Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical study and design of cyclometalated platinum complexes bearing innovatively highly-rigid terdentate ligand with carboranyl as a chelating unit

Yanyan Xu [a], Yafei Luo [a], Wenting Zhang [a], Wenqian Li [a], Ming Li [a], Wei Shen [a] *

[a] *College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China*

E-mail: shenw@swu.edu.cn

* To whom correspondence should be addressed. E-mail: shenw@swu.edu.cn

Table S1. The selected structural parameters at the optimized S_0 geometries for complex **1** at different theoretical levels as well as the experimental data.

	Exp	PBE0	B3LYP	M062X	CAM-B3LYP
Pt-N	2.063	2.063	2.090	2.094	2.072
Pt-C1	2.089	2.093	2.122	2.115	2.108
Pt-C2	2.062	2.058	2.079	2.054	2.070
Pt-P	2.242	2.288	2.322	2.258	2.306
C1-Pt-N	92.55	82.20	81.98	81.63	82.01
N-Pt-C2	81.28	81.36	81.07	81.02	81.09
C1-Pt-C2	163.82	163.51	162.97	162.52	162.94
average relative error		1.9%	2.8%	2.4%	2.4%

Table S2. The three main absorption bands (nm) calculated at optimized S_0 geometry of complex **2** with different functionals along with the experimental data.

Exp	TPSSH	B3LYP	PBE0	M062X
320	326	220	210	205
275	281	270	260	265
250	250	310	300	330

Table S3. The calculated emission wavelengths at the optimized T_1 geometries of complexes **1** and **2** with different functionals as well as the experimental data.

	Exp	M062X	M052X	B3LYP	PBE0
1	508	519	547	576	588
2	511	521	547	582	590

The properties of frontier molecular orbitals

As well known, the frontier molecular orbitals, especially the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), are closely associated with the photophysical properties of transition metal complexes. Moreover, the HOMO−LUMO energy gap can also be used to predict the direction of emission color-tuning for the new materials designed theoretically. Therefore, the properties of frontier molecular orbitals at the optimized S_0 geometries were analyzed in this research. The electron density distributions of HOMO and LUMO were depicted in **Figure S1**, the energy levels as well as HOMO−LUMO energy gaps were plotted in **Figure S2**. Detailed contributions of ligand and metal to the molecular orbitals were summarized in **Tables S4−S9**.

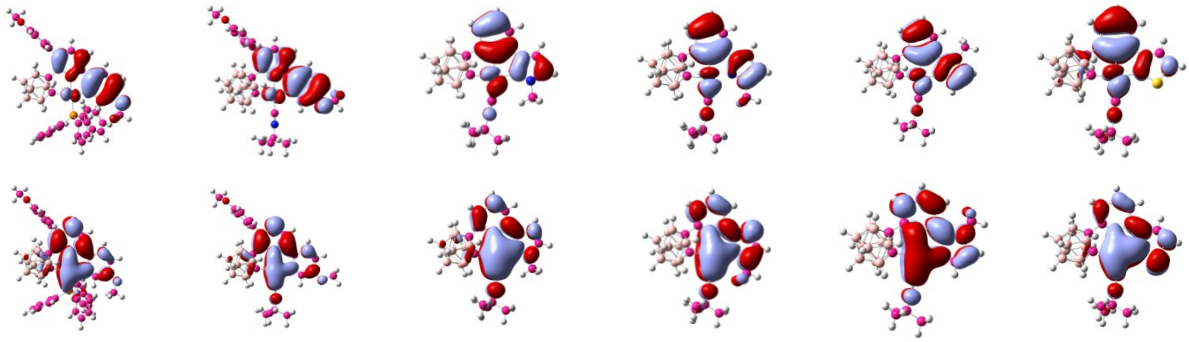

Figure S1 The electron density distributions of HOMO and LUMO at the optimized S_0 geometry.

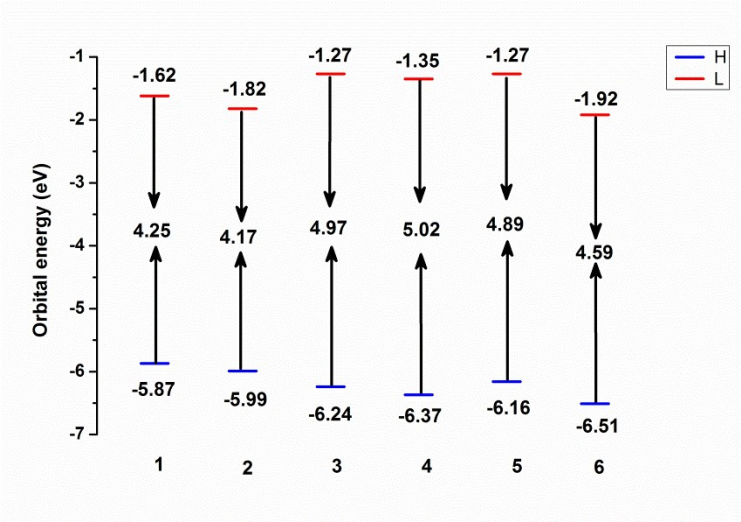

Figure S2 The energy levels of HOMO and LUMO as well as HOMO−LUMO energy gaps for all the studied complexes.

As revealed by **Figure S1**, all the investigated complexes have the similar electron density distributions at HOMO and LUMO, an indicator that modifications in the ancillary ligand and cyclometalating ligand have few effects on the molecular compositions of HOMO and LUMO. Obviously, HOMOs and LUMOs are mainly distributed on the metal atom and the cyclometalating ligand, while ancillary ligand contributes little to the frontier molecular orbitals, therefore, the excited state properties are mainly controlled by the cyclometalating ligand. According to **Tables S4−S9**, the d orbitals of metal atom Pt contribute more to HOMO than LUMO, demonstrating a considerable metal to ligand charge transfer (MLCT) character in the electronic transitions, especially those arising from HOMO to LUMO.

As discussed above, since the frontier molecular orbitals are mainly located at the cyclometalating ligand, it can be inferred that modifications in the ancillary ligand hardly influence the energy levels of HOMO and LUMO. This prediction was well justified in **Figure S2**, with HOMO and LUMO energy levels at complex **2** remaining

the same with the counterpart at complex 1. While for complexes **3** to **5**, by contrast with **2**, the incorporation of azole groups at the cyclometalating ligand leads to the decrease in HOMO energy level and increase in LUMO energy level. As a result, the energy gap between HOMO and LUMO are all widened. Unlike **3**-**5**, for complex **6**, both the energy levels of HOMO and LUMO are lowered, which may be ascribed to the electron-withdrawing effect of S atom added into the cyclometalating ligand. Notably, owing to the different extent of decrease in HOMO and LUMO, the energy gap is also enlarged. Generally, for all the theoretically-designed complexes **3**-**6**, the phosphorescence emission bands are all predicted to exhibit blue-shifted behavior compared with that of the parent complex **2**.

Table S4. Molecular orbital composition at the optimized S_0 geometry for complex **1**

1	MO composition		
	Ancillary ligand(A)	Cyclometalating ligand(C)	Pt
LUMO+1	2%	98%	0%
LUMO	4%	89%	7%
HOMO	0%	92%	8%

Table S5. Molecular orbital composition at the optimized S_0 geometry for complex **2**

2	MO composition		
	Ancillary ligand	Cyclometalating ligand	Pt
LUMO	6%	87%	7%
HOMO	0%	93%	6%
HOMO-6	15%	24%	60%

Table S6. Molecular orbital composition at the optimized S_0 geometry for complex **3**

3	MO composition

	Ancillary ligand	Cyclometalating ligand	Pt
LUMO+6	22%	48%	30%
LUMO	18%	57%	25%
HOMO	2%	68%	30%
HOMO-8	1%	59%	40%

Table S7. Molecular orbital composition at the optimized S_0 geometry for complex **4**

4	MO composition		
	Ancillary ligand	Cyclometalating ligand	Pt
LUMO+1	12%	79%	9%
LUMO	12%	74%	14%
HOMO	3%	79%	18%
HOMO-3	0%	40%	59%

Table S8. Molecular orbital composition at the optimized S_0 geometry for complex **5**

5	MO composition		
	Ancillary ligand	Cyclometalating ligand	Pt
LUMO+1	16%	71%	13%
LUMO	9%	82%	9%
HOMO	2%	80%	18%
HOMO-3	0%	46%	54%

Table S9. Molecular orbital composition at the optimized S_0 geometry for complex **6**

6	MO composition		
	Ancillary ligand	Cyclometalating ligand	Pt
LUMO+1	0%	99%	0%
LUMO	7%	77%	16%
HOMO	3%	75%	22%

The electronic absorption spectra in 2-methyltetrahydrofuran

As widely known, to achieve highly-efficient energy transfer from host materials to guest materials in OLED devices, a good match between the emission of the host and the absorption of the guest is necessary, thus a detailed learning of the absorption properties of the phosphors is crucial. Here, forty singlet−singlet excited states were calculated based on TDDFT/TPSSH method with PCM using the parameters of 2-methyltetrahydrofuran. The corresponding results were depicted in **Figure S3**. Moreover, the excitation energies, oscillator strengths, main configurations as well as the orbitals involved at the lowest and the strongest absorptions for complexes **1-6** were listed in **Table S10.**

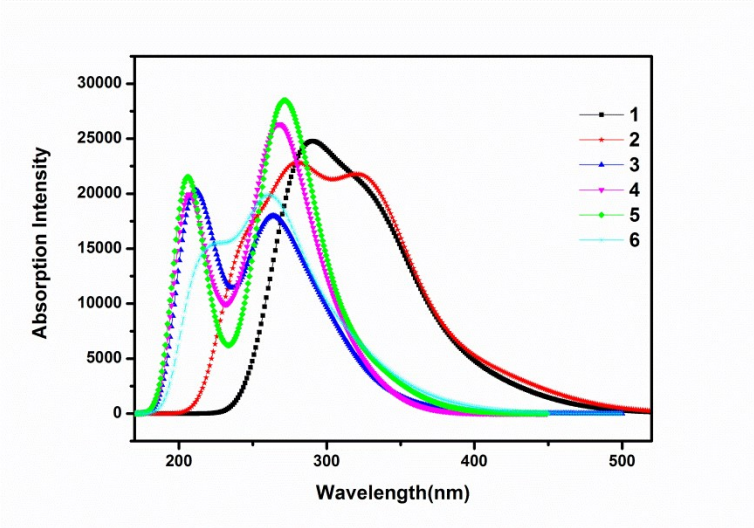

Figure S3. Absorption spectra simulated at the equilibrium geometry of S_0 for all the studied complexes 1-6.

As clearly demonstrated by **Figure S3**, the investigated complexes **1-6** show strong absorption bands in the range between 200 to 350 nm. The main bands at complexes **3-6** blue shift compared with those of **2**. Based on Table 2, the strongest absorption energy for complexes **1**, **2**, **3** and **6** is located at 331, 282, 214 and 267 nm, respectively, with large involvement of metal d orbitals in the electronic transitions. The main characters can be assigned as MLCT (metal to ligand charge transfer) with d(Pt)→π^*(C) transition (C represents the cyclometalating ligand). For complex **4**, the

strongest absorption band with the oscillator strength as high as 0.49 is located at 266 nm, the transition character can be simply described as MLCT with d(Pt)→π*(A+C) (A denotes the ancillary ligand) dominating the electron transfer. While for complex **5**, the main configurations contributing to the strongest electronic absorption are H-3→L(42%) and H→L+1(25%), the transition character is a mix of MLCT/LLCT(ligand to ligand charge transfer) [d(Pt)+ π(C)→π*(A+C)].

Table S10. The excitation energies, oscillator strengths, main configurations as well as the orbital involved at the lowest and the strongest absorptions for complexes 1-6.

	State	λ (nm)	E(eV)	*f*	Configuration[a]	Orbital involved[b]	Character
1	S_1	404	3.07	0.06	H→L(91%)	π(C)→π*(A)	LLCT
	S_6	331	3.74	0.30	H→L+1(66%)	d(Pt)→π*(C)	MLCT
2	S_1	412	3.01	0.07	H→L(93%)	π(C)→π*(A)	LLCT
	S_{12}	282	4.39	0.36	H-6→L(92%)	d(Pt)→π*(C)	MLCT
3	S_1	337	3.68	0.03	H→L(98%)	d(Pt)→π*(A)	MLCT
	S_{24}	214	5.79	0.12	H-8→L(22%) H→L+6(19%)	d(Pt)→π*(C)	MLCT
4	S_1	317	3.90	0.06	H→L(91%)	d(Pt)→π*(A) π(C)→π*(A)	MLCT/LLCT
	S_6	266	4.66	0.49	H-3→L(41%) H→L+1(40%)	d(Pt)→π*(A+C)	MLCT
5	S_1	333	3.72	0.06	H→L(93%)	d(Pt)→π*(A)	MLCT
	S_6	268	4.62	0.51	H-3→L(42%) H→L+1(25%)	d(Pt)→π*(A+C) π(C)→π*(A)	MLCT/LLCT
6	S_1	366	3.38	0.02	H→L(88%)	d(Pt)→π*(A)	MLCT
	S_6	267	4.65	0.29	H→L+1(76%)	d(Pt)→π*(C)	MLCT

[a] H and L represent HOMO and LUMO, respectively.

[b] C and A represent cyclometalating ligand and ancillary ligand, respectively.

For all the investigated complexes, the lowest energy absorptions are mainly contributed by HOMO to LUMO transition. The excitation energy follows the order, 4> 5> 3> 6> 1> 2, which is not strictly in accordance with the sequence observed in HOMO-LUMO energy gap. The cause of this phenomenon may be due to the common character of multiple configurations exhibited in the one-electron excitation. For complexes **1** and **2**, the transition character can be assigned as LLCT [π(C)→π*(A)], while for complexes 3 to 6, it is the MLCT [d(Pt)→π*(A)] that

accounts for the transition. With regarding to complex **4**, the transition character is a mix of MLCT/LLCT [d(Pt)+ π(C)$\rightarrow\pi^*$(A)].

Table S11. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **1**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
12.4078	4.20E+01	0.049995
19.9562	1.04E+01	0.004969
27.9084	5.80E+01	0.214293
29.9274	-4.43E+01	0.134079
36.6606	4.80E+01	0.192847
41.0954	-2.42E+01	0.055069
44.3474	1.24E+01	0.015585
46.5337	1.75E+01	0.032481
51.4405	-1.71E+01	0.034565
57.6625	-3.07E+01	0.124167
63.0348	-1.32E+01	0.025241
69.5017	4.24E+00	0.00285
76.3793	-1.09E+01	0.020683
83.7735	3.01E+00	0.001732
94.8352	7.88E+00	0.013446

97.5492	7.07E+00	0.011144
98.2683	6.78E+00	0.010327
105.2425	-1.26E+00	0.000383
113.1331	2.10E+00	0.001136
115.1783	-2.54E+00	0.001698
126.9322	-2.12E+00	0.001299
148.2411	5.56E+00	0.010466
163.854	2.05E+00	0.001581
177.715	-2.66E-01	2.87E-05
181.2898	1.58E+01	0.103574
196.259	1.03E+01	0.047656
201.6346	4.78E+00	0.010531
215.5393	-5.42E-01	0.000145
221.3481	-3.35E+00	0.00569
225.1306	2.09E+00	0.002239
240.1472	-2.37E+00	0.00308
242.4369	-2.06E+00	0.002355
245.8608	-4.82E+00	0.013054
252.753	-2.71E+00	0.004246
257.2042	2.89E+00	0.004921
259.8184	-2.23E+00	0.002941
261.9417	2.54E+00	0.003868
269.2588	8.50E-01	0.000445
280.656	1.97E+00	0.002489

285.9741	5.17E-01	0.000175
309.2443	6.66E+00	0.031374
345.9692	-8.68E-01	0.000595
357.1519	3.08E+00	0.007718
387.7441	-2.73E+00	0.006601
403.2258	-3.09E+00	0.008805
407.3575	5.39E-02	2.7E-06
410.3055	-1.72E-01	2.77E-05
419.6476	-3.09E-01	9.14E-05
425.0911	-1.88E-01	3.44E-05
430.7155	1.36E+00	0.001821
442.6947	-2.96E-01	8.85E-05
458.5469	-3.10E+00	0.010073
460.5292	-1.49E+00	0.002321
468.7147	2.57E+00	0.00708
472.6785	6.66E-01	0.00048
480.6066	-3.55E-01	0.000138
483.0808	-4.36E-01	0.00021
508.4713	1.74E+00	0.003506
525.8521	-3.21E+00	0.012375
529.9942	1.55E+00	0.002902
540.3425	1.41E-01	2.46E-05
545.006	-1.91E+00	0.004538
549.2132	3.33E+00	0.013931

557.4765	-5.02E-01	0.000321
574.7385	-1.51E-01	3.01E-05
580.8142	-3.58E-01	0.00017
584.1459	-2.85E-01	0.000109
590.4315	2.94E+00	0.011635
602.7012	5.48E-01	0.000413
608.5575	-7.35E-02	7.52E-06
609.1549	-2.45E-02	8.37E-07
612.7996	-6.04E-03	5.1E-08
628.5739	-1.17E-01	1.96E-05
629.5079	1.51E-01	3.26E-05
631.0372	1.02E-01	1.49E-05
637.1755	1.83E-02	4.86E-07
643.2164	-1.10E+00	0.00177
648.1073	6.18E-01	0.000566
664.1215	4.92E-02	3.67E-06
666.975	4.67E+00	0.033244
673.2413	3.18E+00	0.015599
685.0381	-3.78E-01	0.000223
697.2366	1.11E+00	0.001981
703.2554	1.15E+00	0.002113
707.3155	2.05E-01	6.77E-05
709.9182	7.73E-03	9.7E-08
711.5963	2.15E-01	7.52E-05

715.7104	6.43E-01	0.000676
716.8698	-5.00E-01	0.000409
718.5044	-2.08E-01	7.1E-05
724.1655	-1.43E-01	3.37E-05
728.0195	-2.84E-02	1.34E-06
741.806	-1.96E-01	6.48E-05
746.9446	2.72E-01	0.000127
753.117	-3.39E+00	0.019823
754.4882	1.95E+00	0.006552
762.2942	-4.92E-03	4.21E-08
763.8676	-3.85E-01	0.000259
764.6931	-4.53E+00	0.035852
765.5603	2.78E+00	0.013501
766.012	4.98E-01	0.000434
769.4504	-8.65E-01	0.001317
771.8529	-1.91E-01	6.41E-05
772.1487	5.30E-01	0.000496
780.3671	1.68E-01	5.02E-05
781.239	1.88E+00	0.006284
788.7124	-7.09E-01	0.000906
793.8986	-7.96E-01	0.001148
796.2795	-7.60E-01	0.00105
798.7648	8.14E-01	0.00121
818.4967	7.34E-01	0.001009

826.5654	4.10E-02	3.17E-06
829.2773	-9.22E-02	1.61E-05
832.5559	2.76E+00	0.014458
845.0766	-5.51E+00	0.058575
856.9276	-2.27E+00	0.010068
862.5329	-1.08E+01	0.229768
863.2619	-2.09E+00	0.008657
865.6729	-2.31E-01	0.000105
866.3581	-8.06E-01	0.001286
869.0812	1.51E+00	0.004507
873.9471	4.56E-01	0.000415
881.7705	5.73E+00	0.066169
902.8257	-4.29E-01	0.00038
905.3377	-8.50E-01	0.001494
927.2589	-3.23E+00	0.022103
934.6516	-2.61E-01	0.000146
935.1371	-5.81E-01	0.00072
937.1603	-8.37E-03	1.5E-07
940.8225	2.51E-01	0.000135
942.1509	-6.27E-02	8.46E-06
942.6734	2.94E-02	1.87E-06
946.0891	-2.03E-01	8.93E-05
948.6223	3.17E-01	0.000218
949.3442	1.79E-01	6.98E-05

949.9536	-1.99E-01	8.6E-05
951.5894	2.20E-01	0.000105
955.2033	-2.96E-02	1.91E-06
956.2514	1.51E-01	4.97E-05
957.2036	-2.10E-01	9.62E-05
958.955	9.54E-02	2E-05
960.8679	3.81E-01	0.000319
963.3426	-2.78E-01	0.00017
965.1223	3.52E-03	2.73E-08
966.1724	8.52E-02	1.6E-05
972.5915	9.55E-02	2.03E-05
985.9629	-2.61E-01	0.000153
989.8684	1.66E+00	0.006268
993.7917	-1.44E-03	4.69E-09
995.6528	7.75E-02	1.37E-05
997.6955	5.56E-03	7.04E-08
1010.295	1.45E+00	0.004887
1011.017	-8.05E-02	1.5E-05
1014.516	-1.29E-01	3.84E-05
1017.341	-4.51E-01	0.000472
1017.969	4.89E-01	0.000557
1019.743	-6.53E-01	0.000994
1028.606	4.17E+00	0.040875
1034.163	1.49E+00	0.00528

1058.104	-2.94E+00	0.020848
1061.004	-3.08E+00	0.023017
1066.065	3.43E-01	0.000287
1066.451	-2.78E+00	0.018841
1067.304	-1.21E-02	3.59E-07
1067.753	-4.07E-01	0.000404
1080.434	-6.84E-02	1.16E-05
1094.844	1.13E+00	0.003203
1114.594	-2.94E-01	0.00022
1119.219	2.81E+00	0.020169
1120.616	-7.12E-01	0.0013
1124.244	-1.39E-01	4.99E-05
1126.084	-2.23E-01	0.000128
1131.419	3.10E-02	2.48E-06
1132.77	1.65E-01	7.07E-05
1136.58	3.97E-02	4.09E-06
1144.042	-8.01E-02	1.68E-05
1147.52	1.04E-01	2.84E-05
1178.521	3.30E+00	0.029353
1189.303	2.22E+00	0.013391
1190.701	5.28E-02	7.59E-06
1196.469	1.86E-02	9.45E-07
1196.902	-1.08E-01	3.22E-05
1197.969	7.45E-02	1.52E-05

1197.981	1.94E+00	0.010323
1214.125	1.34E-01	4.97E-05
1222.253	-6.73E-01	0.001264
1223.746	-1.88E+00	0.009924
1225.096	6.65E-02	1.24E-05
1226.072	7.33E-01	0.001507
1229.224	3.00E-02	2.52E-06
1272.998	-1.73E-02	8.71E-07
1287.347	5.52E+00	0.08965
1312.333	-1.58E+00	0.007517
1331.512	5.61E-01	0.000959
1333.617	5.21E-02	8.26E-06
1340.882	2.07E+00	0.013074
1343.137	-9.24E-01	0.002619
1346.892	2.02E-01	0.000125
1348.62	7.87E-02	1.91E-05
1353.668	4.78E-01	0.000708
1377.38	-9.34E-02	2.75E-05
1381.661	-1.46E+00	0.006735
1383.864	6.11E-01	0.001181
1384.084	-5.90E-02	1.1E-05
1385.53	-4.64E-02	6.83E-06
1388.449	2.10E-03	1.4E-08
1428.876	-4.16E-01	0.000564

1469.712	-5.58E+00	0.104701
1472.716	-4.01E-01	0.00054
1487.633	9.12E-01	0.002827
1490.507	-1.22E-02	5.05E-07
1492.112	5.18E-02	9.15E-06
1493.291	2.82E-02	2.71E-06
1501.076	3.03E+00	0.031434
1519.109	-5.01E-01	0.000873
1522.844	-3.98E+00	0.055103
1522.993	7.26E-02	1.83E-05
1532.393	-1.15E-01	4.63E-05
1535.019	9.98E-01	0.003495
1536.054	-1.52E+00	0.008118
1536.995	2.37E+00	0.019705
1538.716	9.69E-02	3.3E-05
1541.354	1.59E-01	8.94E-05
1586.07	4.69E-03	7.97E-08
1628.482	-4.36E+00	0.07069
1638.699	-2.04E+00	0.015592
1652.147	1.67E+00	0.010518
1655.997	2.84E-01	0.000306
1658.974	2.94E-01	0.000329
1660.241	4.36E-01	0.000721
1671.099	-4.25E-01	0.000691

1673.136	1.20E+01	0.554963
1674.4	3.56E-01	0.000485
1675.867	-2.43E-01	0.000226
1681.872	-1.13E-01	4.88E-05
1701.959	4.30E-01	0.000718
2682.887	-5.58E-03	1.91E-07
2683.879	7.18E-03	3.16E-07
2689.431	-4.88E-04	1.46E-09
2696.147	3.09E-02	5.89E-06
2715.519	2.00E-02	2.47E-06
2718.434	-4.10E-02	1.04E-05
2733.994	-5.49E-03	1.89E-07
2749.698	-3.25E-03	6.64E-08
2753.698	-1.02E-02	6.59E-07
2763.046	2.25E-02	3.19E-06
3044.375	-4.45E-01	0.001376
3045.951	9.91E-03	6.83E-07
3112.2	-1.54E-02	1.68E-06
3114.421	-1.78E-02	2.26E-06
3185.436	-8.36E-02	5.09E-05
3187.685	3.64E-03	9.67E-08
3210.064	8.51E-05	5.31E-11
3211.712	1.96E-03	2.83E-08
3213.085	2.11E-03	3.27E-08

3215.586	1.69E-02	2.11E-06
3216.623	1.12E-01	9.19E-05
3221.437	3.48E-03	8.93E-08
3222.019	-9.09E-02	6.08E-05
3222.471	1.55E-03	1.77E-08
3225.863	6.63E-03	3.25E-07
3227.086	-1.09E-02	8.74E-07
3229.271	-1.67E-01	0.000205
3231.614	7.18E-03	3.81E-07
3235.252	-1.08E-03	8.62E-09
3236.075	-2.43E-02	4.35E-06
3237.811	-7.75E-02	4.44E-05
3242.235	-7.49E-03	4.16E-07
3242.605	9.88E-03	7.24E-07
3243.017	5.87E-04	2.55E-09
3245.235	-2.85E-02	6.01E-06
3245.749	2.74E-01	0.000556
3246.667	5.83E-03	2.52E-07
3252.573	2.26E-03	3.8E-08
3253.848	-2.71E-01	0.000548
3263.925	6.43E-02	3.08E-05

Table S12. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **2**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
15.2992	7.85E+01	0.215636
19.4398	2.77E-01	3.4E-06
22.2955	-7.13E+01	0.259236
27.4377	2.42E+00	0.000368
31.965	-5.19E+01	0.197126
35.6095	-6.83E+01	0.379672
42.8983	7.62E+01	0.56953
73.0203	-1.04E+01	0.017885
84.6999	-1.33E+00	0.000344
88.9555	1.05E+00	0.000223
90.8843	3.98E+00	0.003295
93.9824	-6.87E+00	0.010151
103.211	-3.13E+00	0.002312
108.7252	-7.11E+00	0.01255
124.6763	-3.73E+00	0.003967
152.6726	1.01E+01	0.035788
163.1356	5.44E+00	0.011037
175.0504	4.25E+00	0.007217
197.0017	8.48E+00	0.03241
207.9923	-4.22E+00	0.008477
213.9367	-1.28E+01	0.079804
225.7976	3.25E+00	0.005462
228.604	-1.06E-01	5.84E-06

238.8072	-2.24E+00	0.002736
248.3021	-2.68E+00	0.004081
257.0754	8.53E-01	0.000427
260.219	-1.20E+00	0.000858
269.9696	1.71E+00	0.001797
279.8261	2.40E+00	0.003684
282.1331	-9.85E-02	6.26E-06
284.0669	2.79E-01	5.05E-05
310.342	5.80E+00	0.023888
334.0141	3.47E-01	9.19E-05
341.1312	1.15E+00	0.001029
349.7537	-2.71E+00	0.005862
356.126	-3.27E+00	0.008684
388.5159	-1.15E+00	0.001179
406.1964	-2.57E+00	0.006138
424.3561	-1.70E-02	2.79E-07
428.0228	-5.94E-01	0.000345
443.7743	-1.88E-01	3.58E-05
451.9051	-4.29E+00	0.019008
456.2337	-7.72E-01	0.000621
476.8576	-3.33E+00	0.012083
478.8346	-2.00E+00	0.004367
482.8295	-6.01E-02	3.98E-06
486.0889	-1.62E+00	0.002925

520.2315	-2.22E+00	0.005853
526.3169	2.83E+00	0.009656
537.3992	-1.13E+00	0.001576
540.9271	9.76E-01	0.001178
552.7645	-2.98E+00	0.011246
557.3474	1.30E+00	0.002142
575.1185	-1.71E+00	0.003844
580.7844	1.97E-01	5.15E-05
585.3112	4.37E-01	0.000256
588.9839	3.16E+00	0.013409
603.3099	5.40E-01	0.000401
606.825	-3.93E-02	2.14E-06
608.1339	-2.54E-01	8.97E-05
609.8536	5.44E-02	4.13E-06
636.1313	-7.78E-02	8.8E-06
643.7195	8.72E-01	0.001119
647.4429	7.81E-01	0.000901
664.3919	5.01E-01	0.000381
666.9475	3.83E+00	0.022372
673.7303	-4.69E+00	0.033845
689.8149	1.80E-01	5.1E-05
699.8327	-1.24E-01	2.47E-05
705.814	-7.14E-01	0.000823
719.9702	-2.83E-01	0.000132

728.6387	3.65E-01	0.000222
740.9346	-7.13E-02	8.62E-06
745.4166	2.50E-01	0.000107
751.1745	-1.89E+00	0.006105
752.6021	2.32E+00	0.009295
761.2081	-4.02E-01	0.000282
763.3627	-8.25E-02	1.19E-05
766.7826	4.01E+00	0.028243
768.0524	2.93E+00	0.015046
770.5454	-3.65E-01	0.000234
774.9898	1.37E+00	0.003328
777.6236	-2.07E+00	0.00763
779.7318	1.92E+00	0.006561
789.9753	-2.09E+00	0.007898
791.3869	1.49E+00	0.004009
794.8983	3.62E-01	0.000238
806.1147	7.86E-02	1.14E-05
822.5202	6.32E-01	0.000752
828.7708	7.36E-01	0.001025
829.6102	1.65E+00	0.005167
832.7969	-1.50E+00	0.004281
848.1936	-7.34E-01	0.001045
857.126	-2.24E+00	0.009804
857.9303	-3.79E-01	0.000282

863.4083	-1.29E+01	0.326512
869.406	-2.29E+00	0.010444
886.7409	5.22E+00	0.055192
902.8152	-1.07E-01	2.36E-05
913.6664	-1.08E+00	0.002446
925.2922	-4.33E+00	0.039735
932.3487	-2.35E-03	1.18E-08
935.2089	3.93E-01	0.00033
935.7812	-2.33E-02	1.16E-06
939.1732	-1.63E-01	5.71E-05
941.5792	7.49E-02	1.21E-05
944.5733	2.57E-01	0.000142
946.26	-1.67E-02	6.04E-07
948.0553	2.06E-01	9.23E-05
949.2151	6.61E-01	0.000949
949.6485	2.87E-01	0.000178
951.584	2.37E-01	0.000122
951.7607	-5.83E-02	7.38E-06
955.9021	-1.27E-01	3.51E-05
957.5314	1.61E-01	5.7E-05
959.0808	1.40E-01	4.29E-05
961.5493	-3.07E-01	0.000207
962.202	2.68E-01	0.000158
962.8374	-5.18E-03	5.9E-08

964.902	-1.64E-01	5.93E-05
971.8902	-5.01E-01	0.000557
983.2599	-5.89E-02	7.8E-06
996.1923	6.50E-03	9.62E-08
998.3956	9.49E-01	0.002055
1029.188	3.17E-01	0.000236
1033.14	4.41E+00	0.045957
1055.493	-2.55E+00	0.015699
1061.329	-2.70E+00	0.017618
1069.81	2.35E-01	0.000134
1071.105	-2.72E+00	0.018138
1071.503	1.47E-01	5.3E-05
1080.521	-1.48E-02	5.44E-07
1096.145	1.26E+00	0.003953
1113.913	6.09E-01	0.000943
1118.956	3.04E+00	0.023696
1143.146	-1.51E-01	5.93E-05
1147.408	8.34E-01	0.001823
1175.181	4.76E+00	0.060927
1189.492	-1.62E-01	7.14E-05
1189.725	2.79E-02	2.12E-06
1195.072	6.87E-02	1.29E-05
1213.602	1.63E+00	0.007404
1224.082	-1.74E+00	0.008487

1225.174	-1.87E+00	0.009808
1261.184	1.86E+00	0.010004
1266.256	5.44E+00	0.085691
1276.59	6.20E-01	0.001121
1277.213	2.64E-02	2.03E-06
1278.703	-2.79E-01	0.000228
1312.72	-2.09E+00	0.0131
1331.598	1.90E-01	0.00011
1332.497	-8.13E-01	0.002015
1340.009	2.60E+00	0.020672
1345.835	-2.23E-01	0.000152
1373.323	-4.60E-01	0.000665
1377.598	-1.44E+00	0.006513
1383.895	2.99E-01	0.000282
1422.843	-6.81E-02	1.51E-05
1423.913	3.95E-02	5.09E-06
1427.867	1.65E-02	8.86E-07
1453.333	-6.22E+00	0.128349
1472.346	-1.50E-02	7.61E-07
1473.6	-1.21E-01	4.92E-05
1491.543	1.47E+00	0.007394
1496.564	4.32E-02	6.37E-06
1500.8	2.54E+00	0.022191
1508.961	-7.29E-01	0.001834

1509.805	-2.02E-02	1.4E-06
1518.642	7.59E-02	2E-05
1522.842	-3.67E+00	0.046857
1523.633	-3.97E-02	5.48E-06
1523.872	-5.08E-02	8.97E-06
1524.684	7.11E-02	1.76E-05
1531.7	-2.06E-01	0.000148
1535.302	1.81E+00	0.011502
1535.756	-2.44E+00	0.020935
1543.808	8.82E-01	0.002744
1586.141	-7.75E-02	2.18E-05
1625.787	-4.60E+00	0.078468
1637.986	-2.71E+00	0.027415
1652.114	1.79E+00	0.012164
1669.827	7.88E-01	0.002371
1681.125	1.11E+01	0.473755
1702.276	1.05E+00	0.004313
2323.215	3.55E-01	0.000668
2683.856	4.09E-03	1.03E-07
2686.387	7.67E-03	3.61E-07
2688.457	2.63E-03	4.26E-08
2693.6	-7.58E-03	3.53E-07
2694.281	-6.22E-03	2.38E-07
2703.727	6.98E-02	3.01E-05

2724.374	1.18E-02	8.74E-07
2726.907	-2.19E-02	2.99E-06
2756.469	2.78E-02	4.86E-06
2761.956	8.68E-02	4.75E-05
3046.741	-1.08E+00	0.008087
3047.338	1.06E-01	7.89E-05
3081.258	-1.87E-03	2.46E-08
3082.054	3.11E-02	6.79E-06
3086.608	-1.89E-01	0.000252
3115.355	-7.30E-04	3.79E-09
3116.091	1.96E-03	2.75E-08
3169.049	-5.39E-03	2.11E-07
3169.204	7.23E-03	3.79E-07
3171.585	-5.07E-02	1.86E-05
3174.395	-5.92E-02	2.55E-05
3174.995	-2.22E-02	3.57E-06
3177.583	-1.63E-02	1.94E-06
3187.232	-2.43E-01	0.000432
3188.991	1.64E-02	1.95E-06
3208.028	3.26E-01	0.000778
3221.454	-5.87E-03	2.54E-07
3221.917	-2.49E-01	0.000456
3222.459	-1.70E-01	0.000213
3231.375	-1.09E-01	8.7E-05

3246.273	6.30E-01	0.002946
3254.296	-3.91E-02	1.14E-05
3254.329	-6.42E-01	0.003061
3260.85	6.42E-02	3.07E-05

Table S13. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **3**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
23.8154	-6.04E+00	-2.8E-05
27.1766	-1.85E+01	-8.4E-05
34.3214	-2.53E+01	-0.00012
45.3308	2.29E+01	0.000104
71.163	6.48E+01	0.000296
79.2604	-7.64E-01	-3.5E-06
89.3084	6.69E+00	3.06E-05
101.355	-6.61E+00	-3E-05
106.272	-3.46E+01	-0.00016
126.1946	-2.80E+01	-0.00013
138.8687	3.34E+00	1.52E-05
182.6571	-2.02E+01	-9.2E-05
197.4349	1.42E+01	6.48E-05
199.7873	-1.72E+01	-7.9E-05
222.5076	3.16E-01	1.44E-06

232.0195	-5.30E-01	-2.4E-06
249.9317	-8.38E+00	-3.8E-05
263.4701	-1.96E+01	-8.9E-05
276.6933	1.95E+01	8.93E-05
280.6651	-2.52E+00	-1.2E-05
281.5924	-6.59E-01	-3E-06
300.0661	-1.22E+01	-5.6E-05
314.2887	-5.41E+00	-2.5E-05
334.261	8.51E+00	3.89E-05
346.7961	6.89E-01	3.15E-06
347.9898	4.52E+00	2.07E-05
387.7269	3.38E+00	1.54E-05
411.0659	1.74E+00	7.95E-06
435.3703	3.90E+00	1.78E-05
454.9385	-3.46E+00	-1.6E-05
458.5473	-6.47E+00	-3E-05
484.994	-1.59E-01	-7.3E-07
498.1933	6.42E+00	2.93E-05
513.951	1.76E+00	8.05E-06
533.9208	-3.29E+00	-1.5E-05
535.5197	9.97E+00	4.56E-05
548.8858	-2.03E+00	-9.3E-06
564.2639	2.30E+01	0.000105
567.6785	1.55E+00	7.1E-06

584.153	2.20E+00	1.01E-05
598.9943	-4.83E+00	-2.2E-05
602.7756	4.24E+00	1.94E-05
603.4581	4.22E+00	1.93E-05
611.3225	3.05E+00	1.39E-05
632.2607	6.99E+00	3.19E-05
633.5753	-5.27E+00	-2.4E-05
641.5667	3.43E+00	1.57E-05
664.62	-3.25E-02	-1.5E-07
699.9986	6.25E+00	2.86E-05
701.2859	-4.08E+00	-1.9E-05
701.6593	3.48E+00	1.59E-05
707.6699	-1.27E+01	-5.8E-05
717.4417	7.96E+00	3.64E-05
724.8471	5.11E+00	2.34E-05
729.6521	4.10E+00	1.87E-05
737.0476	-1.43E+00	-6.5E-06
740.8604	1.01E+00	4.63E-06
750.2534	-2.24E+00	-1E-05
752.2458	4.41E+00	2.01E-05
754.2432	1.85E+00	8.44E-06
757.1999	-9.85E+00	-4.5E-05
760.2521	6.41E-01	2.93E-06
767.0353	1.04E+00	4.76E-06

767.7209	-6.59E-01	-3E-06
770.6997	6.37E-01	2.91E-06
771.878	-1.10E+00	-5E-06
782.6051	1.70E+00	7.79E-06
790.5181	-2.01E+00	-9.2E-06
808.0953	-1.84E+00	-8.4E-06
808.5915	-5.99E-01	-2.7E-06
814.8262	4.70E-01	2.15E-06
820.5493	-1.62E+00	-7.4E-06
839.2042	-1.20E-01	-5.5E-07
861.1651	-7.10E-01	-3.2E-06
869.8551	-2.69E-01	-1.2E-06
905.4428	1.25E-01	5.69E-07
913.3318	-1.03E+00	-4.7E-06
914.3104	-2.43E+00	-1.1E-05
922.8901	-3.24E-01	-1.5E-06
923.8183	-2.66E-01	-1.2E-06
937.3749	-7.44E-01	-3.4E-06
940.2028	1.78E-02	8.13E-08
942.8299	-1.28E-01	-5.8E-07
944.7511	5.36E-01	2.45E-06
947.1887	-3.73E-02	-1.7E-07
948.1567	3.76E-01	1.72E-06
949.1854	7.87E-01	3.6E-06

949.6571	-4.19E+00	-1.9E-05
952.7157	-5.81E-01	-2.7E-06
952.993	-2.57E+00	-1.2E-05
954.9223	-3.12E-01	-1.4E-06
957.852	9.63E-02	4.4E-07
958.8544	4.80E-01	2.19E-06
960.6321	-4.14E-01	-1.9E-06
962.2688	2.06E-01	9.41E-07
980.1999	9.77E-01	4.46E-06
984.336	3.78E-02	1.73E-07
990.4513	1.45E+00	6.61E-06
1008.01	-1.94E+00	-8.9E-06
1047.978	-1.34E+01	-6.1E-05
1052.928	1.49E+01	6.81E-05
1062.865	1.16E+00	5.3E-06
1070.149	4.10E-01	1.87E-06
1072.238	2.97E-01	1.36E-06
1074.09	-1.17E+00	-5.3E-06
1088.407	-5.62E+00	-2.6E-05
1103.949	-1.08E+01	-4.9E-05
1121.457	-2.07E+01	-9.4E-05
1137.835	-5.98E+00	-2.7E-05
1162.573	2.05E-01	9.39E-07
1166.436	3.69E-01	1.69E-06

1190.574	2.06E+00	9.43E-06
1219.943	-1.46E+00	-6.7E-06
1258.272	-2.61E-01	-1.2E-06
1276.158	1.18E+00	5.4E-06
1277.571	7.92E-01	3.62E-06
1282.922	6.25E+00	2.86E-05
1330.794	2.03E+00	9.27E-06
1362.94	1.04E+01	4.73E-05
1394.341	-2.33E+00	-1.1E-05
1421.755	-2.15E+00	-9.8E-06
1423.137	-7.44E-01	-3.4E-06
1425.153	-2.59E-02	-1.2E-07
1443.1	1.00E+01	4.58E-05
1454.481	-8.43E-02	-3.9E-07
1466.982	1.61E+01	7.34E-05
1496.581	-1.44E+00	-6.6E-06
1498.876	-1.61E+01	-7.4E-05
1508.473	-1.40E-01	-6.4E-07
1510.005	-1.66E+00	-7.6E-06
1516.808	3.25E-01	1.49E-06
1522.277	2.04E-01	9.31E-07
1523.724	3.09E-01	1.41E-06
1525.447	-6.53E+00	-3E-05
1534.238	1.70E+01	7.75E-05

1544.394	-1.53E+00	-7E-06
1549.633	-2.51E-01	-1.1E-06
1635.447	7.76E+00	3.55E-05
1657.384	-2.38E+00	-1.1E-05
1684.504	1.09E+01	4.97E-05
2291.736	2.30E-01	1.05E-06
2678.538	-1.39E-01	-6.3E-07
2682.128	-9.58E-02	-4.4E-07
2684.111	-2.15E-01	-9.8E-07
2689.229	-1.43E-01	-6.5E-07
2690.942	3.45E-01	1.58E-06
2699.281	-7.27E-02	-3.3E-07
2703.924	2.53E-01	1.15E-06
2711.904	7.23E-01	3.31E-06
2736.625	-1.19E-01	-5.4E-07
2739.532	9.80E-02	4.48E-07
3079.538	7.06E-01	3.23E-06
3082.851	8.41E-01	3.84E-06
3087.01	3.18E+00	1.45E-05
3093.183	-3.37E-01	-1.5E-06
3165.201	1.81E-02	8.28E-08
3166.346	9.87E+00	4.51E-05
3168.364	5.03E-01	2.3E-06
3169.27	-1.24E+00	-5.7E-06

3173.649	8.14E-01	3.72E-06
3178.717	-3.51E-01	-1.6E-06
3182.148	9.07E-01	4.15E-06
3214.793	5.00E-01	2.28E-06
3227.034	-7.07E+00	-3.2E-05
3228.807	-1.29E+00	-5.9E-06
3242.532	-4.11E-01	-1.9E-06
3320.146	-3.58E-01	-1.6E-06
3342.688	1.33E+00	6.07E-06

Table S14. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **4**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
25.3944	2.39E+01	0.033037
28.6688	6.77E+00	0.003003
45.7778	-5.31E+00	0.002951
56.376	2.89E-01	1.08E-05
72.9438	-3.71E+00	0.00229
87.8808	-1.41E-01	4E-06
102.5309	-1.07E+00	0.000267
103.6482	4.53E+00	0.004856
117.8603	-1.42E+00	0.000545
134.4902	-2.40E+00	0.001777

174.7363	-2.56E+00	0.002618
192.2887	-5.80E-01	0.000148
200.2587	2.68E+00	0.003287
220.8734	7.55E-01	0.000288
233.6313	9.88E-01	0.000521
250.5286	1.03E+01	0.060753
255.2903	5.79E+00	0.019534
274.6249	-9.79E-02	6.02E-06
280.4835	1.62E+01	0.167884
280.7257	5.91E+00	0.02241
288.983	4.70E-01	0.000146
312.5475	-1.28E+00	0.001177
325.5826	5.06E+00	0.019013
344.4886	-2.41E-01	4.59E-05
346.3008	-1.36E+00	0.001468
378.5745	-7.41E-02	4.74E-06
410.2389	-6.47E-02	3.92E-06
426.9125	-2.31E+00	0.005203
450.3616	-1.42E-01	2.08E-05
454.3825	-7.89E+00	0.064693
482.804	-1.07E+01	0.127126
494.8223	-3.01E-01	0.000103
513.4581	-3.08E+00	0.011152
534.2112	-1.59E-01	3.09E-05

535.7102	-6.18E-02	4.67E-06
548.1095	-3.53E-01	0.000156
561.8975	-8.11E-02	8.44E-06
565.7021	1.94E+00	0.004885
584.052	5.62E-02	4.22E-06
596.8538	-3.71E-01	0.000188
601.8364	-1.13E+00	0.001742
603.7582	5.35E-01	0.000395
609.5576	1.10E+00	0.001686
631.4906	-5.28E-01	0.000403
644.8338	1.02E-01	1.54E-05
647.3876	5.44E-01	0.000437
663.2482	6.58E+00	0.065611
681.168	3.30E-01	0.00017
691.4569	-2.54E-02	1.02E-06
700.6546	1.46E+00	0.003426
703.4918	1.49E+00	0.003585
715.9209	-6.16E+00	0.062058
728.2507	3.71E-01	0.000229
737.0168	6.12E-01	0.00063
739.4349	3.55E-01	0.000213
748.201	-2.40E+00	0.009832
749.3724	1.27E-01	2.77E-05
751.7948	4.40E-02	3.33E-06

756.8128	-5.08E-01	0.000446
757.8456	3.19E-01	0.000176
766.7698	1.69E+00	0.005014
768.5915	8.85E+00	0.137676
770.2352	2.74E-02	1.32E-06
770.7511	-7.39E-01	0.000961
771.552	8.44E-01	0.001256
782.6719	8.11E-02	1.18E-05
790.0019	1.95E-01	6.87E-05
804.4605	3.36E-01	0.000208
806.8739	-1.35E-01	3.34E-05
816.8735	-2.48E-02	1.15E-06
837.8375	-1.46E-02	4.08E-07
857.3531	-5.21E-03	5.31E-08
861.8578	2.52E-01	0.000125
879.7275	3.11E-02	1.95E-06
904.2472	-2.10E+00	0.009124
912.8767	-6.39E+00	0.085127
915.0155	1.44E-01	4.32E-05
922.8062	7.65E+00	0.123405
925.0483	1.24E-01	3.27E-05
937.2781	1.88E-01	7.54E-05
939.3058	-3.73E-02	2.98E-06
942.1377	9.97E-02	2.14E-05

944.393	3.36E-01	0.000243
946.516	1.07E+00	0.002454
947.1414	-2.70E-02	1.58E-06
949.0215	-7.36E-01	0.001174
949.4254	-2.72E-01	0.00016
951.8894	-2.25E-01	0.00011
952.1649	1.73E-01	6.52E-05
953.9268	-8.17E-02	1.46E-05
957.5354	3.29E-01	0.000236
958.432	1.75E+00	0.006707
959.5024	-4.71E-01	0.000486
961.0643	4.57E-01	0.000458
980.9076	9.53E-02	2.03E-05
983.9107	-6.49E-01	0.000948
992.0229	7.23E+00	0.118414
1003.926	-2.64E-02	1.59E-06
1013.297	-1.41E+00	0.004589
1048.735	2.41E+00	0.013863
1062.322	-2.56E+00	0.015956
1069.908	-7.09E+00	0.122996
1071.562	-1.39E-01	4.74E-05
1072.675	2.55E-01	0.000159
1075.79	-2.11E+00	0.010973
1079.786	-1.17E+00	0.003403

1093.349	2.63E+00	0.017298
1103.782	1.59E-01	6.4E-05
1106.988	3.20E+00	0.025964
1152.14	-9.05E+00	0.215705
1183.145	1.78E+00	0.008607
1215.884	3.50E+00	0.034125
1258.96	-4.02E+00	0.046543
1274.819	1.11E+00	0.003593
1276.07	-2.11E+00	0.013039
1277.904	-2.46E-01	0.000177
1326.223	1.85E-01	0.000103
1357.03	5.77E-01	0.001032
1399.726	-7.21E-01	0.001664
1422.822	1.93E+00	0.012057
1424.438	7.84E+00	0.2001
1427.758	1.11E-01	4E-05
1446.651	1.10E-01	4.03E-05
1453.822	-3.33E+00	0.036857
1456.711	1.09E-01	3.99E-05
1495.967	4.02E-01	0.000553
1496.421	-2.48E+00	0.020973
1505.611	5.18E-02	9.23E-06
1508.666	6.99E-02	1.69E-05
1509.724	7.09E-02	1.74E-05

1523.4	3.12E-01	0.000339
1524.114	1.75E+00	0.010639
1529.183	-9.95E-02	3.46E-05
1534.387	1.74E-01	0.000106
1543.828	-7.84E-01	0.002171
1579.854	-5.51E-01	0.001096
1604.767	3.52E+00	0.04531
1657.904	-6.02E+00	0.13745
1678.803	1.61E+01	0.992891
2305.622	-3.21E-01	0.000542
2682.153	-4.68E-03	1.34E-07
2687.104	4.88E-03	1.46E-07
2688.299	-1.75E-03	1.89E-08
2693.226	-3.52E-03	7.61E-08
2694.768	2.35E-03	3.41E-08
2703.433	2.68E-02	4.45E-06
2706.33	1.92E-02	2.27E-06
2714.464	1.09E-02	7.33E-07
2742.509	7.94E-03	3.95E-07
2745.136	-3.69E-02	8.52E-06
3080.453	3.14E-01	0.000694
3082.616	-6.17E-01	0.00268
3083.119	-1.15E-01	9.33E-05
3086.964	-2.22E+00	0.034782

3154.129	2.56E-02	4.73E-06
3166.986	-6.50E-02	3.06E-05
3168.922	-3.15E-02	7.19E-06
3170.056	-4.29E-02	1.33E-05
3174.2	3.24E-01	0.00076
3177.004	1.37E+00	0.013641
3179.841	-1.53E-01	0.00017
3180.168	-7.72E-01	0.004332
3217.785	1.09E-01	8.79E-05
3230.673	4.69E-03	1.62E-07
3243.932	2.20E-01	0.00036
3308.716	1.02E-01	7.94E-05
3327.519	-2.37E-01	0.000426

Table S15. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **5**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
22.9186	-1.30E+01	0.008813
23.895	-1.94E+01	0.020491
27.2306	-1.49E+01	0.013736
39.0814	-2.20E+00	0.000434
80.959	-7.38E-02	1.01E-06
87.463	1.20E+00	0.000288

95.7407	3.55E-01	2.76E-05
98.4123	6.08E-01	8.32E-05
122.3104	1.39E+01	0.054368
134.0852	-1.04E+00	0.000333
166.9332	1.41E+00	0.000758
189.1238	-1.03E+00	0.000463
191.8393	8.06E+00	0.028503
206.4695	1.66E+01	0.129592
222.351	1.19E+00	0.000725
235.0324	1.11E-01	6.63E-06
242.0309	1.64E+00	0.001486
251.0315	-6.34E+00	0.023087
266.368	-1.04E+01	0.066163
276.075	-3.59E+00	0.008144
281.1573	6.50E-02	2.72E-06
282.9468	-1.08E-01	7.5E-06
313.6745	-3.92E-01	0.00011
323.1749	1.17E+01	0.100499
342.2326	-5.35E-03	2.24E-08
346.8382	-1.17E+00	0.001091
393.2452	3.31E+00	0.009839
409.2335	2.00E-01	3.75E-05
429.4801	-4.36E+00	0.018663
444.4667	-9.31E+00	0.088025

450.6873	1.29E+00	0.001726
483.7549	-6.44E-02	4.58E-06
495.2177	-1.41E-01	2.25E-05
513.5655	-5.87E-01	0.000405
533.256	1.01E-01	1.25E-05
536.5836	9.10E-02	1.01E-05
545.3932	-5.80E-01	0.000419
553.9335	-4.18E-01	0.000221
560.0838	1.63E-02	3.4E-07
584.1428	-1.33E-01	2.35E-05
594.3244	-6.47E-01	0.000569
601.8658	-1.26E-01	2.19E-05
602.7318	6.91E-01	0.000658
607.3636	3.74E-01	0.000194
632.117	-6.52E-02	6.14E-06
633.8211	4.09E-02	2.43E-06
645.0441	3.46E-02	1.77E-06
664.212	4.05E-01	0.000249
700.845	-1.04E+00	0.001745
702.964	-5.80E+00	0.053969
713.3446	1.81E+00	0.005315
713.5971	-9.95E+00	0.161389
720.2076	-6.15E-02	6.23E-06
728.049	-2.62E+00	0.011422

737.1755	1.17E-01	2.3E-05
740.0009	5.87E-01	0.000582
747.5977	-5.32E+00	0.04839
750.8818	7.85E-01	0.001056
755.0225	-3.23E+00	0.018055
756.9227	5.16E-01	0.000461
758.5999	2.07E+00	0.007408
763.3782	-3.30E-01	0.00019
767.1497	2.17E-02	8.28E-07
768.4743	5.80E-01	0.00059
771.1684	6.45E-01	0.000734
771.2092	1.41E+00	0.003521
782.8504	-2.41E-02	1.04E-06
789.9079	1.93E-01	6.76E-05
809.0791	2.69E-01	0.000134
815.5476	5.53E-02	5.7E-06
822.036	3.05E-01	0.000174
839.3501	-7.59E-02	1.1E-05
844.3853	6.67E-01	0.000858
861.0594	-2.55E-02	1.28E-06
879.2749	-1.02E-02	2.07E-07
904.8232	-1.30E+00	0.003494
914.2287	3.28E-01	0.000225
921.5674	1.16E+00	0.002839

926.7407	4.08E+00	0.035248
931.5838	-2.67E-01	0.000151
937.9762	1.02E+00	0.002222
939.4408	-3.90E-02	3.26E-06
942.2764	8.15E-04	1.43E-09
944.635	2.44E-01	0.000129
946.8539	8.64E-01	0.001614
947.4121	-1.05E-01	2.4E-05
949.1884	-5.09E-01	0.000562
949.527	-4.15E-01	0.000374
951.802	-9.03E-02	1.77E-05
952.0069	-1.11E-01	2.69E-05
953.9133	1.99E-01	8.61E-05
958.264	-3.11E-02	2.11E-06
958.5674	1.23E+00	0.003288
959.9135	-3.10E-01	0.00021
961.5423	-3.25E-01	0.000232
976.469	-6.30E-01	0.000887
983.6459	1.16E-02	3.04E-07
985.4911	-6.61E+00	0.098248
999.3627	4.36E-03	4.35E-08
1036.158	1.26E+00	0.003783
1062.674	1.48E+00	0.005345
1064.969	-7.23E+00	0.127333

1070.091	-3.95E+00	0.038154
1071.596	-1.98E-01	9.63E-05
1077.768	6.77E-02	1.13E-05
1088.857	6.27E-02	9.77E-06
1095.755	-4.73E+00	0.056122
1122.241	8.52E-01	0.001864
1150.288	1.80E+00	0.008494
1159.823	5.38E-01	0.000768
1169.761	9.19E+00	0.225853
1216.919	-1.59E+00	0.007071
1226.442	3.23E+00	0.029316
1260.176	7.21E+00	0.149696
1275.852	3.56E-01	0.00037
1278.366	-1.39E-01	5.63E-05
1301.876	-2.35E-01	0.000164
1334.771	4.20E+00	0.053755
1365.022	1.82E+00	0.010383
1386.49	-2.41E+00	0.018467
1418.213	-1.68E+00	0.009094
1422.496	-1.35E+00	0.005963
1424.133	8.09E-03	2.13E-07
1453.525	-4.24E-03	5.96E-08
1454.572	-1.89E+00	0.01187
1474.919	4.12E-02	5.73E-06

1496.464	-2.55E+00	0.022257
1498.086	-2.24E-01	0.000172
1509.028	2.75E-03	2.61E-08
1510.18	-2.03E-02	1.42E-06
1512.358	2.38E-02	1.96E-06
1523.435	-2.74E-02	2.61E-06
1524.279	-6.12E-02	1.3E-05
1534.718	2.10E-02	1.55E-06
1544.137	1.73E+00	0.010535
1556.947	-3.38E+00	0.040603
1567.208	-1.65E-01	9.7E-05
1609.061	3.51E+00	0.045216
1649.326	-2.18E+00	0.017906
1669.28	-1.77E+01	1.197629
2303.79	-2.24E-01	0.000264
2680.662	-2.05E-03	2.58E-08
2685.258	2.75E-03	4.66E-08
2686.855	1.03E-03	6.5E-09
2691.619	6.18E-03	2.35E-07
2693.148	-5.34E-03	1.75E-07
2701.974	-3.64E-03	8.2E-08
2703.749	1.32E-03	1.07E-08
2712.065	7.75E-03	3.72E-07
2740.86	7.45E-03	3.48E-07

2743.528	-5.12E-02	1.64E-05
3080.409	2.05E-01	0.000297
3082.115	-7.19E-04	3.64E-09
3086.623	-2.90E-03	5.93E-08
3092.911	-2.53E-02	4.53E-06
3167.251	-1.81E-03	2.38E-08
3168.53	-2.08E-03	3.14E-08
3169.989	2.54E-03	4.69E-08
3173.399	-1.78E-03	2.29E-08
3173.796	-1.03E-02	7.63E-07
3176.497	5.55E-04	2.24E-09
3179.571	-2.02E-03	2.97E-08
3199.497	-3.96E-02	1.15E-05
3219.844	1.62E-01	0.000192
3233.771	1.71E-02	2.15E-06
3244.499	2.50E-01	0.000462
3313.852	5.77E-02	2.52E-05
3334.198	-5.69E-02	2.46E-05

Table S16. Vibrational frequencies ω_i at the optimized singlet ground states, Shift vector ΔQ_i and Huang-Rhys factor S_i of different normal modes for complex **6**.

ω_i (cm^{-1})	ΔQ_i (a.u.)	S_i
21.9702	2.07E-01	2.14566E-06

24.4602	-1.25E+00	8.67872E-05
26.3311	-3.64E+00	0.000795738
44.2761	-8.25E-01	6.88535E-05
82.5683	3.61E-01	2.46566E-05
87.5903	-1.60E+00	0.000510398
96.1778	-3.87E+00	0.003298244
117.9551	-8.53E+00	0.019605433
124.1896	1.19E+01	0.040468121
135.7107	1.38E+00	0.000593441
186.9934	-1.06E+00	0.000481621
203.6047	1.33E+01	0.081925955
213.7241	7.26E+00	0.025774458
222.2471	8.08E-01	0.000331506
231.9282	-6.93E-01	0.000254881
252.2589	1.80E+01	0.187074899
269.9049	1.24E+01	0.094125733
275.5316	3.52E-02	7.79052E-07
282.0806	-8.35E-02	4.49036E-06
312.1672	-4.08E-01	0.000118529
312.6401	6.95E+00	0.034491049
337.3697	2.77E-02	5.92292E-07
344.7404	-2.41E+00	0.004591972
347.9456	7.05E-01	0.000395224
407.2562	4.52E-02	1.90152E-06

412.5869	6.36E+00	0.038165388
431.4903	-1.79E-01	3.14429E-05
451.6493	-4.64E+00	0.022251381
484.439	8.17E-01	0.000738892
491.8559	-5.84E-02	3.8306E-06
503.6425	-7.75E+00	0.069039325
516.4558	6.25E+00	0.046079074
531.3377	-1.41E+01	0.240296584
537.4936	-2.85E+00	0.009961599
547.6202	5.53E-01	0.000382836
548.8006	-6.04E+00	0.045681136
561.0393	-2.27E-02	6.6042E-07
584.4445	-3.10E-01	0.000128759
595.9468	-2.22E+00	0.006729816
603.0711	1.43E+00	0.002828533
603.4689	4.30E+00	0.025549152
608.1279	5.82E-01	0.0004705
629.532	5.09E-01	0.000373227
640.1732	1.00E+01	0.147547451
656.4004	4.27E+00	0.027406778
667.3019	-3.06E+00	0.014267914
670.3145	-6.55E-02	6.56578E-06
700.9205	-7.70E+00	0.094938105
702.5579	4.32E+00	0.029984572

714.1995	-4.52E+00	0.033294404
725.2959	1.24E+00	0.002556596
726.3801	1.64E-01	4.45398E-05
726.9665	-7.73E-02	9.93638E-06
739.719	-8.91E-02	1.34211E-05
743.8734	-6.53E-02	7.23968E-06
749.0443	9.99E-02	1.70692E-05
753.4092	-1.52E-02	3.99362E-07
755.5404	3.11E-01	0.000166654
757.2078	-1.19E+00	0.002433812
766.9675	-1.60E-02	4.50706E-07
768.2236	-2.22E-02	8.63972E-07
770.0931	5.02E-01	0.000444286
770.4113	3.82E-01	0.000256918
781.8242	-6.56E-01	0.00076813
789.2851	-3.81E-01	0.000261806
806.7138	4.71E-02	4.08638E-06
808.5849	6.31E-01	0.00073552
819.7622	4.88E-01	0.000446929
831.2979	-4.82E-02	4.41238E-06
839.1411	7.61E-01	0.001111846
861.1085	3.49E-02	2.39647E-06
869.2238	-7.15E+00	0.101546426
871.0778	3.42E-02	2.32976E-06

904.2577	-5.20E+00	0.055773518
907.6766	3.78E-02	2.9686E-06
913.7468	2.54E-01	0.000135056
916.3444	4.25E-01	0.000377569
924.0103	-8.36E-02	1.47689E-05
937.6727	-2.42E+00	0.012522806
940.3921	9.57E-02	1.96713E-05
942.4534	-2.69E-01	0.000155768
944.179	-9.37E-01	0.001896238
947.5861	-1.27E-01	3.50743E-05
948.0148	4.90E-01	0.000520451
949.4938	1.14E-01	2.79685E-05
949.6135	-6.85E-01	0.001019102
952.0109	-1.79E-02	6.96371E-07
953.5042	1.14E+00	0.002840812
955.0021	1.16E-01	2.9513E-05
956.0951	1.01E-01	2.21869E-05
959.1465	-1.42E-01	4.44307E-05
961.2653	-2.19E-02	1.05698E-06
962.4302	4.09E-01	0.000367494
972.9535	-2.73E-01	0.000166009
983.6204	-5.31E-01	0.000633889
983.8398	2.07E-02	9.67014E-07
994.1511	-6.53E-06	9.67314E-14

1025.763	-2.03E+00	0.00962737
1043.615	-4.98E+00	0.059098248
1062.211	-7.11E+00	0.122858634
1070.139	-5.81E+00	0.082505103
1071.445	4.64E-01	0.000526748
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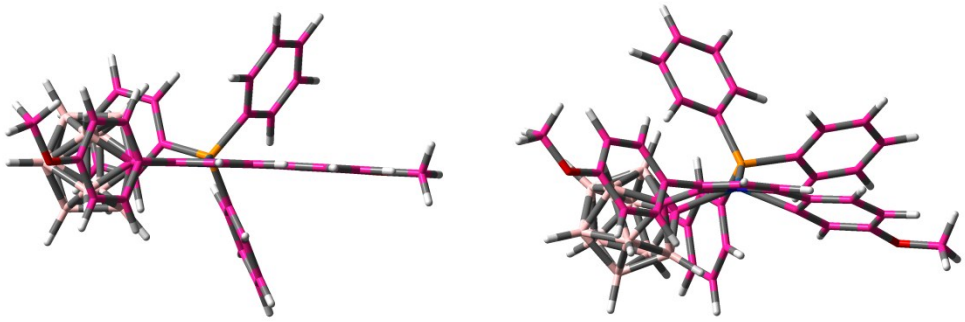
1094.591	9.04E-03	2.04528E-07
1095.572	3.64E+00	0.033245974
1137.388	-3.20E+00	0.026596609
1153.61	9.45E+00	0.23522838
1187.44	-6.50E+00	0.114731754
1216.712	1.99E+00	0.01104878
1259.379	5.44E+00	0.085222974
1276.093	1.55E-01	7.03279E-05
1278.566	2.66E-02	2.06766E-06
1301.222	9.32E-02	2.58151E-05
1336.009	5.12E+00	0.080109224
1368.196	-6.85E+00	0.14651836
1395.958	-8.21E-01	0.002150191
1413.436	4.40E-02	6.25362E-06
1422.65	-2.35E-02	1.80047E-06
1423.763	5.05E-01	0.000829834
1453.516	-9.64E+00	0.308926492
1496.411	-2.32E-01	0.000184147

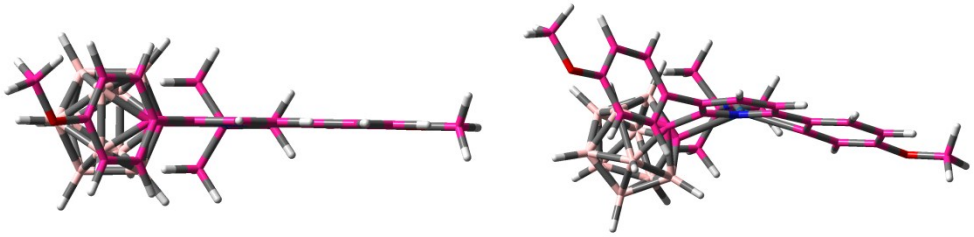
1497.989	1.64E-03	9.16187E-09
1508.928	1.98E-01	0.000135238
1510.088	1.87E-01	0.000120834
1523.554	-1.32E+01	0.6048387
1524.06	-4.85E-01	0.000819042
1530.239	-1.76E-02	1.08481E-06
1544.058	2.36E-03	1.95907E-08
1614.801	-3.40E+00	0.042676405
1654.889	-1.65E+00	0.010243359
1682.078	-2.10E+00	0.016950899
2310.452	-2.49E-01	0.000328008
2681.052	-1.17E-02	8.36956E-07
2684.404	7.32E-03	3.28248E-07
2685.428	2.33E-03	3.32186E-08
2690.689	-1.07E-03	7.09219E-09
2692.232	5.43E-03	1.8128E-07
2700.519	-8.29E-03	4.24042E-07
2703.72	6.29E-02	2.44487E-05
2711.822	2.74E-02	4.64775E-06
2735.614	3.25E-03	6.62337E-08
2738.461	-2.33E-02	3.40248E-06
3081.126	6.80E-03	3.25414E-07
3082.572	7.90E-04	4.40084E-09
3087.047	-1.54E-02	1.67045E-06

3168.317	9.74E-04	6.87166E-09
3169.312	4.50E-03	1.46938E-07
3171.006	5.36E-04	2.08143E-09
3174.48	-1.76E-02	2.23774E-06
3176.512	3.48E-03	8.7803E-08
3179.559	-4.08E-03	1.21222E-07
3216.639	1.24E-01	0.000113006
3230.216	-2.78E-02	5.70639E-06
3243.871	9.64E-02	6.88991E-05
3302.257	-4.50E-02	1.53146E-05
3322.396	4.56E-02	1.57931E-05



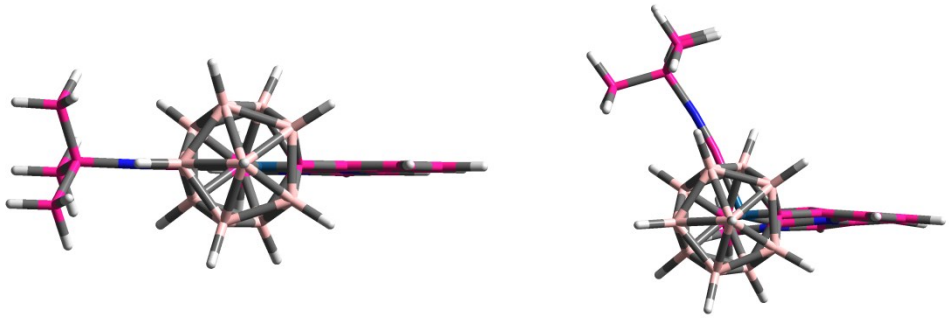
S_0 ^3MC

Figure S4 The comparison between the optimized geometries of S_0 and ^3MC for complex 1



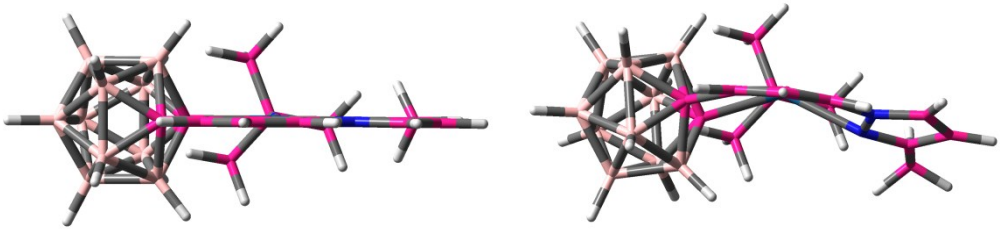
S_0 ^3MC

Figure S5 The comparison between the optimized geometries of S_0 and ^3MC for complex 2



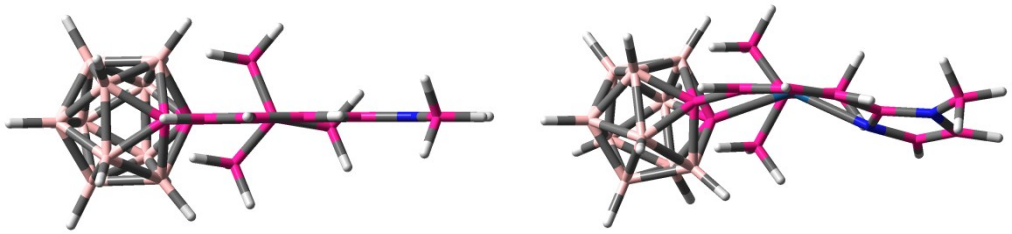
S_0 ^3MC

Figure S6 The comparison between the optimized geometries of S_0 and ^3MC for complex 3



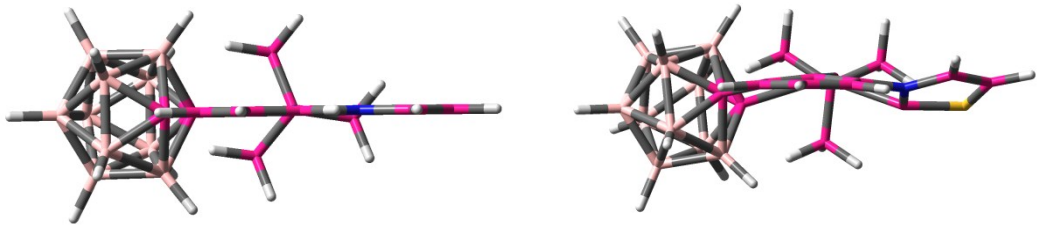
S_0 ^3MC

Figure S7 The comparison between the optimized geometries of S_0 and ^3MC for complex 4



S_0 ^3MC

Figure S8 The comparison between the optimized geometries of S_0 and ^3MC for complex 5



S_0 ^3MC

Figure S9 The comparison between the optimized geometries of S_0 and ^3MC for complex 6

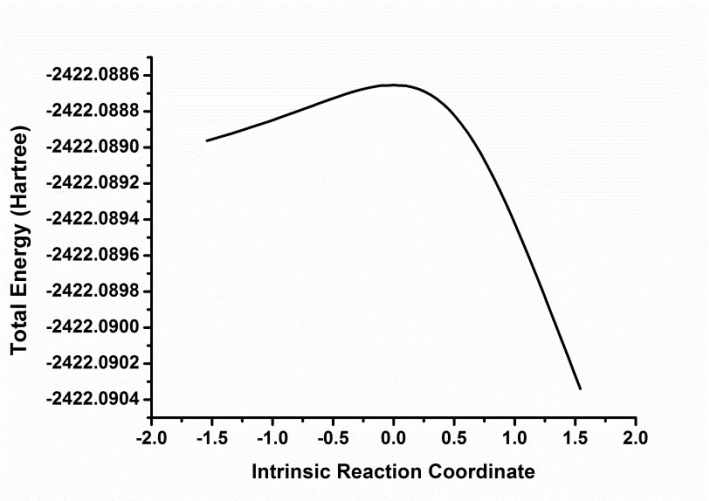


Figure S10 The curve of intrinsic reaction coordinate of TS [T_1-^{3}MC] for complex **1**.

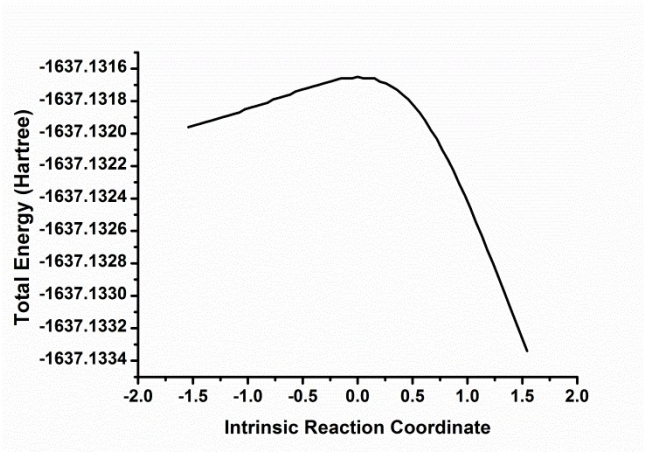


Figure S11 The curve of intrinsic reaction coordinate of TS [T_1-^{3}MC] for complex **2**

.

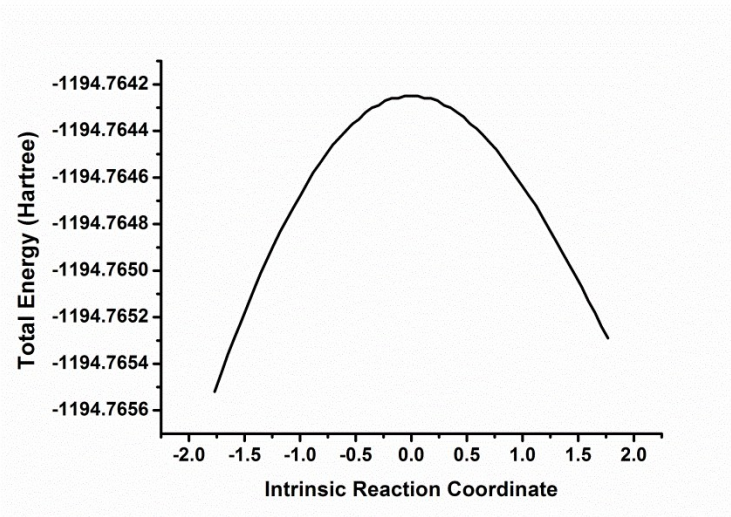


Figure S12 The curve of intrinsic reaction coordinate of TS [T_1-^{3}MC] for complex **4**

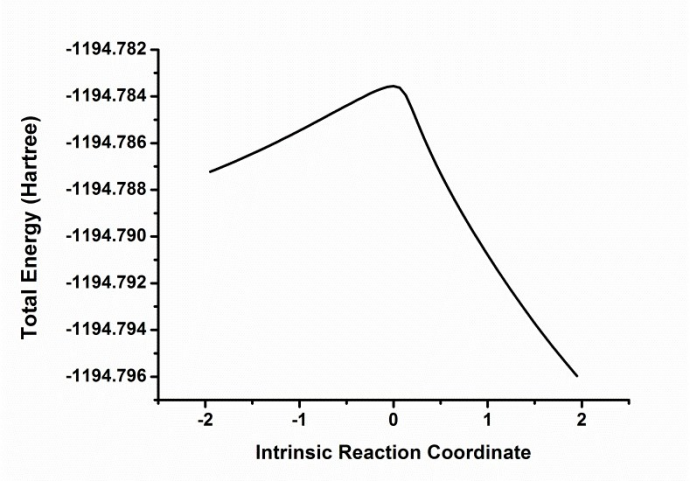
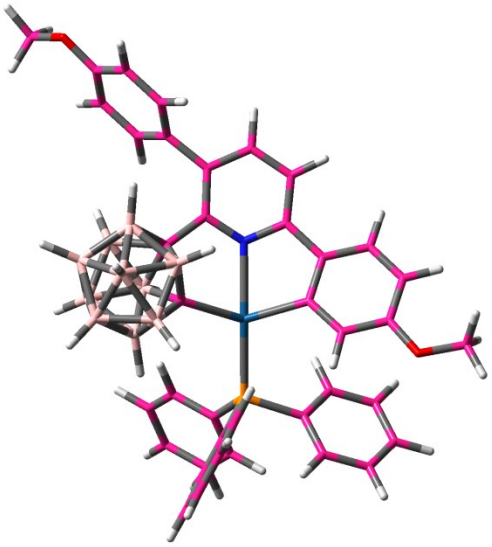
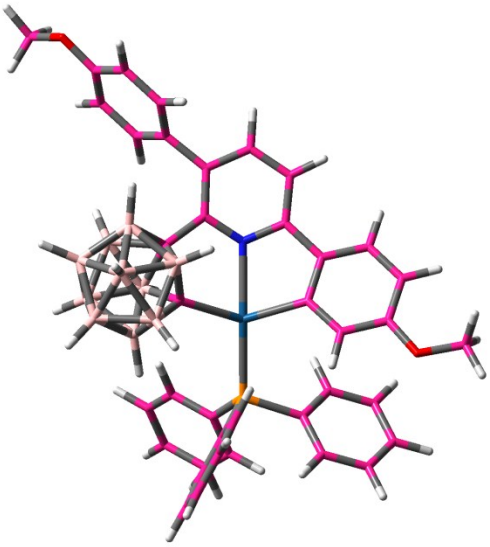


Figure S13 The curve of intrinsic reaction coordinate of TS [T_1-^{3}MC] for complex **5**

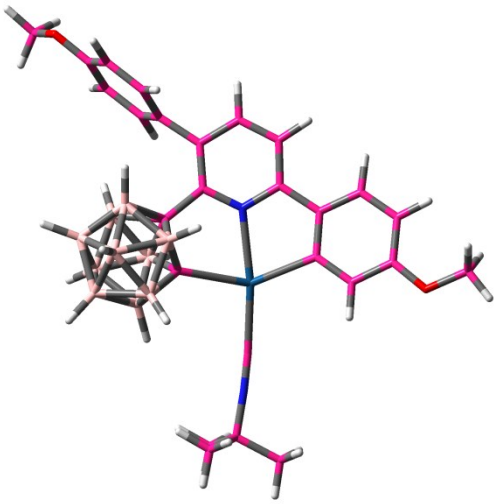


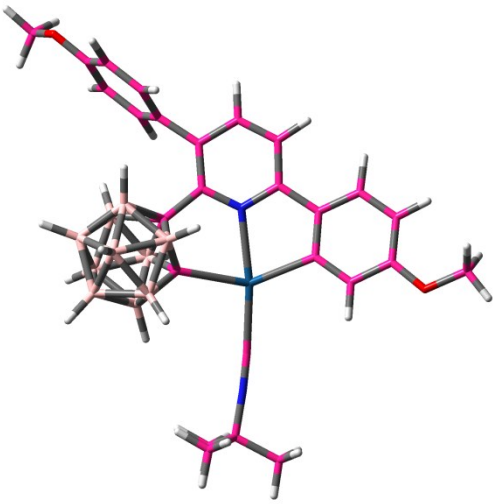


S_0^{MECP} $^3MC^{MECP}$

E= -2422.08951750a.u. E= -2422.08951813a.u.

Figure S14 The structures of S_0 and ^{3}MC at MECP for complex **1**.

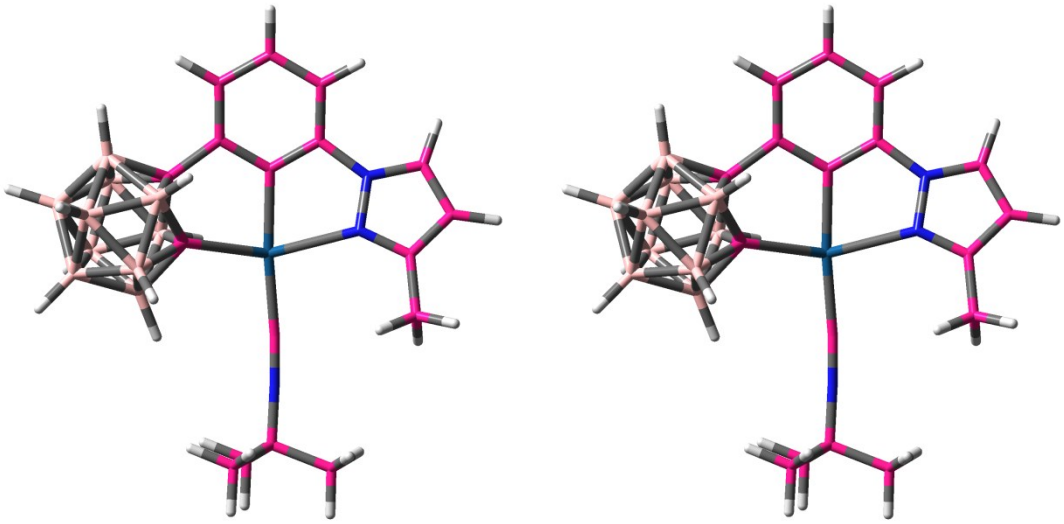




S_0^{MECP} $^3MC^{MECP}$

E= -1637.12530438a.u. E= -1637.12530359a.u.

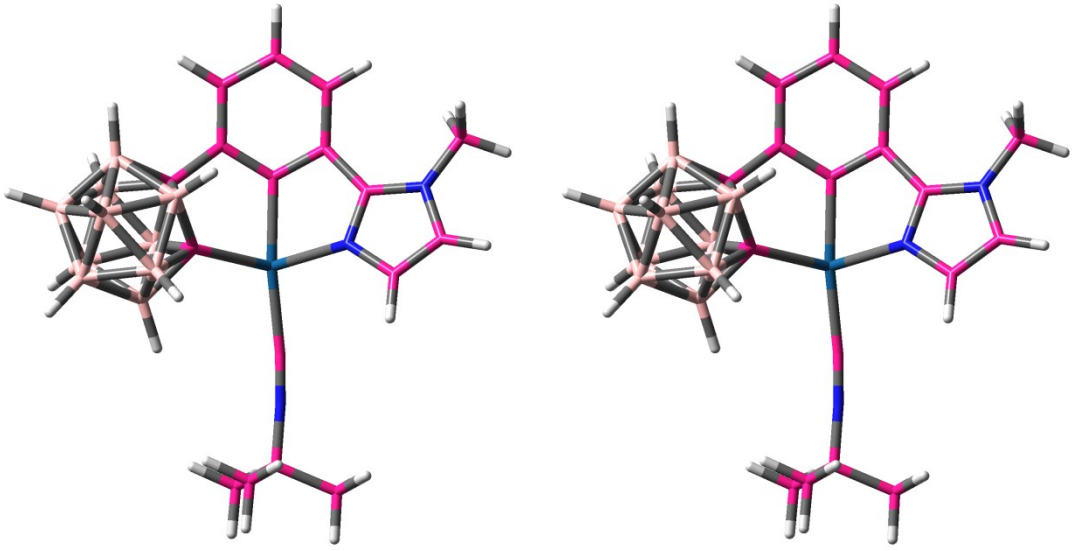
Figure S15 The structures of S_0 and ^{3}MC at MECP for complex **2**.



S_0^{MECP} $^3MC^{MECP}$

E= -1194.7560342a.u. E= -1194.75759651a.u.

Figure S16 The structures of S_0 and ^3MC at MECP for complex **4**.



S_0^{MECP} $^3MC^{MECP}$

E= -1194.77292358a.u. E= -1194.77296507a.u.

Figure S17 The structures of S_0 and ^3MC at MECP for complex **5**.

Cartesian coordinates of the structures for complex **1**

S_0

78	7.307513	2.440492	14.092485
15	7.963389	4.620303	13.861608
6	7.723804	5.849978	15.204027
6	6.510170	6.536487	15.322550
6	6.311114	7.439671	16.361371
6	7.321407	7.670542	17.291128
6	8.534947	6.998923	17.174487
6	8.736981	6.093037	16.137901
6	7.188809	5.454861	12.424743
6	6.440956	4.699404	11.515737
6	5.841218	5.310887	10.417555
6	5.979871	6.680734	10.217131
6	6.710553	7.444575	11.125273
6	7.305484	6.838673	12.226825
6	5.639019	0.936394	16.203734
6	6.132522	2.511274	15.822945
6	8.181900	0.394452	12.233622
6	8.289322	1.806726	12.398350
6	8.986917	2.488918	11.407455
6	9.567105	1.839629	10.309102
6	9.461241	0.453500	10.171474
6	8.764075	-0.252855	11.140962
5	4.887546	3.580020	16.261648

5	6.315426	3.383924	17.269405
5	6.811652	1.701226	17.178594
5	5.513639	0.708974	17.887093
5	4.073829	0.908971	16.875117
5	3.577568	2.601746	16.946146
5	5.918389	2.275565	18.593457
5	4.214526	1.792470	18.400295
5	4.498766	2.023249	15.553443
5	4.711003	3.452667	18.022943
1	5.716759	6.368797	14.601157
1	5.360801	7.959207	16.445446
1	7.162900	8.373433	18.104411
1	9.329390	7.176441	17.894077
1	6.332387	3.630812	11.676800
1	5.260449	4.712219	9.721473
1	5.510093	7.157031	9.360712
1	6.808753	8.517327	10.982800
1	7.839858	7.449408	12.949456
1	9.123324	3.564669	11.439586
1	6.463149	2.345930	19.651451
1	7.164615	4.209972	17.320057
1	4.714290	4.542633	15.589142
1	7.932535	1.312528	17.106779
1	3.368757	-0.008307	16.620136
1	3.521468	1.510211	19.328444

1	2.433654	2.909514	16.813451
1	5.807676	-0.343664	18.342808
1	4.135316	1.843585	14.436592
1	4.378787	4.390259	18.680532
6	5.916190	-1.475185	15.307035
6	6.478450	-2.260720	14.288947
6	7.224023	-1.713772	13.268731
6	7.427961	-0.333145	13.243287
6	6.151645	-0.093859	15.236359
1	6.309808	-3.333348	14.323845
1	7.646852	-2.346707	12.497682
7	6.886354	0.425215	14.225637
1	8.678283	-1.330181	11.025254
1	9.903246	-0.072343	9.332833
6	9.785178	4.693944	13.629799
6	10.418391	5.699317	12.893685
6	10.563022	3.725940	14.275439
6	11.807123	5.735375	12.805647
1	9.831138	6.446777	12.369720
6	11.951930	3.774008	14.198125
1	10.070764	2.927577	14.825980
6	12.576028	4.777448	13.461335
1	12.288166	6.514141	12.220071
1	12.545220	3.018387	14.705696
1	13.660097	4.809104	13.392537

8	10.211959	2.643781	9.431519
6	10.826636	2.046198	8.315092
1	11.287684	2.859915	7.752526
1	11.603089	1.330412	8.616194
1	10.095200	1.534840	7.675144
6	5.135363	-2.223861	16.333259
6	5.765979	-2.773595	17.447890
6	3.789824	-2.544624	16.110149
6	5.078434	-3.587511	18.345768
1	6.815820	-2.558264	17.628246
6	3.092746	-3.352945	16.991929
1	3.282306	-2.146442	15.235663
6	3.730846	-3.876060	18.122254
1	5.602004	-3.985176	19.208141
1	2.046907	-3.593604	16.828666
8	2.965840	-4.652004	18.925744
6	3.558393	-5.176978	20.090404
1	3.914373	-4.379913	20.756235
1	2.776419	-5.745632	20.596386
1	4.394727	-5.847642	19.851709
1	9.687187	5.574163	16.059156
	T_1		
78	7.326471	2.425022	14.102007
15	7.968182	4.618757	13.870627
6	7.736605	5.844102	15.218651

6	6.520885	6.524568	15.349442
6	6.325680	7.422219	16.393738
6	7.342222	7.654329	17.316286
6	8.558179	6.989484	17.186737
6	8.756197	6.088712	16.144952
6	7.179090	5.461017	12.443874
6	6.421613	4.709608	11.539803
6	5.809568	5.325189	10.450497
6	5.944854	6.695993	10.254517
6	6.684696	7.456303	11.158365
6	7.292043	6.845917	12.250663
6	5.656558	0.927449	16.218023
6	6.139804	2.504253	15.827651
6	8.199223	0.340745	12.269873
6	8.303822	1.806934	12.421479
6	8.977567	2.472993	11.423797
6	9.574095	1.816006	10.323077
6	9.512585	0.401561	10.208628
6	8.849395	-0.318605	11.159472
5	4.886776	3.567843	16.256273
5	6.314526	3.388450	17.267964
5	6.822435	1.708711	17.189265
5	5.530228	0.714049	17.902367
5	4.090483	0.893990	16.886900
5	3.582492	2.584901	16.946755

5	5.922001	2.287415	18.598575
5	4.222410	1.790917	18.406380
5	4.508815	2.004020	15.559486
5	4.708564	3.452213	18.018059
1	5.722095	6.355274	14.634565
1	5.373208	7.936021	16.487959
1	7.186658	8.352622	18.134085
1	9.357584	7.167959	17.900588
1	6.313477	3.640735	11.700659
1	5.219883	4.729491	9.759245
1	5.464530	7.175980	9.406011
1	6.779734	8.529926	11.020109
1	7.833373	7.453776	12.970593
1	9.098941	3.551220	11.438151
1	6.465539	2.368241	19.656624
1	7.158426	4.219956	17.315768
1	4.707734	4.524123	15.575758
1	7.946655	1.329307	17.124320
1	3.393185	-0.031647	16.637366
1	3.530491	1.510803	19.336198
1	2.436836	2.884622	16.809575
1	5.831803	-0.329345	18.371958
1	4.147138	1.816118	14.443843
1	4.368804	4.392357	18.668443
6	5.901411	-1.473517	15.282385

6	6.407542	-2.283304	14.210090
6	7.163153	-1.742496	13.217224
6	7.445845	-0.350812	13.217498
6	6.171740	-0.091477	15.239161
1	6.180066	-3.343930	14.225257
1	7.547074	-2.367786	12.418351
7	6.901983	0.443476	14.247366
1	8.810255	-1.399395	11.071664
1	9.987675	-0.110801	9.378630
6	9.787764	4.711518	13.613634
6	10.403214	5.708826	12.851813
6	10.583548	3.762382	14.266082
6	11.790634	5.755801	12.745289
1	9.803069	6.442407	12.322813
6	11.970950	3.821815	14.170928
1	10.105780	2.969961	14.837557
6	12.576835	4.817270	13.408277
1	12.256892	6.528948	12.140487
1	12.577399	3.081786	14.685986
1	13.659711	4.858216	13.326182
8	10.194909	2.615432	9.434954
6	10.839049	2.032950	8.322588
1	11.266704	2.861954	7.757116
1	11.643158	1.355004	8.634770
1	10.129198	1.489481	7.686541

6	5.128183	-2.221136	16.307634
6	5.728921	-2.690679	17.474965
6	3.816698	-2.634970	16.030099
6	5.042330	-3.510197	18.368992
1	6.756604	-2.415736	17.694916
6	3.119328	-3.443641	16.910544
1	3.334443	-2.299724	15.115639
6	3.726413	-3.883951	18.092384
1	5.543280	-3.846346	19.270188
1	2.097137	-3.747765	16.707689
8	2.964757	-4.670718	18.889410
6	3.525952	-5.115906	20.101581
1	3.804191	-4.275049	20.750386
1	2.752107	-5.708359	20.592682
1	4.408881	-5.746528	19.931002
1	9.708285	5.574845	16.056879

TS

78	0.474800	0.215697	-0.131275
15	2.510444	-0.892799	-0.130790
6	2.616086	-2.588086	-0.818267
6	2.508859	-3.709973	0.011627
6	2.525266	-4.989854	-0.534164
6	2.641170	-5.164082	-1.909995
6	2.744572	-4.051389	-2.741543
6	2.733105	-2.770401	-2.200609

6	3.227606	-1.066251	1.544565
6	2.594972	-0.440790	2.623998
6	3.116693	-0.558290	3.910123
6	4.270045	-1.304204	4.131200
6	4.899190	-1.944042	3.064559
6	4.379571	-1.832182	1.779514
6	-2.469753	-0.709307	0.131392
6	-0.904344	-1.319900	0.209367
6	0.305590	3.068271	-0.165017
6	1.238826	2.047359	0.249956
6	2.520810	2.430322	0.666742
6	2.953828	3.739735	0.528700
6	2.082555	4.712925	-0.024234
6	0.791291	4.375118	-0.369918
5	-0.824077	-2.590124	1.324288
5	-0.879732	-2.902285	-0.412960
5	-1.886846	-1.667442	-1.157864
5	-3.538722	-1.855702	-0.528258
5	-3.488508	-1.539312	1.216479
5	-2.465153	-2.772039	1.972802
5	-2.546678	-3.281274	-0.862430
5	-3.535153	-3.202813	0.616378
5	-1.808618	-1.166347	1.652748
5	-1.887586	-3.861669	0.688154
1	2.394769	-3.588642	1.083863

1	2.433856	-5.851748	0.120695
1	2.647172	-6.164230	-2.334383
1	2.835585	-4.179078	-3.816651
1	1.687058	0.131902	2.449776
1	2.612988	-0.070398	4.739705
1	4.674185	-1.398075	5.135513
1	5.790946	-2.541089	3.234577
1	4.856363	-2.365666	0.961545
1	3.232689	1.713307	1.061486
1	-2.790762	-3.995367	-1.784874
1	0.070314	-3.264605	-1.019681
1	0.183684	-2.718608	1.945578
1	-1.649449	-1.125226	-2.187547
1	-4.349214	-0.930318	1.756392
1	-4.508734	-3.875697	0.760514
1	-2.657630	-3.118703	3.096655
1	-4.434073	-1.472897	-1.201476
1	-1.522386	-0.299095	2.411195
1	-1.654659	-5.014007	0.887520
6	-3.627229	1.577568	-0.159440
6	-3.434187	2.979560	-0.327489
6	-2.166171	3.516470	-0.369243
6	-1.058890	2.674328	-0.302534
6	-2.500700	0.769393	-0.112797
1	-4.310618	3.617553	-0.365911

1	-2.021899	4.591584	-0.415683
7	-1.247282	1.301837	-0.270548
1	0.135925	5.141148	-0.776348
1	2.416571	5.735754	-0.162603
6	3.727554	0.030148	-1.155014
6	5.091317	0.094360	-0.856006
6	3.252121	0.670573	-2.306045
6	5.963510	0.777468	-1.699395
1	5.478204	-0.367757	0.046310
6	4.128539	1.339228	-3.154914
1	2.185759	0.661675	-2.520633
6	5.486761	1.394293	-2.852567
1	7.019748	0.829231	-1.449514
1	3.745147	1.829626	-4.045478
1	6.170748	1.925250	-3.509179
8	4.221529	4.005949	0.935833
6	4.718816	5.310332	0.761775
1	5.742826	5.294351	1.139279
1	4.732172	5.604119	-0.296615
1	4.139667	6.048311	1.333390
6	-5.048523	1.145417	-0.051625
6	-5.771475	0.760643	-1.179267
6	-5.741289	1.279652	1.159689
6	-7.134046	0.473940	-1.109789
1	-5.262909	0.679834	-2.136125

6	-7.094422	0.998643	1.246301
1	-5.203161	1.599840	2.048016
6	-7.801109	0.587458	0.110613
1	-7.657332	0.166893	-2.008688
1	-7.630184	1.088063	2.186316
8	-9.120255	0.334378	0.294679
6	-9.864021	-0.105989	-0.816045
1	-9.471392	-1.049907	-1.216863
1	-10.881518	-0.264917	-0.454503
1	-9.879682	0.645436	-1.617112
1	2.819316	-1.911418	-2.859313

^{3}MC

78	7.507978	2.450587	14.180235
15	8.309680	4.640778	14.205238
6	8.900006	5.390084	15.775420
6	8.306191	5.011520	16.983609
6	8.724747	5.580032	18.183006
6	9.747644	6.524763	18.189931
6	10.350680	6.901419	16.992110
6	9.931581	6.338459	15.789948
6	7.101910	5.835741	13.532702
6	6.256250	5.403918	12.504010
6	5.352682	6.287990	11.922843
6	5.276190	7.603911	12.373076
6	6.106295	8.035221	13.405042

6	7.018880	7.157298	13.983240
6	5.250568	0.867933	15.722497
6	5.538995	2.359022	14.990162
6	8.679194	0.235118	12.688055
6	8.285250	1.583588	12.453637
6	8.737085	2.222186	11.305865
6	9.618638	1.584153	10.425863
6	10.062945	0.282206	10.695862
6	9.585168	-0.379359	11.819528
5	4.076466	3.043570	14.474657
5	4.872680	3.591055	15.945208
5	5.655075	2.198764	16.696228
5	4.387890	1.051009	17.177472
5	3.587877	0.495628	15.696137
5	2.808291	1.888254	14.928830
5	4.114887	2.792320	17.334386
5	2.826641	1.733399	16.703562
5	4.362611	1.316485	14.317434
5	3.121371	3.313119	15.950959
1	7.516800	4.267230	16.985483
1	8.252260	5.277303	19.113352
1	10.078725	6.963225	19.127553
1	11.153298	7.634216	16.991432
1	6.297924	4.366723	12.179225
1	4.696627	5.942367	11.128869

1	4.562375	8.290793	11.926386
1	6.041031	9.057959	13.766366
1	7.660247	7.498688	14.790696
1	8.447199	3.241407	11.068064
1	4.076689	3.309127	18.408019
1	5.431707	4.641127	15.971607
1	4.086379	3.705384	13.487941
1	6.732611	2.201219	17.201549
1	3.275068	-0.641102	15.560943
1	1.845883	1.485712	17.333987
1	1.824654	1.749511	14.270565
1	4.615800	0.312221	18.073741
1	4.612629	0.747830	13.306493
1	2.355762	4.223151	16.029537
6	6.261695	-1.534869	15.687720
6	7.147853	-2.355074	14.963671
6	7.972291	-1.853690	13.976225
6	8.000285	-0.471341	13.769215
6	6.297193	-0.167263	15.378316
1	7.136159	-3.421374	15.172660
1	8.572656	-2.519293	13.365502
7	7.231394	0.312493	14.545277
1	9.926776	-1.394729	12.009038
1	10.762037	-0.219952	10.036615
6	9.779834	4.824073	13.124174

6	9.850336	5.771585	12.099892
6	10.867898	3.970160	13.344528
6	10.993945	5.862270	11.307496
1	9.012220	6.437752	11.916776
6	12.010361	4.071398	12.560455
1	10.810575	3.216749	14.126874
6	12.073973	5.016145	11.536751
1	11.036446	6.598168	10.509033
1	12.848619	3.403996	12.741181
1	12.963889	5.088842	10.917212
8	9.991265	2.303879	9.341320
6	10.878851	1.710858	8.424212
1	11.038499	2.450345	7.637502
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1	10.455523	0.799510	7.981120
6	5.407169	-2.199168	16.704412
6	5.641183	-2.022372	18.067597
6	4.434243	-3.132222	16.317276
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1	6.411974	-1.328470	18.391726
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8	3.167699	-4.362039	19.467593
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