Supplementary Information

Phosphorescent heterobimetallic complexes involving platinum(IV) and rhenium(VII) centers connected by an unsupported *μ*-oxido bridge

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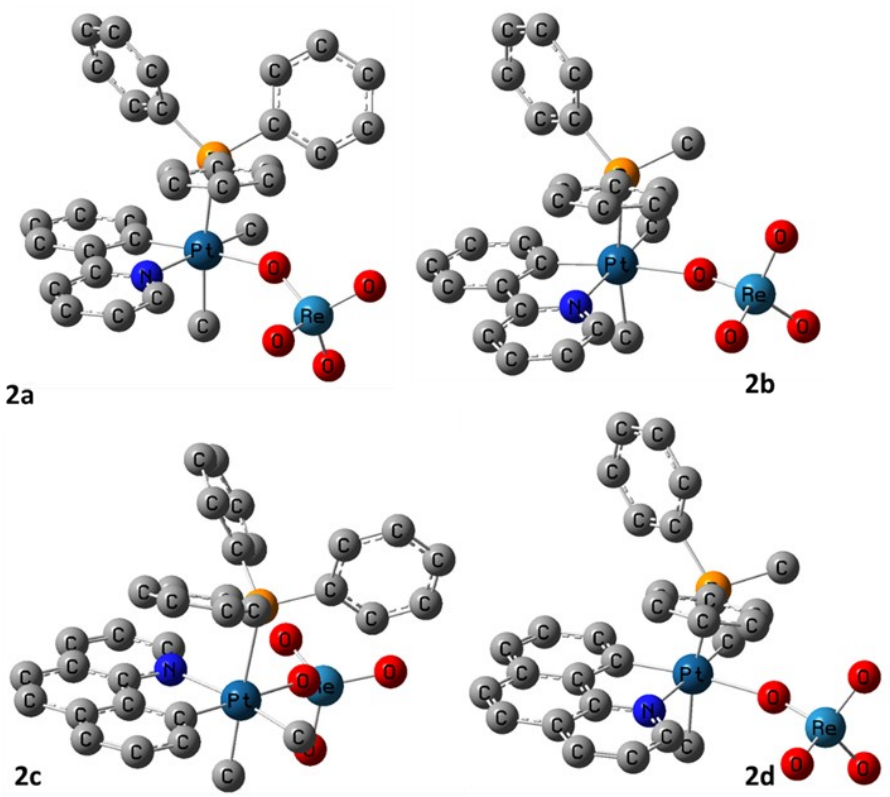


Fig. S1 Gas phase DFT optimized structures of complexes **2a** – **2d** in S_0 geometry

Table S1 Selected calculated bond lengths and angles for complexes **2a**-**2d** in S_0 and T_1 geometries compared to the experimental data of complex **2d**

Bond lengths(Å) and angles (º)	**2a** (S_0)	**2a** (T_1)	**2b** (S_0)	**2b** (T_1)	**2c** (S_0)	**2c** (T_1)	**2d** (exp)	**2d** (S_0)	**2d** (T_1)
Pt1-$C_{(trans\ to\ O)}$	2.006	1.987	2.005	1.986	2.010	2.014	2.000(3)	2.001	1.996
Pt1-$C_{(trans\ to\ P)}$	2.095	2.096	2.094	2.096	2.095	5.005	2.081(3)	2.094	2.104
Pt1-$C_{(trans\ to\ N)}$	2.078	2.082	2.080	2.083	2.078	2.067	2.058(3)	2.077	2.079
Pt1-N	2.224	2.205	2.216	2.205	2.259	2.237	2.142(2)	2.237	2.234
Pt1-O	2.222	2.218	2.228	2.225	2.231	2.197	2.167(2)	2.222	2.220
Pt1-P	2.624	2.643	2.580	2.596	2.600	2.579	2.4020(7)	2.577	2.549
N-Pt1-$C_{(trans\ to\ O)}$	79.7	80.8	79.7	80.8	80.2	80.3	81.66(12)	80.4	79.9
N-Pt1-O	94.5	94.0	96.0	95.4	96.5	95.1	92.73(10)	95.5	95.8
$C_{(trans\ to\ O)}$-Pt1-$C_{(trans\ to\ N)}$	95.9	95.7	96.6	96.2	94.6	95.2	93.76(16)	95.8	95.8
$C_{(trans\ to\ P)}$-Pt1-O	90.4	91.0	89.3	89.0	91.2	71.5	89.60(12)	89.5	92.5
O-Pt1-$C_{(trans\ to\ N)}$	88.8	89.4	87.5	87.5	88.5	87.3	91.86(14)	88.1	88.5

Table S2. Energies of selected molecular orbitals of the complexes **2a**-**2d** in S_0 geometry

	E (eV)	Pt	ReO_4	Me trans to P	Me trans to N	PPh_3	ĈN
2a							
LUMO+5	-0.732	2	13	1	0	82	2
LUMO+4	-0.965	10	57	3	1	23	5
LUMO+3	-1.073	7	1	1	1	85	5
LUMO+2	-1.271	16	22	6	1	16	38
LUMO+1	-1.334	10	13	2	1	8	66
LUMO	-1.924	5	1	1	0	6	88
HOMO	-6.287	13	0	12	0	52	23
HOMO-1	-6.566	16	5	3	0	21	55
HOMO-2	-6.929	15	8	1	0	14	62
HOMO-3	-7.022	1	1	0	0	92	6
HOMO-4	-7.055	1	1	0	0	91	6
2c							
LUMO+5	-0.912	4	35	2	1	51	6
LUMO+4	-1.059	1	0	0	1	94	4
LUMO+3	-1.319	12	3	7	1	44	33
LUMO+2	-1.450	30	27	0	6	14	23
LUMO+1	-1.623	12	2	3	1	27	56
LUMO	-1.989	2	1	0	0	3	93
HOMO	-6.185	5	1	7	0	24	62
HOMO-1	-6.442	21	4	10	1	45	19
HOMO-2	-6.827	5	1	0	0	6	88
HOMO-3	-6.954	1	2	1	0	90	6
HOMO-4	-7.072	1	1	0	1	96	1

	E (eV)	Pt	ReO_4	Me trans to P	Me trans to N	$PMePh_2$	ĈN
2b							
LUMO+5	-0.906	9	48	3	3	33	5
LUMO+4	-1.004	10	42	4	1	38	5
LUMO+3	-1.062	7	2	2	1	85	3
LUMO+2	-1.260	15	34	3	2	4	42
LUMO+1	-1.358	9	15	2	1	6	66
LUMO	-1.931	4	1	1	0	5	90
HOMO	-6.363	15	0	11	1	38	36
HOMO-1	-6.668	12	4	6	0	31	47
HOMO-2	-6.991	17	8	1	0	11	62
HOMO-3	-7.138	1	9	1	0	86	3
HOMO-4	-7.241	2	89	0	1	4	3
2d							
LUMO+5	-0.910	13	33	4	3	39	7
LUMO+4	-1.014	7	57	3	1	27	5
LUMO+3	-1.049	6	3	2	1	84	4
LUMO+2	-1.265	20	42	4	3	8	24
LUMO+1	-1.598	6	2	0	0	7	85
LUMO	-2.066	2	0	1	0	2	96
HOMO	-6.191	12	0	6	0	18	63
HOMO-1	-6.632	11	4	11	1	58	15
HOMO-2	-6.872	6	1	0	0	2	91
HOMO-3	-7.121	3	12	1	0	83	2
HOMO-4	-7.248	2	90	0	1	5	2

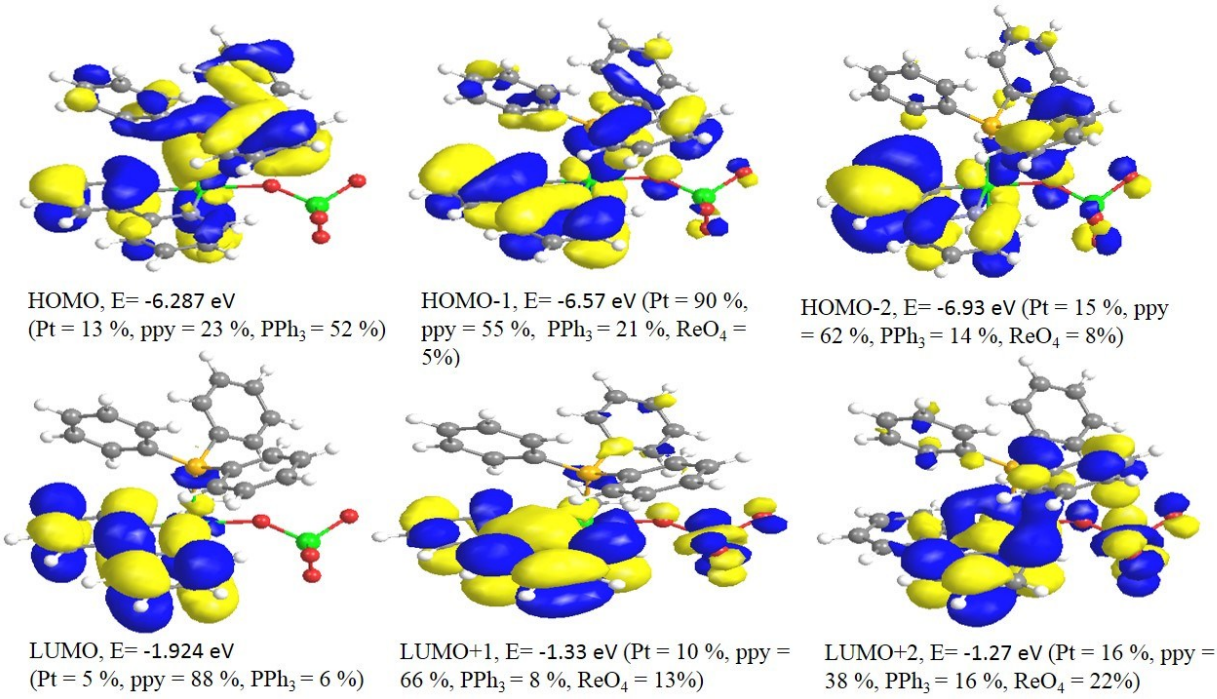


Fig. S2 Representative frontier orbitals and the relative composition energy levels for **2a** in dichloromethane

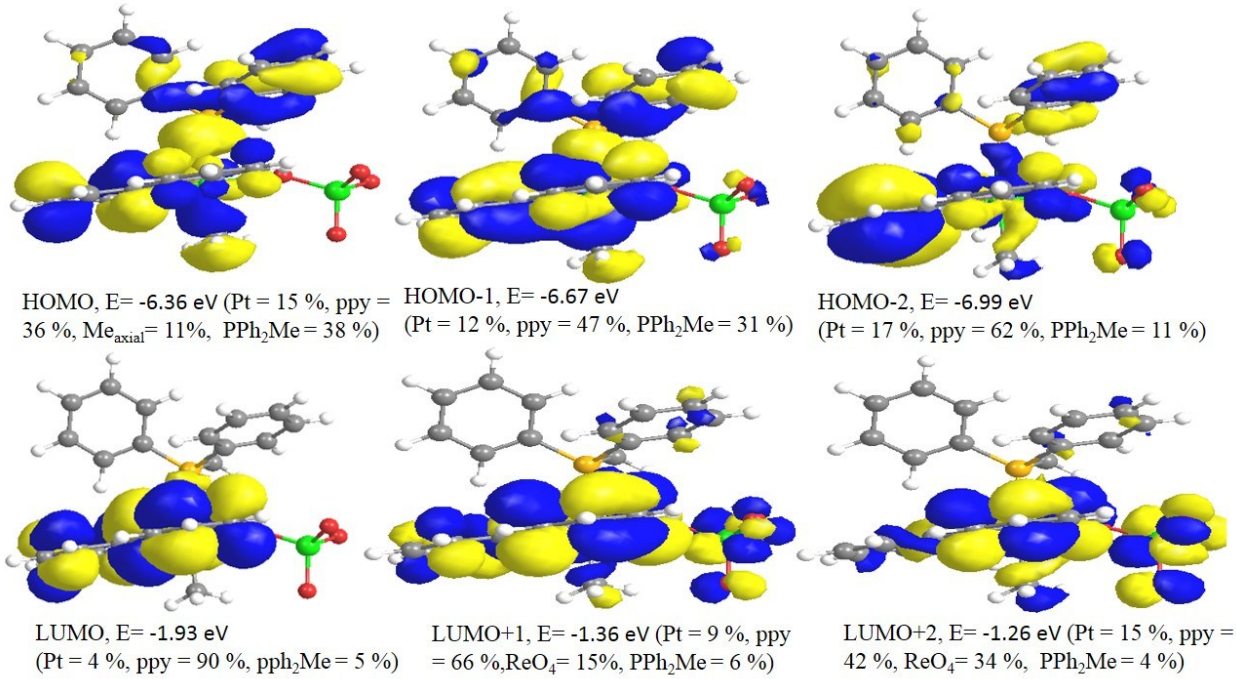


Fig. S3 Representative frontier orbitals and the relative composition energy levels for **2b** in dichloromethane

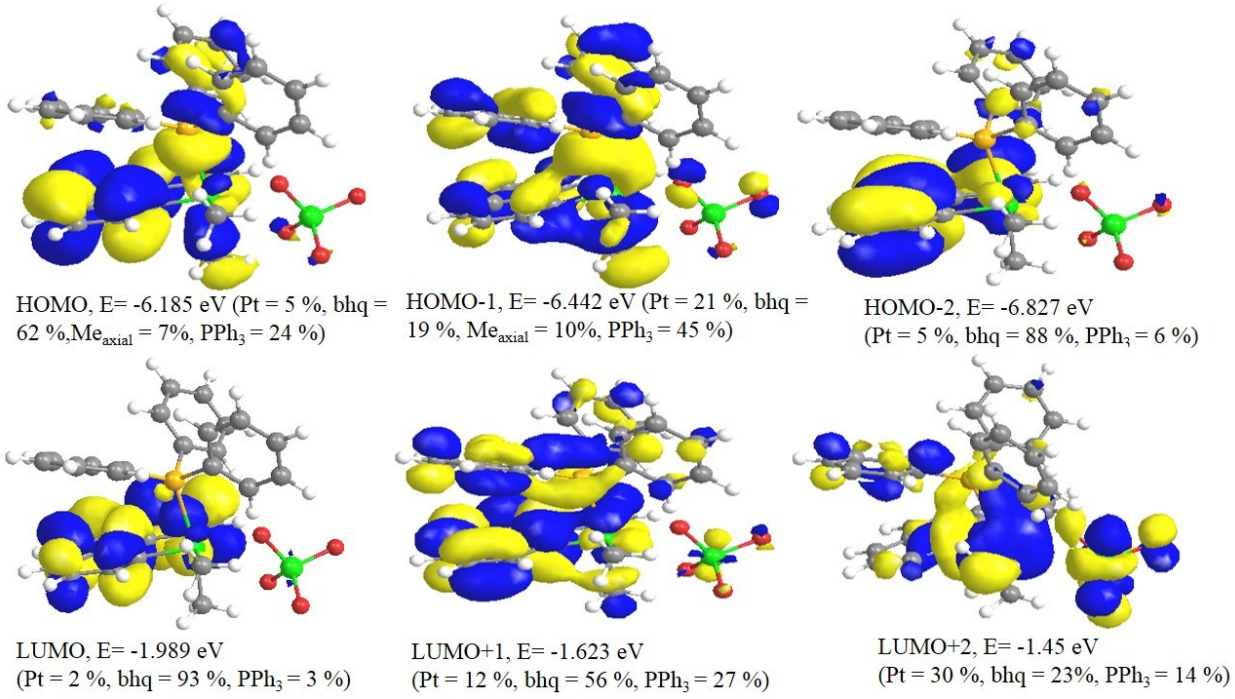


Fig S4 Representative frontier orbitals and the relative composition energy levels for **2c** in dichloromethane

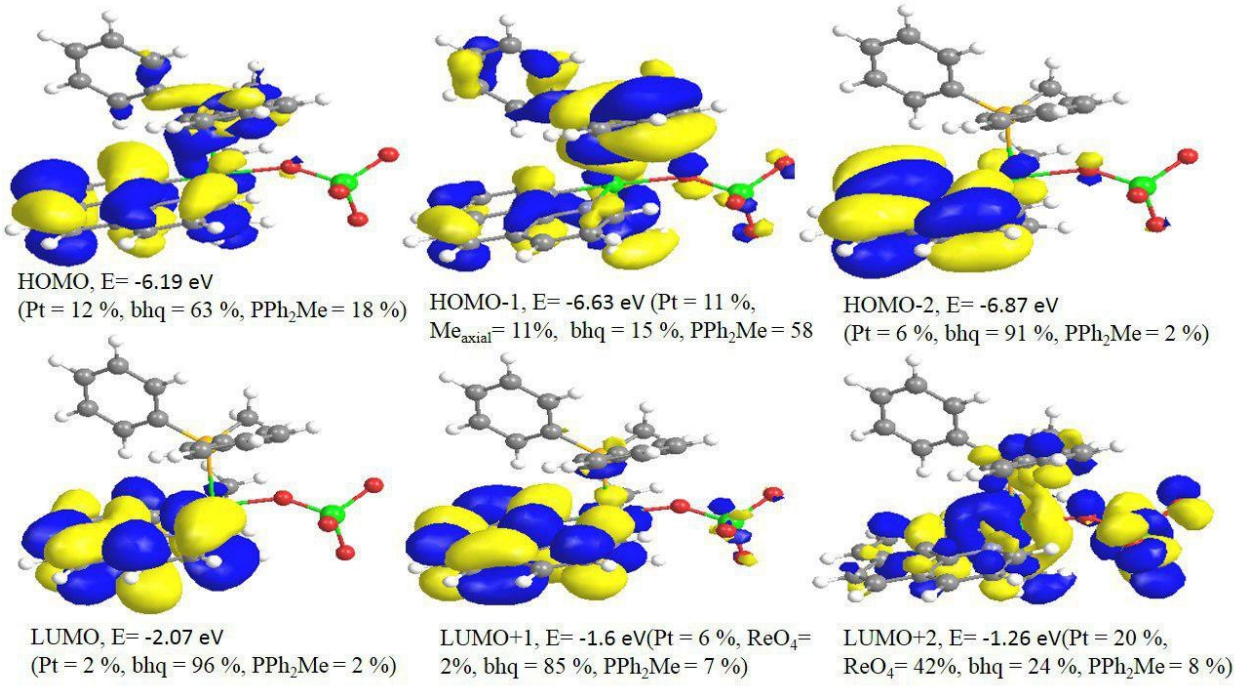


Fig S5 Representative frontier orbitals and the relative composition energy levels for **2d** in dichloromethane

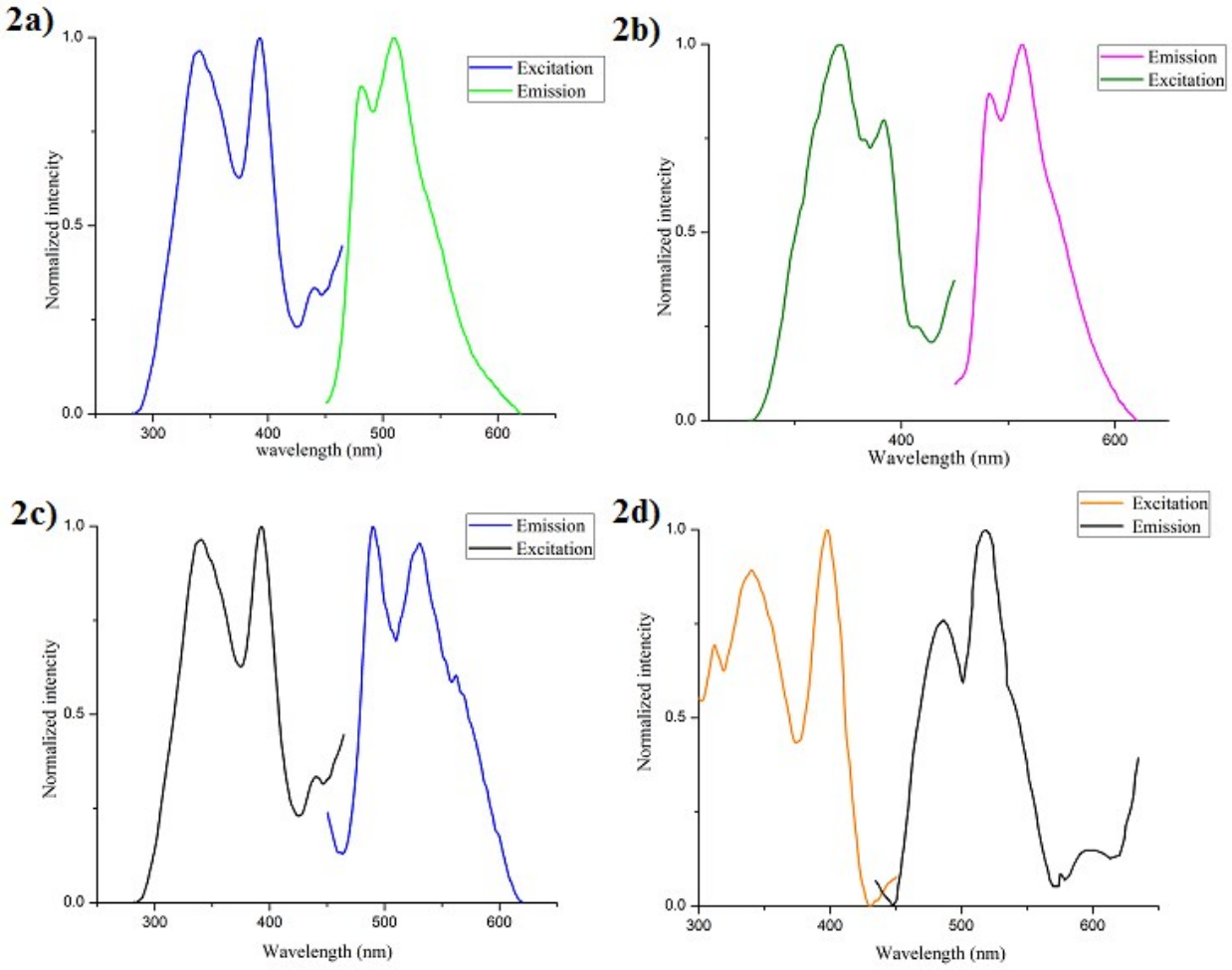


Fig. S6 Excitation and emission spectra of complexes **2a**-**2d** in solid state at 298 K

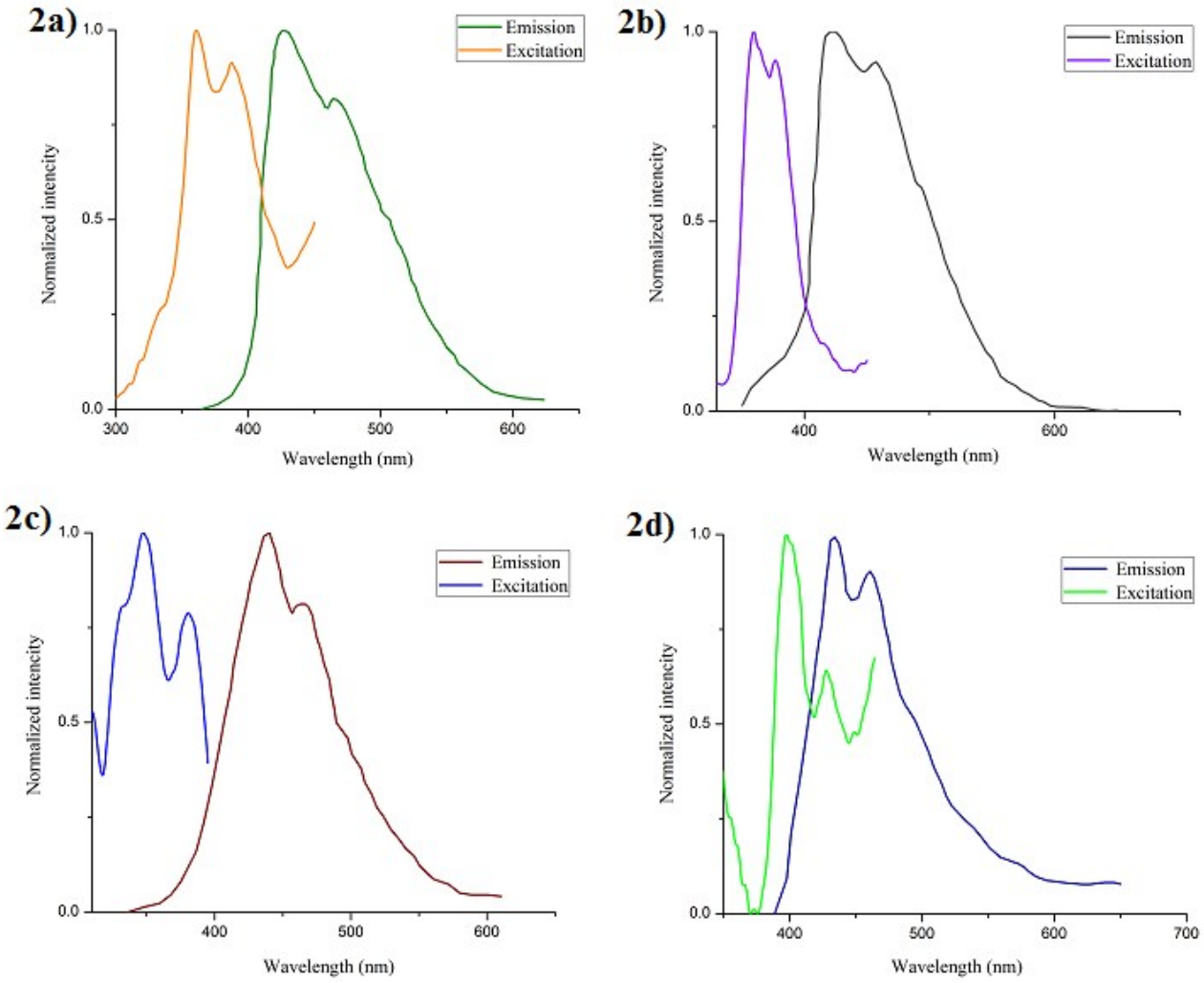
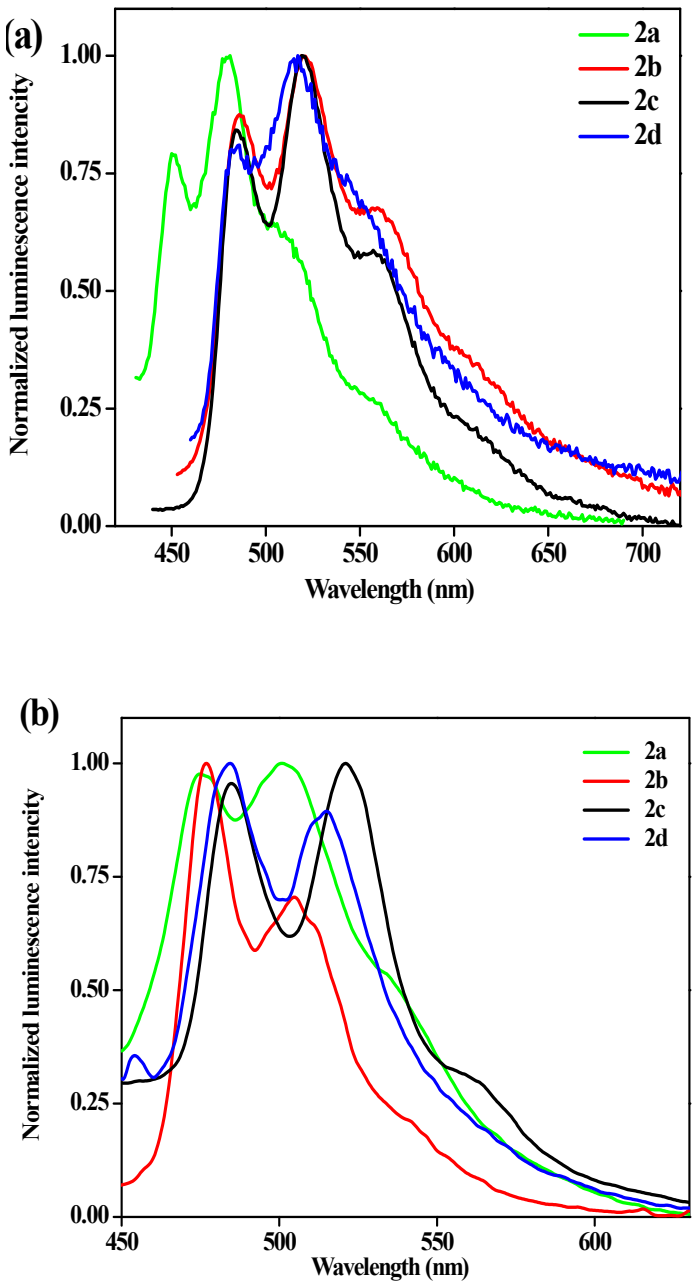


Fig. S7 Normalized excitation and emission spectra of complexes **2a-2d** in THF at 298 K



(B)

Fig. S8 Normalized emission spectra of complexes **2a-2d** in CH_2Cl_2 solution, a) at 298 k and b) at 77 K

XYZ Cartesian and energy of optimized structures

DFT optimized coordinates and energy for ground state (S_0) of **2a**
Charge = 0 Multiplicity = 1 E_{SP} = -2094.1573821 Hartree

Pt	-0.30569300	-0.83692800	-0.96207000
C	-2.53162000	-2.52900600	-0.16057000
C	-2.87412800	-1.64103500	-2.39054000
C	-3.77592900	-3.17688500	-0.24753800
C	-1.64520900	-2.67502300	1.00710200
C	-4.10567800	-2.29716000	-2.46383900
H	-2.53952600	-1.05306500	-3.23791300
C	-4.56357600	-3.06058500	-1.38774100
H	-4.13446300	-3.78284900	0.57929700
C	-1.90143100	-3.48946800	2.11908400
H	-4.70538800	-2.21211600	-3.36666800
H	-5.52150700	-3.56973700	-1.44063400
C	0.43768300	-2.07485900	1.90967300
C	-0.95189200	-3.59359400	3.13105300
H	-2.82660100	-4.05005000	2.18352400
C	0.24396500	-2.88368500	3.02584700
H	1.35162600	-1.50595500	1.77814500
H	-1.14216000	-4.23211800	3.98924300
H	1.01747500	-2.94755200	3.78302800
N	-0.48399300	-1.97312300	0.94114300
C	-2.08143600	-1.72741100	-1.24104800
C	-0.21808100	0.05925400	-2.83520900
H	-0.97991700	0.83772200	-2.93233900
H	0.77416600	0.50671400	-2.93126200
H	-0.35211700	-0.68849000	-3.62017000
P	-1.06699500	1.37675200	0.22396900
C	-0.24593700	1.53255100	1.87090100
C	-0.76531200	0.82331500	2.96839000
C	0.93332100	2.27222800	2.04376100
C	-0.13186300	0.87261700	4.21021300
H	-1.67628300	0.24166900	2.86083600
C	1.57210000	2.30809000	3.28514100
H	1.36009200	2.82590200	1.21524800
C	1.04092100	1.61323500	4.37203600
H	-0.55468000	0.32690000	5.04959200
H	2.48703800	2.88272400	3.39659500
H	1.53799000	1.64597500	5.33757600
C	-0.58353500	2.90097700	-0.70286200
C	-1.45687800	3.99049900	-0.84914400
C	0.69370500	2.96990800	-1.28788900
C	-1.05706000	5.12675600	-1.55493400

H	-2.44962400	3.95847000	-0.41436800
C	1.09170300	4.11351400	-1.98130800
H	1.37257300	2.12868900	-1.20004100
C	0.21777200	5.19360100	-2.11862900
H	-1.74568500	5.96089700	-1.66045700
H	2.08579400	4.15286500	-2.41774800
H	0.52747500	6.08064600	-2.66463100
C	-2.85297000	1.64833700	0.60190700
C	-3.27964000	2.41801100	1.69864800
C	-3.81807400	1.12852700	-0.27415900
C	-4.63835100	2.64909900	1.91590300
H	-2.55048800	2.83632300	2.38457500
C	-5.17693700	1.36389000	-0.05592000
H	-3.51199200	0.53209900	-1.12545100
C	-5.59039800	2.12138900	1.04031100
H	-4.95185000	3.24484600	2.76900100
H	-5.90929700	0.94763700	-0.74208200
H	-6.64820500	2.30106500	1.21269900
C	0.55374500	-2.51613400	-1.87339900
H	1.57645800	-2.23133000	-2.13395100
H	0.55891100	-3.33862000	-1.15384200
H	-0.00320600	-2.80497500	-2.76609000
O	1.69787900	0.01338700	-0.51369000
Re	3.42303400	-0.29290800	-0.19011900
O	4.24303900	1.21945400	-0.11473500
O	4.09426000	-1.26298300	-1.44254400
O	3.56842900	-1.12373100	1.31717900

DFT optimized coordinates and energy for triplet excited state (T_1) of **2a**
Charge = 0 Multiplicity = 3 E_{SP} = -2094.0532483 Hartree

Pt	-0.26459700	-0.82409900	-0.96594500
C	-2.47389200	-2.54032000	-0.12189400
C	-2.76344000	-1.71272100	-2.43737100
C	-3.76853400	-3.19840800	-0.23592300
C	-1.63785500	-2.67218000	0.98108600
C	-3.99467100	-2.39147700	-2.51973400
H	-2.41525800	-1.15831800	-3.30233800
C	-4.48713400	-3.12201400	-1.39177300
H	-4.15563400	-3.76412400	0.60454500
C	-1.89369600	-3.49812400	2.14198100
H	-4.57628200	-2.35429600	-3.43556900
H	-5.44651400	-3.62742600	-1.46487900
C	0.48601900	-2.10852300	1.86647900
C	-0.94547500	-3.62502100	3.12437400
H	-2.83441400	-4.03125000	2.21669500
C	0.28515100	-2.93324900	2.99645000

H	1.41644300	-1.55990400	1.75230400
H	-1.13194300	-4.25508500	3.98900000
H	1.06796900	-3.01261200	3.74134900
N	-0.41566900	-1.96468100	0.91557900
C	-2.00960400	-1.72127900	-1.27928800
C	-0.18339400	0.12404900	-2.81732100
H	-1.00944600	0.83148000	-2.93278500
H	0.76437300	0.66656200	-2.85935000
H	-0.21353900	-0.61123500	-3.62500500
P	-1.09793000	1.37758700	0.23584100
C	-0.40972200	1.48948500	1.94318700
C	-0.95391000	0.67333900	2.95069100
C	0.69252000	2.29960200	2.25246900
C	-0.41778600	0.68184400	4.23789400
H	-1.80652900	0.03586500	2.73483000
C	1.23384300	2.29714200	3.54021000
H	1.13304500	2.93681100	1.49390600
C	0.68061300	1.49203900	4.53597000
H	-0.85679500	0.05079200	5.00595300
H	2.09004900	2.92852500	3.75984000
H	1.10263300	1.49358700	5.53715500
C	-0.56009700	2.92883500	-0.60908400
C	-1.42812400	4.01797500	-0.78780100
C	0.75745900	3.02179200	-1.09246400
C	-0.98482600	5.17608800	-1.42907400
H	-2.44994500	3.96881000	-0.42797900
C	1.19771500	4.18691000	-1.72167900
H	1.43465500	2.18307200	-0.97486500
C	0.32796600	5.26536100	-1.89424700
H	-1.66928500	6.00986400	-1.56131000
H	2.22174500	4.24386400	-2.07984400
H	0.67079900	6.16932200	-2.39046400
C	-2.91114200	1.62371800	0.47134400
C	-3.44606000	2.28764200	1.58856900
C	-3.78450000	1.18921800	-0.53838300
C	-4.82134400	2.49985700	1.69461600
H	-2.78900600	2.63927000	2.37708300
C	-5.15932100	1.40587500	-0.43105200
H	-3.39312000	0.67363700	-1.40777000
C	-5.68131600	2.05885200	0.68639800
H	-5.21930600	3.01388900	2.56546700
H	-5.82023700	1.05819300	-1.22025300
H	-6.75192700	2.22430400	0.77190700
C	0.64397800	-2.47129100	-1.89092200
H	1.66442400	-2.15889900	-2.12631400
H	0.65040000	-3.30343000	-1.18310000

H	0.10775700	-2.75253800	-2.79844100
O	1.71677200	0.03821600	-0.46466300
Re	3.45267300	-0.25842000	-0.18984700
O	4.26538400	1.25868300	-0.13904600
O	4.09303500	-1.22643600	-1.46005700
O	3.64294500	-1.08779300	1.31295900

DFT optimized coordinates and energy for ground state (S_0) of **2b**
Charge = 0 Multiplicity = 1 E_{SP} = -1902.43334723821 Hartree

Pt	-0.41931900	-1.13457400	-0.58106600
C	-2.62373100	-1.86419300	1.16882500
C	-3.19012500	-2.25601200	-1.15648200
C	-3.90353400	-2.31320400	1.53740900
C	-1.60387300	-1.47887000	2.15923100
C	-4.45582300	-2.70704600	-0.77244700
H	-2.92663900	-2.25393600	-2.20842000
C	-4.81907300	-2.72720400	0.57579100
H	-4.18803700	-2.34906700	2.58491100
C	-1.76870900	-1.52137000	3.55069600
H	-5.15657300	-3.04718700	-1.53082100
H	-5.80323300	-3.07449000	0.87639800
C	0.61229000	-0.75262600	2.42986200
C	-0.70830800	-1.17334000	4.38109200
H	-2.71399000	-1.83384300	3.97884700
C	0.50717200	-0.78607200	3.81686900
H	1.53684400	-0.46078300	1.94289200
H	-0.82977600	-1.21004200	5.46008000
H	1.36170800	-0.51471700	4.42661200
N	-0.41511200	-1.08523000	1.63498800
C	-2.26941700	-1.80898700	-0.20358600
C	-0.52486600	-1.29595000	-2.65225900
H	-1.33985900	-0.68671100	-3.05522700
H	0.43258500	-0.93978000	-3.04239600
H	-0.67146400	-2.33739800	-2.94846700
P	-0.81457000	1.41178500	-0.71723900
C	-0.29408700	2.30533000	0.80363100
C	-1.19079600	2.40058500	1.88269000
C	0.99950700	2.83166900	0.94561000
C	-0.80580600	3.01863200	3.07116600
H	-2.19795000	2.00334300	1.78874500
C	1.38119600	3.44681600	2.14156800
H	1.72359300	2.76354100	0.14013900
C	0.48261000	3.54426600	3.20368500
H	-1.51325300	3.09223900	3.89292700
H	2.38654800	3.84763300	2.23465600
H	0.78256700	4.02612800	4.13034600

C	-2.46782100	2.14491100	-1.08461500
C	-2.65702300	3.53667500	-1.00954400
C	-3.53646800	1.33694100	-1.49431700
C	-3.88636200	4.10271500	-1.34114100
H	-1.84486600	4.17870500	-0.68012800
C	-4.76893500	1.90709400	-1.82637600
H	-3.41454700	0.26138400	-1.54487300
C	-4.94580100	3.28792900	-1.75161400
H	-4.01862700	5.17946500	-1.27776600
H	-5.58919000	1.26662900	-2.13892800
H	-5.90444000	3.73057200	-2.00850500
C	0.19135200	-3.13772300	-0.54664600
H	1.19735600	-3.13961400	-0.97374700
H	0.21532400	-3.48347500	0.48990600
H	-0.47799700	-3.76810300	-1.13493600
O	1.70764400	-0.51841700	-0.83344300
Re	3.38612900	-0.06024900	-0.48957000
O	3.59712400	1.58570300	-0.97487700
O	4.47933800	-1.06984100	-1.35004300
O	3.67029300	-0.19764800	1.20861100
C	0.22898500	2.12652800	-2.06424700
H	0.12573000	3.21498800	-2.10138000
H	1.27924800	1.86238800	-1.92304200
H	-0.11008000	1.70403800	-3.01439400

DFT optimized coordinates and energy for triplet excited state (T_1) of **2b**
Charge = 0 Multiplicity = 3 E_{SP} = -1902.3290945 Hartree

Pt	-0.39844200	-1.15231200	-0.58042200
C	-2.60831600	-1.77906900	1.22487600
C	-3.13607800	-2.32589700	-1.13205900
C	-3.96242300	-2.18269400	1.58239600
C	-1.63933800	-1.42086700	2.15409800
C	-4.42248700	-2.74733500	-0.73929200
H	-2.85995200	-2.39918000	-2.17857200
C	-4.82123400	-2.64879500	0.63192900
H	-4.28113000	-2.12342800	2.61740500
C	-1.80420000	-1.42331500	3.59179700
H	-5.11645800	-3.13658200	-1.47759800
H	-5.82385700	-2.95766600	0.91569100
C	0.62701600	-0.78917900	2.42811400
C	-0.74690100	-1.12058400	4.41057000
H	-2.76775800	-1.68354000	4.01450600
C	0.50796800	-0.80083500	3.83592400
H	1.57840600	-0.53886200	1.96670400
H	-0.86787000	-1.13097200	5.48971200
H	1.37167500	-0.55781100	4.44329300

N	-0.37820200	-1.06931000	1.62253200
C	-2.23850800	-1.80686700	-0.22005300
C	-0.49937900	-1.33071500	-2.65324900
H	-1.32512100	-0.74186200	-3.06414600
H	0.45161800	-0.95841000	-3.04421500
H	-0.62349600	-2.37718900	-2.94252500
P	-0.81490200	1.40607600	-0.73278900
C	-0.32926900	2.29659300	0.79882200
C	-1.23567000	2.35270900	1.87270800
C	0.95155900	2.84846800	0.95928600
C	-0.87264800	2.95690400	3.07483400
H	-2.23151000	1.93126000	1.76545100
C	1.31134000	3.44931700	2.16903500
H	1.68299800	2.80829500	0.15859200
C	0.40360300	3.50656000	3.22654800
H	-1.58644600	2.99852100	3.89323900
H	2.30710200	3.86973700	2.27748900
H	0.68726300	3.97591400	4.16467400
C	-2.47351700	2.11050400	-1.12823600
C	-2.71184600	3.49050700	-0.99937900
C	-3.49571400	1.28899000	-1.62229000
C	-3.94474900	4.03186400	-1.35886500
H	-1.93564500	4.14185500	-0.60773400
C	-4.73097900	1.83460000	-1.98311000
H	-3.33392100	0.22134600	-1.71458400
C	-4.95736700	3.20422800	-1.85289200
H	-4.11583200	5.09975600	-1.25277900
H	-5.51500100	1.18440700	-2.36162800
H	-5.91842500	3.62786400	-2.13181800
C	0.23527100	-3.14928400	-0.52528300
H	1.24116100	-3.14001100	-0.95181300
H	0.26059700	-3.48070200	0.51546100
H	-0.42739200	-3.79017100	-1.10948900
O	1.72242500	-0.52855600	-0.83480400
Re	3.38885400	-0.03313600	-0.48208600
O	3.56208500	1.62285900	-0.94804800
O	4.50558700	-1.00613400	-1.35423300
O	3.67683800	-0.18475800	1.21402000
C	0.23878600	2.13377000	-2.06424100
H	0.11829900	3.22051100	-2.10367400
H	1.29096100	1.88658700	-1.90688400
H	-0.07993600	1.70514900	-3.01868200

DFT optimized coordinates and energy for ground state (S_0) of **2c**
Charge = 0 Multiplicity = 1 E_{SP} = -2170.3893722 Hartree

Pt	0.18448700	-0.52919700	-1.04287300

C	-0.35433400	-2.22724600	-2.14547100
H	-0.10027500	-3.11929100	-1.56800100
H	-1.43669200	-2.16591500	-2.28722700
P	0.76042100	1.62598600	0.29325000
C	2.53523000	2.05745500	0.07262900
C	3.52469500	1.32235200	0.74935400
C	2.93922500	3.00941300	-0.87728300
C	4.87745800	1.55837700	0.50702800
H	3.24134100	0.56243000	1.47099000
C	4.29484000	3.23863100	-1.12265600
H	2.19703200	3.58305200	-1.42261100
C	5.26754100	2.51952300	-0.42807200
H	4.58674000	3.98478100	-1.85681300
H	6.32190800	2.70257600	-0.61626600
C	-0.16267300	3.16437600	-0.14319200
C	0.26468200	4.41844400	0.32920700
C	-1.35883800	3.08034300	-0.86963200
C	-0.47827900	5.56520000	0.05676100
H	1.17721000	4.50071500	0.91226000
C	-2.10432500	4.23291200	-1.13421900
H	-1.72150800	2.11550200	-1.20345700
C	-1.66427500	5.47463900	-0.67821400
H	-0.13572600	6.52859600	0.42496900
H	-3.03249900	4.15072300	-1.69250000
H	-2.24521300	6.36940000	-0.88514100
C	0.47619300	1.53136500	2.11518700
C	1.35461900	2.04949000	3.07854000
C	-0.74438500	0.97651700	2.53396500
C	1.02228800	1.99688800	4.43406600
H	2.29723900	2.49538000	2.77865500
C	-1.07680500	0.93418700	3.88783300
H	-1.44387600	0.58932200	1.80067200
C	-0.19103200	1.43959000	4.84176800
H	1.71288000	2.39917200	5.17068400
H	-2.02787200	0.50360300	4.18812700
H	-0.44663400	1.40377700	5.89737600
C	0.00788600	0.53097900	-2.82108600
H	-1.05374900	0.75062800	-2.95893400
H	0.57792700	1.46318300	-2.77957600
H	0.36248700	-0.07601400	-3.65656400
H	0.16074300	-2.24802800	-3.10712200
C	2.10001100	-1.05226600	-1.35551800
C	2.61550900	-1.95280600	-0.38460000
C	2.93504000	-0.65165200	-2.38770200
C	1.77603600	-2.38537600	0.69511500
C	3.94848100	-2.44372700	-0.46070000

C	4.26199300	-1.12633700	-2.46425800
H	2.58381600	0.03575000	-3.14865900
C	2.24584300	-3.30785700	1.66395900
C	4.40640300	-3.36571200	0.54292200
C	4.76638400	-2.00796700	-1.52534200
H	4.89357900	-0.79154300	-3.28322800
C	1.34505700	-3.70733700	2.67335500
C	3.59577100	-3.78426300	1.55717600
C	-0.32561800	-2.27803700	1.69414300
H	5.42653400	-3.73544000	0.47312200
H	5.78713300	-2.37405400	-1.59942700
C	0.05940100	-3.19897200	2.68397500
H	1.66892500	-4.41744700	3.43033400
H	3.95826600	-4.48822200	2.30166500
H	-1.33100900	-1.86979100	1.68142900
H	-0.66099100	-3.49373800	3.43930500
N	0.51144700	-1.87870600	0.73880000
Re	-3.55209500	-0.74969500	-0.21775400
O	-4.76579300	0.43637100	-0.50017500
O	-3.52874400	-1.19271800	1.45503900
O	-3.85688300	-2.14496900	-1.17741800
O	-1.95775200	-0.06685300	-0.62240000
H	5.62622100	0.98514500	1.04663800

DFT optimized coordinates and energy for triplet excited state (T_1) of **2c**
Charge = 0 Multiplicity = 3 E_{SP} = -2170.3060323 Hartree

Pt	0.12605500	-0.45634800	-0.95621000
C	-2.74371700	-4.36538800	-2.14233100
H	-2.54897500	-5.08901800	-1.35946800
H	-3.37358500	-3.50535000	-1.94703500
P	1.06177100	1.63028000	0.23391200
C	1.88487000	2.79339000	-0.92566300
C	2.86665700	2.31331600	-1.81119900
C	1.53332200	4.15166800	-0.97317300
C	3.49686900	3.17885500	-2.70477800
H	3.13429500	1.26169300	-1.80632000
C	2.15985500	5.01095100	-1.87774600
H	0.77286200	4.54165000	-0.30612500
C	3.14372700	4.52994900	-2.74211500
H	1.87592900	6.05938900	-1.90284800
H	3.62922100	5.20150800	-3.44478100
C	-0.14584500	2.65877900	1.15877200
C	0.20483000	3.32768400	2.34565200
C	-1.44087400	2.81606200	0.63946000
C	-0.73049300	4.12980500	2.99901100
H	1.20258800	3.22461700	2.75893900

C	-2.37492200	3.61447300	1.30243100
H	-1.72953300	2.29295600	-0.26386300
C	-2.02136400	4.27041900	2.48241200
H	-0.44963200	4.64201500	3.91539900
H	-3.38056000	3.69305700	0.90203200
H	-2.75079100	4.88518500	3.00269400
C	2.33079900	1.17059500	1.48160800
C	3.69981200	1.42578800	1.30931300
C	1.90786800	0.50091100	2.64494700
C	4.62197700	1.01987500	2.27628800
H	4.05206200	1.95255400	0.42971400
C	2.83097700	0.10511000	3.61054400
H	0.85321600	0.30045300	2.80428100
C	4.19276600	0.35927400	3.42729000
H	5.67778600	1.22968600	2.12838000
H	2.48489800	-0.40439700	4.50551600
H	4.91251900	0.04681700	4.17880300
C	-0.08611100	0.46113100	-2.79623000
H	-0.99679200	1.06732900	-2.76435000
H	0.76536800	1.08870000	-3.06961500
H	-0.21217700	-0.33185800	-3.54318200
H	-2.33100200	-4.52754000	-3.13113500
C	1.88595200	-1.33498900	-1.39032400
C	2.31692100	-2.26897900	-0.40305800
C	2.67799900	-1.19094800	-2.52514700
C	1.48999500	-2.50628000	0.74397300
C	3.52079800	-3.01093700	-0.54508300
C	3.87570900	-1.92354900	-2.67611700
H	2.37660900	-0.51718300	-3.32058800
C	1.85297600	-3.45740600	1.72994700
C	3.88428400	-3.94955200	0.48228800
C	4.30235600	-2.81061200	-1.70412500
H	4.46781300	-1.78753000	-3.57794200
C	0.95614000	-3.66035200	2.79963200
C	3.09102400	-4.16620500	1.57065700
C	-0.51526600	-2.02007800	1.82928900
H	4.81295900	-4.50317600	0.36659300
H	5.22618500	-3.36962700	-1.82872600
C	-0.22979200	-2.94897800	2.84510000
H	1.19958600	-4.38556700	3.57243100
H	3.37692000	-4.89013500	2.32933500
H	-1.44707500	-1.46249100	1.83095200
H	-0.94988600	-3.09728000	3.64270200
N	0.32699700	-1.80032700	0.82028800
Re	-3.64624500	-0.30143400	-0.09617000
O	-4.52236600	1.17872000	0.01412100

O	-3.63006600	-1.08543300	1.44383700
O	-4.39005100	-1.33501000	-1.25518400
O	-1.97351400	0.06644500	-0.57096900
H	4.25711800	2.79386800	-3.37894500

DFT optimized coordinates and energy for ground state (S_0) of **2d**
Charge = 0 Multiplicity = 1 E_{SP} = -1978.6660687 Hartree

Pt	-0.30879600	-0.75889800	-1.02085600
C	-2.69566000	-1.75967000	0.26205500
C	-3.11926800	-1.38526900	-2.08077600
C	-4.03152900	-2.20307700	0.46108200
C	-1.78287800	-1.78478600	1.36722300
C	-4.44930300	-1.82194200	-1.89113900
H	-2.79984900	-1.09506400	-3.07607800
C	-4.90721000	-2.21640000	-0.64659400
C	-2.18881600	-2.23772800	2.64642600
H	-5.12043200	-1.85121400	-2.74593700
H	-5.93225200	-2.55225000	-0.51367700
C	0.40139700	-1.41261300	2.09214000
C	-1.21336900	-2.25973800	3.66593700
C	0.07908400	-1.85334100	3.38795600
H	1.40914800	-1.09377400	1.84430800
H	-1.48578500	-2.60369500	4.66079700
H	0.85324000	-1.86763100	4.14734600
N	-0.50746400	-1.37665100	1.12061100
C	-2.23632200	-1.32591900	-1.01165900
C	-0.23850700	-0.28456600	-3.04158800
H	-0.97329100	0.48647200	-3.29203100
H	0.77132700	0.08712400	-3.23606500
H	-0.42259700	-1.17195300	-3.65215500
P	-0.49245100	1.73524700	-0.39660300
C	-0.04231600	2.07762500	1.35312800
C	-1.02342000	1.94834200	2.35213300
C	1.27239600	2.39613200	1.72800400
C	-0.69864200	2.14516100	3.69322000
H	-2.04752500	1.70695600	2.08020100
C	1.59310000	2.58841300	3.07497700
H	2.05901900	2.49052400	0.98647400
C	0.61181200	2.46649100	4.05845500
H	-1.47004800	2.05016500	4.45286300
H	2.61583200	2.83324500	3.34713000
H	0.86464600	2.62015800	5.10406800
C	-2.04173700	2.70982200	-0.63024800
C	-2.13252600	4.02680500	-0.14461300
C	-3.12449500	2.17303500	-1.33900700
C	-3.27955600	4.78586900	-0.36800800

H	-1.30947400	4.45702600	0.41922900
C	-4.27397100	2.93657700	-1.56218400
H	-3.07893800	1.15502600	-1.70739800
C	-4.35348400	4.24185000	-1.07898400
H	-3.33635500	5.80164900	0.01389500
H	-5.10677800	2.50461000	-2.11042000
H	-5.24791900	4.83454300	-1.25103900
C	0.13878500	-2.73312300	-1.55856500
H	1.18426700	-2.71746300	-1.87683000
H	0.01428700	-3.37631900	-0.68380900
H	-0.50496600	-3.07673200	-2.37015900
O	1.86571900	-0.31496800	-0.91497500
Re	3.52450900	-0.20317800	-0.29662200
O	3.97070600	1.46633900	-0.27409400
O	4.60577500	-1.08453300	-1.30094200
O	3.57350900	-0.83073400	1.31214000
C	-3.55178400	-2.65454500	2.82001500
C	-4.42806100	-2.63606000	1.77415900
H	-3.87003500	-2.99476400	3.80198800
H	-5.45462900	-2.96366900	1.91842500
C	0.72590500	2.70611100	-1.39108900
H	1.73348400	2.30148400	-1.27186000
H	0.44318800	2.62617600	-2.44470000
H	0.71593800	3.76004800	-1.09812700

DFT optimized coordinates and energy for triplet excited state (T_1) of **2d**
Charge = 0 Multiplicity = 3 E_{SP} = -1978.568584 Hartree

Pt	0.08170600	-0.29095800	-0.87795800
Re	-3.55814100	-0.66438500	0.22799000
P	0.66770500	1.56921600	0.76379100
N	0.67115100	-1.79571400	0.66417700
O	-1.95759100	0.06534800	-0.07562100
O	-4.05270000	-1.60240600	-1.12662700
O	-3.44022200	-1.68019800	1.61897600
O	-4.69161500	0.59755300	0.51919500
C	2.95513100	1.58793400	2.45303300
H	2.28988500	1.34322800	3.27403100
C	1.91570300	-2.21644200	0.44152800
C	-0.06593400	-2.32835400	1.69841000
H	-1.08887800	-1.98351600	1.79476400
C	1.93644400	-0.70733800	-1.48646800
C	-0.58647100	-1.83425500	-2.14238600
H	-0.28684300	-2.79120600	-1.70853800
H	-0.16802200	-1.72967500	-3.14511900
H	-1.67625900	-1.75430100	-2.17377300
C	-0.15550200	1.25457700	2.38496600

H	-1.22827800	1.18503700	2.19403500
H	0.03417600	2.06430600	3.09549500
H	0.17627200	0.29999900	2.80235900
C	4.57410600	-2.99554900	-0.17666000
H	5.58975100	-3.31836200	-0.38372900
C	5.20231000	2.03549900	1.67212500
H	6.26567500	2.13638700	1.87101800
C	4.32320500	1.71498400	2.70612900
H	4.69754300	1.56600100	3.71522000
C	2.44838100	1.77484000	1.15796900
C	3.34652700	2.08610900	0.12129300
H	2.97988900	2.22403500	-0.89172100
C	2.60889600	-1.64271100	-0.69783600
C	3.95821400	-2.05487500	-0.99125900
C	2.56083800	-3.20430600	1.27254800
C	0.05215500	3.24901400	0.32728600
C	0.48016400	-3.28762600	2.54613900
H	-0.13257600	-3.68783400	3.34793400
C	4.70964400	2.22292500	0.37802100
H	5.38778100	2.46879800	-0.43444300
C	4.59482300	-1.46539000	-2.13457800
H	5.61217300	-1.75936400	-2.37854400
C	3.86406100	-3.57383100	0.96217900
H	4.37033900	-4.31545000	1.57343900
C	3.91862500	-0.54255100	-2.92045000
H	4.41220700	-0.11335200	-3.78864800
C	-1.02491500	5.76534500	-0.29567700
H	-1.44139200	6.73955600	-0.53693400
C	-1.30278600	3.37536500	-0.02949200
H	-1.93920300	2.49621200	-0.07112800
C	1.78577200	-3.73119900	2.36090600
H	2.22365300	-4.47932800	3.01488100
C	0.85929400	4.39562900	0.36466400
H	1.90546400	4.32004700	0.64202100
C	2.60478100	-0.15787700	-2.61870200
H	2.09727800	0.55835700	-3.25399700
C	0.32119500	5.64582700	0.05137200
H	0.95734400	6.52636400	0.08419700
C	-0.36127800	1.01755800	-2.43247500
H	-1.41580800	1.28487300	-2.32807600
H	-0.20547800	0.53144800	-3.39819800
H	0.25075100	1.92138900	-2.36853400
C	-1.83536700	4.62803300	-0.33236300
H	-2.88461000	4.71134300	-0.60133000

DFT optimized coordinates and energy for ground state (S_0) of **1a**
Charge = 0 Multiplicity = 1 E_{SP} = -1725.4610969 Hartree

Pt	-0.58798600	-0.81174500	-0.95606300
C	-3.17444300	0.29870600	-0.11231000
C	-2.57635600	1.11033200	-2.31275200
C	-4.35630500	1.05910100	-0.17287300
C	-2.87070000	-0.58656400	1.02521100
C	-3.75766100	1.85453300	-2.36371800
H	-1.90095100	1.14076600	-3.16115100
C	-4.64761900	1.83802300	-1.28699400
H	-5.06245500	1.04173800	0.65223600
C	-3.70986800	-0.78398700	2.13341000
H	-3.98282900	2.44623100	-3.24793400
H	-5.56579100	2.41761800	-1.32015500
C	-1.35657300	-2.15814300	1.88273000
C	-3.35168300	-1.69648100	3.11931000
H	-4.64170100	-0.23730500	2.21509900
C	-2.15712800	-2.40684300	2.99296500
H	-0.41281500	-2.67000600	1.72230400
H	-4.00352700	-1.85650600	3.97377600
H	-1.84556700	-3.13721300	3.73203900
N	-1.70003200	-1.26999000	0.93845600
C	-2.25280500	0.34211800	-1.18893700
C	0.17968400	-0.33657000	-2.83158100
H	0.39014300	0.73485000	-2.89113800
H	1.09904800	-0.90017800	-2.99318300
H	-0.54994800	-0.61013000	-3.59801600
P	0.90291700	0.98846600	0.25562200
C	1.69497700	0.38035000	1.80996100
C	0.87430200	0.08700000	2.91287100
C	3.07552300	0.17081400	1.92495200
C	1.42249600	-0.39980500	4.09881700
H	-0.19624200	0.25617000	2.85423600
C	3.62137100	-0.32390900	3.11144500
H	3.73087900	0.38920300	1.08974700
C	2.79938700	-0.61123200	4.20057200
H	0.77188000	-0.61593400	4.94222100
H	4.69390500	-0.48435000	3.17931900
H	3.22673400	-0.99644200	5.12242800
C	2.30799700	1.60658700	-0.77885400
C	2.58215200	2.97648000	-0.91954600
C	3.12181200	0.68025300	-1.45540100
C	3.64470100	3.40906200	-1.71559000
H	1.96991600	3.71171600	-0.40974000
C	4.18873900	1.11820600	-2.24070900
H	2.92500700	-0.38377200	-1.36204200
C	4.45170700	2.48277100	-2.37673700

H	3.84035900	4.47362600	-1.81421000
H	4.80904600	0.38723500	-2.75226800
H	5.27881300	2.82142400	-2.99514000
C	0.09191800	2.56003800	0.81203000
C	0.40776500	3.18933900	2.02814900
C	-0.83196700	3.18204700	-0.04300200
C	-0.19872200	4.39562500	2.38362800
H	1.12973500	2.74153300	2.70165500
C	-1.43366100	4.39003100	0.31181700
H	-1.08809700	2.72199500	-0.98931100
C	-1.12311200	4.99839400	1.52901500
H	0.05771000	4.86486000	3.32987300
H	-2.15071700	4.84849400	-0.36360300
H	-1.59555400	5.93634700	1.80868800
C	-1.66062200	-2.32672200	-1.94495500
H	-0.94291200	-2.93472100	-2.49493100
H	-2.15735600	-2.93117800	-1.18214900
H	-2.39694700	-1.88819700	-2.62173600
I	1.48599600	-2.77181400	-0.49349200

DFT optimized coordinates and energy for ground state (S_0) of **1b**
Charge = 0 Multiplicity = 1 E_{SP} = -1533.738453 Hartree

Pt	0.46876500	-1.08953300	-0.49145800
C	-1.45641700	-1.88422300	1.58081300
C	-2.09170500	-2.79784000	-0.56915800
C	-2.58814900	-2.49253200	2.15342700
C	-0.46802400	-1.14761700	2.38733200
C	-3.20813200	-3.40311900	0.01379200
H	-1.90953200	-2.94158600	-1.62918100
C	-3.46550700	-3.24149400	1.37714800
H	-2.78479000	-2.39227400	3.21696300
C	-0.54752700	-0.95398300	3.77493900
H	-3.87477400	-4.00519500	-0.59906600
H	-4.33367800	-3.70758600	1.83430200
C	1.58118000	-0.01136300	2.33774900
C	0.47029300	-0.27846700	4.43871700
H	-1.39567000	-1.33628000	4.33043200
C	1.56015700	0.20113600	3.71213200
H	2.39723200	0.33400100	1.71134600
H	0.41348600	-0.13140800	5.51378100
H	2.37773700	0.72963500	4.19026400
N	0.59753800	-0.66140000	1.70027200
C	-1.21718900	-2.01232500	0.18930900
C	0.17124400	-1.64048900	-2.47971700
H	-0.81509700	-1.30609300	-2.81750500
H	0.94754700	-1.18045100	-3.09348700

H	0.23433800	-2.72763600	-2.57534300
P	-0.49102900	1.25598200	-0.94042500
C	0.01676300	2.50726600	0.31173700
C	-0.75268700	2.68211700	1.47482700
C	1.20224000	3.24462600	0.16814900
C	-0.35390300	3.58351800	2.46134200
H	-1.67432500	2.12184100	1.60490400
C	1.59790300	4.14770700	1.15765200
H	1.82922800	3.10548400	-0.70521800
C	0.82174000	4.32180200	2.30396800
H	-0.96473400	3.71179000	3.35111200
H	2.51660500	4.71342600	1.02826700
H	1.13043300	5.02728900	3.07086200
C	-2.30687200	1.58075000	-1.10677300
C	-2.78641600	2.90042500	-1.19961500
C	-3.21978200	0.52405500	-1.21161900
C	-4.14375700	3.15097100	-1.39159400
H	-2.09876100	3.73674800	-1.11052200
C	-4.58120400	0.77689300	-1.40523300
H	-2.87331200	-0.49871300	-1.13225500
C	-5.04587300	2.08789200	-1.49561100
H	-4.49806900	4.17623000	-1.45916300
H	-5.27466500	-0.05640200	-1.48003400
H	-6.10441500	2.28435600	-1.64402300
C	1.41907800	-2.94717600	-0.22034400
H	2.18904500	-3.03908500	-0.98606100
H	1.87758000	-2.94480900	0.77165500
H	0.69417500	-3.76005700	-0.30096300
I	3.08503800	-0.00548800	-1.11738700
C	0.12314900	1.93477200	-2.54755600
H	-0.31268900	1.33667400	-3.35311400
H	-0.17426500	2.97951200	-2.67714800
H	1.20975500	1.83526100	-2.59597900

DFT optimized coordinates and energy for ground state (S_0) of **1c**
Charge = 0 Multiplicity = 1 E_{SP} = -1801.6943859 Hartree

Pt	-0.21823800	-0.83391500	-1.06838400
C	-2.92545800	0.07984600	-0.47748200
C	-2.20036000	1.02202000	-2.56855100
C	-4.18413000	0.73455800	-0.58995300
C	-2.69882600	-0.79405200	0.63790300
C	-3.44535900	1.67606900	-2.69067900
H	-1.46752600	1.14727500	-3.35956400
C	-4.42154100	1.54826600	-1.71835700
C	-3.70177800	-1.01036700	1.61816300
H	-3.63696400	2.28771600	-3.56928200

H	-5.37785400	2.05486200	-1.82037100
C	-1.24936000	-2.29813600	1.67174200
C	-3.41441000	-1.92512800	2.65290800
C	-2.19362000	-2.57580400	2.67521100
H	-0.27586500	-2.77831200	1.64778200
H	-4.16177200	-2.11872100	3.41880500
H	-1.95001600	-3.29444500	3.45072300
N	-1.49366900	-1.42720300	0.69641200
C	-1.91048100	0.23821600	-1.46022400
C	0.70183100	-0.26036200	-2.84539200
H	0.88419900	0.81793900	-2.84832800
H	1.65025200	-0.79090500	-2.94171700
H	0.05557600	-0.52343800	-3.68670900
P	0.97967700	1.01990100	0.33193500
C	1.50795900	0.47436900	2.01481200
C	0.53112000	0.14703600	2.97150300
C	2.85951200	0.32946600	2.35724700
C	0.89956500	-0.29958900	4.24040700
H	-0.52231700	0.25486900	2.73366300
C	3.22516700	-0.12701700	3.62504400
H	3.63179900	0.56789300	1.63484700
C	2.24912000	-0.44115100	4.57040100
H	0.12973400	-0.54062600	4.96876900
H	4.27806900	-0.23647600	3.87001100
H	2.53628800	-0.79480300	5.55695800
C	-0.00928000	2.55316000	0.65718300
C	-0.13596100	3.14755000	1.92228600
C	-0.62586300	3.17732100	-0.44046500
C	-0.87533400	4.32183500	2.08572700
H	0.34616000	2.70235200	2.78502500
C	-1.35846000	4.35200100	-0.27688700
H	-0.53487200	2.74385700	-1.42942500
C	-1.49051400	4.92605500	0.98933900
H	-0.96270500	4.76514700	3.07423000
H	-1.83066200	4.81379200	-1.13961700
H	-2.06587400	5.83884500	1.11890100
C	-1.09353700	-2.38403100	-2.19059800
H	-0.29804200	-2.89144700	-2.73586700
H	-1.56140100	-3.07381800	-1.48433500
H	-1.83845200	-1.97887600	-2.87895500
I	1.88653900	-2.68896400	-0.40492400
C	-5.17208900	0.52503700	0.43353200
C	-4.94684900	-0.30770200	1.49002400
H	-5.71177300	-0.46296200	2.24649000
H	-6.12422000	1.04215000	0.34153700
C	2.51954000	1.71253000	-0.42924100

C	2.83048700	3.08034700	-0.34800900
C	3.41289600	0.85355500	-1.09152600
C	4.00296700	3.57629500	-0.91980000
H	2.15906800	3.76360600	0.16009600
C	4.58804500	1.35397800	-1.65501900
H	3.19805100	-0.20834200	-1.15445300
C	4.88461300	2.71549600	-1.57557200
H	4.22562400	4.63780600	-0.84970900
H	5.26769300	0.67379000	-2.16112800
H	5.79663900	3.10362500	-2.02148900

DFT optimized coordinates and energy for ground state (S_0) of **1d**
Charge = 0 Multiplicity = 1 E_{SP} = -1609.9714703 Hartree

Pt	0.41512300	-0.92051800	-0.86017600
C	-2.10397400	-1.56446300	0.46591100
C	-2.43175100	-1.55430100	-1.91793900
C	-3.47066600	-1.89942200	0.67808300
C	-1.22890400	-1.47210200	1.59898000
C	-3.78972600	-1.88630600	-1.71898500
H	-2.06401300	-1.44914700	-2.93404700
C	-4.31055400	-2.04588300	-0.44705200
C	-1.70643500	-1.69458200	2.91572400
H	-4.43284200	-2.02209000	-2.58534900
H	-5.35724700	-2.30129000	-0.30321000
C	0.94523200	-1.12472400	2.35698000
C	-0.77173800	-1.61594100	3.96904400
C	0.55329700	-1.33385900	3.69030000
H	1.97341800	-0.90350200	2.08833800
H	-1.10182300	-1.78423100	4.99140800
H	1.29592100	-1.27148500	4.47862900
N	0.07988000	-1.18944800	1.34945100
C	-1.57938800	-1.36136700	-0.83918200
C	0.50294000	-0.77682800	-2.93571500
H	-0.23624200	-0.05422200	-3.29655100
H	1.50488100	-0.45683000	-3.22715100
H	0.29410800	-1.75398100	-3.37881000
P	0.28188100	1.63646000	-0.61725800
C	0.73968000	2.23174200	1.06387000
C	-0.23932400	2.28334500	2.07131400
C	2.06268400	2.56755600	1.38940900
C	0.09419800	2.67650200	3.36691600
H	-1.26980600	2.02822800	1.84013000
C	2.39321800	2.96180300	2.68830600
H	2.84263300	2.50811900	0.63852900
C	1.41217000	3.01981900	3.67867200
H	-0.67706200	2.71762200	4.13154900

H	3.42199000	3.22194400	2.92226800
H	1.67186300	3.32930900	4.68758100
C	-1.26786600	2.58934600	-0.96546600
C	-1.37691600	3.94056800	-0.58976900
C	-2.31996000	2.00242700	-1.68004700
C	-2.51243500	4.67938000	-0.91777100
H	-0.57621900	4.41467000	-0.02948400
C	-3.45746300	2.74493200	-2.00984600
H	-2.25990900	0.96070000	-1.96956400
C	-3.55699400	4.08242200	-1.62952700
H	-2.58225900	5.72150800	-0.61717200
H	-4.26595900	2.27062400	-2.55962700
H	-4.44274600	4.65884300	-1.88312900
C	0.71195200	-2.99104800	-1.09530800
H	1.63756400	-3.12818600	-1.65398100
H	0.80627600	-3.43114400	-0.09935800
H	-0.13150600	-3.43724000	-1.62661300
I	3.28082700	-0.65812500	-0.60936500
C	1.45936700	2.49564400	-1.75622300
H	1.11265300	2.33161800	-2.78077800
H	1.48695600	3.57107400	-1.55691100
H	2.45536500	2.05918300	-1.65749600
C	-3.93654200	-2.09600600	2.02427000
C	-3.09794700	-1.99858000	3.09577400
H	-3.46793500	-2.16126400	4.10483400
H	-4.98574400	-2.33899600	2.17438900