027
C	4.75592	-0.58328	-0.00003
C	5.33864	1.80209	-0.00029
H	3.70715	3.22996	-0.00039
C	5.71320	0.44422	-0.00017
H	5.06967	-1.62908	0.00006
H	6.10726	2.58090	-0.00041
H	6.77534	0.17722	-0.00017
C	-2.66261	4.80125	-0.00024
N	-3.56308	5.57292	-0.00031
H	3.83430	-2.87872	1.37690
H	2.58305	-4.14658	1.30558
H	2.58358	-4.14690	-1.30462
H	3.83473	-2.87897	-1.37595
H	1.06855	-2.68422	0.00001

Coordinates for the optimized triplet state of **4**.

Pt	-0.74918	-0.46688	-0.01328
C	1.14492	0.01245	-0.01670
N	1.42435	1.40280	-0.00318
N	2.38470	-0.59729	-0.02211
O	-0.52131	-2.60762	0.02267
C	-3.46112	-1.84080	0.00046
C	-1.50681	-3.44477	0.04145
C	-2.88041	-3.13105	0.02927
H	-3.57445	-3.97577	0.04421
C	-4.97361	-1.70790	-0.01199
H	-5.48344	-2.68398	0.00814
H	-5.29997	-1.11216	0.85920
H	-5.28875	-1.15524	-0.91520
C	-1.08298	-4.90404	0.07980
H	-0.45021	-5.13001	-0.79741
H	-0.46786	-5.08773	0.97928
H	-1.94159	-5.59376	0.08805
O	-2.83684	-0.71358	-0.01684
C	2.51461	-2.05010	-0.15103
C	2.79985	1.60565	-0.00120
C	3.41260	0.36564	-0.01673
C	0.34348	2.24018	0.00154
C	0.38392	3.66517	0.01641
C	-0.93926	1.48870	-0.01062
C	-0.80547	4.35592	0.01760
C	-2.12241	2.22176	-0.01000
C	-2.09902	3.64739	0.00344
H	-3.08131	1.69565	-0.01960
H	3.23504	2.59949	0.01996
H	3.25628	-2.43752	0.56371
H	1.53163	-2.49785	0.05797
H	2.81611	-2.32360	-1.17698
C	-3.29316	4.39727	0.00430
N	-4.29064	5.04192	0.00522
H	1.33797	4.20355	0.02648
H	-0.81459	5.44977	0.02865
C	4.91093	0.09044	0.01755
C	5.66390	1.44100	-0.08255
H	5.42357	2.10533	0.76635
H	6.75212	1.25632	-0.06308
H	5.42703	1.96993	-1.02273
C	5.31202	-0.57726	1.36246
H	4.84901	-1.56867	1.50145
H	6.40803	-0.71701	1.39497
H	5.01977	0.05687	2.21751
C	5.36351	-0.79331	-1.17609
H	4.96387	-1.81842	-1.12214
H	5.05202	-0.35059	-2.13865
H	6.46585	-0.86988	-1.17676

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

Pt	-0.60272	-0.48562	-0.05005
C	-1.33848	-2.29756	-0.08339
C	-0.60020	-3.48410	-0.12821
C	-2.81972	-2.38822	-0.06121
C	-1.24858	-4.74470	-0.14115
H	0.49192	-3.43099	-0.15583
C	-3.47610	-3.65175	-0.07142
C	-2.71457	-4.80040	-0.10907
H	-4.56430	-3.73311	-0.05056
H	-3.19787	-5.78176	-0.11714
C	-2.50863	-0.03394	-0.03015
N	-3.40493	-1.14796	-0.03280
N	-3.30368	1.09448	0.00202
O	0.18949	1.50666	-0.02345
C	2.45253	-0.52904	-0.03877
C	1.45440	1.79729	0.00183
C	2.52834	0.88911	-0.01253
H	3.53159	1.32309	0.02512
O	1.36989	-1.23147	-0.05484
C	-2.75971	2.47579	0.01324
C	-3.11984	3.20351	1.32074
C	-3.16726	3.24273	-1.25742
H	-2.78818	2.61652	2.19414
H	-2.86519	2.68465	-2.16012
C	-4.73438	-0.68614	-0.00300
C	-4.65520	0.73692	0.01941
C	-5.96959	-1.34775	0.00652
C	-5.82812	1.51260	0.05189
C	-7.13711	-0.56480	0.03927
H	-6.04388	-2.43615	-0.01100
C	-7.06182	0.84158	0.06159
H	-5.79256	2.60354	0.06948
H	-8.11299	-1.05976	0.04737
H	-7.98435	1.43123	0.08717
C	-0.51177	-5.95104	-0.18049
N	0.08979	-6.97238	-0.21102
H	-4.20223	3.39284	1.42247
H	-2.60241	4.17818	1.34619
H	-2.65410	4.21995	-1.27008
H	-4.25305	3.43101	-1.31517
H	-1.66726	2.34141	-0.00816
C	1.75754	3.27630	0.05421
C	1.81586	4.02065	-1.15001
C	1.94565	3.91171	1.30640
C	2.07310	5.40185	-1.07801
C	2.19865	5.29567	1.32905
C	2.26505	6.06044	0.15026
H	2.12535	5.97850	-2.01096
H	2.34798	5.78901	2.29857
C	3.72784	-1.32508	-0.00156
C	4.66528	-1.24194	-1.06467
C	3.97387	-2.17720	1.10993
C	5.83703	-2.01760	-0.99289
C	5.16895	-2.91518	1.14243
C	6.11157	-2.85841	0.09931
H	6.55424	-1.96624	-1.82262
H	5.36699	-3.55807	2.00998
C	1.61742	3.34648	-2.49317
H	2.39825	2.58704	-2.68484
H	0.64731	2.82031	-2.54178
H	1.65161	4.08150	-3.31503
C	1.87954	3.12481	2.60068
H	0.92394	2.57743	2.69215
H	2.68434	2.36891	2.65888
H	1.97723	3.79117	3.47437
C	2.50900	7.55461	0.20367
H	3.02655	7.91344	-0.70328
H	1.55716	8.11561	0.27880
H	3.12061	7.83415	1.07940
C	4.43335	-0.36880	-2.28456
H	3.39029	-0.42343	-2.64133
H	4.64794	0.69684	-2.07863
H	5.09280	-0.68112	-3.11254
C	2.99608	-2.28699	2.26362
H	2.63295	-1.29630	2.59150
H	2.10264	-2.87229	1.98368
H	3.46949	-2.78197	3.12851
C	7.36722	-3.70349	0.13925
H	7.17319	-4.72403	-0.24377
H	8.16982	-3.26815	-0.48119
H	7.75014	-3.81222	1.16939

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

Pt	0.55794	-0.57014	-0.34851
C	2.48761	-0.39610	0.00320
N	3.19946	-1.57308	0.08403
N	3.39911	0.59289	0.26087
O	0.06300	1.48863	-0.55488
C	-2.43147	-0.22415	-0.22991
C	-1.10832	2.00491	-0.20741
C	-2.28400	1.18957	-0.07775
H	-3.21205	1.73202	0.12585
O	-1.44487	-1.02763	-0.61112
C	2.99568	2.00123	0.34770
C	4.52937	-1.32331	0.37611
C	4.68422	0.04211	0.49083
C	2.45408	-2.76682	-0.11461
C	3.00338	-4.05299	-0.09748
C	1.07655	-2.50488	-0.34186
C	2.15243	-5.14507	-0.32339
C	0.24699	-3.60696	-0.58640
C	0.77805	-4.92581	-0.57254
H	-0.81428	-3.44830	-0.80093
H	5.25946	-2.12056	0.47815
H	3.65849	2.62991	-0.26572
H	1.95943	2.07850	-0.02038

H	3.02992	2.34399	1.39475
C	-0.08335	-6.04812	-0.81131
N	-0.78790	-6.97219	-1.00461
H	4.07108	-4.21870	0.08299
H	2.54679	-6.16512	-0.31415
C	5.97348	0.81118	0.75329
C	7.10066	-0.21150	1.04285
H	7.27231	-0.88429	0.18371
H	8.04421	0.32761	1.23657
H	6.87319	-0.82581	1.93216
C	6.38436	1.63420	-0.49882
H	5.64715	2.41450	-0.75279
H	7.34919	2.13999	-0.31207
H	6.50333	0.97882	-1.37923
C	5.85120	1.74460	1.98773
H	5.15024	2.57874	1.82231
H	5.51822	1.18444	2.87931
H	6.83856	2.18724	2.21211
C	-1.22531	3.48233	-0.15082
C	-0.66979	4.28547	-1.20072
C	-1.87637	4.12909	0.94689
C	-0.79092	5.68091	-1.13194
C	-1.96419	5.53198	0.96493
C	-1.43598	6.33294	-0.06205
H	-0.37955	6.28322	-1.95335
H	-2.44654	6.01667	1.82450
C	-3.72213	-0.86302	0.13012
C	-3.74333	-1.89548	1.12292
C	-4.94587	-0.47131	-0.49873
C	-4.96780	-2.48682	1.46624
C	-6.14210	-1.10173	-0.12060
C	-6.18209	-2.11332	0.85745
H	-4.97787	-3.25955	2.24640
H	-7.07388	-0.80738	-0.62181
C	-2.42962	3.35923	2.13186
H	-3.45373	2.97673	1.95271
H	-1.80316	2.48607	2.38499
H	-2.48794	4.01100	3.02130
C	-1.57045	7.84012	-0.03452
H	-2.36699	8.18732	-0.72148
H	-1.82683	8.20549	0.97518
H	-0.63599	8.33864	-0.35072
C	-0.00810	3.67224	-2.41931
H	1.00197	3.28620	-2.19756
H	-0.58447	2.81330	-2.80615
H	0.07995	4.42150	-3.22539
C	-2.48963	-2.32367	1.85635
H	-1.86625	-3.00352	1.24969
H	-1.84724	-1.46080	2.10852
H	-2.74937	-2.84853	2.79204
C	-4.98830	0.56954	-1.60164
H	-5.00071	1.60627	-1.21117
H	-4.11502	0.49050	-2.27227
H	-5.90163	0.44956	-2.20986
C	-7.47978	-2.80102	1.22027
H	-8.35177	-2.14959	1.03454
H	-7.62656	-3.72177	0.62204
H	-7.49559	-3.10194	2.28297

In the following section the triplet state geometries for the complexes **3**-**6** are given, which were used for the spin density calculations (B3LYP/6-31G(d)).

Coordinates for the optimized triplet state of **3**.

Pt	-0.83088	-0.34669	0.00002
C	-0.71504	1.60239	-0.00006
C	-1.77930	2.49422	-0.00015
C	0.66934	2.15856	0.00000
C	-1.56367	3.88513	-0.00014
H	-2.79154	2.10533	-0.00021
C	0.89243	3.56045	0.00011
C	-0.18245	4.40310	0.00004
H	1.89111	3.97688	0.00029
H	-0.03757	5.47813	0.00014
C	1.12577	-0.15655	0.00008
N	1.60952	1.16619	0.00000
N	2.22392	-0.97447	0.00011
O	-0.97466	-2.49295	0.00010
C	-3.72891	-1.29363	-0.00036
C	-2.06203	-3.16805	-0.00003
C	-3.36593	-2.65347	-0.00034
H	-4.17585	-3.37310	-0.00050
C	-5.19704	-0.92225	-0.00063
H	-5.85194	-1.79674	-0.00072
H	-5.41690	-0.30878	0.88051
H	-5.41659	-0.30883	-0.88187
C	-1.86546	-4.67098	0.00040
H	-1.28211	-4.96285	-0.88063
H	-1.28614	-4.96282	0.88415
H	-2.81051	-5.21924	-0.00164
O	-2.93671	-0.29390	-0.00016
C	2.13961	-2.45158	0.00028
C	2.73434	-3.04234	1.28587
C	2.73436	-3.04263	-1.28516
H	2.25188	-2.60658	2.16668
H	2.25193	-2.60706	-2.16608
C	3.01492	1.15207	-0.00008
C	3.38990	-0.21027	-0.00001
C	3.97124	2.16676	-0.00028
C	4.74074	-0.57260	-0.00009
C	5.31703	1.79734	-0.00035
H	3.69935	3.21353	-0.00041
C	5.69219	0.44670	-0.00025
H	5.05103	-1.60962	-0.00004
H	6.07939	2.56987	-0.00050
H	6.74587	0.18361	-0.00031
C	-2.63871	4.79582	-0.00025
N	-3.52047	5.56780	-0.00034
H	3.81338	-2.88007	1.37031
H	2.55748	-4.12326	1.30142
H	2.55749	-4.12355	-1.30048
H	3.81340	-2.88039	-1.36962
H	1.07121	-2.66423	0.00029

Coordinates for the optimized triplet state of **4**.

Pt	-0.75453	-0.47025	-0.00993
C	1.15142	0.01758	-0.01225
N	1.42069	1.38482	-0.00117
N	2.37692	-0.58955	-0.01852
O	-0.54544	-2.61123	0.01594
C	-3.45843	-1.85367	0.00332
C	-1.51603	-3.44508	0.03092
C	-2.88458	-3.13866	0.02360
H	-3.57168	-3.97637	0.03513
C	-4.96707	-1.72069	-0.00386
H	-5.47480	-2.68804	0.01107
H	-5.28446	-1.13461	0.86606
H	-5.27846	-1.16540	-0.89594
C	-1.09008	-4.89974	0.05880
H	-0.46394	-5.11345	-0.81525
H	-0.47677	-5.08291	0.94885
H	-1.93900	-5.58747	0.06488
O	-2.83693	-0.73957	-0.01000
C	2.50888	-2.04097	-0.13007
C	2.79303	1.59443	-0.00159
C	3.40384	0.37098	-0.01465
C	0.34837	2.22938	0.00341
C	0.39961	3.64823	0.01594
C	-0.94424	1.48301	-0.00759
C	-0.77347	4.34277	0.01565
C	-2.11147	2.22394	-0.00813
C	-2.07861	3.63989	0.00244
H	-3.06729	1.71143	-0.01646
H	3.21712	2.58330	0.01430
H	3.23927	-2.41560	0.58852
H	1.53576	-2.48636	0.07343
H	2.81845	-2.32103	-1.14155
C	-3.26066	4.39949	0.00169
N	-4.23745	5.04995	0.00131
H	1.35021	4.17424	0.02538
H	-0.77706	5.42747	0.02485
C	4.90059	0.09835	0.01758
C	5.64932	1.44551	-0.09230
H	5.41030	2.11055	0.74460
H	6.72910	1.26522	-0.07276
H	5.41243	1.96338	-1.02813
C	5.30665	-0.55853	1.36045
H	4.85031	-1.54189	1.50551
H	6.39410	-0.69417	1.39158
H	5.01762	0.07475	2.20593
C	5.35107	-0.78749	-1.16897
H	4.96292	-1.80671	-1.10662
H	5.03236	-0.35709	-2.12478
H	6.44484	-0.85573	-1.17741

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

Pt	-0.62141	-0.44694	-0.34797
C	-1.48212	-2.24739	-0.24889
C	-0.84586	-3.47466	-0.41532
C	-2.87829	-2.25066	-0.04003
C	-1.58097	-4.67696	-0.35729
H	0.22194	-3.50320	-0.60258
C	-3.62338	-3.42661	0.01185
C	-2.96624	-4.64734	-0.14236
H	-4.69540	-3.42239	0.15627
H	-3.52718	-5.57500	-0.10288
C	-2.49825	0.08797	-0.06278
N	-3.40743	-0.93655	0.08375
N	-3.17676	1.25056	0.09185
O	0.29806	1.47291	-0.57463
C	2.40383	-0.67575	-0.21300
C	1.51348	1.76042	-0.16782
C	2.51310	0.73879	-0.03944
H	3.51315	1.09457	0.18559
O	1.28258	-1.26814	-0.54419
C	-2.54637	2.59151	0.01162
C	-2.60991	3.31321	1.36334
C	-3.12129	3.40742	-1.15305
H	-2.16982	2.69336	2.15105
H	-3.03799	2.85108	-2.09231
C	-4.67858	-0.42333	0.34350
C	-4.52976	0.97964	0.34543
C	-5.92293	-1.01216	0.58401
C	-5.61961	1.82066	0.58024
C	-7.00623	-0.16690	0.81725
H	-6.06073	-2.08455	0.59985
C	-6.85879	1.22780	0.81426
H	-5.51618	2.89811	0.58612
H	-7.98283	-0.60201	1.00643
H	-7.72226	1.85929	0.99967
C	-0.91479	-5.93605	-0.52053
N	-0.37786	-6.96055	-0.64956
H	-3.63121	3.57280	1.65972
H	-2.03118	4.24054	1.30036
H	-2.54627	4.33373	-1.25510
H	-4.17094	3.68115	-1.00797
H	-1.49911	2.38350	-0.20892
C	1.89199	3.18646	-0.02803
C	1.59018	4.10894	-1.06771
C	2.54827	3.65442	1.14037
C	1.95216	5.44813	-0.91722
C	2.88776	5.00752	1.24079
C	2.59989	5.92513	0.22858
H	1.73691	6.14087	-1.72931
H	3.37956	5.35599	2.14739
C	3.58560	-1.53782	0.04699
C	4.78220	-1.37691	-0.69488
C	3.51330	-2.54385	1.04614
C	5.87135	-2.20994	-0.42209
C	4.62956	-3.34753	1.28207
C	5.81867	-3.20409	0.55814
H	6.78180	-2.08923	-1.00635
H	4.57309	-4.10455	2.06212
C	0.93943	3.67281	-2.36236
H	1.38334	2.74767	-2.74618
H	-0.12953	3.47052	-2.23971
H	1.05303	4.44910	-3.12609
C	2.85901	2.74747	2.31345
H	2.05950	2.01996	2.48998
H	3.78649	2.17611	2.17219
H	2.98890	3.33607	3.22763
C	2.95097	7.38737	0.37187
H	3.28687	7.81433	-0.58009
H	2.08450	7.97770	0.70070
H	3.74629	7.53863	1.10932
C	4.90610	-0.35836	-1.80902
H	3.99981	-0.31604	-2.42248
H	5.08836	0.65811	-1.43421
H	5.74635	-0.60903	-2.46448
C	2.27826	-2.73321	1.89804
H	1.87183	-1.77377	2.23823
H	1.47358	-3.23409	1.35072
H	2.51006	-3.33710	2.78112
C	6.99541	-4.11670	0.81050
H	6.88469	-5.06619	0.26923
H	7.93540	-3.66140	0.48103
H	7.09138	-4.36282	1.87407

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

Pt	0.55965	-0.60329	0.00272
C	2.52252	-0.46562	0.02592
N	3.20801	-1.67825	-0.02210
N	3.49442	0.49558	0.07251
O	0.09365	1.49614	0.02103
C	-2.44252	-0.13781	-0.01330
C	-1.09103	1.98437	0.01616
C	-2.29431	1.26346	0.00098
H	-3.20851	1.84622	0.00685
O	-1.50299	-1.00333	-0.01469
C	3.16405	1.90988	0.24466
C	4.57648	-1.44578	-0.00675
C	4.77112	-0.09356	0.05387
C	2.45664	-2.81657	-0.06818
C	2.95442	-4.14560	-0.11911
C	0.99432	-2.51702	-0.05835
C	2.06135	-5.17443	-0.15958
C	0.12091	-3.58803	-0.10220
C	0.60089	-4.92002	-0.15178
H	-0.94849	-3.40591	-0.10015
H	5.29085	-2.24949	-0.04885
H	3.74373	2.52572	-0.44419
H	2.10176	2.03957	0.04182

H	3.36579	2.22721	1.27229
C	-0.27809	-6.01549	-0.19300
N	-0.99414	-6.94458	-0.22656
H	4.02268	-4.34333	-0.12556
H	2.40063	-6.20400	-0.19850
C	6.10686	0.63533	0.04811
C	7.24045	-0.41302	0.10933
H	7.21901	-1.08385	-0.75637
H	8.20913	0.09735	0.10838
H	7.18076	-1.01795	1.02069
C	6.28152	1.44225	-1.26265
H	5.54502	2.24381	-1.36742
H	7.27501	1.90529	-1.28124
H	6.19397	0.78828	-2.13682
C	6.26171	1.56619	1.27462
H	5.56593	2.40808	1.25641
H	6.10819	1.01468	2.20880
H	7.27589	1.98139	1.29071
C	-1.16191	3.49053	0.01712
C	-0.99674	4.18839	-1.19486
C	-1.35621	4.18715	1.22487
C	-1.04771	5.58584	-1.17841
C	-1.39390	5.58539	1.19500
C	-1.24993	6.30390	0.00430
H	-0.92461	6.12658	-2.11504
H	-1.53824	6.12593	2.12871
C	-3.83447	-0.71058	0.00045
C	-4.30960	-1.31905	1.18060
C	-4.63837	-0.66122	-1.15406
C	-5.60089	-1.85224	1.18766
C	-5.92031	-1.22095	-1.10346
C	-6.42160	-1.81884	0.05522
H	-5.97326	-2.31088	2.10179
H	-6.54012	-1.19127	-1.99750
C	-1.51190	3.45308	2.53933
H	-2.44050	2.87056	2.56971
H	-0.68957	2.74764	2.70622
H	-1.53018	4.15579	3.37811
C	-1.33423	7.81294	-0.00680
H	-2.37189	8.15222	-0.12810
H	-0.96124	8.24287	0.92923
H	-0.75476	8.24162	-0.83159
C	-0.76919	3.44929	-2.49534
H	0.15370	2.85893	-2.46348
H	-1.58452	2.74627	-2.70540
H	-0.69974	4.14644	-3.33587
C	-3.45309	-1.39423	2.42559
H	-2.59987	-2.06601	2.28131
H	-3.04194	-0.41313	2.69332
H	-4.03481	-1.76063	3.27688
C	-4.14483	-0.03814	-2.44289
H	-4.08598	1.05492	-2.37209
H	-3.14369	-0.39608	-2.70807
H	-4.81858	-0.28050	-3.27065
C	-7.79857	-2.44089	0.07867
H	-8.43741	-2.03108	-0.71070
H	-7.74534	-3.52717	-0.07386
H	-8.29794	-2.27474	1.03990