Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Supporting Information

for

The cyclometalated (C^C*) platinum(II) NHC complex decorated via different carboranes to tune the photodeactivation mechanism: a theoretical investigation

Yafei Luo,[a] Zhongzhu Chen,[a] Jin Zhang,[a,b] Ying Tang,[b] Zhigang Xu,[a] and Dianyong Tang*[a,b]

[a] Yafei Luo, Zhongzhu Chen, Jin Zhang, Ying Tang, Zhigang Xu, Dianyong Tang

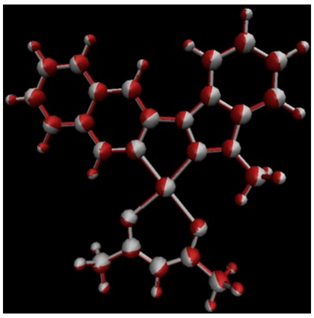
International Academy of Targeted Therapeutics and Innovation, Chongqing University of Arts and Sciences, Chongqing 402160 (P.R. China), E-mail:tangdy2008@163.com

[b] Jin Zhang, Ying Tang, Dianyong Tang

Chongqing Key Laboratory of Environmental Materials and Remediation Technologies and Research Institute for New Materials Technology, Chongqing University of Arts and Sciences, Chongqing 402160 (P.R. China)

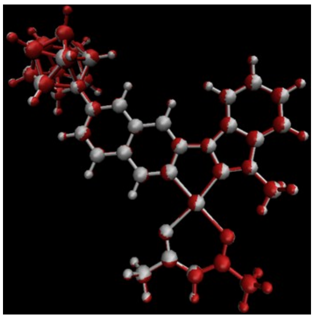
Computational details

The T_1 state geometry was obtained by performing geometry optimization along the triplet state potential energy surface (PES) using the ground state as the initial geometry. For the ^{3}MC state, the electron densities are mainly located on the central metal atom, leading to the weak chelating interaction between central metal and ligands. Therefore, the geometry optimization of ^{3}MC state was performed via unrestricted density functional theory (UDFT), starting with a distorted geometry. As for the distorted geometry, the metal-ligand bonds are largely elongated, and thus, the associated energy is expected to be far away from the global minimum along the PES. S_0, the optimization can fall into the presumably shallow local minimum associated with the ^{3}MC excited state. The reliability of obtained ^{3}MC excited state structure is confirmed by checking the spin density plots and the spin density at the Pt atom. In addition, for the transition sate, it connects the ^{3}ES and ^{3}MC states and the geometry was achieved with the help of keyword “opt=TS” beginning with the initial guess structure. The resulting transition state structure was then confirmed by the number of imaginary frequency and vibration form according to the frequency analysis. Finally, the MECP configurations, a ^{3}MC/S_0 crossing point, was obtained via using the sobMECP program, which was a modified version of Harvey’s MECP program. This calculation starts with the optimized ^{3}MC minimum geometry, in case we are interested in the MECP between ^{3}MC and S_0.



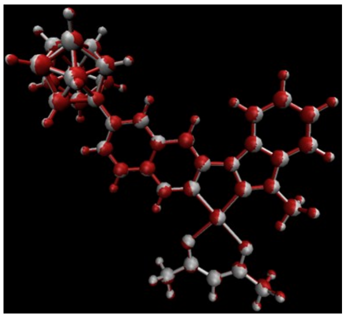
1

RMSD =0.028



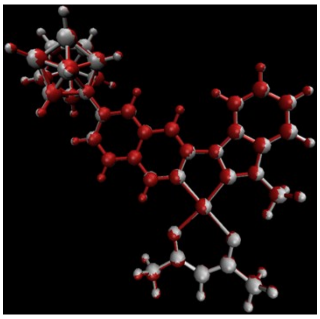
1a

RMSD =0.037



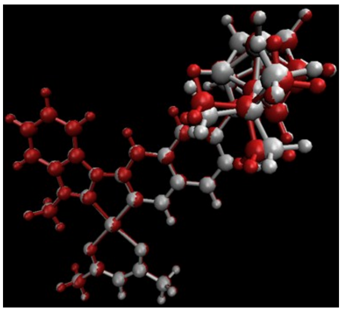
1b

RMSD =0.033



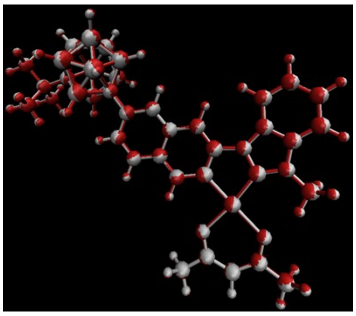
1c

RMSD =0.040



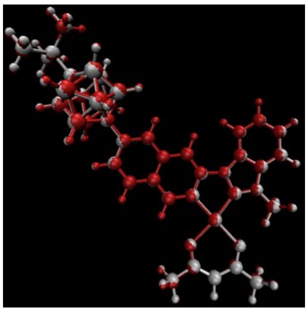
2a

RMSD =0.203



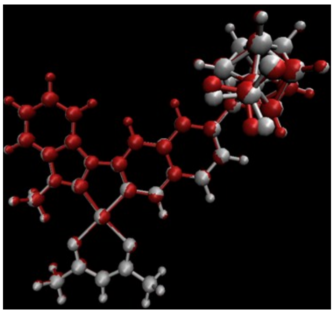
2b

RMSD =0.037



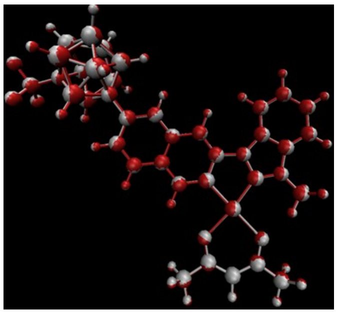
2c

RMSD =0.045



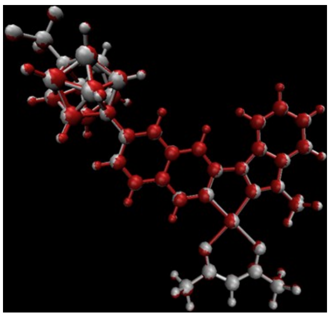
3a

RMSD =0.102



3b

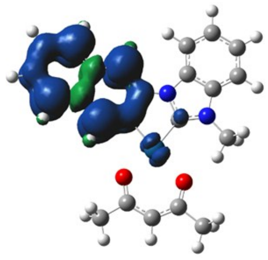
RMSD =0.034



3c

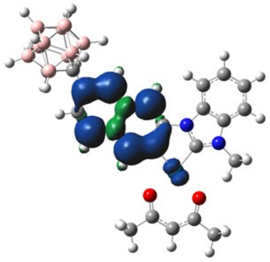
RMSD =0.039

Figure S1. The structural comparison between S_0 and T_1 states, together with the RMSD (root mean square displacement/deviation) valves. (red(S_0), white(T_1))



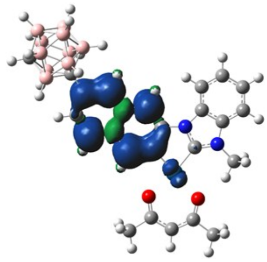
0.05

1



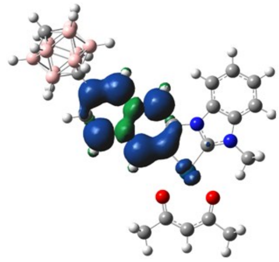
0.07

1a



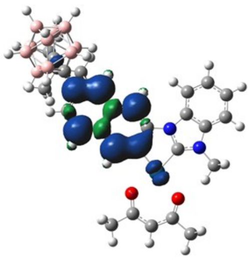
0.06

1b



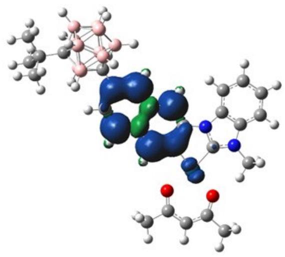
0.06

1c



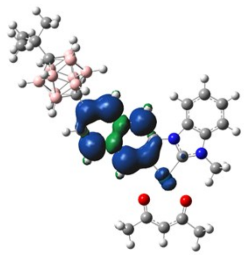
0.07

2a



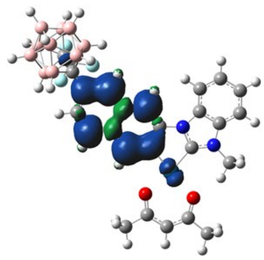
0.06

2b



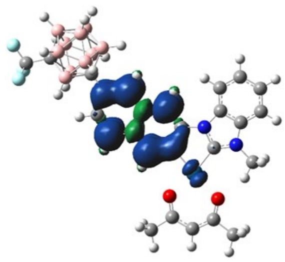
0.06

2c



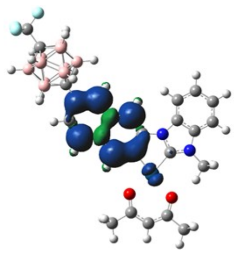
0.07

3a



0.06

3b



0.06

3c

Figure S2. Spin densities calculated on the lowest-lying triplet excited state for all investigated complexes with spin density at the Pt atom (isovalue=0.002).

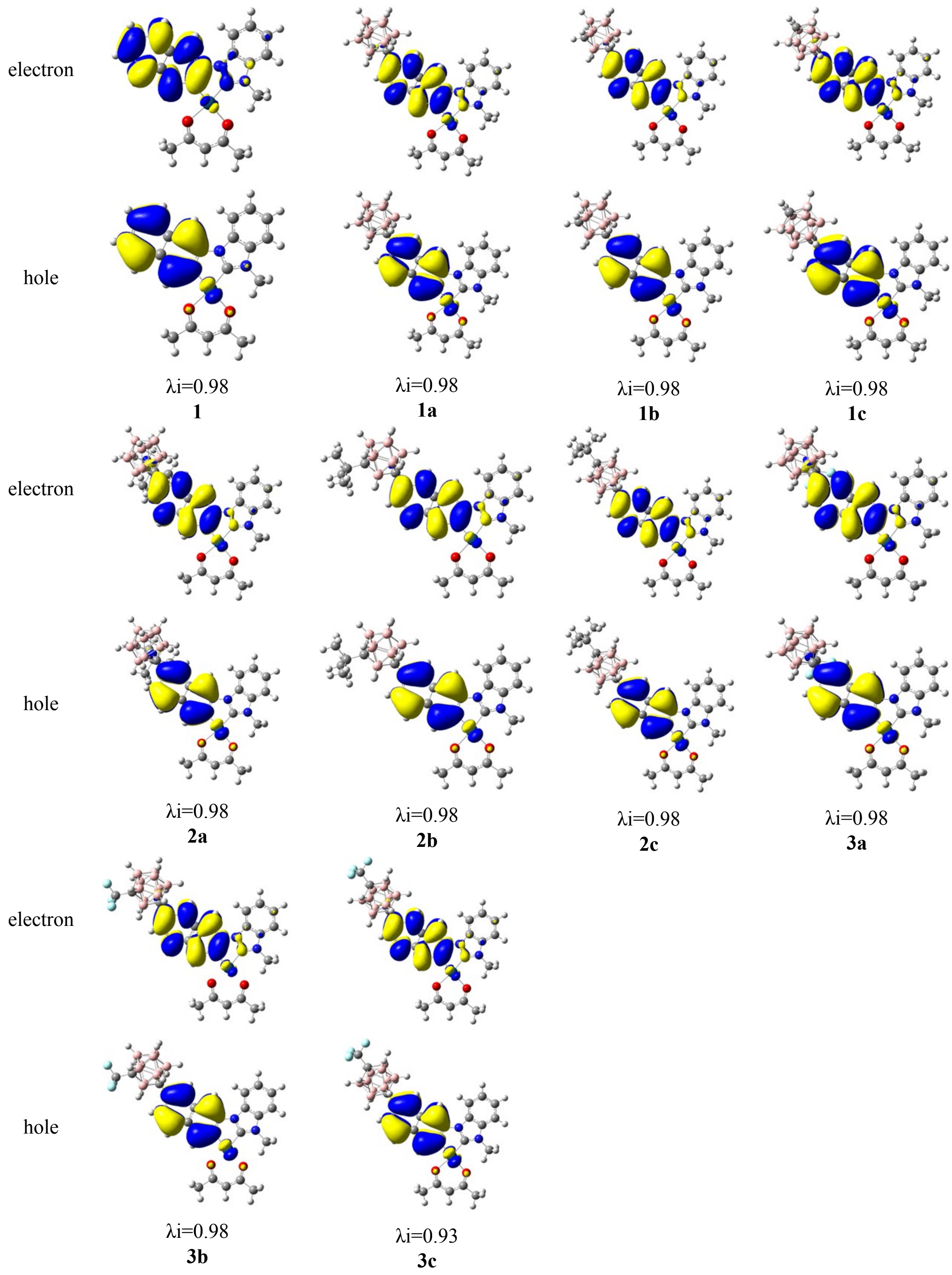
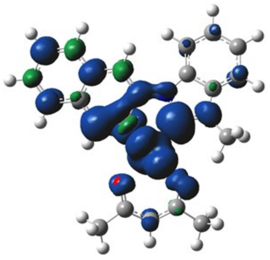
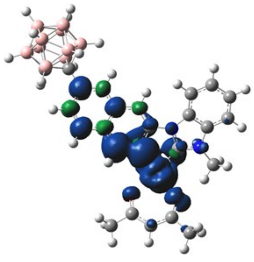


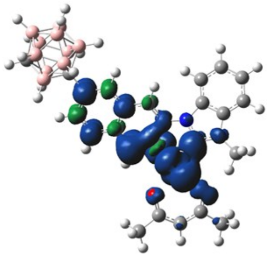
Figure S3. NTO plots of the studied complexes at the lowest-lying triplet excited states (isovalue = 0.02).



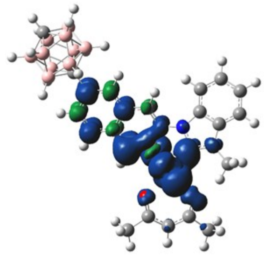
1



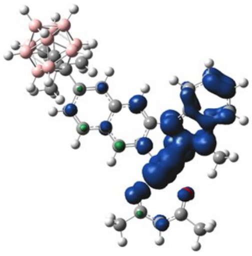
1a



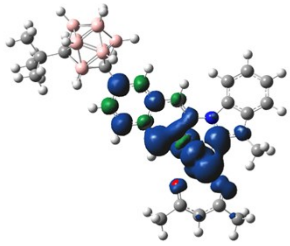
1b



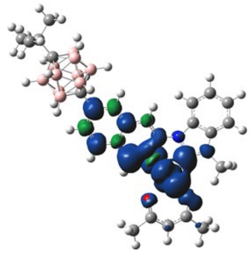
1c



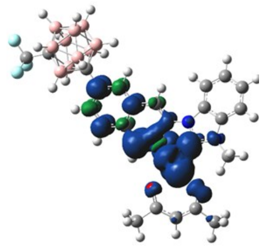
2a



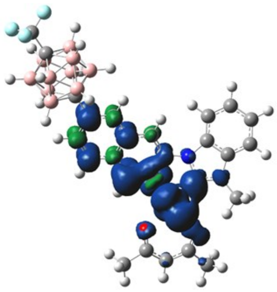
2b



2c

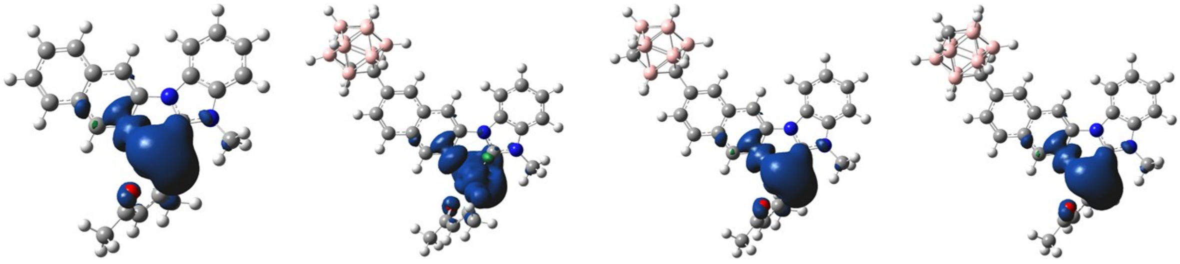


3b

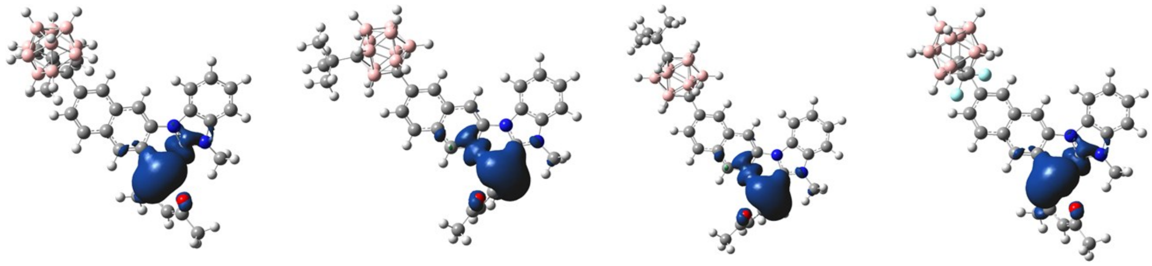


3c

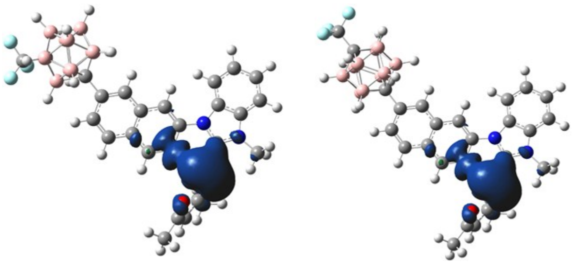
Figure S4. Spin densities calculated on the TS[^{3}ES-^{3}MC] for all investigated complexes (isovalue=0.002).



1 **1a** **1b** **1c**



2a **2b** **2c** **3a**



3b **3c**

Figure S5. Spin densities calculated on the ^{3}MC states for all investigated complexes (isovalue=0.002).

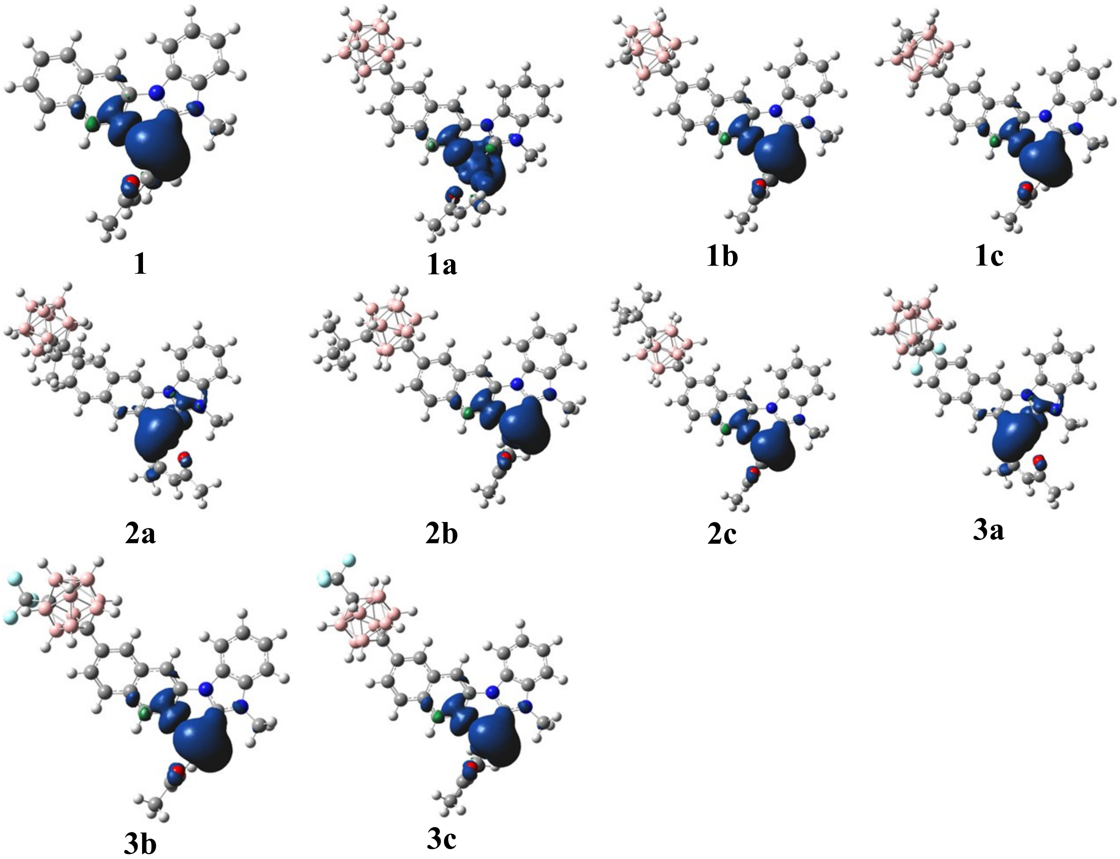


Figure S6. Spin densities calculated on the MECP[^{3}MC/S_0] for all investigated complexes (isovalue=0.002).

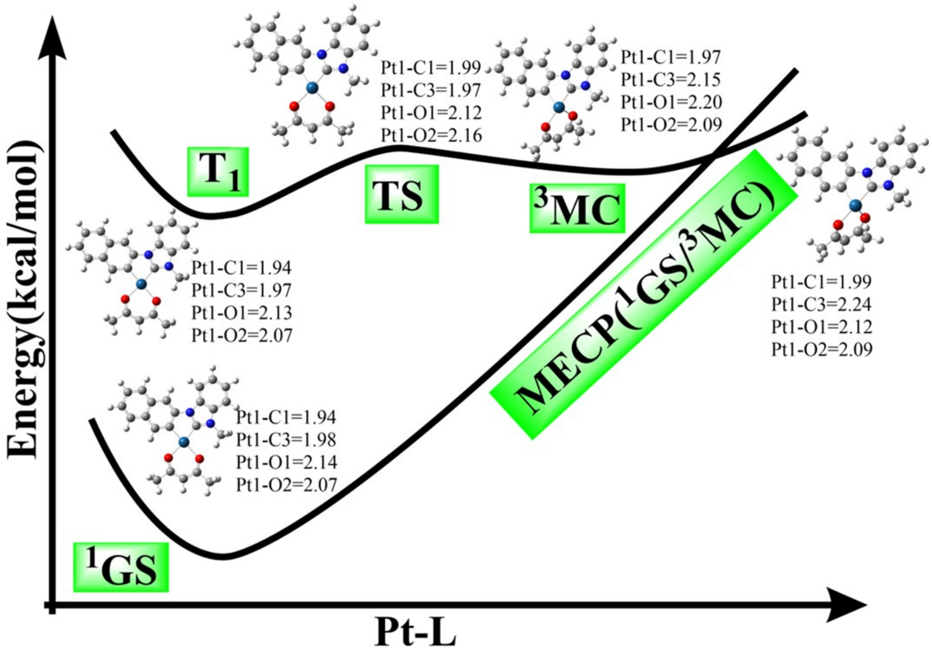


Figure S7. The potential energy surface for complex **1** with detailed geometric parameters.

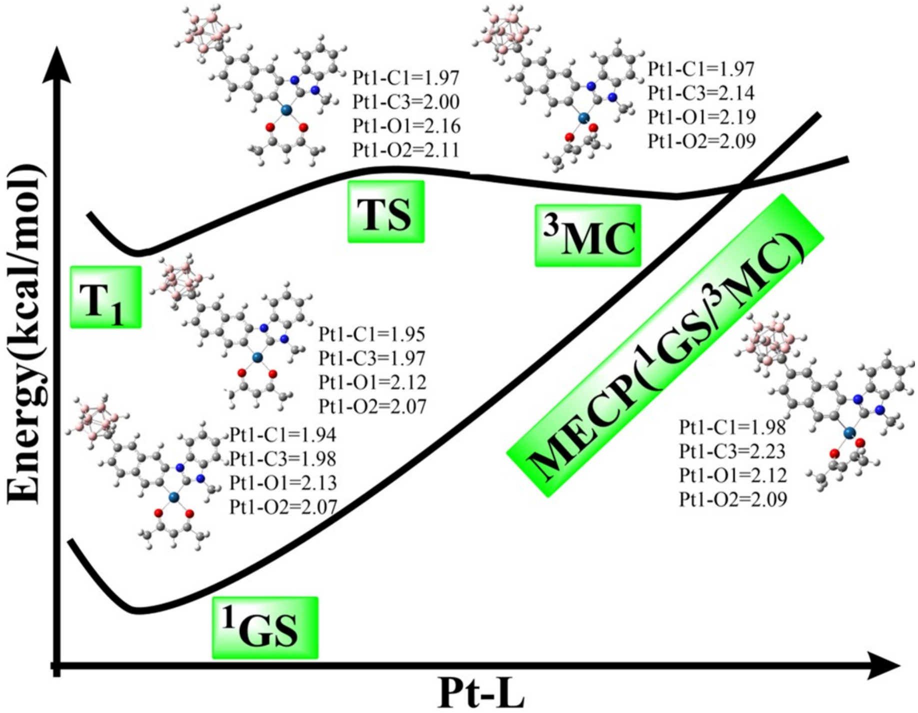


Figure S8. The potential energy surface for complex **1a** with detailed geometric parameters.

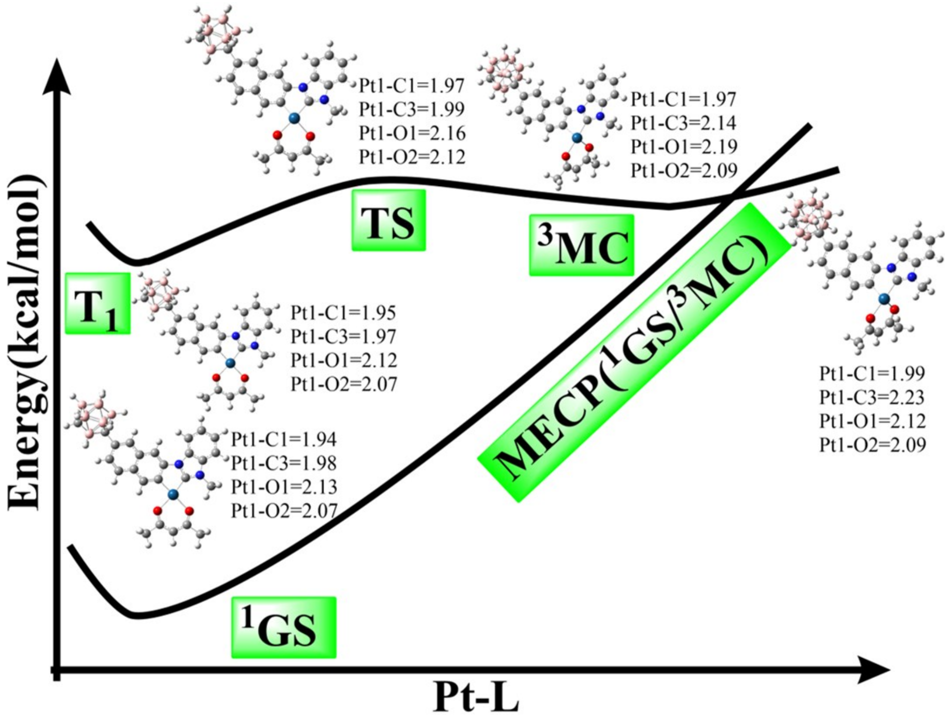


Figure S9. The potential energy surface for complex **1b** with detailed geometric parameters.

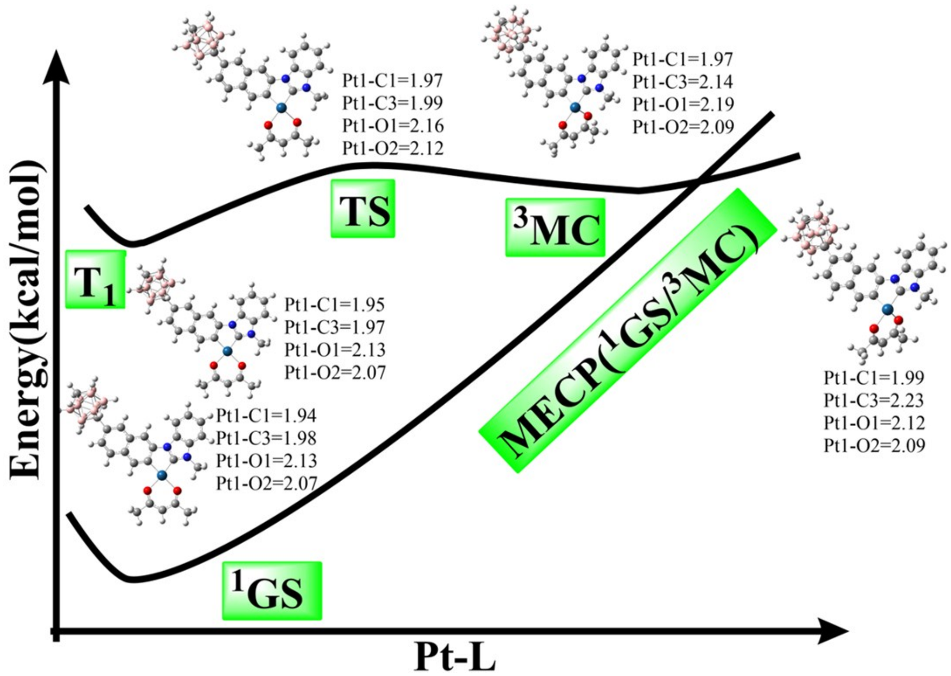


Figure S10. The potential energy surface for complex **1c** with detailed geometric parameters.

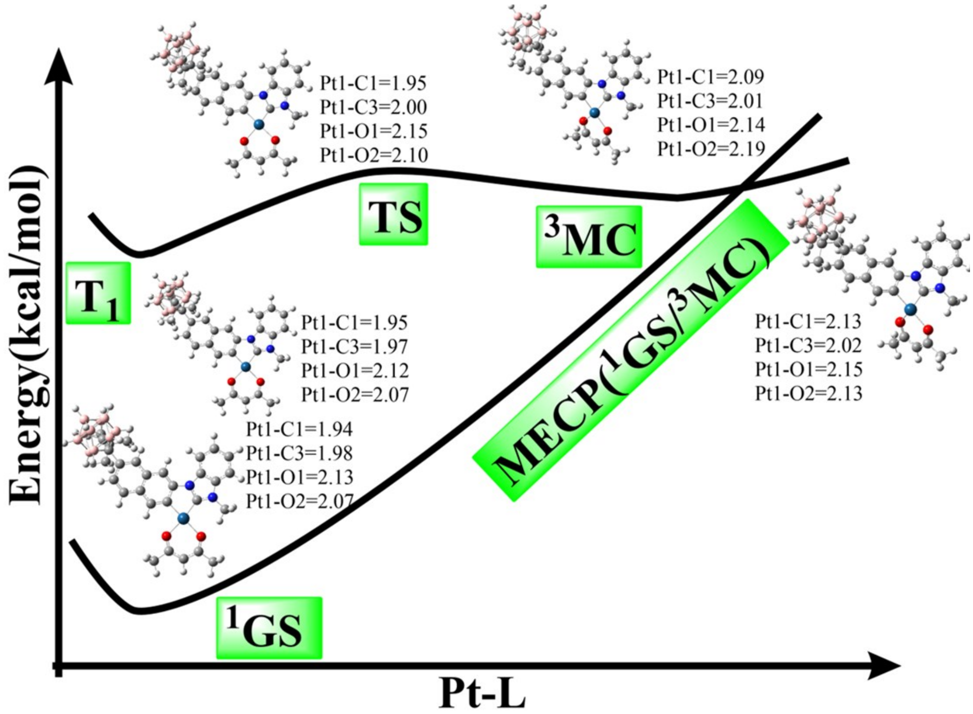


Figure S11. The potential energy surface for complex **2a** with detailed geometric parameters.

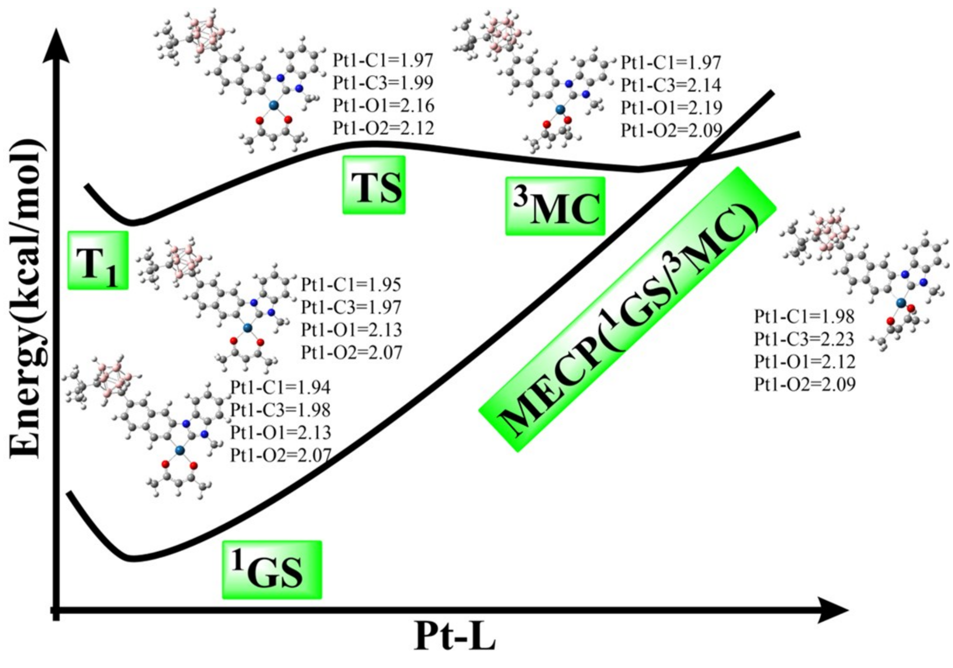


Figure S12. The potential energy surface for complex **2b** with detailed geometric parameters.

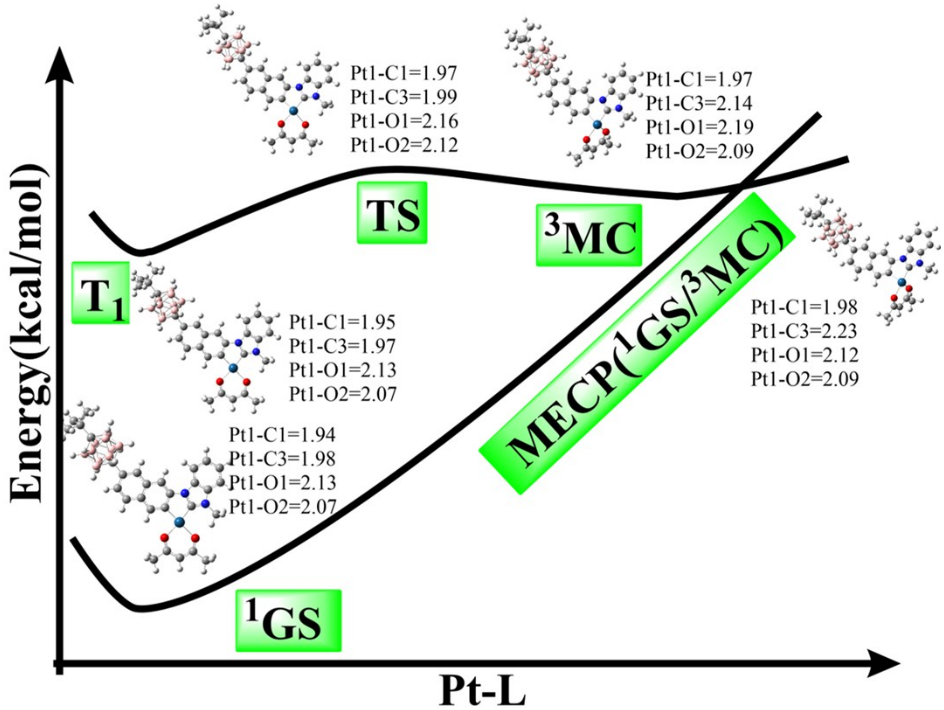


Figure S13. The potential energy surface for complex **2c** with detailed geometric parameters.

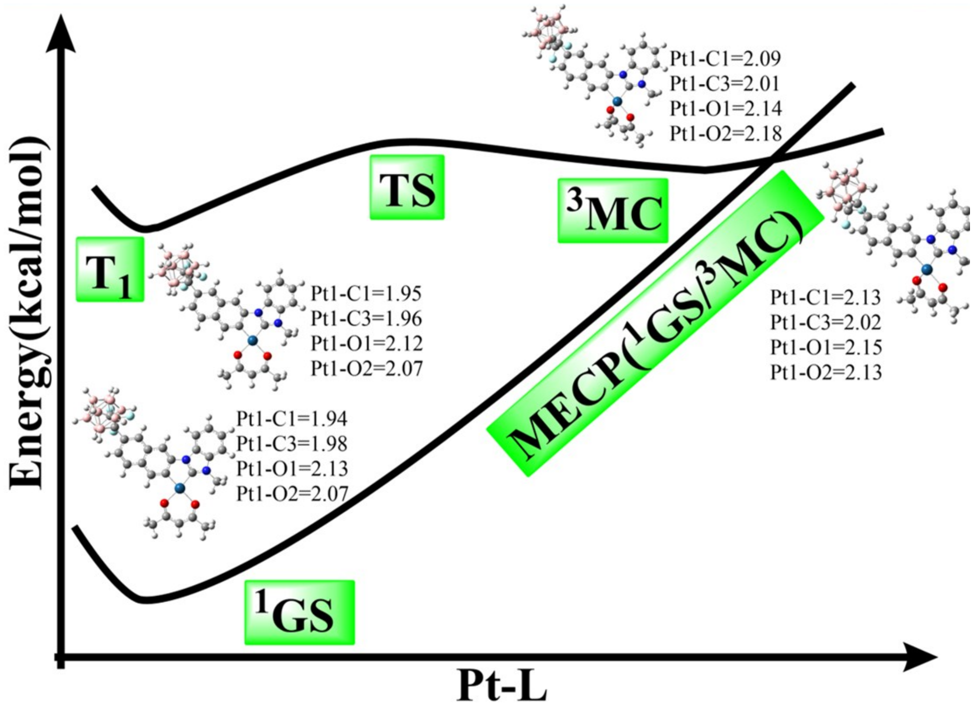


Figure S14. The potential energy surface for complex **3a** with detailed geometric parameters.

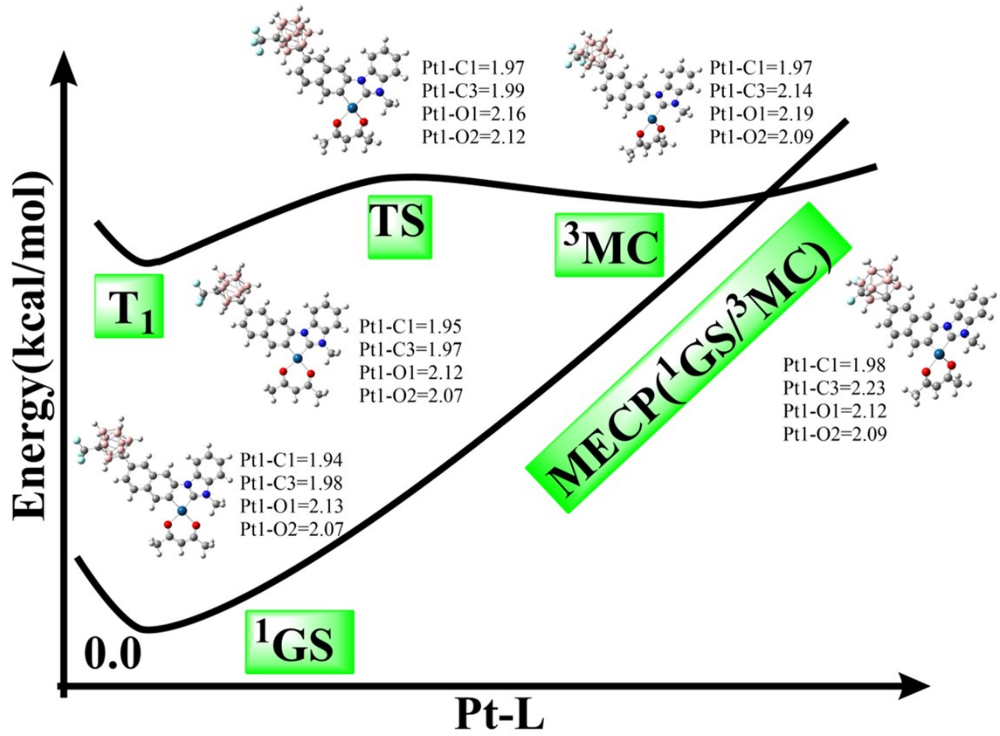


Figure S15. The potential energy surface for complex **3b** with detailed geometric parameters.

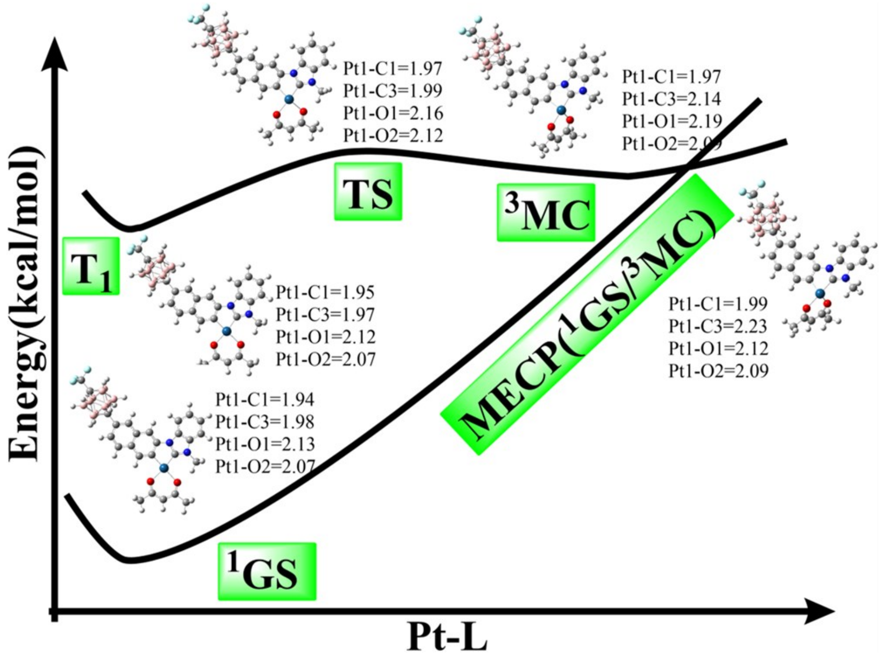


Figure S16. The potential energy surface for complex **3c** with detailed geometric parameters.

Table S1. Selected metal-related bond lengths (Å), bond angles, and dihedral angles (deg) of all investigated complexes at the ground and lowest-lying triplet states optimized geometries.

	1		**1a**		**1b**		**1c**		**2a**	
	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
Pt1-C1	1.936	1.944	1.937	1.946	1.937	1.946	1.936	1.946	1.937	1.946
Pt1-C3	1.980	1.971	1.978	1.966	1.979	1.967	1.979	1.968	1.978	1.965
Pt1-O1	2.138	2.130	2.131	2.123	2.133	2.125	2.134	2.126	2.130	2.122
Pt1-O2	2.072	2.072	2.069	2.069	2.070	2.069	2.071	2.070	2.069	2.069
O1-Pt1-O2	88.2	88.4	88.4	88.5	88.3	88.5	88.3	88.5	88.4	88.6
C1-Pt1-C3	80.2	79.7	80.3	79.7	80.3	79.7	80.3	79.7	80.3	79.7
C2-N1-C1-Pt1	0.1	0.1	-0.5	-0.5	0.2	0.2	0.3	0.3	-0.4	-0.4
N1-C1-Pt1-O1	-180.0	-179.8	179.8	179.7	-180.0	-180.0	-179.1	-179.1	179.7	-179.8
	2b		**2c**		**3a**		**3b**		**3c**	
	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
Pt1-C1	1.937	1.946	1.936	1.945	1.937	1.946	1.937	1.946	1.937	1.946
Pt1-C3	1.979	1.967	1.979	1.968	1.977	1.965	1.979	1.966	1.979	1.967
Pt1-O1	2.134	2.126	2.135	2.126	2.130	2.122	2.132	2.123	2.133	2.125
Pt1-O2	2.070	2.070	2.071	2.070	2.069	2.068	2.069	2.069	2.070	2.070
O1-Pt1-O2	88.3	88.5	88.3	88.5	88.4	88.6	88.3	88.5	88.3	88.5
C1-Pt-C3	80.3	79.7	80.3	79.7	80.3	79.6	80.3	79.7	80.3	79.7
C2-N1-C1-Pt1	0.4	0.4	0.4	0.4	-0.2	-0.3	0.5	0.4	0.4	0.3
N1-C1-Pt1-O1	179.8	179.9	-179.2	-179.1	179.9	-179.8	-179.9	-179.8	-179.6	-179.5

Table S2 MO composition of 5d(Pt) and ^{3}MLCT character in the hole–electron pairs of natural transition orbitals (NTOs) based on the T_1 optimized geometry

Complex	5d(Pt)% in hole	5d(Pt)% in electron	^{3}MLCT%
1	3.01	0.70	2.31
1a	3.80	1.09	2.71
1b	3.57	1.00	2.57
1c	3.50	0.97	2.53
2a	3.86	1.23	2.63
2b	3.50	0.95	2.55
2c	3.44	0.95	2.49
3a	3.86	1.25	2.61
3b	3.69	1.04	2.65
3c	3.63	1.01	2.62

Table S3 Transition dipole moments $\mu(S_n)$ (Debye) for S_0–S_n transitions, singlet–triplet splitting energies $\Delta E(S_n–T_1)$ (eV) and the SOC matrix elements $\langle T_1| H_{SOC}| S_n\rangle$ (cm^{-1}) of studied complexes at their respective T_1 optimized geometries.

	1			**1a**		
S_n	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|Sn\rangle$	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$
S_1	0.81	1.30	53.75	0.79	1.33	47.22
S_2	0.62	1.56	40.37	1.39	1.52	58.34
S_3	0.71	1.67	26.02	0.66	1.75	38.62
S_4	1.60	1.85	47.54	1.54	1.86	66.52
S_5	0.54	1.98	57.60	0.99	2.01	143.94
S_6	0.35	1.99	160.29	0.75	2.02	189.86
	1b			**1c**		
	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$
S_1	0.68	1.32	50.64	0.67	1.31	52.11
S_2	1.38	1.51	46.39	1.34	1.51	43.46
S_3	0.67	1.69	33.73	0.68	1.69	32.86
S_4	1.51	1.85	58.97	1.47	1.85	56.80
S_5	0.96	1.99	32.39	0.89	1.98	34.17
S_6	0.33	2.03	170.34	0.34	2.03	155.47
	2a			**2b**		
S_n	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$
S_1	1.04	1.35	41.34	0.66	1.31	51.02
S_2	1.66	1.49	61.35	1.39	1.51	44.91
S_3	0.73	1.76	43.63	0.67	1.68	32.96
S_4	1.40	1.85	56.22	1.57	1.85	58.07
S_5	1.25	2.03	24.45	0.91	1.99	33.38
S_6	0.26	2.06	237.70	0.33	2.03	163.92
	2c			**3a**		
S_n	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1\|H_{SOC}\|S_n\rangle$
S_1	0.66	1.31	52.43	1.91	1.36	35.91
S_2	1.36	1.51	41.59	1.48	1.49	69.63
S_3	0.69	1.68	32.22	0.93	1.79	53.16
S_4	1.51	1.85	55.59	1.44	1.84	53.42
S_5	0.83	1.98	34.93	1.37	2.02	13.65

S_6	0.34	2.03	148.33	0.20	2.04	307.29
	3b			**3c**		
S_n	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1 \| H_{SOC} \| S_n \rangle$	$\mu(S_n)$	$\Delta E(S_n–T_1)$	$\langle T_1 \| H_{SOC} \| S_n \rangle$
S_1	0.78	1.32	46.94	0.09	1.33	49.27
S_2	1.39	1.51	55.09	1.39	1.51	51.93
S_3	0.66	1.73	38.26	0.66	1.73	36.57
S_4	1.58	1.84	62.29	1.52	1.85	60.57
S_5	1.13	2.01	28.62	1.09	2.00	29.16
S_6	0.31	2.02	213.08	0.32	2.03	196.40

Table S4. Cartesian coordinates of the structures for **3b** reported in the main text.

	S_0		
78	-1.032290	-0.368918	0.045535
6	-0.548122	-2.287229	0.055895
6	-1.413687	-3.352715	0.111541
6	0.851438	-2.571995	-0.011650
6	-0.943818	-4.691542	0.098425
1	-2.483469	-3.168281	0.163957
6	1.354181	-3.845890	-0.028558
6	0.456914	-4.943334	0.025764
1	2.416288	-4.051367	-0.086782
6	0.896385	-0.219703	-0.052367
7	1.617557	-1.387680	-0.063500
7	1.791770	0.788385	-0.109400
6	1.487195	2.202913	-0.122100
6	2.978907	-1.120052	-0.122874
6	3.082340	0.280105	-0.153121
6	4.126100	-1.909645	-0.149615
6	4.306803	0.932330	-0.213016
6	5.354613	-1.257888	-0.209095
1	4.087457	-2.990540	-0.123284
6	5.448106	0.137713	-0.241105
1	4.370044	2.015661	-0.235695
1	6.425473	0.608220	-0.287534
1	6.262569	-1.853049	-0.230418
1	1.879118	2.654980	-1.039101
1	0.404969	2.329668	-0.080348
1	1.951584	2.686995	0.743307
6	-1.816737	-5.803002	0.153263
6	0.924036	-6.276465	0.007268
6	-1.338608	-7.090008	0.132896
1	-2.887600	-5.624504	0.212375
6	0.053637	-7.345070	0.055356
1	1.994449	-6.445988	-0.045802
1	-2.037057	-7.919180	0.177545
5	1.006612	-11.076805	1.512925
5	0.684422	-11.173953	-1.342790
5	2.338182	-10.649369	-0.998392
5	1.105496	-9.458483	-1.452005
5	1.576051	-11.867946	0.028403
5	-0.211002	-9.881651	1.056720
1	1.604832	-8.632058	2.326787
1	3.022039	-8.222280	-0.263045

1	3.578448	-10.808023	1.307679
1	1.805473	-13.029889	0.042079
6	0.564467	-8.763640	0.036524
5	2.241152	-9.106727	-0.142194
1	0.302782	-11.858634	-2.233468
1	1.068762	-8.794261	-2.434448
1	0.841283	-11.695920	2.511171
1	3.235430	-10.911755	-1.733909
1	-1.167261	-9.619445	1.701229
1	-1.481973	-9.718674	-1.149705
5	1.427173	-9.361757	1.408120
5	2.538425	-10.588174	0.773958
6	-0.046476	-11.330951	0.191827
5	-0.407458	-9.940196	-0.710998
6	-1.156413	-12.367100	0.350438
9	-2.104344	-12.205483	-0.579521
9	-0.682703	-13.608256	0.233756
9	-1.743147	-12.264824	1.548123
8	-1.539323	1.701508	0.023238
6	-4.010818	0.036096	0.188723
6	-2.720201	2.171252	0.068748
6	-3.907461	1.432472	0.145942
1	-4.834276	1.993546	0.176422
6	-5.376362	-0.594458	0.272715
1	-6.180993	0.143693	0.297577
1	-5.522258	-1.256247	-0.588083
1	-5.432047	-1.217996	1.171697
6	-2.799388	3.676606	0.034075
1	-2.240157	4.089487	0.881090
1	-2.321005	4.044556	-0.880434
1	-3.826588	4.045750	0.071990
8	-3.052615	-0.800938	0.163878
		T_1	
78	-1.018693	-0.345965	0.046704
6	-0.502677	-2.243382	0.061697
6	-1.40842	-3.36355	0.122374
6	0.84661	-2.521452	-0.003977
6	-0.951225	-4.686287	0.106935
1	-2.473888	-3.161741	0.18045
6	1.354754	-3.840764	-0.023913
6	0.464868	-4.944461	0.029389
1	2.417249	-4.041578	-0.086727
6	0.917803	-0.180055	-0.051735
7	1.633216	-1.346499	-0.060278

7	1.810946	0.829868	-0.109074
6	1.503024	2.243504	-0.1236
6	2.993279	-1.081198	-0.117894
6	3.100299	0.320206	-0.150601
6	4.14018	-1.87316	-0.141063
6	4.327106	0.969174	-0.210097
6	5.369037	-1.224372	-0.200042
1	4.097565	-2.954126	-0.111837
6	5.466097	0.172243	-0.234951
1	4.393146	2.052391	-0.234703
1	6.444727	0.640107	-0.280827
1	6.275953	-1.821264	-0.218537
1	1.894389	2.696332	-1.040425
1	0.420478	2.367409	-0.083471
1	1.964461	2.730323	0.741813
6	-1.826234	-5.79582	0.165004
6	0.920901	-6.263204	0.008256
6	-1.339408	-7.129116	0.142682
1	-2.896483	-5.620528	0.226466
6	0.003929	-7.384933	0.061218
1	1.986487	-6.450682	-0.04636
1	-2.054238	-7.944409	0.190079
5	1.008241	-11.099361	1.507761
5	0.670377	-11.197004	-1.345299
5	2.320312	-10.657504	-1.01126
5	1.076278	-9.479084	-1.457652
5	1.577751	-11.883744	0.019856
5	-0.223848	-9.914516	1.060689
1	1.590658	-8.650377	2.322355
1	2.985809	-8.225188	-0.277271
1	3.576408	-10.806407	1.288111
1	1.817635	-13.043664	0.031078
6	0.531117	-8.787748	0.037008
5	2.212287	-9.115076	-0.152388
1	0.289277	-11.884036	-2.234556
1	1.027591	-8.814306	-2.439569
1	0.853929	-11.720085	2.506937
1	3.216578	-10.911699	-1.751025
1	-1.177061	-9.663462	1.713861
1	-1.509006	-9.763558	-1.14084
5	1.41384	-9.381224	1.403937
5	2.53073	-10.595425	0.761689
6	-0.05122	-11.361406	0.193319
5	-0.430354	-9.973664	-0.706568

6	-1.149538	-12.408032	0.357223
9	-2.101178	-12.260165	-0.571671
9	-0.663632	-13.645027	0.244348
9	-1.73624	-12.308222	1.555496
8	-1.539841	1.712341	0.016958
6	-3.999639	0.029848	0.186274
6	-2.725012	2.174719	0.060113
6	-3.906127	1.426816	0.138973
1	-4.83721	1.980901	0.166838
6	-5.359578	-0.611461	0.271045
1	-6.170111	0.120222	0.292518
1	-5.499385	-1.277298	-0.587656
1	-5.411377	-1.232259	1.172172
6	-2.813909	3.678697	0.019589
1	-2.255334	4.098648	0.863516
1	-2.340002	4.04602	-0.897509
1	-3.843379	4.041276	0.058281
8	-3.033774	-0.799495	0.164963

TS[T_1/^{3}MC]

78	-1.05663	-0.45563	-0.35808
6	-0.5307	-2.25161	0.327633
6	-1.40644	-3.35032	0.448494
6	0.868404	-2.54824	0.12297
6	-0.95088	-4.67433	0.314416
1	-2.45785	-3.16997	0.656224
6	1.346741	-3.81924	0.017086
6	0.448173	-4.92611	0.128936
1	2.390528	-4.01795	-0.20805
6	0.906081	-0.27823	-0.46338
7	1.628945	-1.39033	-0.10815
7	1.796723	0.737443	-0.56752
6	1.4792	2.0854	-0.98059
6	2.976868	-1.08809	0.005022
6	3.080308	0.279539	-0.30352
6	4.099622	-1.82743	0.360818
6	4.304176	0.936581	-0.30715
6	5.326661	-1.1663	0.362524
1	4.030486	-2.87164	0.642099
6	5.430265	0.187201	0.027113
1	4.381127	1.990052	-0.55711
1	6.404733	0.66616	0.032684
1	6.221466	-1.71854	0.633514
1	1.844908	2.269855	-1.99687

1	0.397708	2.213876	-0.93754
1	1.947858	2.797135	-0.29415
6	-1.81562	-5.79517	0.42175
6	0.908821	-6.24743	0.043845
6	-1.33567	-7.08001	0.34249
1	-2.87896	-5.62227	0.567325
6	0.043928	-7.32952	0.147717
1	1.970994	-6.41451	-0.10078
1	-2.0277	-7.91166	0.42627
5	1.061025	-11.1051	1.441521
5	0.634949	-11.1012	-1.40313
5	2.298424	-10.5818	-1.10047
5	1.047377	-9.38123	-1.46607
5	1.57734	-11.8401	-0.09068
5	-0.17527	-9.89924	1.071974
1	1.680906	-8.68792	2.32054
1	3.003165	-8.1808	-0.30092
1	3.622512	-10.818	1.152061
1	1.810485	-13.0008	-0.12763
6	0.55771	-8.74142	0.065125
5	2.228525	-9.07142	-0.18565
1	0.2229	-11.7548	-2.30352
1	0.972775	-8.68201	-2.4218
1	0.932083	-11.7599	2.422164
1	3.169376	-10.8147	-1.87634
1	-1.10657	-9.66672	1.762453
1	-1.52835	-9.65862	-1.07661
5	1.47287	-9.38555	1.383457
5	2.562803	-10.5835	0.665397
6	-0.03929	-11.3151	0.150621
5	-0.43742	-9.89475	-0.68811
6	-1.14089	-12.3595	0.313742
9	-2.11493	-12.1778	-0.58499
9	-0.66673	-13.5954	0.152665
9	-1.69433	-12.2899	1.529642
8	-1.49743	1.614494	0.056022
6	-4.04914	0.020407	-0.1248
6	-2.66449	2.06581	0.307688
6	-3.87168	1.364893	0.253133
1	-4.76782	1.922106	0.50035
6	-5.4509	-0.53138	-0.19365
1	-6.20571	0.18821	0.131005
1	-5.66678	-0.83607	-1.22374
1	-5.5172	-1.43053	0.427949

6	-2.68723	3.525181	0.690351
1	-2.05423	3.676715	1.571457
1	-2.25804	4.121158	-0.12269
1	-3.69479	3.888718	0.904271
8	-3.14228	-0.80605	-0.43787

^{3}MC

78	-0.841485	-0.215410	-1.124704
6	-0.481295	-2.264811	-0.618703
6	-1.349812	-3.324583	-0.601700
6	0.912180	-2.535960	-0.502384
6	-0.889464	-4.662830	-0.469762
1	-2.421101	-3.154191	-0.697523
6	1.411398	-3.810956	-0.413517
6	0.511595	-4.907598	-0.381010
1	2.475683	-4.018724	-0.401553
6	1.112302	-0.194652	-0.885391
7	1.722867	-1.369365	-0.537788
7	2.047991	0.772686	-0.802051
6	1.817601	2.169204	-1.088795
6	3.055858	-1.141465	-0.211612
6	3.259217	0.237376	-0.391331
6	4.093950	-1.949170	0.248336
6	4.487044	0.843374	-0.156374
6	5.323915	-1.343233	0.486804
1	3.961544	-3.005713	0.440587
6	5.523707	0.026668	0.281853
1	4.628293	1.909950	-0.300518
1	6.499675	0.460577	0.476883
1	6.147121	-1.953188	0.846463
1	2.530078	2.518850	-1.842699
1	0.798610	2.264978	-1.470258
1	1.923681	2.767365	-0.178500
6	-1.764634	-5.772738	-0.433957
6	0.975370	-6.237617	-0.268505
6	-1.289128	-7.056146	-0.321391
1	-2.835611	-5.597113	-0.501357
6	0.102771	-7.305836	-0.236142
1	2.046345	-6.406963	-0.204004
1	-1.989724	-7.883100	-0.301207
5	1.818536	-10.592312	1.554332
5	0.413890	-11.386148	-0.823126
5	2.017492	-10.81611	-1.306593
5	0.603927	-9.757049	-1.484776

5	1.829627	-11.731958	0.191218
5	0.420482	-9.524823	1.367114
1	2.478051	-8.044452	1.478448
1	2.688634	-8.265543	-1.492245
1	4.072412	-10.416276	0.277818
1	2.145956	-12.85751	0.380938
6	0.636868	-8.710411	-0.111128
5	2.129338	-9.105830	-0.867859
1	-0.225885	-12.263175	-1.301379
1	0.124485	-9.356289	-2.493524
1	2.115366	-10.942832	2.648206
1	2.569792	-11.266477	-2.258895
1	-0.229854	-9.087721	2.252517
1	-1.622101	-9.932984	-0.09717
5	2.013448	-8.966176	0.893363
5	2.891788	-10.320918	0.168174
6	0.363636	-11.149328	0.869722
5	-0.444434	-10.023733	-0.103624
6	-0.497381	-12.099334	1.699022
9	-1.693441	-12.288193	1.130779
9	0.083656	-13.292511	1.829406
9	-0.704586	-11.612200	2.927600
8	-1.285374	0.658596	0.837245
6	-3.813012	0.105023	-0.767005
6	-2.477585	0.83242	1.239422
6	-3.670859	0.586409	0.544200
1	-4.588217	0.810783	1.076023
6	-5.200933	-0.039124	-1.338871
1	-5.983250	0.201619	-0.615793
1	-5.301764	0.620472	-2.207994
1	-5.340994	-1.064305	-1.697457
6	-2.566013	1.380154	2.645281
1	-2.084336	0.678904	3.335102
1	-2.011216	2.322563	2.702749
1	-3.596439	1.549094	2.965849
8	-2.883421	-0.227445	-1.564849
		MECP	
78	-0.861159	-0.148905	-1.214625
6	-0.547803	-2.237663	-0.493158
6	-1.404915	-3.305738	-0.425691
6	0.849074	-2.508228	-0.470937
6	-0.931392	-4.643859	-0.34411
1	-2.482758	-3.145946	-0.436611
6	1.361875	-3.781717	-0.451217

6	0.473331	-4.8843	-0.370789
1	2.426520	-3.976642	-0.533939
6	1.106261	-0.179349	-0.955528
7	1.674095	-1.349501	-0.541871
7	2.066777	0.764641	-0.896112
6	1.878439	2.153830	-1.242564
6	3.001812	-1.141961	-0.185047
6	3.250988	0.219470	-0.424915
6	3.992484	-1.954200	0.363376
6	4.487561	0.801852	-0.174604
6	5.230363	-1.371940	0.616171
1	3.810867	-2.991848	0.613582
6	5.480968	-0.021516	0.342769
1	4.665991	1.855930	-0.363212
1	6.462389	0.394266	0.549296
1	6.020834	-1.982985	1.041357
1	2.642436	2.466239	-1.960914
1	0.886554	2.250506	-1.689442
1	1.937458	2.779624	-0.346521
6	-1.796104	-5.758370	-0.245595
6	0.949276	-6.213399	-0.311697
6	-1.308696	-7.040625	-0.183456
1	-2.869323	-5.586434	-0.219999
6	0.086480	-7.285424	-0.217057
1	2.022541	-6.378081	-0.332794
1	-2.001478	-7.870961	-0.105693
5	1.836564	-10.558535	1.541125
5	0.437111	-11.363221	-0.836225
5	2.034412	-10.777451	-1.320041
5	0.610719	-9.731006	-1.496810
5	1.857017	-11.696346	0.177069
5	0.428015	-9.505761	1.355120
1	2.469590	-8.001070	1.462840
1	2.683488	-8.225126	-1.507485
1	4.087425	-10.359613	0.261686
1	2.183808	-12.819102	0.365231
6	0.634784	-8.686301	-0.119827
5	2.129611	-9.066844	-0.880214
1	-0.194614	-12.246322	-1.314120
1	0.126831	-9.336437	-2.505938
1	2.136263	-10.906349	2.635085
1	2.590397	-11.221993	-2.272926
1	-0.226525	-9.073577	2.239696
1	-1.612575	-9.929431	-0.113406

5	2.015398	-8.930033	0.881097
5	2.905684	-10.275392	0.154431
6	0.385935	-11.129085	0.856765
5	-0.433982	-10.009645	-0.116062
6	-0.464217	-12.087713	1.686556
9	-1.659603	-12.287895	1.120611
9	0.128036	-13.275738	1.815526
9	-0.674008	-11.602874	2.915791
8	-1.237298	0.535789	0.758756
6	-3.809597	0.175775	-0.847929
6	-2.427912	0.688192	1.192057
6	-3.633968	0.515598	0.506722
1	-4.537824	0.692888	1.078018
6	-5.209805	0.083934	-1.396849
1	-5.972962	0.339687	-0.658724
1	-5.301896	0.751169	-2.259973
1	-5.387918	-0.934087	-1.760133
6	-2.473437	1.129066	2.634189
1	-1.960774	0.388875	3.256812
1	-1.928573	2.072921	2.741102
1	-3.495791	1.261817	2.994402
8	-2.896722	-0.060998	-1.692051