How do the Ligands Influence Quantum Yields of Cyclometalated Platinum(II) Complexes, A Theoretical Research

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Contents

1. The optimized structures of complexes 1-4 on the ground state. S2
2. The frontier molecular orbitals of complexes 1-4 on the ground state. S3
3. The optimized structures of complexes 1-4 on the lowest energy singlet excited state. S4
4. The optimized structures of complexes 1−4 on the lowest energy triplet excited state. S5
5. The spin density distributions of complexes 1−4 at the lowest energy triplet excited state. S6
6. The schematic diagram of reorganization energy. S7
7. The phosphorescent emissions of complex 1 in CH_2Cl_2 calculated with different functionals. S8
8. The compositions of platinum in frontier molecular orbitals for complexes 1−4 on the ground state. S9
9. The first 10 singlet excited states of complexes 1-4 computed by TDDFT/PCM (CH_2Cl_2) at the optimized T_1 state geometry. S10
10. The Cartesian coordinates of important geometries. S11

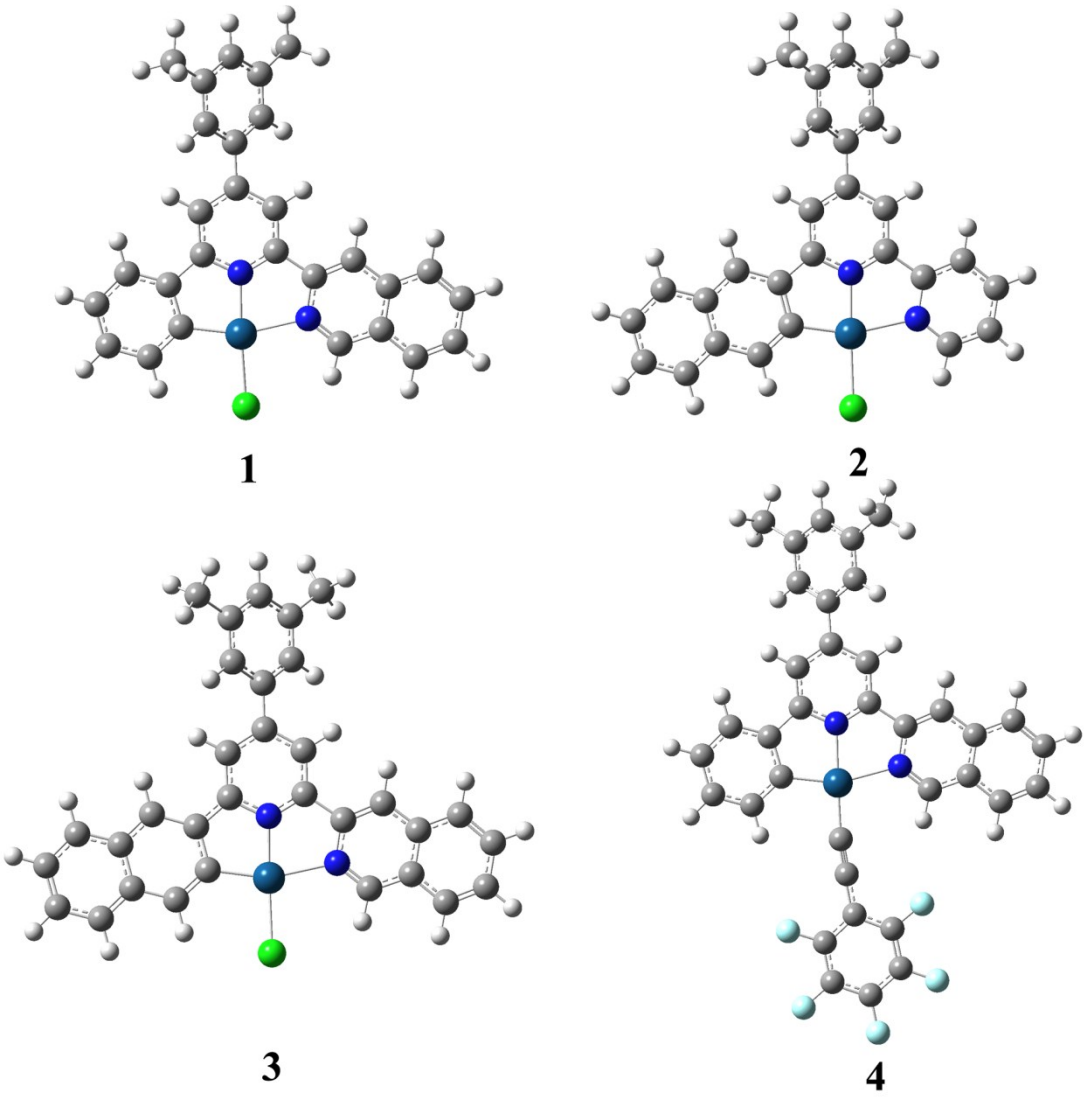

Fig. S1. The optimized structures of complexes 1–4 on the ground state.

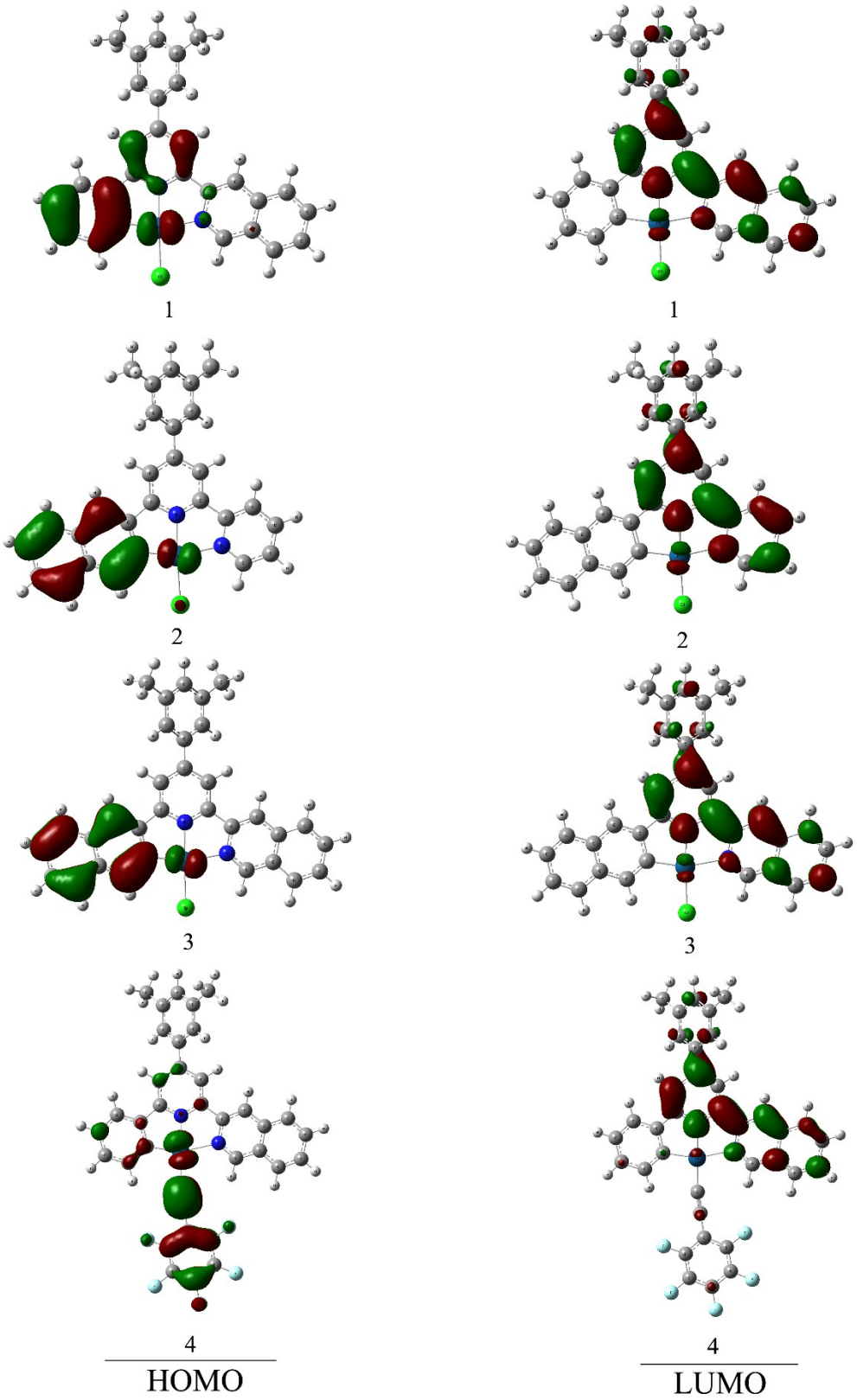

Fig. S2. The frontier molecular orbitals of complex 1-4 on the ground state.

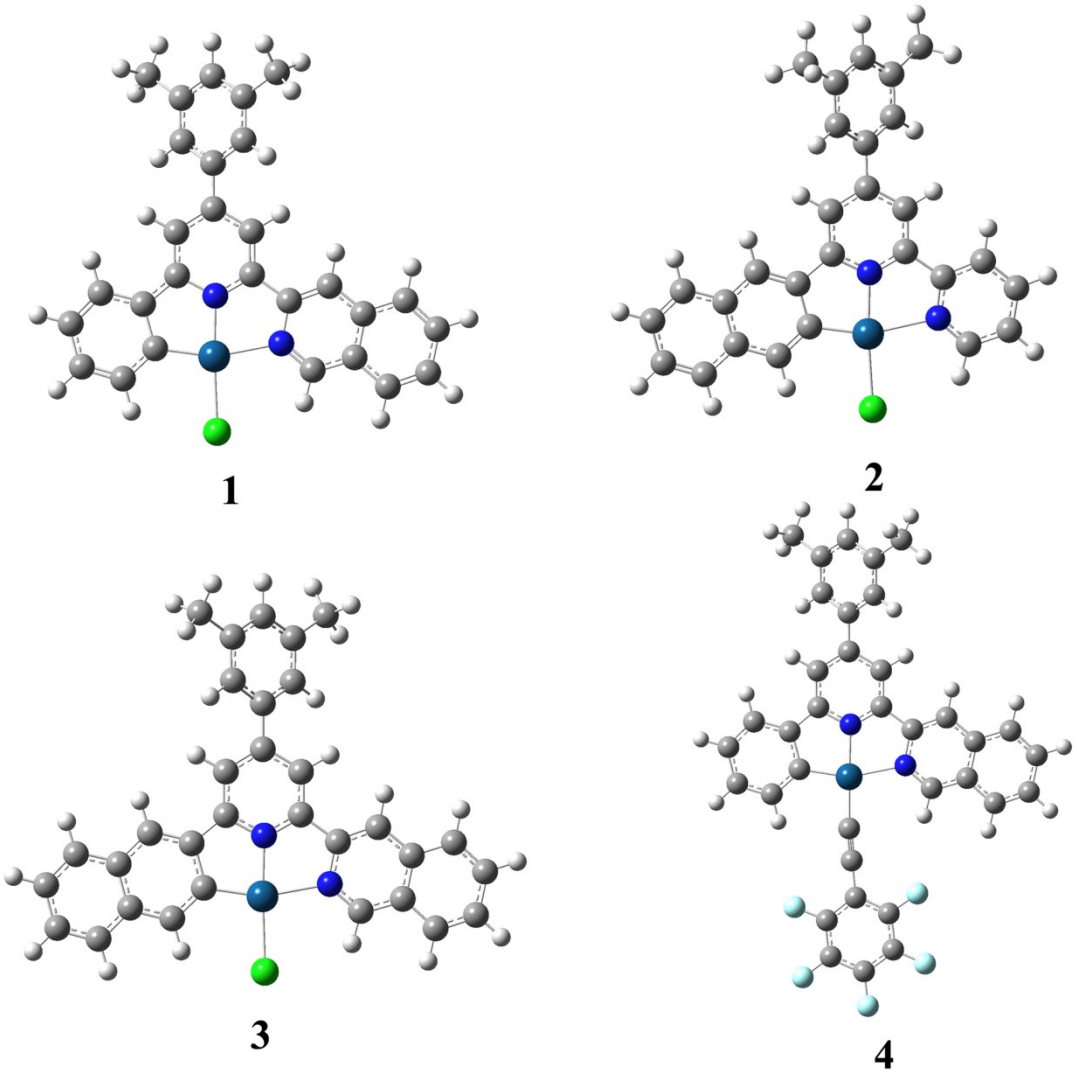

Fig. S3. The optimized structures of complexes 1–4 on the lowest energy singlet excited state.

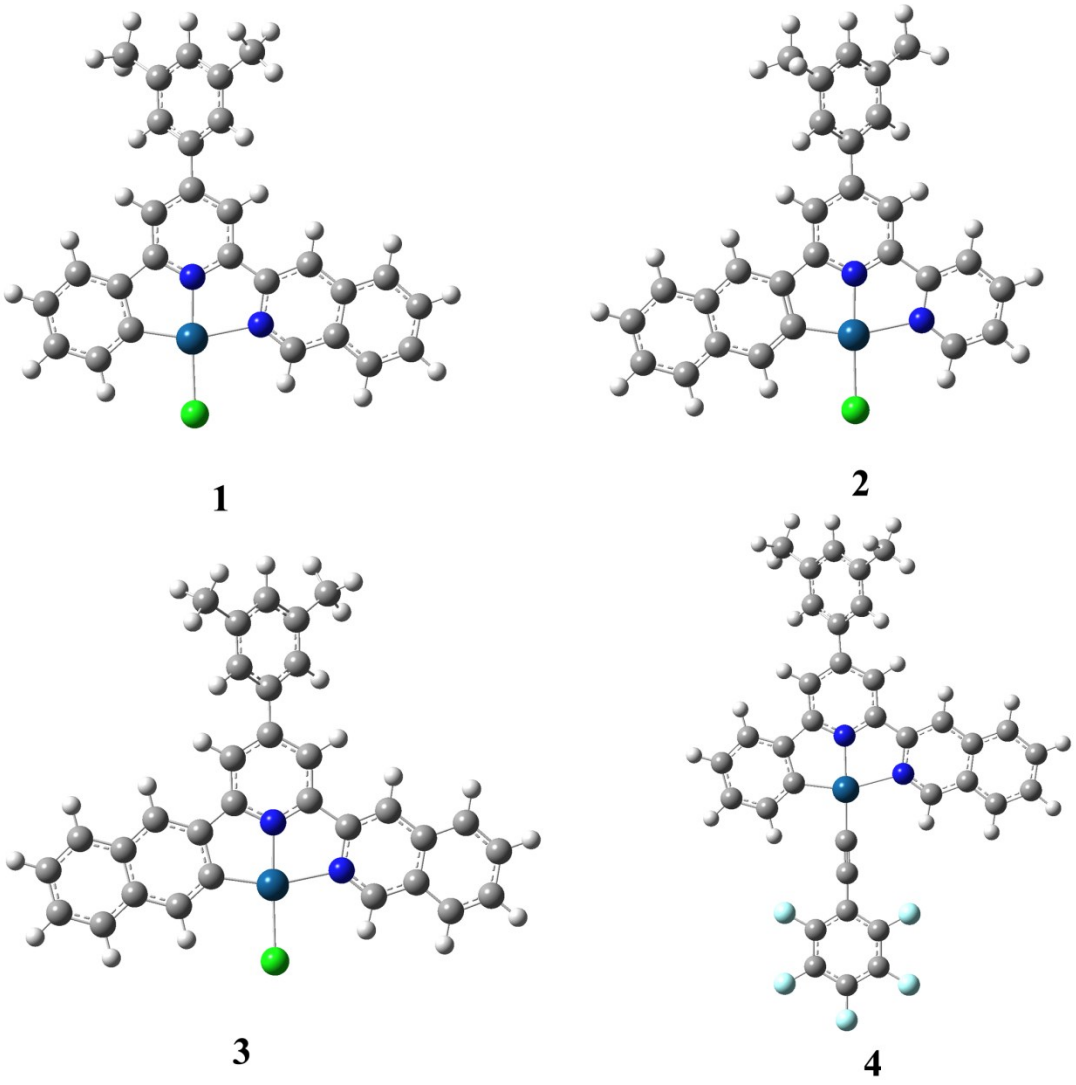

Fig. S4. The optimized structures of complexes 1–4 on the lowest energy triplet excited state.

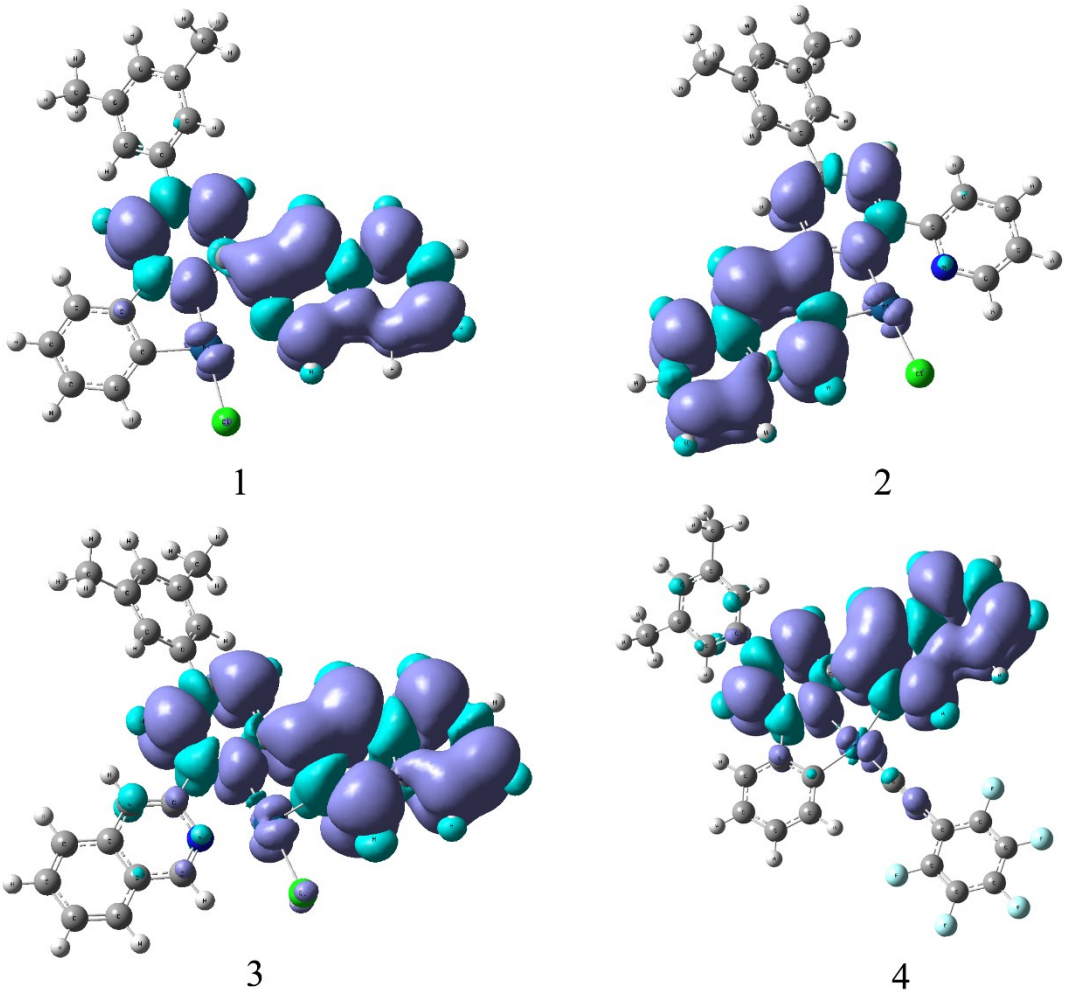

Fig. S5. The spin density distributions of complexes 1−4 at the lowest energy triplet excited state.

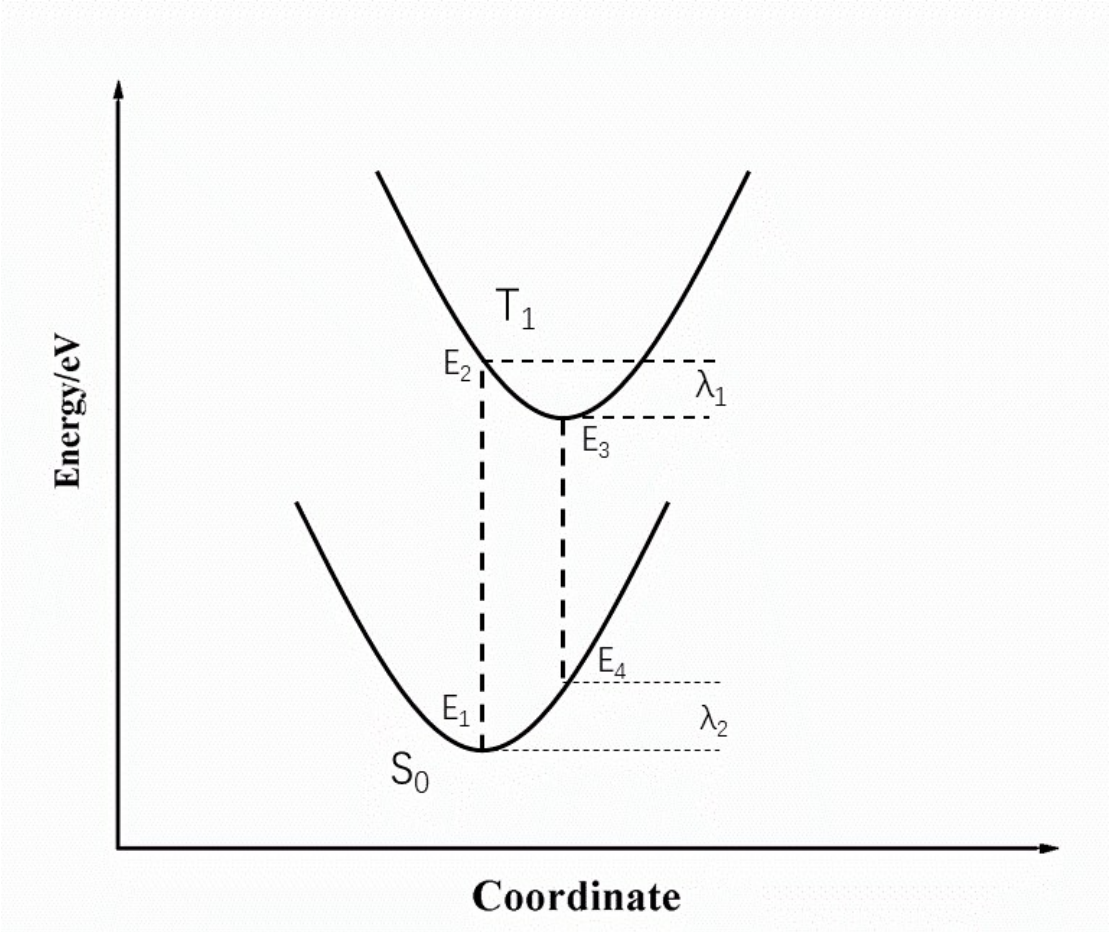

Fig. S6. The schematic diagram of reorganization energy(λ), $\lambda=\lambda_1+\lambda_2=(E_2-E_3)+(E_4-E_1)$

Table S1. The Phosphorescent Emissions of Complex 1 in CH_2Cl_2 Calculated with Different Functionals. (H = HOMO and L = LUMO)

Functional	*E*/nm (/eV)	Excitation (coeff)	Experimental/nm
PBE0	696 (1.78)	H−1 → L (0.43) H−2 → L (0.40)	530
M06−2x	548 (2.26)	H → L (0.49) H−1→ L (0.43)	
ωB97xd	712 (1.74)	H−1→ L (0.51)	

Table S2. The Compositions and Characters of Platinum d orbitals for Complexes 1−4 on the T_1 State. (H = HOMO and L = LUMO)

Orbital	1(%)	2(%)	3(%)	4(%)
L+1	4.77 P			4.37 P
L	1.89 d_{xz}	1.76 d_{xz}	3.62 d_{xz}	1.18 d_{yz}
H	18.6 d_{yz}	7.81 d_{yz}	4.59 d_{yz}	25.3 d_{xz}
H–1	27.2 d_{yz}	19.8 d_{yz}+6.92 d_{xz}	25.4 d_{yz}	15.9 d_{yz}+10.4d_{xz}
H–2	36.1 d_{xz}	35.1 d_{xz}	27.5 d_{xz}+9.8 d_{yz}	17.5 d_{yz}
H–3	47.1 d_{z^2}	41.5 d_{z^2}+10.5 d_{xy}	29.7 d_{z^2}+6.68d_{xy}	30.1d_{xy}+7.1 d_{z^2}
H–4			20.3 d_{z^2}	
H–5		20.1 d_{z^2}+23.5 d_{xy}		53.9 d_{z^2}
H–6	23.3 d_{z^2}+19.3 d_{xy}	19.9 d_{xz}	20.7 d_{z^2}+20.4d_{xy}	
H–7	15.5 d_{xz}	7.37 d_{yz}	18.8 d_{xz}	

Table S3. The First 10 Singlet Excited States (S_n) of complex 1 Computed by TDDFT/PCM (CH_2Cl_2) at the Optimized T_1 State Geometry.

S_n	Excitation[a]	Contribution	E^b/eV	f	Pt(%)[c]
S_1	H → L	74%	3.32	0.2385	
S_2	H–1→ L	74%	3.62	0.4570	
S_3	H–3 → L	72%	3.82	0.0051	47.1
S_4	H → L+1	27%	3.88	0.0267	
	H–2 → L	23%			34.2
S_5	H → L+1	34%	3.95	0.2677	
	H–2 → L	41%			34.2
S_6	H–1→ L+1	29%	4.05	0.0584	
S_7	H–6 → L	20%	4.14	0.0025	42.6
S_8	H–1→ L+1	27%	4.15	0.0208	
S_9	H–6 → L	25%	4.25	0.0006	42.6
S_{10}	H–6 → L	19%	4.29	0.0006	42.6

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).
[b] Vertical excitation energies. [c] Contributions of d orbitals that are different from d orbital in T_1 excitation.

Table S4. The First 10 Singlet Excited States (S_n) of complex 2 Computed by TDDFT/PCM (CH_2Cl_2) at the Optimized T_1 State Geometry.

S_n	Excitation[a]	Contribution	E^b/eV	f	Pt(%)[c]
S_1	H → L	74%	3.31	0.2385	
S_2	H–1→ L	82%	3.45	0.2242	5.16
S_3	H → L+1	79%	3.75	0.0250	
S_4	H–3 → L	82%	3.88	0.0065	52.0
S_5	H–1 → L+1	34%	3.94	0.0039	6.92
	H–2 → L	30%			33.3
S_6	H–1 → L+1	28%	4.04	0.6382	6.92
S_7	H–2 → L	42%	4.15	0.2485	33.3
S_8	H–5 → L	27%	4.19	0.0025	43.6
S_9	H–2 → L+8	20%	4.22	0.0002	
S_{10}	H–5 → L+8	19%	4.30	0.0035	

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).
[b] Vertical excitation energies. [c] Contributions of d orbitals that are different from d orbital in T_1 excitation.

Table S5. The First 10 Singlet Excited States (S_n) of Complex 3 Computed by TDDFT/PCM (CH_2Cl_2) at the Optimized T_1 State Geometry.

S_n	Excitation[a]	Contribution	E^b/eV	f	Pt(%)[c]
S_1	H → L	87%	3.33	0.3238	
S_2	H–1→ L	85%	3.51	0.2926	
S_3	H → L+1	74%	3.81	0.0413	
S_4	H–2 → L	29%	3.98	0.1236	23.9
S_5	H–3 → L	52%	4.02	0.0083	36.4
S_6	H–1 → L+1	61%	4.08	0.3076	
S_7	H–2 → L+8	14%	4.16	0.0268	
S_8	H–2 → L	26%	4.17	0.1377	23.9
S_9	H–2 → L+7	26%	4.23	0.0024	
S_{10}	H–6 → L+9	30%	4.30	0.0155	

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).
[b] Vertical excitation energies. [c]Contributions of d orbitals that are different from d orbital in T_1 excitation.

Table S6. The first 10 Singlet Excited States (S_n) of Complex 4 Computed by TDDFT/PCM (CH_2Cl_2) at the Optimized T_1 State Geometry.

S_n	Excitation[a]	Contribution	E^b/eV	f	Pt(%)[c]
S_1	H–1 → L	42%	3.39	0.2404	25.1
	H → L	29%			25.3
S_2	H→ L	41%	3.59	0.3386	25.3
	H–1 → L	20%			25.1
S_3	H–2 → L	65%	3.84	0.6097	16.3
S_4	H → L+1	35%	3.89	0.0593	25.3
	H–1 → L+1	19%			25.1
S_5	H–3 → L	56%	3.90	0.0056	37.2
	H–3 → L+1	22%			37.2
S_6	H–1 → L+1	27%	4.04	0.0061	26.3
S_7	H–5 → L	58%	4.08	0.0045	53.9
S_8	H–2 → L+1	33%	4.21	0.5766	17.5
S_9	H–3 → L+1	46%	4.35	0.0024	37.2
	H–3 → L	32%			37.2
S_{10}	H → L+2	25%	4.49	0.2612	25.3
	H–7 → L	18%			

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).
[b] Vertical excitation energies. [c]Contributions of d orbitals that are different from d orbital in T_1 excitation.

Table S7. Cartesian coordinates of complexes 1-4 on the ground state (S_0).

Complex 1	X	Y	Z
C	0.37141400	0.72940300	-0.02531100
C	1.70762600	1.10882000	-0.02878100
N	0.05066700	-0.57527300	0.01483300
C	2.70410900	0.12460500	0.00854700
H	1.98887100	2.15378000	-0.08511800
C	0.97403900	-1.56318000	0.04990800
C	2.32467900	-1.21841200	0.04709500
H	3.08073900	-1.99352600	0.10473800
C	0.37301300	-2.90226300	0.09584500
C	-1.05032600	-2.93399700	0.09829700
C	1.12476900	-4.07933000	0.13274500
C	-1.67495000	-4.18148900	0.13940200
C	0.47779100	-5.30697000	0.17242600
H	2.21137700	-4.04165700	0.13033800
C	-0.91754600	-5.35166700	0.17574200
H	-2.75969900	-4.22605600	0.14268400
H	1.05550600	-6.22514300	0.20058700
H	-1.42176800	-6.31370500	0.20763300
C	-3.11578000	1.80057300	-0.07565900
C	-3.08366700	3.21831600	-0.14204700
C	-1.81428800	3.84903900	-0.17503200
C	-0.65890100	3.02728700	-0.13664600
C	-0.78646300	1.66443200	-0.06974600
H	-5.22789400	3.49745900	-0.14880800
H	-4.05830800	1.25352700	-0.05099400
C	-4.26428600	3.99799100	-0.17638600
C	-1.75250700	5.26293500	-0.24502200
H	0.31979800	3.49515700	-0.16353100
C	-2.91042700	5.99960000	-0.27795100
C	-4.17644600	5.36594000	-0.24283700
H	-0.78206400	5.75009300	-0.27291000
H	-2.85963500	7.08246600	-0.33192400
H	-5.07727700	5.96980100	-0.26851200
N	-2.03036600	1.06972200	-0.04187500
Pt	-1.85234200	-1.14375100	0.03908300
Cl	-4.14268600	-1.68881900	0.06950100
C	4.13640400	0.50697100	0.00824800
C	5.06486800	-0.23456000	-0.72651900
C	4.57307900	1.61326200	0.74221500
C	6.41430500	0.11709500	-0.73908400
H	4.72722300	-1.08004600	-1.32194300
C	5.91804900	1.97999400	0.75446100

H	3.85995400	2.17759300	1.33954400
C	6.82208800	1.22403400	0.00656200
H	7.87309600	1.50515100	0.00511800
C	7.40133000	-0.68190000	-1.55179500
H	7.41983900	-1.72810300	-1.23009300
H	7.13523600	-0.67110100	-2.61365100
H	8.41261200	-0.28017800	-1.45287200
C	6.38031200	3.15533900	1.57798900
H	5.77629400	4.04448300	1.37219500
H	6.29397000	2.94096200	2.64848100
H	7.42462200	3.39921400	1.36832400

Complex 2	X	Y	Z
C	0.35296600	0.75872500	-0.02934700
C	1.68648100	1.16531500	-0.03448400
N	0.07603800	-0.56336000	0.01370600
C	2.70943400	0.21685000	0.00526500
H	1.92923900	2.22048800	-0.09350900
C	1.03013100	-1.51049300	0.05077700
C	2.36843800	-1.14282900	0.04719200
H	3.15175400	-1.88931000	0.10708800
C	0.52166700	-2.91079600	0.10351200
C	1.35426300	-4.02570300	0.14311500
C	-1.37397700	-4.26061300	0.15702200
C	0.78134300	-5.29299600	0.19142300
H	2.43183500	-3.91169000	0.13607300
C	-0.60218500	-5.41870000	0.19949900
H	-2.46143100	-4.27338600	0.15915600
H	1.41522300	-6.17315600	0.22194300
H	-1.08228500	-6.38956700	0.23807000
C	-3.27529300	1.59387100	-0.08373000
C	-3.26429400	3.01552200	-0.14283600
C	-2.02297400	3.71437100	-0.16610900
C	-0.82148200	2.96723400	-0.12831300
C	-0.85658300	1.59359800	-0.07084900
H	-5.41267900	3.23553500	-0.16121300
H	-4.22986700	1.07363900	-0.06701200
C	-4.46665000	3.76970600	-0.17967200
C	-2.02284900	5.13291600	-0.22655900
H	0.12344900	3.50718500	-0.14749200
C	-3.20148300	5.83200900	-0.26101300
C	-4.43722800	5.14005100	-0.23687400
H	-1.06917000	5.65499300	-0.24548000
H	-3.19294500	6.91640700	-0.30732100
H	-5.36542900	5.70257100	-0.26416900

Pt	-1.84323700	-1.07386600	0.03162700
Cl	-4.07600200	-1.81050800	0.06659600
C	4.13089600	0.63652600	0.00578200
C	5.08079800	-0.07922400	-0.72752100
C	4.53407100	1.75623600	0.73830500
C	6.41884600	0.31306200	-0.74198100
H	4.76852300	-0.93382000	-1.32410300
C	5.86741200	2.16359300	0.74844300
H	3.80335600	2.30106500	1.33214600
C	6.79322100	1.43310200	0.00181500
H	7.83522800	1.74577200	-0.00103600
C	7.42870900	-0.45423000	-1.55730400
H	7.46263400	-1.50578000	-1.25469700
H	7.17457100	-0.42801400	-2.62191000
H	8.43150600	-0.03665200	-1.44002600
C	6.29224200	3.35856600	1.56368000
H	5.69568600	4.24047200	1.31069400
H	6.15934000	3.16948200	2.63395400
H	7.34390800	3.60068600	1.39275500
C	-2.11038800	0.86836000	-0.04774200
N	-0.82190600	-3.04962800	0.11030700

Complex 3	X	Y	Z
C	-0.57596700	1.26302200	-0.01530100
C	0.21494800	2.41051700	-0.01756200
N	0.02714000	0.05372300	0.00934600
C	1.60638600	2.30125800	0.00676200
H	-0.25091700	3.38837900	-0.06839800
C	1.36294900	-0.09745300	0.03473900
C	2.18218900	1.02427600	0.03473700
H	3.26011800	0.92378100	0.08154800
C	1.84104900	-1.50649400	0.06546700
C	3.16553700	-1.85637300	0.10471400
C	1.16591000	-3.73955900	0.07099700
C	3.53904600	-3.22398900	0.12705900
H	3.94297200	-1.09941900	0.11934000
C	2.50892900	-4.19804500	0.10849100
H	0.32726600	-4.43568700	0.05748700
C	-3.94309900	-0.32692300	-0.07619700
C	-4.81453100	0.79760700	-0.10588800
C	-4.27142800	2.11480300	-0.10504100
C	-2.86552400	2.27042500	-0.07502200
C	-2.04286200	1.16895000	-0.04701000
H	-6.63929700	-0.35695400	-0.13739700
H	-4.37103700	-1.32640600	-0.07713400

C	-6.22600500	0.64799300	-0.13667100
C	-5.14844700	3.23071100	-0.13445900
H	-2.45754200	3.27946800	-0.07534100
C	-6.50728600	3.05252900	-0.16380900
C	-7.05061700	1.74408000	-0.16500200
H	-4.72134800	4.23075800	-0.13367000
H	-7.17094200	3.91110100	-0.18595400
H	-8.12806400	1.61229300	-0.18862000
Pt	-1.16327100	-1.53751300	-0.00301900
Cl	-2.45999500	-3.50229300	-0.01701600
C	2.46363200	3.51035800	0.00062800
C	3.64652600	3.53226300	-0.74487800
C	2.10054900	4.63968900	0.73789600
C	4.46271500	4.66131400	-0.76109400
H	3.91895900	2.66772200	-1.34576500
C	2.90068600	5.78273500	0.73930500
H	1.19622600	4.61967100	1.34157200
C	4.07519800	5.77540300	-0.01313400
H	4.70595200	6.66239300	-0.01895700
C	5.74603100	4.67826700	-1.55209000
H	6.60616900	4.47861600	-0.90337800
H	5.73820500	3.91839600	-2.33791200
H	5.90822200	5.65259700	-2.02126300
C	2.49112400	7.00608300	1.51938100
H	1.85362000	7.65807700	0.91206200
H	1.92670800	6.73471300	2.41548000
H	3.36240600	7.59008200	1.82704000
C	-2.57836700	-0.17735800	-0.04666100
N	0.85311700	-2.46838000	0.05055000
C	4.15111000	-5.96350500	0.16278700
C	2.83537500	-5.57510400	0.12675000
C	4.88898700	-3.65246200	0.16528600
C	5.18278700	-4.99324700	0.18241200
H	4.40849600	-7.01732800	0.17629400
H	2.03348900	-6.30763800	0.11114900
H	5.68062700	-2.90877100	0.18076500
H	6.21776400	-5.31890500	0.21096700

Complex 4	X	Y	Z
C	2.30841200	0.74578000	0.00091300
C	3.69549100	0.83309900	0.00876300
N	1.72119200	-0.45646200	-0.03923500
C	4.45108900	-0.34809700	-0.02260500
H	4.19940200	1.79069500	0.07106600
C	2.39771800	-1.62090600	-0.07369500

C	3.79202200	-1.57976800	-0.06532200
H	4.36761600	-2.49719500	-0.11535400
C	1.51388100	-2.80085400	-0.12052600
C	0.10863700	-2.54756300	-0.11193700
C	2.01049800	-4.10536400	-0.17127000
C	-0.74774900	-3.64959900	-0.15426300
C	1.13313600	-5.18125600	-0.21364800
H	3.08244000	-4.28625500	-0.17929500
C	-0.24177200	-4.94807500	-0.20450300
H	-1.82074000	-3.48362700	-0.14788000
H	1.51780500	-6.19512900	-0.25425500
H	-0.92911600	-5.78879900	-0.23726600
C	-0.89107100	2.50840600	0.08474400
C	-0.57020800	3.88946100	0.13574700
C	0.80119700	4.24837100	0.13862200
C	1.76320500	3.20674400	0.09237400
C	1.36180700	1.89744600	0.04634900
H	-2.61438200	4.59394800	0.18072200
H	-1.92808900	2.17404400	0.07916800
C	-1.56910300	4.89056600	0.18292900
C	1.14905700	5.62081100	0.18783600
H	2.81761700	3.46367900	0.09507400
C	0.16430100	6.57665400	0.23243600
C	-1.20458700	6.21283200	0.23093800
H	2.19808900	5.90232400	0.19009100
H	0.43413200	7.62731900	0.26999000
H	-1.96357800	6.98715700	0.26884500
N	0.02001300	1.56815300	0.04224100
Pt	-0.31863100	-0.62643200	-0.03987900
C	5.93278200	-0.29050900	-0.00434900
C	6.66187800	-1.20237400	0.76225400
C	6.61474700	0.67890500	-0.74558100
C	8.05537000	-1.15599300	0.79856700
H	6.13497600	-1.93773100	1.36586100
C	8.00676800	0.74130400	-0.73312300
H	6.05283700	1.37625400	-1.36280800
C	8.70915700	-0.17833900	0.04848700
H	9.79627800	-0.12919600	0.07489900
C	8.83628600	-2.15119900	1.61843800
H	8.26326700	-2.48501300	2.48755400
H	9.08183500	-3.03769400	1.02326100
H	9.77695100	-1.72182300	1.97335300
C	8.74424200	1.75943500	-1.56497100
H	9.09406600	1.31558600	-2.50346600

H	8.10280400	2.60733200	-1.81884400
H	9.62191800	2.14082100	-1.03543700
C	-2.25455300	-0.73555600	-0.03375400
C	-3.47542700	-0.66001100	-0.02246500
C	-4.88832600	-0.54403300	-0.00906300
C	-5.51763500	0.70729900	0.01563800
C	-5.73077100	-1.66374300	-0.01901700
C	-6.89669600	0.84466400	0.02934100
C	-7.11291400	-1.54672600	-0.00499400
C	-7.70103200	-0.28826200	0.01911300
F	-5.20552200	-2.88132200	-0.04134200
F	-7.88106000	-2.62938800	-0.01424600
F	-4.77916200	1.81644700	0.02727600
F	-7.45483000	2.05014500	0.05171700
F	-9.02168500	-0.16900700	0.03368300

Table S8. Cartesian coordinates of complexes 1-4 on the lowest triplet excited state (T_1).

Complex 1	X	Y	Z
C	-0.33707165	0.73171007	-0.00469946
C	-1.71289654	1.09168484	-0.01133920
N	-0.01777118	-0.60650544	0.03216989
C	-2.69174677	0.10821286	0.02758408
H	-1.99905872	2.13429492	-0.07433688
C	-0.93658483	-1.57850023	0.06888555
C	-2.29997305	-1.24548623	0.07136769
H	-3.04745312	-2.02725619	0.13426036
C	-0.33781095	-2.91916388	0.10759643
C	1.08765033	-2.94310031	0.09264893
C	-1.08423237	-4.09859743	0.15479473
C	1.71535855	-4.18904080	0.12587649
C	-0.43083705	-5.32544616	0.18806770
H	-2.17019655	-4.06520573	0.16588911
C	0.96367172	-5.36563579	0.17331284
H	2.80014629	-4.23903960	0.11505582
H	-1.00487676	-6.24536339	0.22493924
H	1.47306599	-6.32495519	0.19963080
C	3.07258039	1.86090632	-0.07357905
C	3.00775039	3.30644503	-0.13602606
C	1.70699653	3.91204913	-0.14855138
C	0.58696864	3.09197549	-0.09896332
C	0.74680717	1.63578424	-0.04317126
H	5.12448401	3.60595745	-0.17317118
H	4.04044820	1.36236876	-0.06185619

C	4.14851859	4.08266269	-0.18407093
C	1.63408630	5.33377879	-0.21244423
H	-0.40456271	3.52638095	-0.10469471
C	2.79793081	6.09995855	-0.26115953
C	4.05033801	5.49638242	-0.24764737
H	0.65884532	5.81035201	-0.22386136
H	2.72073600	7.18105211	-0.31069343
H	4.95148879	6.09692774	-0.28446581
N	2.02147892	1.09036188	-0.03166961
Pt	1.87672015	-1.13858248	0.03200871
Cl	4.21687884	-1.69208361	0.03403233
C	-4.12935547	0.46926646	0.01721888
C	-5.04640415	-0.31617908	-0.68212681
C	-4.58203513	1.60347620	0.70421682
C	-6.40402337	0.01591590	-0.70860782
H	-4.70127173	-1.18410821	-1.23961884
C	-5.92894460	1.95369892	0.69543715
H	-3.87798481	2.20400951	1.27502106
C	-6.82586167	1.14986871	-0.01767675
H	-7.88057453	1.41828238	-0.03099786
C	-7.38115790	-0.84620930	-1.46680460
H	-7.01926289	-1.05373747	-2.47834537
H	-7.52046010	-1.81038624	-0.96641380
H	-8.35815536	-0.36328780	-1.54463141
C	-6.42410454	3.16840491	1.43837287
H	-5.60870193	3.67354194	1.96144725
H	-6.88321597	3.88591958	0.75058314
H	-7.18421024	2.89317808	2.17645492

Complex 2	X	Y	Z
C	0.33118246	0.76261631	-0.01643590
C	1.68322456	1.17533920	-0.02163557
N	0.07026777	-0.58828550	0.02557880
C	2.70208850	0.23619705	0.01837537
H	1.91927290	2.23177230	-0.08300466
C	1.03419341	-1.51719301	0.06092598
C	2.37147601	-1.13875944	0.05947136
H	3.15822311	-1.87996235	0.12126080
C	0.54098952	-2.92207568	0.10658360
C	1.38713687	-4.02507184	0.14336207
C	-1.33484832	-4.29695316	0.14871517
C	0.83208575	-5.30138759	0.18507169
H	2.46257000	-3.89650150	0.13847502
C	-0.54926155	-5.44529353	0.18906148
H	-2.42010396	-4.33951907	0.14780781

H	1.47776357	-6.17229068	0.21343143
H	-1.01804304	-6.42144876	0.22236979
C	-3.25834473	1.58402494	-0.08265226
C	-3.27405233	3.03396852	-0.14115006
C	-2.02267717	3.74512470	-0.15602709
C	-0.82930466	3.02523691	-0.11384194
C	-0.84105674	1.55824976	-0.05726408
H	-5.40173743	3.20249583	-0.17129471
H	-4.21480881	1.06674486	-0.07136120
C	-4.45936911	3.74335161	-0.18297597
C	-2.05426996	5.16414249	-0.21411107
H	0.11580588	3.55969552	-0.12424634
C	-3.27413170	5.86155880	-0.25640111
C	-4.46863173	5.17191399	-0.24169412
H	-1.11483000	5.70904828	-0.22620026
H	-3.26730010	6.94571222	-0.30115109
H	-5.41516736	5.69972740	-0.27459765
Pt	-1.83126497	-1.10028929	0.03233759
Cl	-4.13659055	-1.79826168	0.04708869
C	4.12276610	0.66031602	0.01356250
C	5.07925224	-0.07850619	-0.68935276
C	4.51982858	1.80802880	0.70690425
C	6.41613693	0.31991746	-0.71458594
H	4.77591620	-0.95885032	-1.25167040
C	5.85127408	2.22309501	0.70366061
H	3.78636345	2.37160921	1.27912824
C	6.78373604	1.46990607	-0.01318108
H	7.82437729	1.78699545	-0.02435189
C	7.43171417	-0.47303328	-1.49789805
H	7.44692203	-1.51908861	-1.17612472
H	7.19422889	-0.46454897	-2.56669174
H	8.43633273	-0.06263146	-1.37133430
C	6.26868608	3.44924474	1.47573091
H	5.64765774	4.31079012	1.21218644
H	6.16139074	3.28754588	2.55346763
H	7.31168756	3.70593944	1.27542313
C	-2.08465235	0.85142800	-0.04248689
N	-0.80410213	-3.07493476	0.10831440

Complex 3	X	Y	Z
C	0.82618513	1.10675422	0.06517402
C	0.26441929	2.40331292	0.06663732
N	-0.03138975	0.03026058	0.03620453
C	-1.11226790	2.56910014	0.02525378
H	0.91579709	3.26814276	0.11774934

C	-1.36277288	0.15942340	0.00279874
C	-1.94189530	1.42609512	-0.00503113
H	-3.01626496	1.54152358	-0.07093040
C	-2.11686762	-1.12089132	-0.03631198
C	-3.48505793	-1.19271628	-0.04417026
C	-1.91388879	-3.44350465	-0.09186296
C	-4.13143941	-2.45475898	-0.07910927
H	-4.09020286	-0.29302632	-0.02108087
C	-3.32152179	-3.61876999	-0.10317790
H	-1.24661118	-4.30310323	-0.10838207
C	3.79034556	-1.07945584	0.07487574
C	4.90013055	-0.14440564	0.11589999
C	4.62141856	1.26793916	0.13947365
C	3.29634389	1.70113375	0.12436553
C	2.19305084	0.73443834	0.08596794
H	6.41974952	-1.64376889	0.11256061
H	4.02352757	-2.14119602	0.05370367
C	6.21259610	-0.57722988	0.13070462
C	5.71635188	2.17174795	0.17712129
H	3.08450923	2.76583026	0.14071277
C	7.04192046	1.70480606	0.19181611
C	7.30009900	0.34966552	0.16929463
H	5.51375224	3.23861978	0.19449561
H	7.85900299	2.41832393	0.22130690
H	8.31875309	-0.02149534	0.18033925
Pt	0.82064917	-1.74776231	-0.00441616
Cl	1.79285169	-3.94781673	-0.10922970
C	-1.71044540	3.92574097	0.00517958
C	-2.90950009	4.18416997	0.67709033
C	-1.08174204	4.96322556	-0.69101695
C	-3.47951332	5.45692442	0.66342777
H	-3.39384986	3.39037285	1.24065187
C	-1.63064933	6.24462555	-0.71935924
H	-0.16546037	4.76341206	-1.24106037
C	-2.82837565	6.47352467	-0.03871416
H	-3.26644786	7.47005301	-0.05716630
C	-4.78037360	5.73022426	1.37519020
H	-5.61371853	5.75741624	0.66459442
H	-4.99753337	4.95564083	2.11503779
H	-4.75483788	6.69694960	1.88603906
C	-0.94094155	7.36565152	-1.45490144
H	-0.38924648	8.00564256	-0.75749403
H	-0.22768382	6.97936160	-2.18727312
H	-1.66359384	7.99840670	-1.97781191

C	2.46842608	-0.66947267	0.05951311
N	-1.34212399	-2.26470675	-0.06069465
C	-5.28858998	-5.01099432	-0.14362331
C	-3.91989861	-4.90069650	-0.13557724
C	-5.54065439	-2.59664781	-0.08875381
C	-6.10117492	-3.85053354	-0.12024927
H	-5.75611600	-5.98952942	-0.16878479
H	-3.28627556	-5.78225201	-0.15294705
H	-6.16323021	-1.70748874	-0.07142827
H	-7.18083769	-3.95892470	-0.12758870

Complex 4	X	Y	Z
C	2.34818793	0.73172551	0.04351328
C	3.76518371	0.68195703	0.03135113
N	1.65686325	-0.44544867	0.01129147
C	4.40956313	-0.55135216	-0.01514833
H	4.34865251	1.59310593	0.08132959
C	2.23902024	-1.64422219	-0.03069386
C	3.64135500	-1.73064113	-0.04471655
H	4.13155325	-2.69476278	-0.11112595
C	1.26420915	-2.75133363	-0.07026917
C	-0.11554691	-2.37728477	-0.06537545
C	1.64666842	-4.09380958	-0.11052460
C	-1.06178298	-3.40306627	-0.10357633
C	0.67893151	-5.09241094	-0.14773019
H	2.69857499	-4.36592375	-0.11215496
C	-0.67050010	-4.74322415	-0.14473839
H	-2.11799483	-3.15000055	-0.10033187
H	0.97623340	-6.13548248	-0.17858785
H	-1.42815970	-5.52146944	-0.17467850
C	-0.60053137	2.79935718	0.12085080
C	-0.12287151	4.16539064	0.16345112
C	1.29742199	4.37116976	0.17187579
C	2.13148404	3.26123371	0.13710719
C	1.55716944	1.91110780	0.09005358
H	-2.06325636	5.06165382	0.18793093
H	-1.67063763	2.60447317	0.11514396
C	-0.99135574	5.23686262	0.19544589
C	1.77628508	5.71246496	0.21570222
H	3.20648166	3.38881574	0.14502865
C	0.88050867	6.78519906	0.24861567
C	-0.48914646	6.56847214	0.23884763
H	2.84716079	5.88858912	0.22254975
H	1.26727600	7.79829864	0.28211914
H	-1.18047085	7.40244294	0.26417670

N	0.18544869	1.75321998	0.08720418
Pt	-0.37932170	-0.42139437	0.00345464
C	5.89057735	-0.62500280	-0.03524915
C	6.55649289	-1.62208757	0.68282489
C	6.63506332	0.30585287	-0.76719001
C	7.95009519	-1.69560853	0.68184267
H	5.98478413	-2.33079133	1.27737075
C	8.02763374	0.24886199	-0.79053370
H	6.12208313	1.07095888	-1.34498554
C	8.66757117	-0.75330888	-0.05663319
H	9.75520864	-0.79868726	-0.05914785
C	8.66553760	-2.77749446	1.45049813
H	8.06528994	-3.12654483	2.29467597
H	8.86824212	-3.64117632	0.80757358
H	9.62518789	-2.42014492	1.83332750
C	8.83063471	1.22980058	-1.60650143
H	9.18049326	0.76744769	-2.53591984
H	8.23501417	2.10612175	-1.87391680
H	9.71407855	1.56729289	-1.05701643
C	-2.32629879	-0.43294388	-0.01450081
C	-3.55137614	-0.41355881	-0.02504820
C	-4.97123987	-0.43038178	-0.03461109
C	-5.72978996	0.74667512	-0.03358042
C	-5.69116759	-1.63179984	-0.04396077
C	-7.11574995	0.73424138	-0.04138812
C	-7.07661501	-1.66496380	-0.05154176
C	-7.79480998	-0.47662447	-0.05030449
F	-5.03879998	-2.79012484	-0.04530680
F	-7.72215130	-2.82631549	-0.05978680
F	-5.11579707	1.92654304	-0.02475061
F	-7.79969720	1.87381731	-0.04015937
F	-9.12130531	-0.49785019	-0.05791603

Table S9. Cartesian coordinates of complexes 1-4 on the Metal-center excited state (^{3}MC).

Complex 1	X	Y	Z
C	-0.23335394	0.68634342	0.31395557
C	-1.62316231	0.98770299	0.32559271
N	0.14444105	-0.62027829	0.10384945
C	-2.55763165	-0.02139622	0.13753475
H	-1.95384517	2.01092329	0.45428861
C	-0.73052813	-1.61539558	-0.08192034
C	-2.10697425	-1.34175855	-0.06607678
H	-2.82015066	-2.14893430	-0.18309480

C	-0.24042798	-2.98340872	-0.29581379
C	1.10729440	-3.21096552	0.10989371
C	-1.01393377	-4.00383180	-0.85336393
C	1.63083803	-4.49198828	-0.07002920
C	-0.46531032	-5.27056624	-1.01946050
H	-2.03988040	-3.81604161	-1.15787051
C	0.85242041	-5.50902039	-0.62803550
H	2.65482193	-4.69540455	0.22907025
H	-1.06096017	-6.06767281	-1.45183906
H	1.27987709	-6.49939096	-0.75809721
C	2.95129296	2.28572080	-0.13944826
C	2.65892200	3.68197720	-0.38979355
C	1.28053168	4.08059954	-0.39360468
C	0.30574380	3.11948930	-0.15802344
C	0.69319680	1.72590472	0.08063127
H	4.69885320	4.28273625	-0.61209350
H	3.98451577	1.94255835	-0.12783705
C	3.66108528	4.60345206	-0.61941785
C	0.98383311	5.45215394	-0.64164382
H	-0.74053911	3.39724227	-0.15351802
C	2.01029727	6.36712046	-0.87217724
C	3.34071873	5.96347622	-0.86433642
H	-0.05322465	5.77277397	-0.64951216
H	1.76317838	7.40670874	-1.06023043
H	4.13440152	6.67919798	-1.04292051
N	2.03641958	1.38217975	0.07718632
Pt	2.03867493	-1.11311482	0.30680956
Cl	4.37279217	-1.62143455	0.58288980
C	-4.00907488	0.27937437	0.14342344
C	-4.86919641	-0.38979672	-0.72800608
C	-4.53200520	1.24026024	1.01895778
C	-6.23899606	-0.11121136	-0.74052323
H	-4.46937813	-1.11896646	-1.42919874
C	-5.89244000	1.53358583	1.02769291
H	-3.87253710	1.74498897	1.72073730
C	-6.73123251	0.84984120	0.13996791
H	-7.79608689	1.07506909	0.13936306
C	-7.15396205	-0.84641266	-1.68668898
H	-6.75379398	-0.83939418	-2.70505408
H	-7.26440081	-1.89406402	-1.38725033
H	-8.14895392	-0.39541129	-1.70626325
C	-6.46303066	2.56087392	1.97201977
H	-5.68669906	2.98564238	2.61274811
H	-6.93362269	3.38020911	1.41893852

H	-7.23121505	2.11852566	2.61427849

Complex 2	X	Y	Z
C	-0.18276935	0.61501562	-0.43213302
C	-1.57355512	0.86799780	-0.42218449
N	0.23716931	-0.68280905	-0.24752477
C	-2.47271617	-0.17030141	-0.23478907
H	-1.93266115	1.88459439	-0.53668786
C	-0.60855119	-1.70411902	-0.06056328
C	-1.98070462	-1.48366272	-0.04903198
H	-2.67422633	-2.30674184	0.06818343
C	-0.07832935	-2.99211686	0.46760007
C	-0.89095192	-3.99417537	0.98667797
C	1.82881699	-4.26231054	0.86788985
C	-0.30268251	-5.16523404	1.45717105
H	-1.96592735	-3.86799358	1.02689226
C	1.07761761	-5.30720065	1.39832813
H	2.91144221	-4.30864636	0.79461573
H	-0.92191832	-5.95631645	1.86572023
H	1.57152943	-6.20381001	1.75313300
C	2.90648964	2.58715657	-0.07026786
C	2.41470193	3.85514675	0.43302627
C	0.99523476	4.09244835	0.45957245
C	0.13041362	3.10499619	-0.01072431
C	0.64506283	1.74835189	-0.23442605
H	4.34647407	4.64775902	0.87617094
H	3.98237789	2.42994489	-0.08697240
C	3.27565109	4.83097764	0.89829002
C	0.52859304	5.33379075	0.96878543
H	-0.94068612	3.28217955	0.00771011
C	1.42601733	6.30952428	1.43656171
C	2.78475347	6.07364722	1.40732414
H	-0.54091705	5.52133911	0.99306620
H	1.04048259	7.24827043	1.82069359
H	3.48572917	6.81895263	1.76614547
Pt	2.09413377	-0.98668167	-0.51085978
Cl	4.43533880	-1.44563340	-0.84256925
C	-3.93297814	0.08607174	-0.22326994
C	-4.76706943	-0.61294865	0.65449806
C	-4.49054522	1.03496804	-1.08602147
C	-6.14036113	-0.36855185	0.68579572
H	-4.33948893	-1.33531846	1.34628989
C	-5.86125294	1.29217940	-1.07960784
H	-3.85179917	1.56198783	-1.79120837
C	-6.66926955	0.58437467	-0.18699219

H	-7.73939877	0.77984745	-0.17219057
C	-7.02360188	-1.11224062	1.65561993
H	-6.92457429	-2.19467797	1.52707589
H	-6.74974471	-0.88078696	2.69013605
H	-8.07429124	-0.84696036	1.51639339
C	-6.45134484	2.30091665	-2.03250314
H	-5.92929719	3.26012609	-1.96339841
H	-6.36504661	1.95670590	-3.06847979
H	-7.50959297	2.47194410	-1.82101110
C	2.05567634	1.51201921	-0.26016947
N	1.26630052	-3.14087388	0.41777062

Complex 3	X	Y	Z
C	0.91245081	1.06615669	-0.09248695
C	0.43836620	2.39599393	-0.03396683
N	-0.01523766	0.05054066	-0.14753991
C	-0.92465522	2.65380538	-0.04706238
H	1.14653659	3.21333941	0.03868074
C	-1.33539096	0.26853840	-0.15474836
C	-1.82890854	1.57007525	-0.10634240
H	-2.89399894	1.75863856	-0.15065518
C	-2.17355269	-0.95675564	-0.22914804
C	-3.54346876	-0.93770103	-0.21768447
C	-2.12650354	-3.28390732	-0.37396162
C	-4.27289250	-2.15204957	-0.28896888
H	-4.08697348	-0.00153567	-0.15156271
C	-3.54270833	-3.36525562	-0.36915087
H	-1.51825027	-4.18445216	-0.43303156
C	3.72426587	-1.30985128	-0.21139837
C	4.89432333	-0.45238463	-0.15359158
C	4.71065014	0.97336493	-0.07323601
C	3.41729015	1.49339746	-0.05099946
C	2.25163755	0.60384892	-0.10745844
H	6.31051119	-2.04763284	-0.23688461
H	3.88589988	-2.38310000	-0.27563361
C	6.17512384	-0.97120377	-0.17591545
C	5.86376335	1.80079071	-0.01972191
H	3.27708516	2.56836760	0.00818161
C	7.15536278	1.24709191	-0.04362961
C	7.32237429	-0.12030368	-0.12048466
H	5.73293116	2.87728064	0.04041750
H	8.01848209	1.90344316	-0.00085303
H	8.31409955	-0.55808885	-0.13956150
Pt	0.67239643	-1.84897283	0.40583450
Cl	1.47851912	-4.07582001	-0.02743361

C	-1.43135725	4.04677453	-0.00725132
C	-2.60130782	4.35809744	0.69294491
C	-0.74444867	5.06619164	-0.67454224
C	-3.08541134	5.66531924	0.73560189
H	-3.12976486	3.57716782	1.23441812
C	-1.20711839	6.38119869	-0.64657152
H	0.14894117	4.82735648	-1.24625687
C	-2.37759232	6.66265748	0.06123692
H	-2.74852388	7.68592488	0.08675543
C	-4.35540129	5.99667892	1.47780367
H	-5.19464889	6.10586089	0.78218007
H	-4.61361438	5.21055437	2.19183947
H	-4.25860101	6.93947698	2.02364101
C	-0.45431560	7.48138147	-1.35106043
H	0.14819503	8.05654687	-0.63937312
H	0.22162472	7.07695670	-2.10860253
H	-1.14024468	8.17991608	-1.83849512
C	2.43250399	-0.81316128	-0.19032654
N	-1.47711997	-2.14748965	-0.30833042
C	-5.59850955	-4.62196374	-0.42954693
C	-4.22552849	-4.60269746	-0.43940497
C	-5.68843000	-2.20007770	-0.28122702
C	-6.33160102	-3.41209468	-0.35014759
H	-6.13047504	-5.56581434	-0.48343093
H	-3.65232581	-5.52288007	-0.49959783
H	-6.25010455	-1.27304171	-0.22097436
H	-7.41608629	-3.44857775	-0.34415466

Complex 4	X	Y	Z
C	2.27040112	0.67697910	0.02654988
C	3.67508890	0.58555738	0.19683542
N	1.58562777	-0.44778714	-0.33496602
C	4.31477211	-0.63386015	-0.00874677
H	4.24953091	1.44963398	0.50750268
C	2.16320357	-1.63229009	-0.53766366
C	3.55348661	-1.75877880	-0.37853530
H	4.04432920	-2.70564517	-0.57024405
C	1.62464083	-2.96418689	-0.20073492
C	0.21505181	-3.03549723	0.02650437
C	2.42847589	-4.10204021	-0.10442043
C	-0.32420944	-4.28296380	0.34599619
C	1.86016387	-5.33061145	0.21610699
H	3.49901152	-4.03510670	-0.27771063
C	0.48692456	-5.41618153	0.43926316
H	-1.39208648	-4.36852594	0.52475280

H	2.48491370	-6.21456236	0.29131737
H	0.04065880	-6.37490942	0.68885807
C	-0.24832754	3.25096339	-0.05493177
C	0.47057246	4.50703756	-0.01643995
C	1.90313941	4.44935565	0.04739682
C	2.51944675	3.20492126	0.06675730
C	1.70870593	1.98207202	0.01952188
H	-1.27129966	5.74384597	-0.08831386
H	-1.33503588	3.25528359	-0.10169146
C	-0.18651699	5.71990599	-0.03932845
C	2.61862356	5.68092785	0.08759630
H	3.59849314	3.13361780	0.11711116
C	1.93492497	6.90005804	0.06446914
C	0.55013161	6.93767302	0.00158594
H	3.70259289	5.65805840	0.13585620
H	2.49995451	7.82569965	0.09627480
H	0.02360131	7.88451981	-0.01644101
N	0.33244979	2.07806265	-0.03756523
Pt	-0.75029079	-0.31484406	-0.55476456
C	5.78386500	-0.74913771	0.15771599
C	6.33939422	-1.88956178	0.74429309
C	6.62666496	0.28428778	-0.26443146
C	7.71926570	-2.00572518	0.91748116
H	5.68769232	-2.68360018	1.10120304
C	8.00869284	0.18878769	-0.10975665
H	6.20213675	1.16476305	-0.74079523
C	8.53627409	-0.95893268	0.48763154
H	9.61348635	-1.03748957	0.62351209
C	8.31646339	-3.24083282	1.54280516
H	7.60318167	-3.73118645	2.21030299
H	8.60325365	-3.96575644	0.77298402
H	9.21489788	-2.99727634	2.11611208
C	8.92133204	1.28608751	-0.59542918
H	9.39530975	1.00647555	-1.54261042
H	8.37220904	2.21654463	-0.75952387
H	9.72102787	1.47954466	0.12524303
C	-2.72243015	-0.33658848	-0.28963141
C	-3.93505780	-0.32624836	-0.11433457
C	-5.34223854	-0.35086568	0.07440867
C	-6.02970752	0.70359460	0.68789232
C	-6.12018730	-1.43784073	-0.34400490
C	-7.40286956	0.68250530	0.87519620
C	-7.49392086	-1.47772906	-0.16543721
C	-8.14082629	-0.41279159	0.44724421

F	-5.53682865	-2.47627541	-0.93446934
F	-8.19596444	-2.52831470	-0.57644495
F	-5.35780799	1.77033603	1.11188236
F	-8.01849691	1.70377082	1.46208605
F	-9.45559044	-0.44133118	0.62240029

Table S10. Cartesian coordinates of complexes 1-4 on the transition state (TS) between ^{3}MC and T_1.

Complex 1	X	Y	Z
C	-0.28736106	0.70039484	0.30816891
C	-1.67716943	1.00175441	0.31980605
N	0.09043393	-0.60622687	0.09806279
C	-2.61163877	-0.00734480	0.13174809
H	-2.00785229	2.02497471	0.44850195
C	-0.78453525	-1.60134416	-0.08770700
C	-2.16098137	-1.32770713	-0.07186344
H	-2.87415778	-2.13488288	-0.18888146
C	-0.30701772	-2.97364133	-0.30261625
C	1.03921143	-3.21334508	0.10104879
C	-1.09045016	-3.98697331	-0.85923869
C	1.55099999	-4.49896242	-0.07992092
C	-0.55343448	-5.25853053	-1.02641613
H	-2.11512330	-3.78993788	-1.16218736
C	0.76268560	-5.50885950	-0.63699153
H	2.57356261	-4.71160451	0.21762021
H	-1.15683426	-6.05017536	-1.45808270
H	1.18106675	-6.50298742	-0.76789612
C	2.88007891	2.39161218	0.19562189
C	2.60662673	3.70432338	-0.35182555
C	1.24667349	4.01117476	-0.69130101
C	0.27034115	3.04619611	-0.47908842
C	0.63918968	1.73995614	0.07484461
H	4.63318009	4.38248739	-0.28237725
H	3.89891100	2.11946076	0.46647137
C	3.60963592	4.63301277	-0.54594679
C	0.96917768	5.29971812	-1.23293466
H	-0.76276520	3.25595724	-0.72519099
C	1.99634388	6.22334243	-1.42210600
C	3.30864029	5.90929510	-1.08704807
H	-0.05355971	5.55010032	-1.49687573
H	1.76424546	7.19863939	-1.83695742
H	4.10271296	6.63151888	-1.23511458
N	1.96468794	1.48370538	0.39074976
Pt	2.09268205	-1.12716624	0.31259622

Cl	4.42679929	-1.63548597	0.58867646
C	-4.06308200	0.29342579	0.13763678
C	-4.91800708	-0.35019813	-0.75781828
C	-4.59119963	1.22880576	1.03734465
C	-6.28769900	-0.07109008	-0.77047929
H	-4.51403284	-1.05895376	-1.47732129
C	-5.95165327	1.52203401	1.04640709
H	-3.93591680	1.71298176	1.75729032
C	-6.78515288	0.86430754	0.13437116
H	-7.84997772	1.08967536	0.13389996
C	-7.19702348	-0.77855348	-1.74286701
H	-6.79078343	-0.74229245	-2.75820211
H	-7.30928007	-1.83437107	-1.47438747
H	-8.19186685	-0.32697370	-1.75538070
C	-6.52783897	2.52181726	2.01650566
H	-5.75533276	2.92780059	2.67382103
H	-6.99509582	3.35683553	1.48445172
H	-7.29985716	2.06131264	2.64116471

Complex 2	X	Y	Z
C	-0.18276935	0.61501562	-0.43213302
C	-1.57355512	0.86799780	-0.42218449
N	0.23716931	-0.68280905	-0.24752477
C	-2.47271617	-0.17030141	-0.23478907
H	-1.93266115	1.88459439	-0.53668786
C	-0.60855119	-1.70411902	-0.06056328
C	-1.98070462	-1.48366272	-0.04903198
H	-2.67422633	-2.30674184	0.06818343
C	-0.03263203	-2.97170214	0.46913504
C	-0.80790325	-3.99567308	1.00238604
C	1.91756446	-4.17904975	0.85627386
C	-0.17824494	-5.14489669	1.47314982
H	-1.88583631	-3.90304181	1.05328769
C	1.20514741	-5.24383629	1.40047254
H	3.00028889	-4.19183130	0.77178774
H	-0.76801861	-5.95258592	1.89265182
H	1.73066786	-6.12239497	1.75502385
C	2.93271993	2.49966373	-0.98497610
C	2.59706548	3.81869789	-0.48453209
C	1.23001434	4.10685405	-0.13806273
C	0.26183776	3.11735194	-0.30442406
C	0.68588967	1.73044578	-0.53259359
H	4.59079666	4.57464517	-0.58420488
H	3.97005888	2.30408706	-1.24614225
C	3.56008715	4.79637213	-0.32115502

C	0.91977178	5.39890443	0.36427050
H	-0.77012536	3.33279419	-0.04437565
C	1.91878777	6.37539651	0.52134125
C	3.22628888	6.09058016	0.18671128
H	-0.10907371	5.62506444	0.62874048
H	1.65226981	7.35355956	0.90812786
H	4.00476927	6.83603833	0.30444074
Pt	2.10399293	-0.97445215	-0.44731156
Cl	4.45802151	-1.41798260	-0.69977748
C	-3.93297814	0.08607174	-0.22326994
C	-4.76706943	-0.61294865	0.65449806
C	-4.49054522	1.03496804	-1.08602147
C	-6.14036113	-0.36855185	0.68579572
H	-4.33948893	-1.33531846	1.34628989
C	-5.86125294	1.29217940	-1.07960784
H	-3.85179917	1.56198783	-1.79120837
C	-6.66926955	0.58437467	-0.18699219
H	-7.73939877	0.77984745	-0.17219057
C	-7.02360188	-1.11224062	1.65561993
H	-6.92457429	-2.19467797	1.52707589
H	-6.74974471	-0.88078696	2.69013605
H	-8.07429124	-0.84696036	1.51639339
C	-6.45134484	2.30091665	-2.03250314
H	-5.92929719	3.26012609	-1.96339841
H	-6.36504661	1.95670590	-3.06847979
H	-7.50959297	2.47194410	-1.82101110
C	2.04456016	1.44362601	-0.87624349
N	1.31541699	-3.07849442	0.40588661

Complex 3	X	Y	Z
C	0.91245081	1.06615669	-0.09248695
C	0.43836620	2.39599393	-0.03396683
N	-0.01523766	0.05054066	-0.14753991
C	-0.92465522	2.65380538	-0.04706238
H	1.14653659	3.21333941	0.03868074
C	-1.33539096	0.26853840	-0.15474836
C	-1.82890854	1.57007525	-0.10634240
H	-2.89399894	1.75863856	-0.15065518
C	-2.22773346	-0.91795532	-0.22791535
C	-3.59539337	-0.83760130	-0.21328179
C	-2.28524309	-3.24478203	-0.37416725
C	-4.37861007	-2.01803041	-0.28357802
H	-4.09629102	0.12191150	-0.14537173
C	-3.70365516	-3.26265358	-0.36613713
H	-1.71805125	-4.17161334	-0.43515447

C	3.73136592	-1.28279152	-0.41188895
C	4.89542897	-0.44851974	-0.17403822
C	4.70519523	0.95192903	0.10075085
C	3.41130498	1.47008695	0.13344265
C	2.25163755	0.60384892	-0.10745844
H	6.31713667	-2.02266638	-0.41518591
H	3.89809548	-2.33657870	-0.62128896
C	6.17677717	-0.96539936	-0.20726241
C	5.85260686	1.75717317	0.32921461
H	3.26622533	2.52619126	0.33915171
C	7.14488776	1.20594552	0.28995683
C	7.31819207	-0.13716787	0.02617229
H	5.71683794	2.81459578	0.53655156
H	8.00353169	1.84492113	0.46896099
H	8.31050112	-0.57282184	-0.00649483
Pt	0.67560994	-1.85785464	0.16929099
Cl	1.47851912	-4.07582001	-0.02743361
C	-1.43135725	4.04677453	-0.00725132
C	-2.60130782	4.35809744	0.69294491
C	-0.74444867	5.06619164	-0.67454224
C	-3.08541134	5.66531924	0.73560189
H	-3.12976486	3.57716782	1.23441812
C	-1.20711839	6.38119869	-0.64657152
H	0.14894117	4.82735648	-1.24625687
C	-2.37759232	6.66265748	0.06123692
H	-2.74852388	7.68592488	0.08675543
C	-4.35540129	5.99667892	1.47780367
H	-5.19464889	6.10586089	0.78218007
H	-4.61361438	5.21055437	2.19183947
H	-4.25860101	6.93947698	2.02364101
C	-0.45431560	7.48138147	-1.35106043
H	0.14819503	8.05654687	-0.63937312
H	0.22162472	7.07695670	-2.10860253
H	-1.14024468	8.17991608	-1.83849512
C	2.43917544	-0.78757624	-0.38361646
N	-1.58548777	-2.13861873	-0.30938418
C	-5.81378764	-4.42602996	-0.42251053
C	-4.44134663	-4.46823980	-0.43552373
C	-5.79485718	-2.00264705	-0.27259929
C	-6.49179811	-3.18460975	-0.34072927
H	-6.38759533	-5.34508360	-0.47570714
H	-3.91005184	-5.41311935	-0.49756426
H	-6.31432848	-1.05143711	-0.21052163
H	-7.57681289	-3.17251176	-0.33225630

Complex 4	X	Y	Z
C	2.25475099	0.67700583	0.02798350
C	3.65943877	0.58558411	0.19826904
N	1.56997764	-0.44776041	-0.33353240
C	4.29912198	-0.63383342	-0.00731315
H	4.23388078	1.44966071	0.50893630
C	2.13553215	-1.63206344	-0.53308960
C	3.53783648	-1.75875207	-0.37710168
H	4.02867907	-2.70561844	-0.56881043
C	1.43980714	-2.92080768	-0.40868167
C	0.01204295	-2.86310366	-0.45138736
C	2.10745765	-4.13759724	-0.25439817
C	-0.68564815	-4.06668828	-0.33450394
C	1.38282474	-5.31955021	-0.14038934
H	3.19305337	-4.16869142	-0.22166898
C	-0.00987305	-5.27942806	-0.18150148
H	-1.77132292	-4.05468857	-0.36283196
H	1.90169814	-6.26487513	-0.02010076
H	-0.57796187	-6.20146520	-0.09356669
C	-0.47590792	3.01960604	-0.15021477
C	0.13115138	4.33390494	-0.13932683
C	1.56243491	4.40248410	-0.05948483
C	2.28375193	3.21719089	0.00058418
C	1.58243874	1.92777600	-0.02089019
H	-1.71011441	5.41252481	-0.26301534
H	-1.55825338	2.92835532	-0.20802281
C	-0.62801842	5.48412924	-0.20245791
C	2.16818888	5.69213153	-0.04624496
H	3.36421210	3.24116636	0.06376503
C	1.38197319	6.84627625	-0.11005632
C	0.00000393	6.76188426	-0.18790739
H	3.24939110	5.76471208	0.01354940
H	1.86440615	7.81797639	-0.09823921
H	-0.60616334	7.65864570	-0.23748698
N	0.20385418	1.90241437	-0.09448040
Pt	-0.76491330	-0.33993205	-0.46894881
C	5.76821487	-0.74911098	0.15914961
C	6.32690046	-1.90803550	0.70505880
C	6.60783015	0.30259305	-0.22223379
C	7.70675794	-2.02481244	0.87794555
H	5.67755419	-2.71733203	1.03061309
C	7.98980882	0.20715478	-0.06708189
H	6.18093094	1.19823341	-0.66717059
C	8.52054723	-0.95957343	0.48928012

H	9.59769549	-1.03864257	0.62537070
C	8.30740207	-3.27960889	1.45921877
H	7.59432368	-3.79710051	2.10612872
H	8.59940805	-3.97455451	0.66412720
H	9.20318790	-3.05360228	2.04374752
C	8.89917138	1.32531211	-0.50939281
H	9.37698200	1.08266370	-1.46480308
H	8.34659134	2.25890718	-0.64080481
H	9.69601737	1.49542978	0.22026736
C	-2.70678002	-0.33661521	-0.29106503
C	-3.91940767	-0.32627509	-0.11576819
C	-5.32658841	-0.35089241	0.07297505
C	-6.01405739	0.70356787	0.68645870
C	-6.10453717	-1.43786746	-0.34543852
C	-7.38721943	0.68247857	0.87376258
C	-7.47827073	-1.47775579	-0.16687083
C	-8.12517616	-0.41281832	0.44581059
F	-5.52117852	-2.47630214	-0.93590296
F	-8.18031431	-2.52834143	-0.57787857
F	-5.34215786	1.77030930	1.11044874
F	-8.00284678	1.70374409	1.46065243
F	-9.43994031	-0.44135791	0.62096667

Table S11. Cartesian coordinates of complexes 1-4 at the MECP between ^{3}MC and S_0.

Complex 1	X	Y	Z
C	-0.43175218	0.74063381	0.29651640
C	-1.76952875	1.10358387	0.16351882
N	-0.08643961	-0.53212177	0.44304123
C	-2.74066381	0.09255635	0.16460972
H	-2.06041641	2.13496505	-0.00108932
C	-0.96523991	-1.52876921	0.34388840
C	-2.32668284	-1.24245972	0.23024090
H	-3.06025701	-2.03971875	0.18017134
C	-0.31846319	-2.85788642	0.25490937
C	1.09051722	-2.86476803	0.13267510
C	-1.04764351	-4.04724879	0.20664576
C	1.72534461	-4.09619372	-0.05844163
C	-0.39112987	-5.26265140	0.03130205
H	-2.12936059	-4.03493427	0.30961895
C	0.99390536	-5.28671618	-0.10743785
H	2.80680520	-4.13676493	-0.16417694
H	-0.96101635	-6.18551510	-0.00232634
H	1.50880788	-6.23134403	-0.25420359
C	2.98925285	1.76997727	-0.35567548

C	2.96722487	3.18746258	-0.37378830
C	1.74187626	3.83692169	-0.08294954
C	0.61055161	3.02036018	0.16468697
C	0.72618811	1.65514364	0.14900296
H	5.06759400	3.43547190	-0.83905473
H	3.92020795	1.24357543	-0.54026309
C	4.13331691	3.94876911	-0.63116308
C	1.70190844	5.25275472	-0.05682623
H	-0.34737920	3.48634257	0.37265733
C	2.84398707	5.97221383	-0.31051714
C	4.06886682	5.31966306	-0.59826182
H	0.76510814	5.75343550	0.16842190
H	2.81434866	7.05685360	-0.28781922
H	4.95787751	5.91170305	-0.78837265
N	1.93587115	1.03204699	-0.08375615
Pt	2.19776028	-1.17375193	0.61468047
Cl	4.46370509	-0.41003309	1.46134905
C	-4.17775706	0.43858203	0.04239951
C	-5.04132297	-0.35155435	-0.72278922
C	-4.68037154	1.56605776	0.69844492
H	-4.65259769	-1.21468555	-1.25905431
H	-4.01790461	2.17064229	1.31440762
C	-6.86996354	1.10193434	-0.16680108
H	-7.92410406	1.36007771	-0.24662910
C	-6.02860802	1.90939370	0.60189506
C	-6.39432486	-0.02824764	-0.83492585
C	-6.55429459	3.13281805	1.30803002
H	-6.19839588	3.17158928	2.34179433
H	-6.21074808	4.04609492	0.81052763
H	-7.64689408	3.14686624	1.31819640
C	-7.31980230	-0.89040360	-1.65587679
H	-6.91180508	-1.06345572	-2.65627852
H	-7.45808551	-1.87001233	-1.18664019
H	-8.30325272	-0.42575067	-1.76176975

Complex 2	X	Y	Z
C	0.33598183	0.74710981	-0.05834483
C	1.66708771	1.16412442	-0.08082370
N	0.07507735	-0.57740873	0.02332621
C	2.69690874	0.22509881	-0.01279170
H	1.90117667	2.21872623	-0.17287192
C	1.03574000	-1.51527275	0.07603630
C	2.37133773	-1.13669731	0.06411409
H	3.16155163	-1.87364712	0.14938077
C	0.53535272	-2.91775529	0.15745566

C	1.37212468	-4.02998925	0.16100525
C	-1.35173726	-4.27351758	0.30547005
C	0.80602331	-5.29898041	0.24466320
H	2.44749165	-3.91321369	0.09272839
C	-0.57488482	-5.42882121	0.32334437
H	-2.43822122	-4.28963743	0.35508794
H	1.44289326	-6.17747381	0.24690769
H	-1.04954339	-6.40036466	0.39504688
C	-3.30402840	1.56414600	-0.14571781
C	-3.28773196	2.93862091	-0.29402233
C	-2.06375669	3.66725350	-0.30887826
C	-0.86502119	2.95667541	-0.23834316
C	-0.88122671	1.56340880	-0.11776835
H	-5.42573893	3.25240391	-0.69897982
H	-4.24859906	1.02792980	-0.13156061
C	-4.47636511	3.78675191	-0.58446215
C	-2.11909743	5.11352251	-0.30011810
H	0.07578830	3.50225784	-0.28092275
C	-3.31981958	5.79843375	0.05293667
C	-4.49507408	5.11466357	0.09454302
H	-1.18210733	5.66097448	-0.34334375
H	-3.25364401	6.82987591	0.39104780
H	-5.39195655	5.50855110	0.56145557
Pt	-1.84043176	-1.09456237	0.09721946
Cl	-4.06876130	-1.82956488	0.21375271
C	4.11357889	0.66053091	-0.01764634
C	5.07768418	-0.05630149	-0.73387293
C	4.50445084	1.79928350	0.69523251
H	4.78012698	-0.92687507	-1.31181364
H	3.76731229	2.34536020	1.27715278
C	6.78449629	1.49620394	-0.02999500
H	7.82017952	1.82063455	-0.03675762
C	-2.10287952	0.83979983	-0.05487076
N	-0.80676920	-3.06147383	0.22198537
C	5.83215227	2.21242453	0.69091926
C	6.40415387	0.36141279	-0.74273787
C	7.44891387	-0.42871569	-1.55253632
H	7.61027818	-1.38145628	-1.09302905
H	7.09313814	-0.57029395	-2.55167556
H	8.36922968	0.11661805	-1.57555628
C	6.24594761	3.45937255	1.49434570
H	5.87637635	4.33694893	1.00631211
H	5.83576691	3.40036595	2.48083950
H	7.31320666	3.50718836	1.55411011

Complex 3	X	Y	Z
C	0.80672021	1.14293383	0.07762572
C	0.25374562	2.42111607	0.10446381
N	-0.02249914	0.07169670	0.05930745
C	-1.13351936	2.58415405	0.09297546
H	0.90418679	3.28719643	0.14389526
C	-1.36255106	0.18297571	0.06147474
C	-1.94773446	1.44257078	0.07809820
H	-3.02478259	1.54986537	0.04314682
C	-2.10588425	-1.10356589	0.01826515
C	-3.47362015	-1.18504714	0.00238245
C	-1.88559183	-3.42349855	-0.06513298
C	-4.11002878	-2.45103326	-0.05719383
H	-4.08634674	-0.29057391	0.03034078
C	-3.29148815	-3.60903980	-0.08841820
H	-1.21067020	-4.27708151	-0.09119738
C	3.81502160	-1.04288114	-0.05435377
C	4.86923562	-0.11258351	-0.03442417
C	4.57465951	1.28127992	-0.02654405
C	3.26792469	1.70961397	0.03289629
C	2.22000335	0.76875679	0.04873254
H	6.46727096	-1.58376342	0.04612656
H	4.04558597	-2.10480201	-0.09765760
C	6.24745725	-0.52135470	0.07301393
C	5.77197018	2.13823945	-0.24968278
H	3.05794243	2.77643380	0.03503949
C	6.99433319	1.73086480	0.50297450
C	7.26254745	0.39951130	0.48983652
H	5.96780604	2.31554729	-1.31214175
H	7.63468264	2.45624022	0.99428166
H	8.18967563	0.00315201	0.89586597
Pt	0.83748259	-1.71084171	-0.02284350
Cl	1.80195253	-3.90747050	-0.16368393
C	-1.73375373	3.93896193	0.06823484
C	-2.93922179	4.20093137	0.72732785
C	-1.10185623	4.96876130	-0.63610105
C	-3.51454670	5.47063089	0.68833422
H	-3.42562546	3.41374515	1.29845635
C	-1.65480986	6.24779766	-0.68726123
H	-0.18154977	4.76666190	-1.17768080
C	-2.86001492	6.48001055	-0.02217110
H	-3.30328185	7.47355817	-0.05976775
C	-4.82565935	5.75153493	1.37741344
H	-5.64528193	5.78348697	0.65125123

H	-5.06147060	4.97960468	2.11433791
H	-4.80351909	6.71923073	1.88673065
C	-0.96012182	7.36044581	-1.43005696
H	-0.40582124	8.00198266	-0.73628090
H	-0.24762325	6.96553690	-2.15857841
H	-1.67905995	7.99293003	-1.95839124
C	2.48427863	-0.62814191	-0.01105101
N	-1.32310013	-2.24060834	-0.01761949
C	-5.24767316	-5.01385323	-0.18148715
C	-3.88019342	-4.89458642	-0.14888817
C	-5.51788885	-2.60225600	-0.09235388
C	-6.06875634	-3.85919538	-0.15454507
H	-5.70774507	-5.99482714	-0.23178945
H	-3.24010171	-5.77143079	-0.17093612
H	-6.14686824	-1.71751516	-0.07350149
H	-7.14733779	-3.97470151	-0.18605796

Complex 4	X	Y	Z
C	2.05794750	0.61100380	-0.26916880
C	3.42881280	0.75436160	-0.07383310
N	1.49478660	-0.60073700	-0.37144840
C	4.23684140	-0.38201710	0.02156040
H	3.86808360	1.74411500	-0.02304450
C	2.24475580	-1.71820880	-0.27302050
C	3.61941680	-1.63112900	-0.06025480
H	4.21884240	-2.53452970	-0.05680560
C	1.53923700	-2.99184540	-0.52478870
C	0.33470060	-2.93680010	-1.26333180
C	2.05025170	-4.21342150	-0.07225030
C	-0.30866230	-4.14434520	-1.55607700
C	1.38786490	-5.39903420	-0.36913800
H	2.94963010	-4.23670690	0.53826240
C	0.21394150	-5.36295860	-1.12224020
H	-1.23611810	-4.13797390	-2.12398730
H	1.78025540	-6.34488740	-0.00946240
H	-0.30365780	-6.28718030	-1.36113010
C	-0.75149630	2.68172510	-1.29518060
C	-0.53986610	3.93856890	-0.66312720
C	0.60295350	4.07180020	0.16524550
C	1.45748660	2.95208300	0.28787980
C	1.16472620	1.79123290	-0.38527090
H	-2.28998490	4.93097240	-1.46903370
H	-1.63439550	2.54371520	-1.91766140
C	-1.42382080	5.03503010	-0.82210750
C	0.83420950	5.29693840	0.84108750

H	2.32649280	3.01088530	0.93473330
C	-0.04457270	6.33854480	0.68494470
C	-1.17846570	6.21122140	-0.15736140
H	1.70836370	5.39025010	1.47890340
H	0.12453070	7.27271770	1.21164240
H	-1.85371720	7.05232020	-0.26994670
N	0.05454860	1.65429330	-1.17364360
Pt	-0.44181420	-1.04598270	-1.41240740
C	5.71082880	-0.27238710	0.12570030
C	6.44113280	-1.20359700	0.86901010
C	6.38891480	0.74056940	-0.55905080
H	5.91996550	-1.98273980	1.42064660
H	5.83160030	1.44792480	-1.16906920
C	8.48459420	-0.11428500	0.23786430
H	9.57000140	-0.05530580	0.27832940
C	-2.07420250	-0.76447620	-0.26876980
C	-3.23824810	-0.81495470	0.11159360
C	-4.61670170	-0.91486690	0.44529990
C	-5.44715580	0.21057130	0.49460310
C	-5.23107940	-2.15551090	0.65399360
C	-6.81192150	0.11121760	0.71723270
C	-6.59402340	-2.27448660	0.87869080
C	-7.38996210	-1.13730690	0.90296770
F	-4.50503010	-3.26711620	0.61678980
F	-7.14647920	-3.46953160	1.05659740
F	-4.92908460	1.41948300	0.30150170
F	-7.57235910	1.19981780	0.74041870
F	-8.69650310	-1.24342020	1.09979460
C	7.78016250	0.83129330	-0.50924410
C	7.83279670	-1.13795080	0.92952620
C	8.60933830	-2.17259110	1.70365160
H	8.15002770	-2.36336770	2.67785390
H	8.63188760	-3.12401270	1.16108970
H	9.64227700	-1.85565410	1.86476580
C	8.49763020	1.93169360	-1.24967320
H	8.13542680	2.01472980	-2.27883800
H	8.33026950	2.89956220	-0.76553550
H	9.57491090	1.75202330	-1.27897010