Supporting Information

A computational scheme for evaluating the phosphorescence quantum efficiency: applied to blue-emitting tetradentate Pt(Ⅱ) complexes

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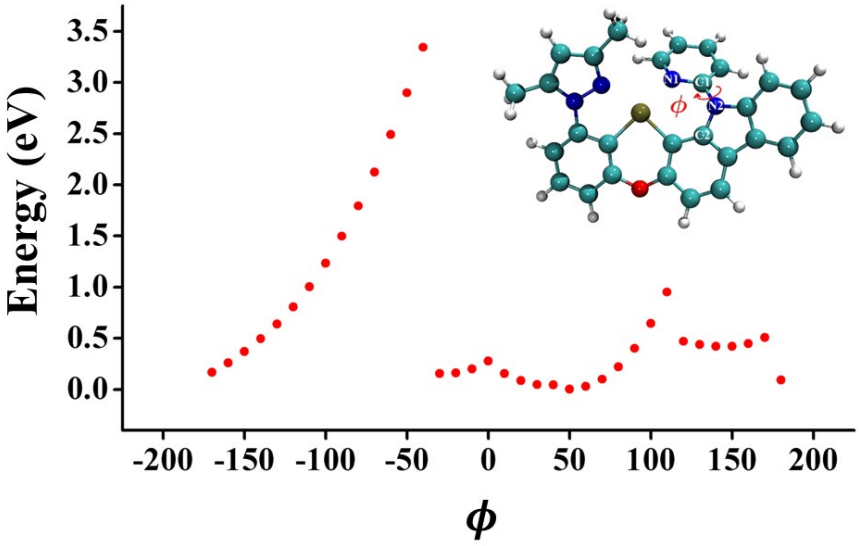

Figure S1. The soft scans of the lowest triplet excited states over N1-C1-N2-C2 dihedral angle ϕ in complex **1**, the energy of optimized ^{3}ES is the reference.

Table S1. The $^3ES \rightarrow S_0$ excitations that coefficients in the configuration interaction expansion are larger than 10 % for selected representative Pt(II) complexes at their optimized ^3ES state geometries. (H = HOMO, L = LUMO)

complex	excitation	coefficient	excitation	coefficient
1	H→L	72.89 %		
2	H→L	44.17 %	H→L+1	30.59 %
6	H→L	70.05 %		
7	H→L	67.41 %	H→L+1	11.67 %
8	H→L	78.56 %		
12	H→L	55.97 %	H-2→L	20.27 %
15	H→L	69.45 %	H→L+1	12.59 %

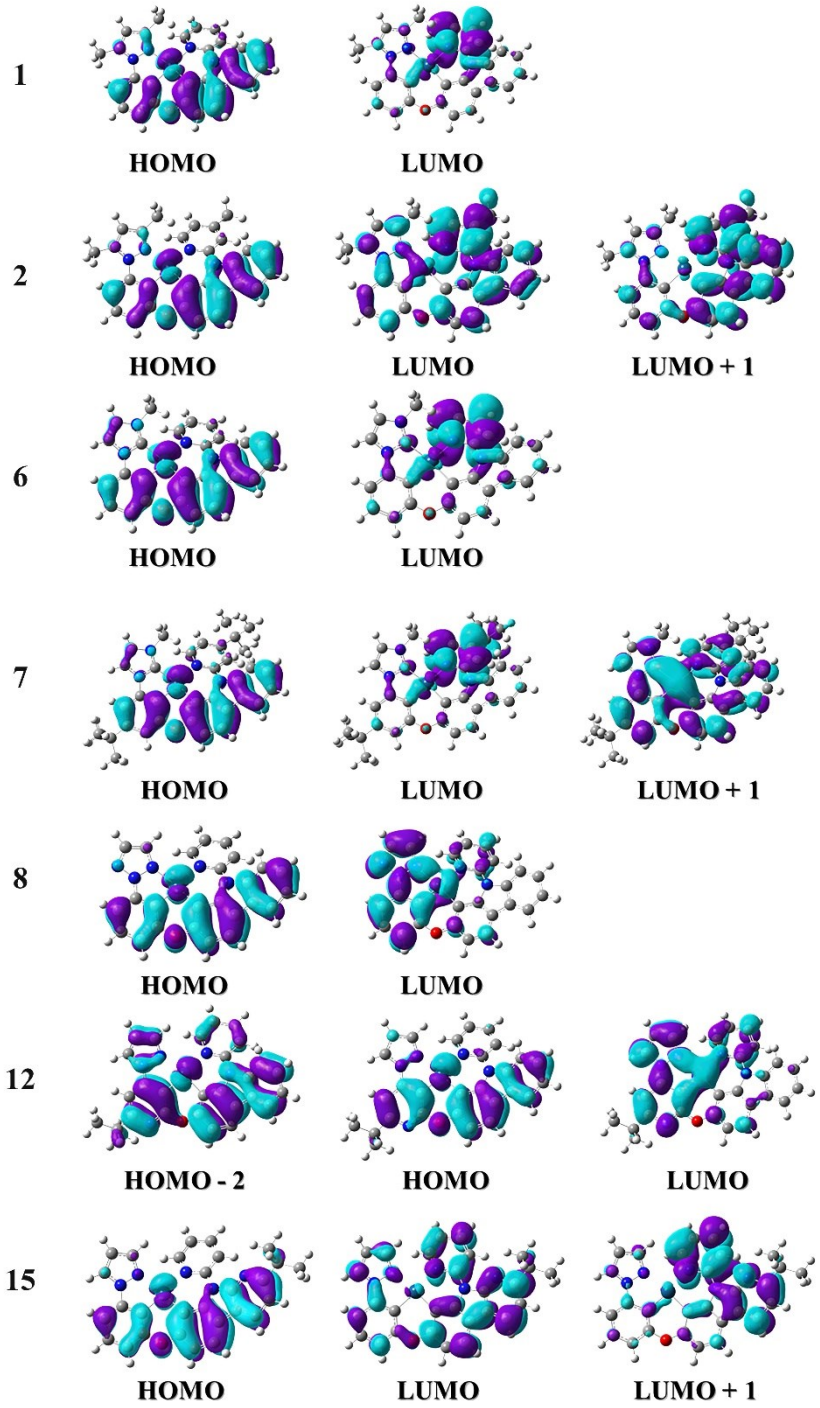

Figure S2. Spatial plots of orbitals listed in Table S1. (isovalue = 0.02)

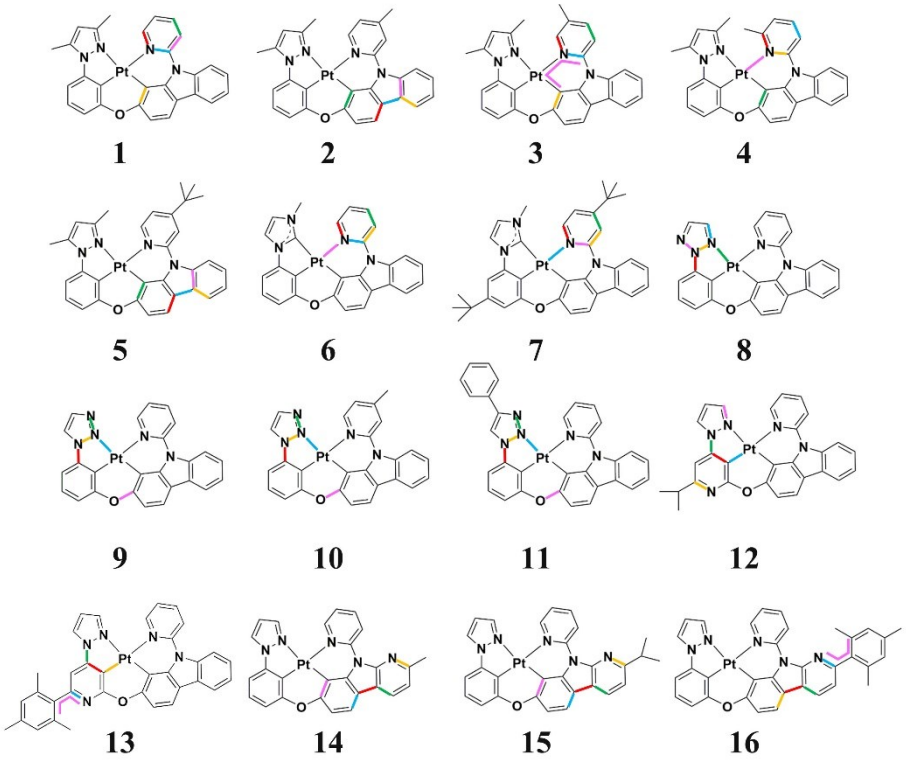

Figure S3. The internal coordinates (bond length, bond angle, and dihedral angle) with the first five largest contributions to the total reorganization energies of $^3ES \rightarrow S_0$ excitations for 16 Pt(Ⅱ) complexes. The colors are sorted by contributions: red > green > blue > yellow > pink.

Table S2. The main orbital transitions of $^3ES \rightarrow S_0$, as well as the calculated proportion of atom Pt in relevant orbitals for complexes **10** ~ **13**. (H = HOMO, L = LUMO)

Complexes	Excitations	Orbitals	Pt %
10	H→L (80.68%)	H-2	26.35%
	H-2→L (4.04%)	H	12.07%
11	H→L (74.89%)	H-2	15.59%
	H-2→L (11.47%)	H	12.40%
12	H→L (55.97%)	H-2	12.92%
	H-2→L (20.27%)	H	17.95%
13	H→L (61.27%)	H-2	6.45%
	H-2→L (11.85%)	H	17.54%

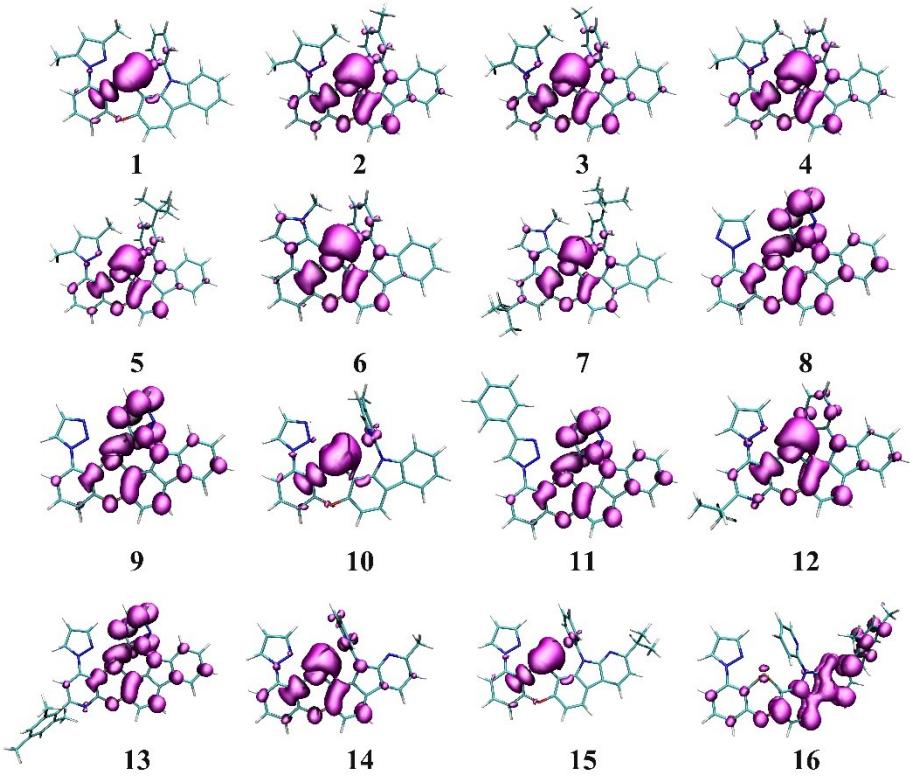

Figure S4. Spin densities of ^{3}MC states for 16 Pt(Ⅱ) complexes by rotating pyridine ring in **L1** part. (isovalue = 0.002)

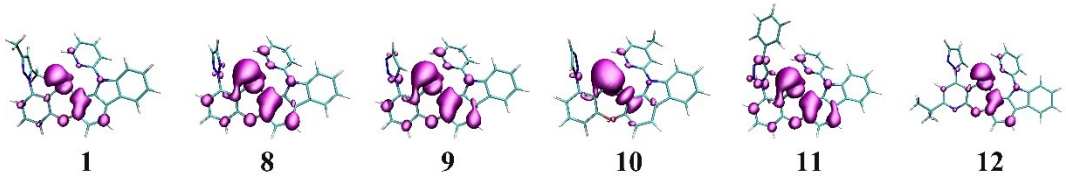

Figure S5. Spin densities of ^{3}MC' states for complexes **1**, **8**~**12** by rotating pyrazole or triazole ring in **L3** part. (isovalue = 0.002)

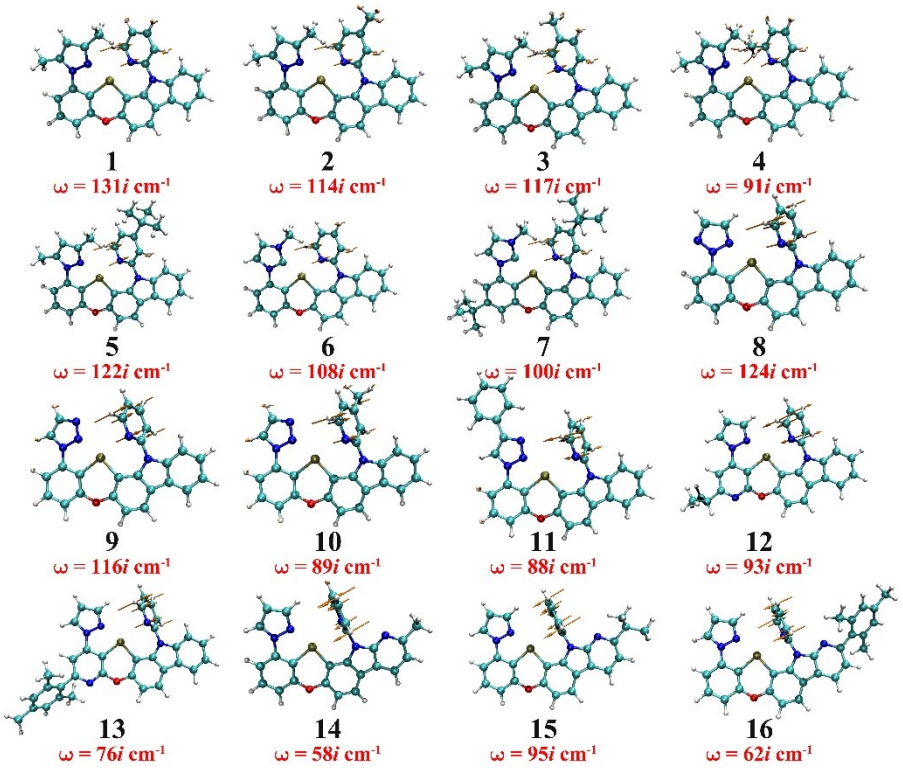

Figure S6. Displacement vectors and imaginary frequency values of ^{3}TS states for 16 Pt(Ⅱ) complexes.

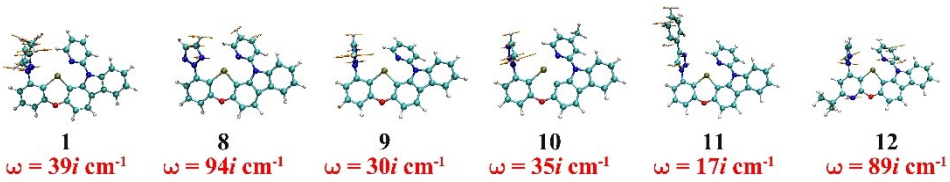

Figure S7. Spin densities of ^{3}MC' states for complexes **1**, **8**~**12** by rotating triazole ring in **L3** part.

Table S3. The calculated electronic energy barriers (E_a, E_b, and E_c), Gibbs free energy ($\Delta G_a^{\neq}$) of activation energy between ^{3}ES and ^{3}TS, and factor A_0 for 16 Pt(Ⅱ) complexes

.

	E_a (eV)	E_b (eV)	E_c [a] (eV)	$\Delta G_a^{\neq}$ (KJ/mol)	A_0 [a]
1	0.41	0.02	0.15	35.93	6.19×10^{-3}
2	0.65	0.03	---	59.43	---
3	0.41	0.04	1.03	36.61	1.60×10^{-17}
4	0.15	0.01	0.30	11.23	1.20×10^{-5}
5	0.65	0.02	---	61.11	---
6	0.46	0.06	0.20	42.09	4.20×10^{-3}
7	0.39	0.04	0.57	37.06	1.02×10^{-9}
8	0.63	0.45	---	56.38	---
9	0.78	0.42	---	61.33	---
10	0.81	0.01	---	71.94	---
11	0.83	0.42	---	75.00	---
12	0.64	0.06	---	49.93	---
13	0.68	0.45	---	62.34	---
14	1.11	0.30	---	103.29	---
15	1.10	0.23	---	101.12	---
16	1.11	0.15	---	103.93	---

[a] "---" means there is no need to consider E_c and A_0 due to the small k_a.

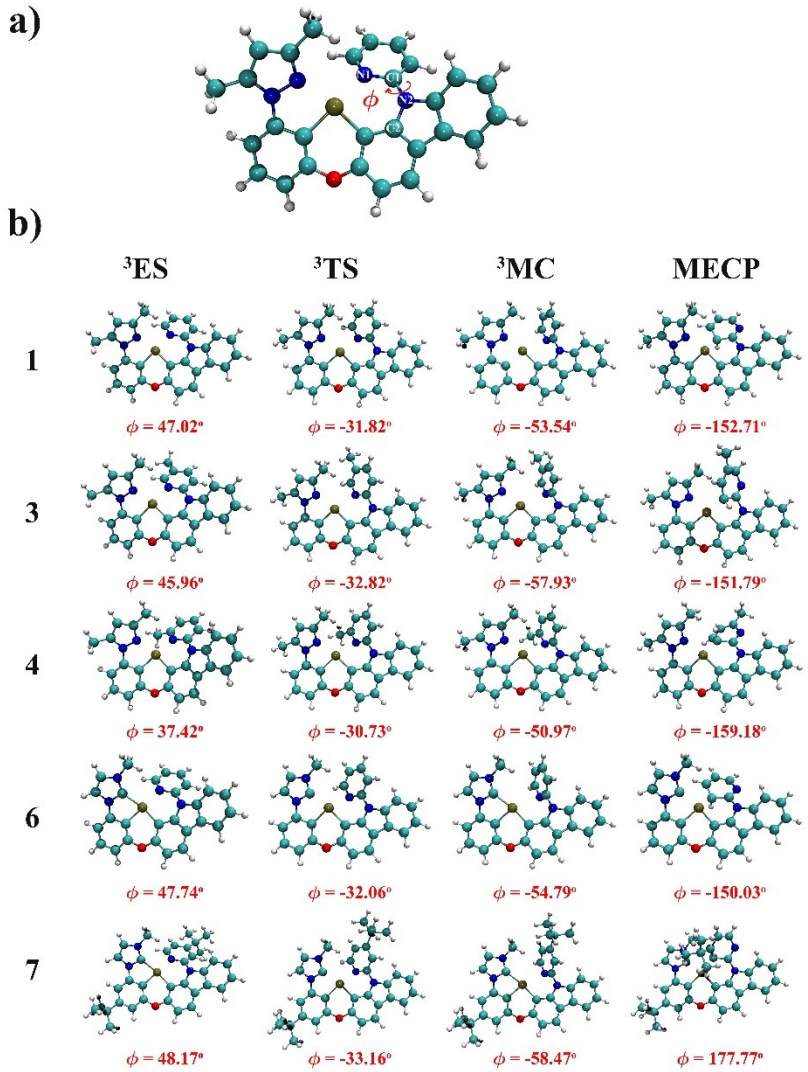

Figure S8. The schematic N1-C1-N2-C2 dihedral angle ϕ; b) structures and N1-C1-N2-C2 dihedral angles of ^{3}ES, ^{3}TS, ^{3}MC, and MECP for complexes **1**, **3**, **4**, **6** and **7**.

Table S4. Calculated Gibbs free energies ($\Delta G_a^{\neq}$) and corresponding rates between ^{3}ES and ^{3}TS' states for complexes **1**, **8**~**12**.

	$\Delta G_a^{\neq}$, (KJ/mol)	k_a, $(s^{-1}, cal.)$
1	36.18	2.85×10^6
8	48.84	1.73×10^4
9	62.81	6.15×10^1
10	62.86	6.03×10^1
11	68.69	5.74×10^0
12	67.28	1.02×10^1

Table S5. The calculated electronic energy barriers (^{E_a}', ^{E_b}', and ^{E_c}') for complex **1** when rotating its pyrazole ring. For comparison, ^{E_a}, ^{E_b}, and ^{E_c}, which are the electronic energy barriers for complex **1** when rotating its pyridine ring, are also listed.

	$\boldsymbol{E_a}$' (eV)	$\boldsymbol{E_b}$' (eV)	$\boldsymbol{E_c}$' (eV)
1	0.42	0.02	1.21
	$\boldsymbol{E_a}$ (eV)	$\boldsymbol{E_b}$ (eV)	$\boldsymbol{E_c}$ (eV)
1	0.41	0.02	0.15

Geometric coordinates of ^{3}ES, ^{3}TS, ^{3}MC, and MECP for complexes **1**, **3**, **4**, **6**, and **7**.

Complex **1**	^{3}ES			^{3}TS		
atoms	x	y	z	x	y	z
Pt	-0.64470	-0.09071	0.12702	0.68788	0.00855	-0.32608
N	-2.31011	-1.25807	-0.42051	2.49404	1.14419	-0.39913
N	-3.48260	-0.55696	-0.39125	3.57904	0.44463	0.04839
N	2.63065	-0.34720	-0.00647	-2.73122	0.40958	-0.02143
N	0.71781	-1.64974	0.51126	-0.99563	1.53965	1.06964
O	-0.70457	3.23283	0.55409	0.58619	-3.29190	0.06965
C	-3.90602	-2.45763	-1.41419	4.21643	2.54053	-0.14815
H	-4.41346	-3.25688	-1.93403	4.81281	3.44112	-0.13694
C	-3.38874	0.79676	0.01026	3.41674	-0.95829	0.18532
C	-4.49557	1.59379	0.28850	4.47232	-1.85788	0.23105
H	-5.50235	1.20114	0.25827	5.50626	-1.54368	0.18197
C	-4.29161	2.93122	0.63618	4.17427	-3.22705	0.30307
H	-5.14847	3.56212	0.84730	4.99147	-3.93947	0.35610
C	-3.01123	3.45569	0.71445	2.86910	-3.68770	0.27086
H	-2.83401	4.49514	0.96974	2.64086	-4.74828	0.30836
C	-1.92345	2.61404	0.46415	1.82654	-2.75295	0.17816
C	-2.06509	1.27385	0.12469	2.07507	-1.38542	0.17311
C	0.73942	1.26264	0.29324	-0.82500	-1.25474	-0.12904
C	0.49769	2.67624	0.33983	-0.61965	-2.65312	-0.01412
C	1.50960	3.64152	0.14410	-1.67234	-3.59428	0.00714
H	1.22987	4.68785	0.19380	-1.41066	-4.64565	0.06278
C	2.79294	3.25361	-0.16378	-2.98460	-3.18330	-0.03382
H	3.55756	3.99662	-0.36732	-3.79319	-3.90757	-0.03098
C	3.09680	1.87692	-0.21536	-3.25191	-1.80753	-0.04412
C	2.09097	0.93863	0.08116	-2.18675	-0.88833	-0.04606
C	3.93948	-0.23565	-0.43756	-4.12736	0.30813	0.00984
C	4.27241	1.14348	-0.56105	-4.47966	-1.06080	-0.02818
C	5.55149	1.51695	-0.99735	-5.82333	-1.44253	0.00028
H	5.81497	2.56587	-1.09421	-6.09477	-2.49365	-0.03543
C	6.46267	0.52523	-1.30903	-6.79852	-0.46016	0.09027
H	7.45814	0.79310	-1.64900	-7.84786	-0.73771	0.11176
C	6.11129	-0.83812	-1.20785	-6.43692	0.89207	0.17266
H	6.83885	-1.59461	-1.48549	-7.21063	1.64797	0.26763
C	4.85980	-1.23676	-0.77313	-5.10706	1.29500	0.14047
H	4.59399	-2.28558	-0.71080	-4.85702	2.34472	0.23040
C	2.08021	-1.48064	0.63977	-2.04025	1.60221	0.23091
C	2.88524	-2.30159	1.39148	-2.45773	2.79627	-0.36008
H	3.93943	-2.06363	1.47670	-3.23372	2.78970	-1.11572

C	2.34545	-3.42469	2.06439	-1.83571	3.97854	0.02367
H	2.97345	-4.08519	2.64866	-2.14883	4.92164	-0.41298
C	0.94395	-3.57227	1.99896	-0.80905	3.93332	0.96190
H	0.43749	-4.37331	2.52991	-0.31139	4.83373	1.30431
C	0.18793	-2.69375	1.27034	-0.40610	2.68739	1.42517
H	-0.89126	-2.78035	1.23591	0.43625	2.58975	2.10512
C	-2.55185	-2.41082	-1.05802	2.87182	2.41523	-0.53249
C	-4.47516	-1.26938	-0.99411	4.64263	1.27728	0.21890
C	-1.49070	-3.41243	-1.33900	1.93630	3.44206	-1.05729
H	-0.51271	-2.92944	-1.39863	1.75698	4.23009	-0.32116
H	-1.43585	-4.17576	-0.55609	2.34948	3.91241	-1.95488
H	-1.70603	-3.91662	-2.28376	0.97835	2.97826	-1.30776
C	-5.87423	-0.80793	-1.18305	5.97489	0.86535	0.73347
H	-6.41272	-0.72691	-0.23345	5.88811	0.21143	1.60562
H	-5.91613	0.16409	-1.68359	6.56497	0.34318	-0.02696
H	-6.40002	-1.53479	-1.80379	6.52979	1.75810	1.02641

Complex **1**	^{3}MC			MECP		
atoms	x	y	z	x	y	z
Pt	0.71198	0.05839	-0.18852	-0.61489	-0.00206	-0.28653
N	2.53588	1.18516	-0.34529	-2.39704	-1.11660	-0.63382
N	3.66548	0.45623	-0.10934	-3.51254	-0.46541	-0.20365
N	-2.76193	0.34970	-0.08579	2.63151	-0.47022	-0.02847
N	-1.65890	1.63124	1.53898	2.59553	-2.51060	1.05690
O	0.65598	-3.27341	0.15685	-0.53621	3.29234	0.33837
C	4.29688	2.54891	-0.38815	-4.15259	-2.46316	-0.87067
H	4.90485	3.43761	-0.47285	-4.75893	-3.32670	-1.10138
C	3.50407	-0.95040	0.07735	-3.34202	0.89529	0.15779
C	4.56253	-1.84579	0.22480	-4.39149	1.74791	0.47695
H	5.59815	-1.53813	0.21979	-5.42011	1.41788	0.49076
C	4.25639	-3.20204	0.37469	-4.09850	3.08447	0.77079
H	5.06946	-3.91139	0.49500	-4.91248	3.75722	1.02099
C	2.94743	-3.66235	0.36284	-2.80421	3.56941	0.73085
H	2.71936	-4.71863	0.46885	-2.57919	4.60985	0.94140
C	1.90725	-2.73625	0.20095	-1.75339	2.70065	0.40076
C	2.17817	-1.38838	0.07819	-2.00873	1.36018	0.12090
C	-0.81452	-1.25331	-0.01590	0.84487	1.28482	0.00986
C	-0.56524	-2.63703	0.07311	0.66835	2.66549	0.14359
C	-1.59592	-3.60373	0.07090	1.74619	3.57011	0.07033
H	-1.30429	-4.64746	0.12729	1.53047	4.63016	0.15418
C	-2.92126	-3.23770	-0.01943	3.03762	3.11379	-0.12014
H	-3.70285	-3.99116	-0.04723	3.86012	3.81788	-0.20095
C	-3.23192	-1.87628	-0.06248	3.26668	1.73483	-0.17573

C	-2.18610	-0.92638	-0.02561	2.17551	0.85986	-0.05394
C	-4.14889	0.21817	-0.14983	4.02970	-0.43309	-0.19947
C	-4.47729	-1.15604	-0.15165	4.44620	0.91441	-0.30231
C	-5.81678	-1.54609	-0.22024	5.79668	1.22157	-0.48332
H	-6.08281	-2.59954	-0.22696	6.11963	2.25621	-0.55662
C	-6.80159	-0.56690	-0.27120	6.71500	0.18345	-0.56654
H	-7.84714	-0.85499	-0.32534	7.76957	0.40407	-0.70485
C	-6.45924	0.79262	-0.24637	6.29006	-1.14863	-0.47302
H	-7.24422	1.54258	-0.27748	7.02230	-1.94827	-0.54289
C	-5.13215	1.20532	-0.18167	4.95154	-1.47724	-0.28483
H	-4.87639	2.25954	-0.15704	4.62805	-2.50387	-0.18614
C	-2.16009	1.56830	0.30441	1.92889	-1.50403	0.61365
C	-2.22069	2.66282	-0.56014	0.44855	-1.29306	0.95355
H	-2.64455	2.54387	-1.55120	0.52457	-0.76736	1.92822
C	-1.71894	3.87989	-0.11654	-0.21597	-2.61658	1.25222
H	-1.75059	4.75331	-0.76056	-1.28328	-2.73099	1.10716
C	-1.16104	3.95214	1.15634	0.54980	-3.61530	1.79540
H	-0.74887	4.87841	1.54164	0.09332	-4.53463	2.15653
C	-1.15101	2.79905	1.93682	1.95137	-3.51853	1.74824
H	-0.73009	2.81870	2.93969	2.58777	-4.32547	2.09629
C	2.90368	2.45335	-0.51750	-2.76752	-2.32178	-1.05752
C	4.75736	1.27093	-0.12839	-4.60499	-1.27692	-0.32716
C	1.89838	3.51040	-0.79724	-1.78699	-3.27758	-1.63838
H	0.92730	3.05442	-1.00656	-0.77958	-2.85673	-1.61085
H	1.78119	4.17807	0.06202	-1.78325	-4.22227	-1.08831
H	2.20304	4.11870	-1.65340	-2.04482	-3.49921	-2.67858
C	6.16325	0.84477	0.09600	-5.99595	-0.93316	0.06974
H	6.28864	0.34130	1.05919	-6.05163	-0.59416	1.10836
H	6.51787	0.17203	-0.69115	-6.42808	-0.15764	-0.57109
H	6.79954	1.73103	0.09130	-6.61394	-1.82745	-0.02637

Complex **3**	^{3}ES			^{3}TS		
atoms	x	y	z	x	y	z
Pt	-0.65020	-0.02153	-0.07765	0.69812	-0.13736	-0.31936
N	-2.30487	1.09758	0.59581	2.50088	1.00435	-0.45932
N	-3.48152	0.40813	0.51248	3.59563	0.32394	-0.00614
N	2.62908	0.18593	0.09829	-2.73773	0.24160	-0.07479
N	0.73256	1.55271	-0.29533	-1.02734	1.47863	0.94436
O	-0.74076	-3.28584	-0.83764	0.62046	-3.42008	0.18889
C	-3.88240	2.20063	1.72253	4.22196	2.41405	-0.28215
H	-4.37924	2.94690	2.32483	4.81494	3.31653	-0.31028
C	-3.40146	-0.89971	-0.02282	3.44093	-1.07402	0.17851
C	-4.51838	-1.65695	-0.36730	4.50090	-1.96767	0.23203

H	-5.52148	-1.26175	-0.28809	5.53216	-1.65097	0.15151
C	-4.32771	-2.95328	-0.84882	4.21103	-3.33517	0.35459
H	-5.19087	-3.55497	-1.11313	5.03243	-4.04217	0.41438
C	-3.05123	-3.47525	-0.99271	2.90756	-3.80129	0.36235
H	-2.88464	-4.48517	-1.35252	2.68428	-4.86083	0.43866
C	-1.95466	-2.67092	-0.67142	1.85980	-2.87347	0.25765
C	-2.08357	-1.37113	-0.19869	2.10023	-1.50537	0.20474
C	0.72147	-1.36523	-0.36921	-0.80763	-1.40251	-0.08845
C	0.46575	-2.76611	-0.55457	-0.58951	-2.79491	0.07867
C	1.46494	-3.75265	-0.44401	-1.63205	-3.74658	0.13205
H	1.17726	-4.78691	-0.59608	-1.35892	-4.79192	0.22967
C	2.75234	-3.40976	-0.08898	-2.94749	-3.35167	0.06777
H	3.50659	-4.17863	0.04633	-3.74873	-4.08355	0.09624
C	3.06988	-2.05164	0.09918	-3.22937	-1.98025	-0.00292
C	2.07581	-1.07839	-0.11386	-2.17521	-1.04811	-0.03852
C	3.93242	0.02091	0.52953	-4.13107	0.12276	-0.04287
C	4.25098	-1.36650	0.52294	-4.46628	-1.25086	-0.02355
C	5.52193	-1.79139	0.93202	-5.80534	-1.64836	0.01789
H	5.77620	-2.84702	0.93105	-6.06340	-2.70343	0.02631
C	6.43890	-0.84188	1.34543	-6.79275	-0.67565	0.06422
H	7.42868	-1.15113	1.66652	-7.83859	-0.96525	0.09553
C	6.10093	0.52784	1.37402	-6.44824	0.68380	0.08975
H	6.83181	1.24701	1.73068	-7.23193	1.43286	0.15153
C	4.85682	0.97735	0.96905	-5.12390	1.10204	0.04299
H	4.59869	2.02919	1.00784	-4.88641	2.15763	0.08827
C	2.09211	1.38551	-0.42524	-2.06939	1.46212	0.10400
C	2.90684	2.27851	-1.08015	-2.50416	2.60900	-0.56144
H	3.96067	2.04648	-1.18405	-3.27480	2.54280	-1.32006
C	0.97415	3.63537	-1.56902	-0.89018	3.88012	0.70583
C	0.21970	2.67709	-0.93921	-0.46956	2.66036	1.23192
H	-0.85981	2.77019	-0.90074	0.37403	2.62377	1.91844
C	-2.53317	2.18351	1.34659	2.87225	2.27148	-0.64107
C	-4.46261	1.06134	1.19523	4.65861	1.16505	0.11992
C	-1.46518	3.14975	1.71232	1.92808	3.27824	-1.18836
H	-0.48841	2.66090	1.71366	0.95877	2.81291	-1.38505
H	-1.41608	3.98569	1.00697	1.78424	4.10636	-0.48965
H	-1.66897	3.55989	2.70402	2.31607	3.69724	-2.12203
C	-5.86092	0.58781	1.35810	6.00030	0.77539	0.62740
H	-6.41418	0.60544	0.41376	5.92964	0.14657	1.51919
H	-5.89966	-0.43018	1.75726	6.58289	0.23482	-0.12591
H	-6.37358	1.24940	2.05778	6.55387	1.67941	0.88647
C	2.37931	3.46813	-1.63052	-0.26444	5.17392	1.12996
H	3.01629	4.18116	-2.14055	-0.01601	5.79702	0.26526

C	0.31270	4.83220	-2.18384	-0.95002	5.75204	1.75920
H	0.68265	5.75954	-1.73053	0.64933	5.00351	1.70529
H	0.53181	4.89514	-3.25603	-1.91143	3.82408	-0.24590
H	-0.77336	4.80318	-2.05939	-2.24305	4.73069	-0.74467

Complex **3**	^{3}MC			MECP		
atoms	x	y	z	x	y	z
Pt	0.72503	-0.12373	-0.28332	-0.64133	-0.07724	0.23363
N	2.46828	1.04672	-0.50046	-2.34803	1.12228	-0.25499
N	3.62554	0.39101	-0.17578	-3.52080	0.40480	-0.29111
N	-2.71426	0.15424	-0.08308	2.63675	0.16013	-0.24915
N	-1.66511	1.56649	1.46550	2.35541	2.42841	-0.68560
O	0.74152	-3.38102	0.36635	-0.72178	-3.41818	0.27713
C	4.16810	2.48917	-0.56614	-4.00571	2.43090	-0.98388
H	4.73838	3.39883	-0.68427	-4.54024	3.29229	-1.35667
C	3.51211	-0.99747	0.11454	-3.42462	-0.99216	-0.07779
C	4.59217	-1.84941	0.31627	-4.52376	-1.82966	0.08706
H	5.61864	-1.51401	0.26750	-5.53746	-1.45466	0.08337
C	4.33276	-3.20237	0.57699	-4.31463	-3.20080	0.27767
H	5.16935	-3.87338	0.74358	-5.17130	-3.85564	0.39705
C	3.04026	-3.69919	0.60932	-3.03289	-3.72100	0.32547
H	2.83890	-4.74869	0.80017	-2.84488	-4.77817	0.48018
C	1.98170	-2.81049	0.37672	-1.97326	-2.82215	0.18818
C	2.18965	-1.46398	0.14758	-2.10263	-1.46536	-0.01965
C	-0.72979	-1.39587	0.02597	0.70907	-1.40363	0.12712
C	-0.46902	-2.79725	0.20439	0.46059	-2.86748	0.22751
C	-1.48529	-3.78054	0.21475	1.50069	-3.82936	0.23858
H	-1.18296	-4.81622	0.32446	1.22747	-4.87131	0.35043
C	-2.80797	-3.43119	0.08151	2.78881	-3.43511	0.00952
H	-3.58058	-4.19399	0.06962	3.58102	-4.17608	-0.03792
C	-3.14259	-2.06996	-0.01545	3.09337	-2.05899	-0.18038
C	-2.12095	-1.10158	0.01105	2.07456	-1.09495	-0.13940
C	-4.09146	-0.00084	-0.16734	3.98861	0.01790	-0.37989
C	-4.39629	-1.38292	-0.14581	4.31970	-1.37139	-0.33846
C	-5.72964	-1.79890	-0.22953	5.66402	-1.78142	-0.42389
H	-5.97902	-2.85602	-0.22072	5.92670	-2.83420	-0.38867
C	-6.72457	-0.83692	-0.31596	6.63166	-0.81248	-0.55572
H	-7.76467	-1.14123	-0.38153	7.67598	-1.09868	-0.63243
C	-6.40542	0.53241	-0.31253	6.29101	0.56571	-0.59312
H	-7.20448	1.26529	-0.37178	7.08821	1.29649	-0.69366
C	-5.09120	0.97128	-0.23394	4.98878	1.00229	-0.51034
H	-4.85182	2.02929	-0.22658	4.71295	2.04701	-0.55893
C	-2.12570	1.40796	0.22767	1.92937	1.42682	-0.06551

C	-2.19538	2.44269	-0.70658	0.81073	1.28559	0.94906
H	-2.59111	2.25251	-1.69820	1.29704	0.75667	1.78758
C	-1.20390	3.88304	0.94963	1.03452	3.80338	0.88058
C	-1.19149	2.76995	1.79263	1.75162	3.72206	-0.39335
H	-0.79345	2.86533	2.80173	2.43912	4.53900	-0.61228
C	2.78896	2.32056	-0.74175	-2.63716	2.35248	-0.69923
C	4.67622	1.25299	-0.20415	-4.54402	1.18641	-0.72766
C	1.75681	3.31132	-1.13768	-1.63900	3.43067	-0.89955
H	0.78601	2.81881	-1.23060	-1.68886	4.16257	-0.08865
H	1.67398	4.10515	-0.38940	-0.61709	3.05767	-0.93459
H	2.01568	3.77950	-2.09207	-1.86831	3.95090	-1.83402
C	6.08625	0.90874	0.11360	-5.95459	0.75686	-0.92134
H	6.17925	0.44422	1.09961	-6.03328	-0.10817	-1.58648
H	6.51859	0.22959	-0.62797	-6.44294	0.50945	0.02635
H	6.67754	1.82551	0.11212	-6.50644	1.58208	-1.37379
C	-1.73760	3.69531	-0.32936	0.52902	2.70660	1.46958
H	-1.77664	4.52368	-1.03179	-0.05831	2.79188	2.38257
C	-0.69228	5.21495	1.40777	0.77828	5.18031	1.43097
H	0.01734	5.63609	0.68865	0.23332	5.79987	0.70587
H	-1.51108	5.93520	1.51213	0.19285	5.14936	2.35581
H	-0.19027	5.13517	2.37501	1.71659	5.71021	1.64196

Complex **4**	^{3}ES			^{3}TS		
atoms	x	y	z	x	y	z
Pt	0.62977	-0.04511	-0.24864	-0.66231	0.07566	-0.35376
N	2.19805	-1.17090	0.56440	-2.48238	-1.03730	-0.52713
N	3.35003	-0.45886	0.73149	-3.56742	-0.34296	-0.07448
N	-2.57882	-0.26454	0.07739	2.74724	-0.36192	-0.11306
N	-0.75976	-1.55659	-0.74549	0.99759	-1.52990	0.91692
O	0.75562	3.22837	-0.89948	-0.53679	3.35895	0.18386
C	3.62481	-2.37333	1.78123	-4.22477	-2.42227	-0.35994
H	4.05317	-3.17570	2.36364	-4.83039	-3.31617	-0.39162
C	3.32313	0.87782	0.26900	-3.39221	1.05171	0.11763
C	4.45779	1.67812	0.15098	-4.43961	1.96153	0.14205
H	5.44454	1.30826	0.39238	-5.47275	1.65998	0.03190
C	4.30886	2.98344	-0.31820	-4.13116	3.32367	0.27124
H	5.18424	3.61745	-0.41220	-4.94194	4.04435	0.30920
C	3.05899	3.47763	-0.66518	-2.82052	3.76907	0.30846
H	2.92706	4.49397	-1.02123	-2.58303	4.82539	0.38674
C	1.94780	2.63938	-0.55179	-1.78327	2.82728	0.22934
C	2.04077	1.32648	-0.10701	-2.04537	1.46162	0.17844
C	-0.72340	1.30768	-0.51526	0.86018	1.32485	-0.11085
C	-0.46671	2.70992	-0.67384	0.66633	2.71434	0.07306

C	-1.47475	3.68666	-0.57324	1.72674	3.64379	0.14311
H	-1.20003	4.72426	-0.72709	1.47460	4.69319	0.25410
C	-2.74886	3.33300	-0.17828	3.03585	3.22434	0.07550
H	-3.50278	4.09725	-0.01761	3.85061	3.94060	0.11497
C	-3.04705	1.97342	0.04685	3.29056	1.84976	-0.01324
C	-2.06406	1.00361	-0.21539	2.21664	0.94178	-0.06167
C	-3.83067	-0.08872	0.65129	4.14559	-0.27490	-0.07736
C	-4.17168	1.29340	0.60731	4.51080	1.09083	-0.04160
C	-5.39566	1.72940	1.13260	5.85731	1.45933	0.00720
H	-5.66303	2.78129	1.10149	6.13687	2.50876	0.02784
C	-6.24329	0.79881	1.70494	6.82481	0.46591	0.04624
H	-7.19454	1.11731	2.11976	7.87636	0.73336	0.08323
C	-5.87558	-0.56039	1.78443	6.45132	-0.88512	0.05793
H	-6.54090	-1.26296	2.27656	7.21803	-1.65193	0.11510
C	-4.67791	-1.02026	1.26463	5.11789	-1.27452	0.00276
H	-4.39518	-2.06188	1.35757	4.85993	-2.32534	0.03870
C	-2.11669	-1.46758	-0.51425	2.04761	-1.56082	0.08149
C	-3.01679	-2.43511	-0.89657	2.46824	-2.72984	-0.55100
H	-4.07539	-2.26712	-0.74835	3.24337	-2.69796	-1.30629
C	-0.35354	-2.60832	-1.57673	0.41085	-2.68631	1.26950
C	2.34771	-2.33625	1.20709	-2.87111	-2.29902	-0.71254
C	4.23974	-1.17035	1.47734	-4.64416	-1.16805	0.04419
C	1.26703	-3.35438	1.25270	-1.92942	-3.32122	-1.23485
H	0.28724	-2.87054	1.25868	-0.97831	-2.85044	-1.49856
H	1.29568	-4.01240	0.37739	-1.73297	-4.09679	-0.48923
H	1.37587	-3.97419	2.14490	-2.34454	-3.80953	-2.12145
C	5.58384	-0.69566	1.89452	-5.98101	-0.75725	0.54757
H	6.27081	-0.60961	1.04652	-5.90235	-0.11978	1.43250
H	5.53343	0.27702	2.39293	-6.55675	-0.21722	-0.21139
H	6.00742	-1.41715	2.59464	-6.54590	-1.65155	0.81579
C	-2.56599	-3.60662	-1.53928	1.85060	-3.92344	-0.19505
H	-3.25763	-4.38620	-1.83372	2.16386	-4.85465	-0.65673
C	-1.21072	-3.62779	-1.91802	0.83929	-3.91174	0.75716
H	-0.82550	-4.43118	-2.54009	0.36514	-4.83136	1.08308
C	1.02752	-2.55609	-2.14847	-0.73962	-2.59158	2.22270
H	1.18653	-1.61097	-2.68638	-0.52565	-1.86224	3.00771
H	1.81634	-2.61642	-1.39296	-1.63920	-2.25190	1.69741
H	1.17107	-3.38024	-2.85184	-0.95610	-3.56001	2.67873

Complex **4**	^{3}MC			MECP		
atoms	x	y	z	x	y	z
Pt	0.70312	-0.08009	-0.38615	0.72834	-0.11252	-0.44211
N	2.47301	1.05511	-0.57324	2.47024	1.09021	-0.72606

N	3.60591	0.38870	-0.19150	3.57099	0.53839	-0.14198
N	-2.72951	0.29539	-0.11438	-2.63557	0.19056	-0.11637
N	-1.46453	1.61727	1.34076	-2.64974	2.40616	0.57867
O	0.64220	-3.32724	0.29625	0.78359	-3.34922	0.39884
C	4.18991	2.47816	-0.56682	4.14364	2.56051	-0.78601
H	4.77538	3.38064	-0.66400	4.70942	3.46126	-0.97354
C	3.46164	-0.99630	0.09946	3.45199	-0.80977	0.27315
C	4.52260	-1.87015	0.30728	4.53148	-1.59117	0.66648
H	5.55587	-1.55474	0.26484	5.53898	-1.20442	0.70598
C	4.23339	-3.21857	0.56021	4.30076	-2.93157	0.99354
H	5.05437	-3.90698	0.73342	5.13797	-3.54823	1.30515
C	2.93093	-3.69018	0.57355	3.03916	-3.49000	0.90517
H	2.70713	-4.73633	0.75773	2.86207	-4.53578	1.13410
C	1.89240	-2.78071	0.33079	1.95825	-2.69005	0.50513
C	2.12957	-1.43652	0.11431	2.14740	-1.34491	0.19824
C	-0.78320	-1.31014	-0.05096	-0.70110	-1.42612	-0.03676
C	-0.55599	-2.71460	0.14249	-0.45319	-2.78577	0.19106
C	-1.59665	-3.67127	0.17736	-1.46944	-3.76027	0.22578
H	-1.31955	-4.71359	0.29112	-1.17903	-4.79310	0.38888
C	-2.91195	-3.28766	0.06857	-2.79174	-3.40333	0.05638
H	-3.70501	-4.02916	0.07740	-3.57272	-4.15751	0.06556
C	-3.21144	-1.91808	-0.02621	-3.10070	-2.04794	-0.08296
C	-2.16547	-0.97669	-0.02910	-2.06548	-1.09400	-0.07750
C	-4.11359	0.17441	-0.16393	-4.03199	0.04669	-0.20267
C	-4.45025	-1.19988	-0.12846	-4.34598	-1.32988	-0.20403
C	-5.79389	-1.58691	-0.17205	-5.67161	-1.74938	-0.32133
H	-6.06507	-2.63848	-0.15182	-5.91413	-2.80841	-0.33091
C	-6.77014	-0.60412	-0.23210	-6.67157	-0.79074	-0.43277
H	-7.81811	-0.88563	-0.26667	-7.70869	-1.09892	-0.52762
C	-6.42026	0.75714	-0.23923	-6.34969	0.57207	-0.42546
H	-7.20372	1.50817	-0.27460	-7.14341	1.30935	-0.51130
C	-5.09469	1.16710	-0.20039	-5.03371	1.01225	-0.30954
H	-4.83511	2.22004	-0.19821	-4.78486	2.06371	-0.28789
C	-2.09074	1.52797	0.17046	-1.96302	1.35051	0.25634
C	-2.24761	2.59463	-0.71477	-0.46004	1.46800	0.22574
H	-2.76477	2.45277	-1.65684	-0.29655	2.22414	-0.57186
C	-0.89778	2.78482	1.66915	-1.99735	3.44925	1.19964
C	2.81829	2.32400	-0.80616	2.80490	2.31487	-1.12852
C	4.66654	1.23852	-0.17447	4.61042	1.42301	-0.15808
C	1.81691	3.32337	-1.25740	1.84742	3.21850	-1.82141
H	0.85818	2.83236	-1.44309	1.09917	2.64914	-2.37780
H	1.66346	4.09395	-0.49633	1.32736	3.86291	-1.10440
H	2.15247	3.81919	-2.17305	2.38193	3.86486	-2.52102

C	6.05450	0.87799	0.21468	5.96438	1.18853	0.40962
H	6.08850	0.38968	1.19289	5.91836	0.82963	1.44181
H	6.52480	0.21322	-0.51696	6.53949	0.46690	-0.17996
H	6.65029	1.79035	0.26784	6.51154	2.13253	0.40291
C	-1.70461	3.81751	-0.34582	-0.02224	2.12158	1.50539
H	-1.80436	4.68003	-0.99766	0.83125	1.76341	2.07206
C	-1.01261	3.91604	0.85656	-0.75498	3.22631	1.85016
H	-0.56598	4.85490	1.16698	-0.46431	3.87780	2.67188
C	-0.12359	2.81163	2.95139	-2.78096	4.71008	1.37455
H	-0.70261	2.35539	3.75868	-2.78783	5.30982	0.45458
H	0.79541	2.22523	2.83879	-3.82626	4.48558	1.61415
H	0.14977	3.82943	3.23737	-2.36023	5.33486	2.16772

Complex **6**	^{3}ES			^{3}TS		
atoms	x	y	z	x	y	z
Pt	-0.81432	-0.15003	0.08519	0.86007	0.08350	-0.26927
N	-3.59868	-0.60795	-0.50039	3.70256	0.50646	0.05216
N	2.47428	-0.30012	0.01841	-2.57650	0.36127	-0.03649
N	0.58217	-1.66642	0.48483	-0.89567	1.49625	1.13316
O	-0.92569	3.20338	0.55241	0.79856	-3.27373	0.09770
C	-4.04649	-2.54437	-1.40833	4.36919	2.57381	-0.19515
H	-4.47971	-3.41782	-1.87011	4.90323	3.50850	-0.26488
C	-3.56073	0.75123	-0.12501	3.58097	-0.89061	0.22989
C	-4.68530	1.54340	0.02379	4.65457	-1.75464	0.33489
H	-5.68303	1.14149	-0.12010	5.68082	-1.40141	0.32459
C	-4.50797	2.88800	0.37266	4.38134	-3.12900	0.42489
H	-5.37466	3.52922	0.49365	5.20638	-3.82761	0.52216
C	-3.23661	3.40672	0.55458	3.08432	-3.61223	0.36006
H	-3.07946	4.45055	0.80529	2.87583	-4.67633	0.41220
C	-2.12396	2.56912	0.39696	2.02072	-2.70469	0.22500
C	-2.23779	1.21775	0.06845	2.23986	-1.32983	0.20174
C	0.55949	1.27045	0.32946	-0.64017	-1.26291	-0.11587
C	0.29836	2.66989	0.39049	-0.41845	-2.65723	-0.01244
C	1.29728	3.66823	0.25062	-1.45132	-3.62145	-0.02789
H	0.99313	4.70690	0.31872	-1.17140	-4.66850	0.02175
C	2.58957	3.31389	-0.04025	-2.76961	-3.23456	-0.09825
H	3.34645	4.07274	-0.21124	-3.56446	-3.97349	-0.12637
C	2.91441	1.93904	-0.12347	-3.06156	-1.86296	-0.09870
C	1.91392	0.97847	0.13078	-2.01061	-0.92844	-0.06123
C	3.78822	-0.15556	-0.38910	-3.97029	0.23896	-0.04825
C	4.10331	1.23227	-0.46814	-4.30064	-1.13524	-0.11123
C	5.38394	1.63817	-0.87491	-5.63908	-1.53595	-0.12983
H	5.63065	2.69389	-0.93680	-5.89402	-2.59035	-0.18537

C	6.31485	0.67189	-1.20354	-6.63098	-0.56862	-0.06165
H	7.31057	0.96420	-1.52186	-7.67629	-0.86138	-0.07723
C	5.98134	-0.69877	-1.14747	-6.29229	0.78794	0.04532
H	6.72369	-1.43644	-1.43685	-7.07985	1.53160	0.12164
C	4.72973	-1.12955	-0.74193	-4.96817	1.21020	0.06007
H	4.48198	-2.18433	-0.71298	-4.73617	2.26257	0.16698
C	1.94029	-1.45793	0.63327	-1.90929	1.55831	0.25699
C	2.75811	-2.28066	1.37031	-2.31788	2.75460	-0.33585
H	3.80188	-2.01000	1.48293	-3.06819	2.74856	-1.11703
C	2.25234	-3.45090	1.98200	-1.71441	3.93728	0.07454
H	2.89349	-4.10620	2.55803	-2.01787	4.88151	-0.36665
C	0.86309	-3.66758	1.85610	-0.71965	3.89207	1.04704
H	0.38161	-4.52267	2.32171	-0.23834	4.79319	1.41039
C	0.08808	-2.78408	1.15655	-0.32863	2.64568	1.51929
H	-0.98512	-2.91404	1.09213	0.48723	2.54837	2.23074
C	-4.61575	-1.37148	-1.02853	4.80754	1.32710	0.11314
H	-5.63457	-1.02891	-1.10761	5.79280	0.97450	0.37194
C	-2.40727	-1.28102	-0.52504	2.57640	1.20983	-0.29689
N	-2.70026	-2.46586	-1.10515	3.01111	2.47985	-0.43923
C	-1.73054	-3.49390	-1.43170	2.17274	3.58511	-0.85240
H	-1.92656	-3.86125	-2.44031	2.60134	4.06700	-1.73399
H	-1.78822	-4.32430	-0.72402	2.07845	4.31605	-0.04648
H	-0.73558	-3.05171	-1.39020	1.18841	3.18211	-1.09394

Complex **6**	^{3}MC			MECP		
atoms	x	y	z	x	y	z
Pt	0.87336	0.09922	-0.23587	-0.78498	-0.07955	-0.23817
N	3.72892	0.53221	-0.13451	-3.63365	-0.56277	-0.26162
N	-2.57070	0.31729	-0.02138	2.48249	-0.39037	0.00502
N	-1.47115	1.54690	1.64067	2.56816	-2.40000	1.13978
O	0.85614	-3.24678	0.22339	-0.80576	3.25947	0.39964
C	4.35400	2.60184	-0.45856	-4.26258	-2.52588	-0.98745
H	4.87511	3.53791	-0.58534	-4.78034	-3.41627	-1.30817
C	3.62849	-0.85986	0.10529	-3.52971	0.79267	0.13240
C	4.70728	-1.70006	0.30364	-4.61591	1.58791	0.44506
H	5.73077	-1.33830	0.30109	-5.62891	1.19926	0.43952
C	4.44367	-3.06587	0.50458	-4.37324	2.93112	0.76411
H	5.27408	-3.74560	0.66736	-5.20905	3.57594	1.01719
C	3.15115	-3.56284	0.48723	-3.09225	3.45248	0.74905
H	2.95075	-4.61992	0.63183	-2.90627	4.49666	0.97881
C	2.08470	-2.67382	0.27306	-1.99998	2.62506	0.42953
C	2.29424	-1.31290	0.09845	-2.20585	1.28082	0.12651
C	-0.60470	-1.24761	0.00151	0.63464	1.29504	0.07397

C	-0.35867	-2.64846	0.08710	0.41832	2.67214	0.18706
C	-1.37556	-3.63325	0.03000	1.45814	3.61648	0.07285
H	-1.07578	-4.67467	0.07670	1.20806	4.67035	0.14400
C	-2.69590	-3.27313	-0.09073	2.75893	3.20341	-0.15032
H	-3.47161	-4.02985	-0.15883	3.55180	3.93607	-0.26911
C	-3.02114	-1.90572	-0.10103	3.03607	1.83193	-0.19269
C	-1.98922	-0.95182	-0.00278	1.97944	0.92344	-0.01982
C	-3.94802	0.18231	-0.13067	3.86931	-0.30940	-0.22200
C	-4.26596	-1.19622	-0.20166	4.23584	1.05016	-0.36149
C	-5.60180	-1.59194	-0.33064	5.56383	1.39667	-0.62264
H	-5.86006	-2.64516	-0.39362	5.84785	2.43991	-0.73048
C	-6.58772	-0.61731	-0.36956	6.50864	0.38738	-0.74655
H	-7.62930	-0.90668	-0.47016	7.54543	0.63871	-0.95125
C	-6.25626	0.74520	-0.27294	6.13413	-0.95667	-0.61108
H	-7.04741	1.48872	-0.29646	6.88608	-1.73378	-0.71443
C	-4.93892	1.16511	-0.14770	4.81974	-1.32442	-0.34278
H	-4.69151	2.21843	-0.06879	4.53740	-2.35984	-0.21377
C	-1.96025	1.52382	0.40086	1.83745	-1.44939	0.66816
C	-2.01945	2.64251	-0.43334	0.34101	-1.34516	0.98882
H	-2.44371	2.55301	-1.42725	0.36116	-0.83309	1.97337
C	-1.50469	3.84035	0.04232	-0.22073	-2.72254	1.25014
H	-1.53055	4.73245	-0.57590	-1.27147	-2.91939	1.07453
C	-0.93373	3.86777	1.31287	0.59923	-3.65598	1.82938
H	-0.50539	4.77708	1.72042	0.20644	-4.60796	2.18153
C	-0.94247	2.69667	2.06501	1.98882	-3.44225	1.83252
H	-0.52275	2.68575	3.06837	2.67638	-4.18934	2.21610
C	4.82723	1.35764	-0.18426	-4.73917	-1.35207	-0.50498
H	5.83589	1.01267	-0.02493	-5.75137	-1.02886	-0.32528
C	2.56933	1.22973	-0.37343	-2.48187	-1.22018	-0.57549
N	2.98146	2.49993	-0.56799	-2.88169	-2.42226	-1.02585
C	2.09061	3.60415	-0.86053	-1.99965	-3.44524	-1.55688
H	2.37879	4.07850	-1.80121	-2.19915	-3.58987	-2.62105
H	2.12262	4.33992	-0.05374	-2.15328	-4.38688	-1.02632
H	1.08164	3.19879	-0.94121	-0.96916	-3.11998	-1.41893

Complex **7**	^{3}ES			^{3}TS		
atoms	x	y	z	x	y	z
Pt	-0.47966	-0.32585	-0.27396	-0.44307	-0.28970	-0.19236
N	-2.74187	-2.01654	-0.85178	-2.58403	-2.21308	0.08185
N	2.45367	1.16891	-0.35968	2.53867	1.42809	0.05659
N	1.49682	-0.99880	-0.14720	1.74055	-0.41443	1.26510
O	-2.15900	2.43637	0.74666	-2.29503	2.53679	-0.11476
C	-2.29465	-3.78604	-2.05294	-1.97233	-4.30984	-0.01495

H	-2.29950	-4.69009	-2.64146	-1.89142	-5.38555	-0.02262
C	-3.32308	-0.87494	-0.26439	-3.27028	-0.97897	0.13577
C	-4.66317	-0.76060	0.03347	-4.64197	-0.85881	0.10470
H	-5.33841	-1.58900	-0.15587	-5.27646	-1.73940	0.07886
C	-5.15771	0.43971	0.59021	-5.22240	0.43081	0.07100
C	-4.26268	1.47474	0.81674	-4.38719	1.53973	0.01337
H	-4.58376	2.42509	1.22598	-4.78685	2.54617	-0.03324
C	-2.90151	1.32551	0.50755	-2.99065	1.38425	0.01552
C	-2.37069	0.15172	-0.03313	-2.39487	0.13074	0.12397
C	0.05167	1.53913	0.20425	0.03292	1.67855	-0.14770
C	-0.84026	2.59869	0.50313	-0.93454	2.70849	-0.14661
C	-0.46245	3.96605	0.54425	-0.62133	4.08537	-0.20059
H	-1.22385	4.69870	0.78892	-1.44266	4.79395	-0.22658
C	0.81564	4.33909	0.21294	0.68878	4.50595	-0.21675
H	1.09750	5.38686	0.18645	0.93243	5.56238	-0.27378
C	1.75319	3.33066	-0.10200	1.69839	3.53728	-0.12726
C	1.35910	1.97828	-0.03334	1.34997	2.17525	-0.05574
C	3.50804	1.99773	-0.71250	3.62297	2.31059	0.07101
C	3.11153	3.35382	-0.54596	3.13153	3.63035	-0.06656
C	4.00627	4.38847	-0.85472	4.01697	4.71123	-0.07627
H	3.70949	5.42567	-0.72953	3.64223	5.72459	-0.18879
C	5.26418	4.06336	-1.32897	5.37481	4.46979	0.07510
H	5.97134	4.84975	-1.57358	6.07709	5.29774	0.06812
C	5.63484	2.71654	-1.51593	5.84663	3.16159	0.25556
H	6.61887	2.48721	-1.91376	6.90966	2.99086	0.39716
C	4.77342	1.67385	-1.21302	4.98568	2.07040	0.26202
H	5.06579	0.64205	-1.37153	5.37381	1.07273	0.42766
C	2.58969	-0.18005	0.04772	2.64576	0.07251	0.40043
C	3.75746	-0.59669	0.62868	3.67276	-0.70116	-0.12865
H	4.53389	0.14167	0.79245	4.30003	-0.28090	-0.90587
C	3.96682	-1.95308	1.02452	3.86037	-2.01412	0.31772
C	2.84006	-2.78317	0.85953	2.97818	-2.47775	1.29523
H	2.86096	-3.82531	1.16239	3.06886	-3.47105	1.71719
C	1.67059	-2.30272	0.32995	1.93053	-1.66204	1.70453
H	0.79560	-2.93513	0.25456	1.18812	-2.02917	2.40861
C	-3.31517	-3.10445	-1.47318	-3.04947	-3.50687	0.17417
H	-4.37549	-3.29728	-1.47168	-4.08066	-3.75112	0.37107
C	-1.38237	-2.00894	-1.01570	-1.23482	-2.18374	-0.17130
N	-1.12793	-3.09807	-1.77390	-0.88048	-3.48601	-0.22259
C	0.17555	-3.46234	-2.29589	0.45592	-3.95366	-0.52316
H	0.07346	-3.73991	-3.34630	0.42356	-4.65759	-1.35780
H	0.60040	-4.29976	-1.73747	0.89824	-4.44137	0.34839
H	0.83391	-2.59862	-2.20805	1.05732	-3.08550	-0.79604

C	5.29216	-2.38151	1.62378	4.97593	-2.86536	-0.27513
C	5.30973	-3.87838	1.93764	5.03398	-4.25493	0.36039
H	5.13803	-4.47839	1.03754	5.22515	-4.20124	1.43705
H	6.28380	-4.16191	2.34967	4.10498	-4.81214	0.20050
H	4.54596	-4.14350	2.67630	5.84705	-4.82909	-0.09367
C	6.43111	-2.07994	0.63464	4.72539	-3.02424	-1.78312
H	6.47780	-1.01374	0.38945	4.71106	-2.05860	-2.29669
H	7.40007	-2.36607	1.06055	5.51882	-3.63188	-2.23071
H	6.28950	-2.63378	-0.29936	3.76728	-3.52059	-1.96890
C	5.55048	-1.60810	2.92877	6.32305	-2.16234	-0.04788
H	5.56566	-0.52702	2.75693	7.13435	-2.76816	-0.46436
H	4.76788	-1.82015	3.66458	6.35785	-1.18243	-0.53345
H	6.51683	-1.89113	3.36298	6.51571	-2.02079	1.02033
C	-6.64571	0.55322	0.90976	-6.74443	0.55317	0.06656
C	-7.02752	-0.53417	1.92621	-7.30585	-0.11410	1.33190
H	-8.09495	-0.46845	2.16291	-8.39880	-0.04215	1.34119
H	-6.83273	-1.53928	1.54035	-7.04005	-1.17400	1.38553
H	-6.46232	-0.41344	2.85584	-6.92277	0.37610	2.23260
C	-7.45606	0.35526	-0.38087	-7.30599	-0.15330	-1.17749
H	-7.27374	-0.62549	-0.83031	-8.39852	-0.07528	-1.19192
H	-8.52759	0.43032	-0.16665	-6.91780	0.30478	-2.09276
H	-7.20052	1.11952	-1.12175	-7.04699	-1.21605	-1.19556
C	-7.00550	1.91639	1.50206	-7.20940	2.00998	0.04357
H	-6.47250	2.10380	2.43980	-6.85118	2.56299	0.91786
H	-6.78104	2.73205	0.80709	-6.86967	2.53008	-0.85784
H	-8.07801	1.94863	1.71681	-8.30326	2.04296	0.05339

Complex **7**	^{3}MC			MECP		
atoms	x	y	z	x	y	z
Pt	0.41622	-0.30401	0.13933	-0.11144	0.31773	-0.65246
N	2.60593	-2.19516	0.02804	-2.67117	1.64830	-0.88828
N	-2.59374	1.44555	-0.14315	3.17635	-0.51884	-0.32997
N	-2.29348	-0.15597	-1.83157	3.91928	1.68154	-0.37284
O	2.23745	2.53982	0.15291	-1.21135	-2.76036	0.26439
C	2.00367	-4.29633	0.02668	-2.60936	3.73456	-1.52452
H	1.93287	-5.37267	0.01090	-2.80122	4.75376	-1.82117
C	3.28040	-0.95147	0.00557	-3.01119	0.34493	-0.45940
C	4.64909	-0.80826	-0.02137	-4.30628	-0.06570	-0.22991
H	5.30155	-1.67571	-0.03689	-5.13438	0.62100	-0.37138
C	5.20797	0.49338	-0.01885	-4.54898	-1.39412	0.18486
C	4.35739	1.58895	0.03074	-3.46558	-2.24780	0.33152
H	4.74023	2.60285	0.04347	-3.59503	-3.27968	0.63695
C	2.96412	1.40271	0.06744	-2.15053	-1.80745	0.09301

C	2.38911	0.14122	0.03783	-1.89166	-0.50546	-0.31761
C	-0.08939	1.65453	0.06958	0.81700	-1.40883	-0.15879
C	0.88102	2.69167	0.15812	0.14951	-2.60995	0.12709
C	0.56764	4.06843	0.27796	0.80015	-3.84727	0.30915
H	1.39152	4.76902	0.36211	0.18931	-4.72064	0.51394
C	-0.73794	4.49160	0.29392	2.17242	-3.93691	0.21498
H	-0.97950	5.54416	0.40667	2.67530	-4.89192	0.33389
C	-1.75195	3.53214	0.14220	2.89634	-2.76564	-0.02124
C	-1.40658	2.17152	-0.00644	2.21705	-1.54180	-0.16419
C	-3.67107	2.31777	-0.08560	4.45568	-1.11296	-0.34554
C	-3.18356	3.63238	0.10743	4.30649	-2.50369	-0.15467
C	-4.08514	4.69783	0.20668	5.42443	-3.33785	-0.12435
H	-3.72482	5.71112	0.36020	5.30699	-4.40774	0.02312
C	-5.44317	4.43802	0.09796	6.68534	-2.77676	-0.28549
H	-6.15677	5.25291	0.17265	7.56726	-3.41049	-0.26664
C	-5.90917	3.12921	-0.11568	6.82399	-1.39679	-0.47411
H	-6.97681	2.95226	-0.20667	7.81565	-0.97157	-0.60135
C	-5.03619	2.05417	-0.21477	5.72157	-0.54637	-0.50726
H	-5.40352	1.04754	-0.38521	5.82934	0.51882	-0.65283
C	-2.74432	0.11479	-0.60584	2.92371	0.83683	-0.24028
C	-3.46771	-0.78116	0.17521	1.56193	1.43375	-0.01914
H	-3.80696	-0.45946	1.15382	1.49769	2.14214	-0.86947
C	-3.73472	-2.06314	-0.31025	1.66040	2.34549	1.19647
C	-3.21344	-2.36654	-1.57089	2.71813	3.22089	1.06546
H	-3.35751	-3.34104	-2.02207	2.88093	4.04294	1.75624
C	-2.50850	-1.39398	-2.27576	3.72580	2.93855	0.11011
H	-2.11476	-1.62142	-3.26410	4.52132	3.65071	-0.09170
C	3.08907	-3.48150	-0.03192	-3.45851	2.75290	-1.13501
H	4.13764	-3.71767	-0.11309	-4.53077	2.75656	-1.02773
C	1.23578	-2.17914	0.12595	-1.35222	1.91702	-1.10592
N	0.89054	-3.48405	0.12061	-1.33047	3.20383	-1.50424
C	-0.47423	-3.95840	0.20707	-0.13519	3.96056	-1.83355
H	-0.58914	-4.61712	1.07104	0.43155	4.19525	-0.92891
H	-0.74736	-4.49763	-0.70305	-0.43232	4.88871	-2.32162
H	-1.11574	-3.08335	0.31529	0.48880	3.38683	-2.52007
C	-4.57284	-3.03569	0.51197	0.79556	2.24810	2.44528
C	-4.64135	-4.42042	-0.13335	1.27142	3.23216	3.52103
H	-5.11470	-4.38735	-1.11970	2.31793	3.06256	3.79261
H	-3.64709	-4.86682	-0.24236	1.16455	4.27268	3.19561
H	-5.23775	-5.08672	0.49706	0.66469	3.10488	4.42383
C	-3.97968	-3.17985	1.92122	-0.68274	2.54677	2.15555
H	-3.94382	-2.22449	2.45180	-1.10588	1.81280	1.46703
H	-4.59569	-3.86530	2.51219	-1.25790	2.50955	3.08790

H	-2.96342	-3.58394	1.88462	-0.80641	3.54477	1.72018
C	-5.99703	-2.46563	0.61671	0.91762	0.82090	3.00832
H	-6.62979	-3.14298	1.19984	0.28545	0.71366	3.89772
H	-6.00212	-1.48923	1.11097	0.60308	0.07749	2.26999
H	-6.44456	-2.34729	-0.37527	1.95144	0.60281	3.29769
C	6.72740	0.63965	-0.06244	-5.98678	-1.84107	0.45118
C	7.26032	-0.02348	-1.34230	-6.81344	-1.68658	-0.83643
H	8.35085	0.06886	-1.38656	-7.84716	-2.00167	-0.65697
H	7.01334	-1.08847	-1.38322	-6.83774	-0.64992	-1.18581
H	6.83966	0.45524	-2.23233	-6.40324	-2.30500	-1.64142
C	7.33783	-0.05270	1.16625	-6.59363	-0.96072	1.55670
H	7.09507	-1.11902	1.19710	-6.60870	0.09677	1.27615
H	8.42898	0.04097	1.14583	-7.62650	-1.26743	1.75444
H	6.97221	0.40404	2.09144	-6.02577	-1.05529	2.48807
C	7.16919	2.10378	-0.05913	-6.06467	-3.30170	0.90185
H	6.78168	2.64569	-0.92785	-5.67380	-3.98398	0.13980
H	6.84263	2.62381	0.84720	-5.51239	-3.46998	1.83232
H	8.26179	2.15407	-0.09571	-7.10977	-3.57124	1.08305