Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Unraveling the marked differences of the phosphorescence efficiencies of blue-emitting iridium complexes with isomerized phenyltriazole ligands

*Chongping Song, Yanan Chen, Jiaqi Li, Fei Zhao and Houyu Zhang**

State Key Laboratory of Supramolecular Structure and Materials,

Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130012, P. R. China

*Corresponding author

Email: houyuzhang@jlu.edu.cn

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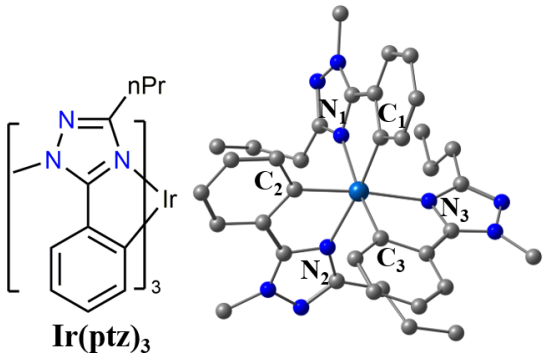
Table S1. Selected bond length (Å) at S_0 optimized geometry by using different functionals as well as experimental data for complex *fac*-tris(1-methyl-5-phenyl-3-propyl-1,2,4-triazolyl)iridium(III) (**Ir(ptz)$_3$**).



Ir(ptz)$_3$

	B3LYP	PBE0	M062X	Cam-B3LYP	EXP
Ir-N_1	2.2200	2.1774	2.2259	2.1941	2.1655
Ir-C_1	2.0338	2.0157	2.0067	2.0282	2.0417
Ir-N_2	2.2163	2.1736	2.2144	2.1909	2.1352
Ir-C_2	2.0315	2.0136	2.0080	2.0267	2.0021
Ir-N_3	2.2234	2.1764	2.2160	2.1920	2.1510
Ir-C_3	2.0304	2.0130	2.0061	2.0260	2.0217
σ	0.051	0.023	0.051	0.033	

Exp: from ref. 44.

σ denotes the standard deviation calculated by the formula $\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - x_{exp})^2}$

Table S2. Calculated absorption wavelengths (nm) by TD-DFT with different functionals in a CH_2Cl_2 solution in comparison to the available experimental absorption spectra for **Ir(ptz)$_3$.**

Compd	State	B3LYP	PBE0	MPW1K	Cam-B3LYP	EXP[a]
Ir(ptz)$_3$	**S_1**	371	352	301	305	350
	S_n	256	248	240	241	248
	T_1	413	412	438	403	
	T_2	408	409	437	403	

[a]Exp: from ref. 44.

Table S3. Compositions (%) and main contribution assignments of the frontier molecular orbitals in the ground states for **1-4**.

Comd	Orbital	Energy (eV)	Ir	L_1	L_2	L_3	Main assignments
1	LUMO+2	-0.72	3.44	18.5	63.1	14.9	π* (L_1) + π* (L_2) + π* (L_3)
	LUMO+1	-0.72	3.44	45.9	1.29	49.5	π* (L_1) + π* (L_3)
	LUMO	-0.90	1.33	32.9	32.9	32.9	π* (L_1) + π* (L_2) + π* (L_3)
	HOMO	-5.35	54.9	15.0	15.0	15.0	d_{z^2}(Ir) + π (L_1) + π (L_2) + π (L_3)
	HOMO-1	-5.52	52.8	8.22	25.4	13.6	$d_{x^2-y^2}$+d_{xy} +d_{yz}(Ir) + π (L_2) + π (L_3)
	HOMO-2	-5.52	52.8	23.2	6.06	17.9	$d_{x^2-y^2}$+d_{xz} +d_{xy}(Ir) + π (L_1) + π (L_3)
2	LUMO+2	-0.28	3.47	4.29	57.0	35.2	π* (L_2) + π* (L_3)
	LUMO+1	-0.28	3.47	60.1	7.31	29.2	π* (L_1) + π* (L_3)
	LUMO	-0.45	1.00	32.9	32.9	32.9	π* (L_1) + π* (L_2) + π* (L_3)
	HOMO	-4.91	54.3	15.2	15.2	15.2	d_{z^2}(Ir) + π (L_1) + π (L_2) + π (L_3)
	HOMO-1	-5.13	52.5	9.62	23.7	14.2	$d_{x^2-y^2}$+d_{xy} +d_{yz} (Ir) + π (L_2) + π
	HOMO-2	-5.13	52.5	22.1	7.99	17.5	$d_{x^2-y^2}$+d_{xz} +d_{xy} (Ir) + π (L_1) + π
3	LUMO+2	0.004	3.39	49.1	46.3	1.20	π* (L_1) + π* (L_2)
	LUMO1	0.004	3.39	15.3	18.1	63.2	π* (L_1) + π* (L_2) + π* (L_3)
	LUMO	-0.14	1.76	32.7	32.7	32.7	π* (L_1) + π* (L_2) + π* (L_3)
	HOMO	-4.93	50.6	16.5	16.5	16.5	d_{z^2}(Ir) + π (L_1) + π (L_2) + π (L_3)
	HOMO-1	-5.06	46.2	5.96	27.1	20.8	$d_{x^2-y^2}$+d_{yz} (Ir) + π (L_2) + π (L_3)
	HOMO-2	-5.06	46.2	29.9	8.78	15.1	d_{xz} +d_{xy} (Ir) + π (L_1) + π (L_3)
4	LUMO+2	-0.97	4.80	50.1	43.3	1.80	π* (L_1) + π* (L_2)
	LUMO+1	-0.97	4.80	13.4	20.1	61.7	π* (L_1) + π* (L_2) + π* (L_3)
	LUMO	-1.06	1.64	32.8	32.8	32.8	π* (L_1) + π* (L_2) + π* (L_3)
	HOMO	-5.73	46.2	17.9	17.9	17.9	d_{z^2}(Ir) + π (L_1) + π (L_2) + π (L_3)
	HOMO-1	-5.80	42.4	6.58	19.5	31.5	$d_{x^2-y^2}$+d_{xz} (Ir) + π (L_2) + π (L_3)
	HOMO-2	-5.80	42.4	31.8	18.9	6.90	d_{yz} +d_{xy} (Ir) + π (L_1) + π (L_2)

L_1, **L_2** and **L_3** denote phenyltriazole ligands.

Figure S1. Orbital interaction diagrams for **1-4**, formed by four fragments at their optimized S_0 geometries.

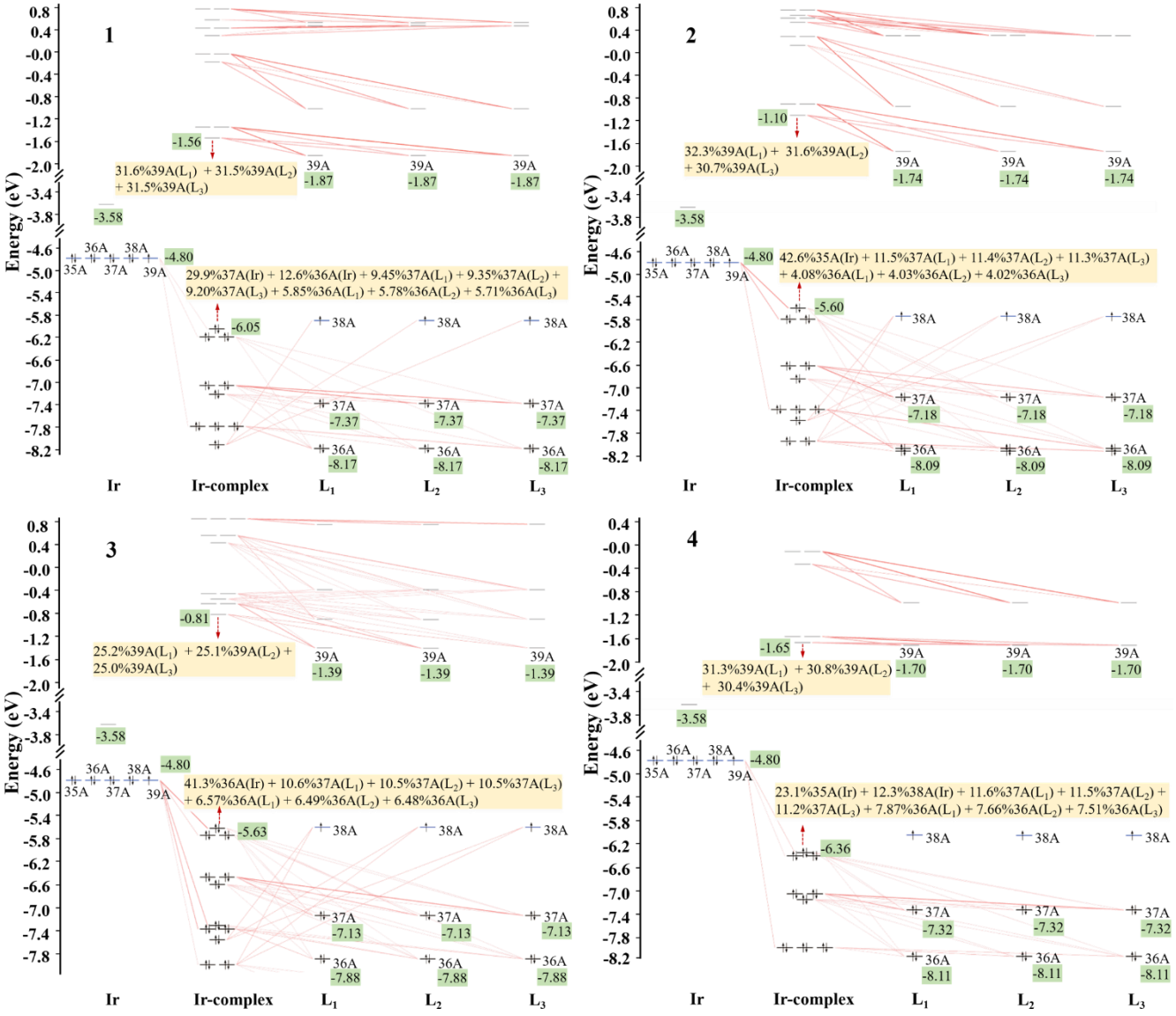


Table S4. Calculated absorption excited energies, dominant orbital excitations, and oscillator strength from **TD-DFT** calculations for the complexes **1-4**.

Comd	State	Excitation	λ(nm)	*f*
1	T_1	HOMO→LUMO (43.9%)	412.9	0.00
		HOMO-2→LUMO+1(9.46%)		
		HOMO-1→LUMO+2(9.46%)		
	T_2	HOMO→LUMO+2(16.9%)	409.6	0.00
		HOMO→LUMO+1(15.8%)		
		HOMO-2→LUMO (14.2%)		
		HOMO-3→LUMO (11.9%)		
	S_1	HOMO→LUMO (97.9%)	353.3	0.0201
	S_4	HOMO-1→LUMO (89.7%)	333.2	0.0364
	S_{28}	HOMO→LUMO+6(39.5%)	231.0	0.1678
	S_{50}	HOMO-2→LUMO+7(22.1%)	217.6	0.2445
		HOMO-1→LUMO+8(22.1%)		
		HOMO-1→LUMO+7(11.6%)		
		HOMO-2→LUMO+8(11.6%)		
2	T_1	HOMO→LUMO (48.4%)	415.7	0.00
		HOMO-1→LUMO+2 (8.38%)		
		HOMO-2→LUMO+1 (8.38%)		
	T_2	HOMO→LUMO+1(24.9%)	411.5	0.00
		HOMO-2→LUMO (12.7%)		
		HOMO→LUMO+2(12.4%)		
		HOMO-3→LUMO (12.0%)		
	S_1	HOMO→LUMO (97.6%)	355.6	0.0217
	S_4	HOMO-1→LUMO (92.8%)	329.4	0.0437
	S_{18}	HOMO-3→LUMO+2(22.9%)	246.1	0.1152
		HOMO-4→LUMO+1(22.9%)		
	S_{28}	HOMO-5→LUMO+1(45.0%)	234.0	0.1003
		HOMO→LUMO+7(13.2%)		
	S_{41}	HOMO-2→LUMO+8(24.5%)	224.9	0.1063
		HOMO-1→LUMO+7(24.5%)		
		HOMO-1-LUMO+8(12.8%)		
		HOMO-2-LUMO+7(12.8%)		
	S_{48}	HOMO-6→LUMO+1(13.2%)	216.8	0.2057
		HOMO-7→LUMO+2(13.2%)		
		HOMO-6→LUMO+2(11.9%)		
		HOMO-7→LUMO+1(11.9%)		
3	T_1	HOMO→LUMO+3(15.2%)	390.9	0.00
		HOMO-3→LUMO+4(8.20%)		
		HOMO-4→LUMO+5(8.20%)		
		HOMO-5→LUMO (8.10%)		
	T_2	HOMO→LUMO+4(15.9%)	390.5	0.00
		HOMO-3→LUMO (8.70%)		
	S_1	HOMO→LUMO+3(64.1%)	316.7	0.0027

		HOMO→LUMO (29.7%)		
	S_{12}	HOMO-1→LUMO+3(27.0%)	293.3	0.0601
		HOMO-1→LUMO+1(15.8%)		
		HOMO-2→LUMO+2(15.8%)		
	S_{43}	HOMO-5→LUMO+5(31.7%)	224.8	0.1139
		HOMO-1→LUMO+6(8.85%)		
	S_{45}	HOMO-6→LUMO (20.7%)	221.3	0.0837
		HOMO-6→LUMO+3(13.5%)		
4	T_1	HOMO→LUMO (27.1%)	404.4	0.00
		HOM-1→LUMO+1(15.3%)		
		HOMO-2→LUMO+2(15.2%)		
	T_2	HOMO→LUMO+2(20.8%)	403.9	0.00
		HOMO-2→LUMO (17.8%)		
	S_1	HOMO→LUMO (91.2%)	336.9	0.0220
	S_7	HOMO-1→LUMO+1(24.8%)	314.2	0.0646
		HOMO-2→LUMO+2(24.8%)		
		HOMO-1→LUMO+2(17.1%)		
		HOMO-2→LUMO+1(17.1%)		
	S_{12}	HOMO-4→LUMO+1(35.6%)	261.1	0.1866
		HOMO-3→LUMO+2(35.6%)		
		HOMO-5→LUMO (11.6%)		
	S_{33}	HOMO-8→LUMO+1(26.1%)	222.9	0.1437
		HOMO-7→LUMO+2(26.1%)		
		HOMO-2→LUMO+5(10.9%)		
		HOMO-1→LUMO+4(10.9%)		

Figure S2. Simulated vibronically-resolved emission spectrum by Franck-Condon calculations for **1-4.**

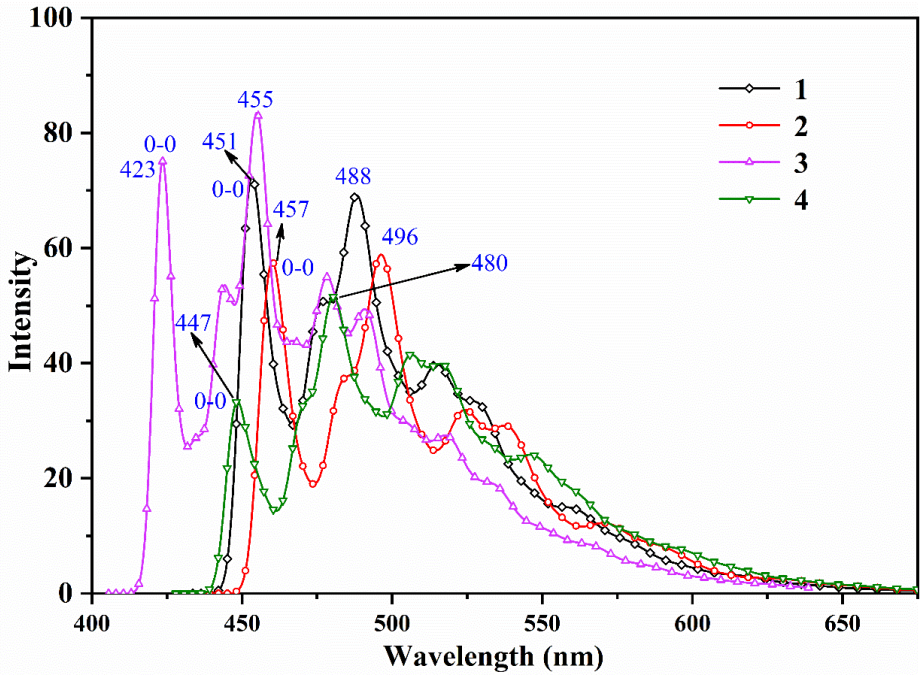


Figure S3. Energy-level diagrams of the T_1 and five S_n states with their dominant excitation in **1- 4**. The values in parentheses are the coefficients of the excited-state configuration and percentage of Ir d in the occupied orbitals, respectively.

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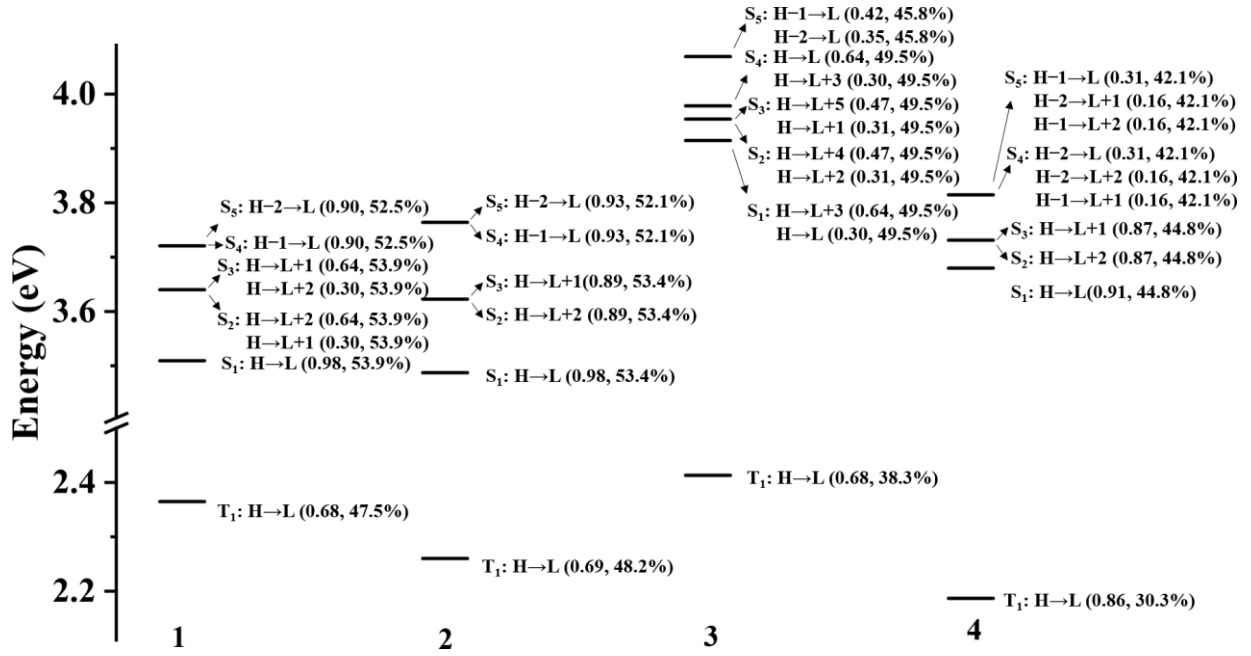

Analysis of the substituent effect:

Considering the effect of the substitution effect on k_{nr1}, we introduced a phenyl substituent on complex **2**, and the value of its k_{nr1} was calculated are listed in the following **Table S5**.

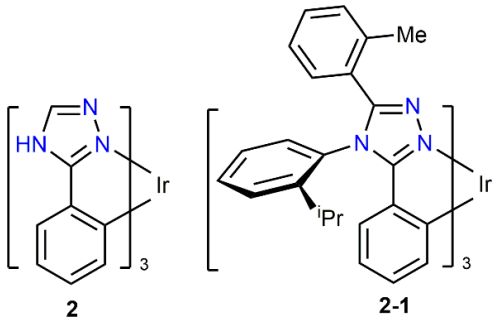

Table S5. Calculated k_{nr1} of the complexes **2-1** with phenyl substituted **ptz2** (Complex **2** as a reference).

Compd.	2	2-1
ΔE_{00}	21856.2	20969.0
SOC[a]	224.6	192.3
S_s	1.571	8.659
S_c	0.488	1.997
S_f	2.020	1.668
λ_s	140.1	350.6
λ_c	227.8	232.7
λ_f	2846.9	2396.0
λ_{total}	3214.8	2979.3
$\hbar\omega_s$	89.2	40.5
$\hbar\omega_c$	466.9	116.5
$\hbar\omega_f$	1409.1	1436.4
γ_0	1.038	1.169
k_{nr1}	4.17×10^4	1.29×10^4

[a] SOC denoted as $\langle T_1|H_{soc}|S_0\rangle$, which were calculated with PySOC package[1,2].

It can be seen from the calculation k_{nr1} that the introduction of the substituent is advantageous for suppressing the temperature-independent non-radiative decay process, which is beneficial for improving the quantum efficiency.

[1] X Gao, S Bai, D Fazzi, T Niehaus, M Barbatti, and W Thiel. *J. Chem. Theory Comput.* 2017, **13**, 515−524.

[2] SG Chiodo, M Leopoldini. *Comput. Phys. Commun.* 2014, **185**, 676–683.

Figure S4. Spin densities of the ^{3}**MC** states for all investigate complexes (isovalue = 0.002).

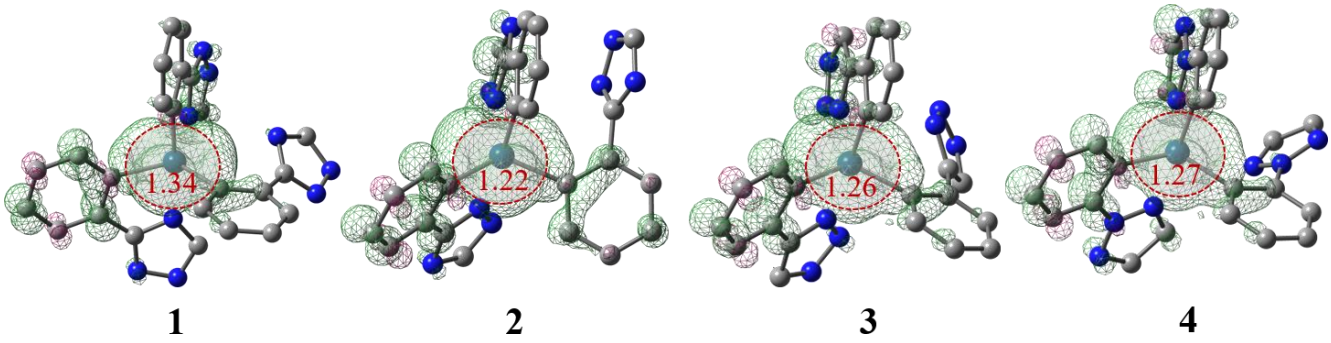

Figure S5. The curve of intrinsic reaction coordinate (IRC) of ^{3}**TS [T$_1$/^{3}MC]** for **1-4**.

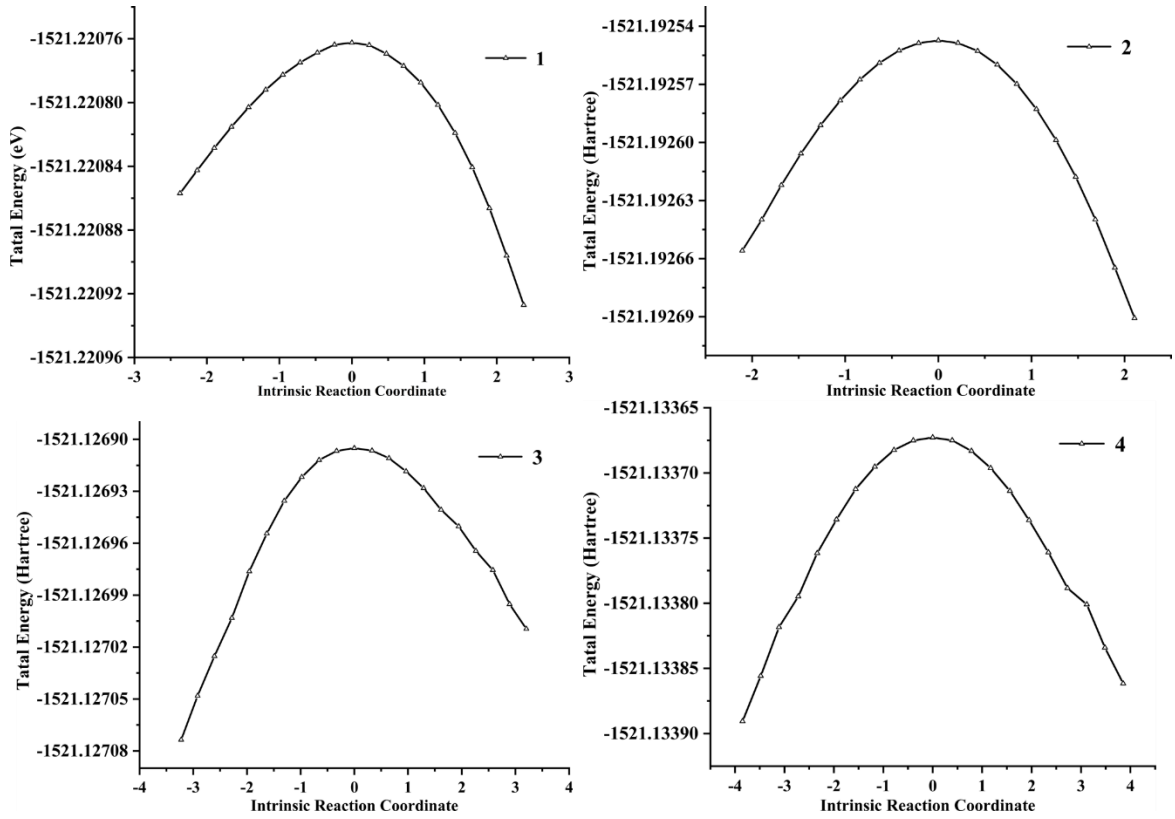

Figure S6. The optimized structures of the ^{3}**TS [T$_1$-^{3}MC]** for **1-4**.

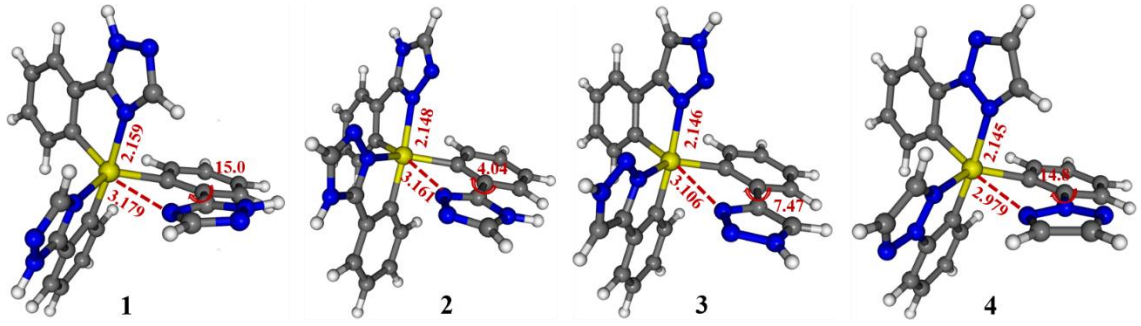

Table S6. Vibrational frequencies (cm^{-1}) at the respective optimized S_0 and T_1 states, dimensionless displacement ΔQ_i, huang-rhys factors S_i and reorganization energy λ_i (cm^{-1}) of **1**.

ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)		ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)
33	-0.126	7.94E-03	0.3	30		1013	-0.355	6.30E-02	63.7	1009
33	0.545	1.49E-01	4.8	34		1013	-0.048	1.15E-03	1.1	1012
34	0.124	7.69E-03	0.3	37		1017	0.109	5.94E-03	6	1013
46	-0.07	2.45E-03	0.1	44		1060	-0.743	2.76E-01	292.5	1014
46	0.683	2.33E-01	10.8	47		1060	0.04	8.00E-04	0.9	1017
54	-0.539	1.45E-01	7.8	52		1068	0.312	4.87E-02	51.9	1061
92	0.022	2.42E-04	0	71		1078	-0.034	5.78E-04	0.6	1065
92	-0.066	2.18E-03	0.2	96		1078	-0.302	4.56E-02	49.1	1072
95	0.306	4.68E-02	4.5	97		1085	-0.326	5.31E-02	57.5	1078
156	0.309	4.77E-02	7.5	142		1130	-0.195	1.90E-02	21.5	1082
159	0.394	7.76E-02	12.4	155		1131	0.238	2.83E-02	31.9	1122
159	0.133	8.84E-03	1.4	159		1131	-0.089	3.96E-03	4.4	1133
173	0.131	8.58E-03	1.5	160		1149	0.057	1.62E-03	1.9	1133
175	-0.606	1.84E-01	32.2	170		1149	-0.006	1.80E-05	0	1148
175	-0.279	3.89E-02	6.8	173		1151	-0.036	6.48E-04	0.7	1150
191	0.104	5.41E-03	1	188		1176	0.112	6.27E-03	7.3	1152
214	0.098	4.80E-03	1	200		1176	0.003	4.50E-06	0	1176
214	0.165	1.36E-02	2.9	211		1177	0.104	5.41E-03	6.3	1177
232	0.34	5.78E-02	13.4	214		1190	0.129	8.32E-03	9.9	1180
232	-0.053	1.40E-03	0.3	228		1190	-0.199	1.98E-02	23.5	1190
260	0.364	6.62E-02	17.2	228		1190	-0.03	4.50E-04	0.5	1191
283	-0.428	9.16E-02	25.9	253		1248	0.088	3.87E-03	4.8	1206
316	-0.044	9.68E-04	0.3	268		1248	-0.074	2.74E-03	3.4	1247
316	0.066	2.18E-03	0.7	279		1249	0.085	3.61E-03	4.5	1248
321	0.402	8.08E-02	25.9	302		1285	0.034	5.78E-04	0.8	1252
321	-0.04	8.00E-04	0.3	314		1285	-0.064	2.05E-03	2.7	1288
325	-0.16	1.28E-02	4.1	320		1286	-0.07	2.45E-03	3.1	1293
404	-0.075	2.81E-03	1.1	323		1345	0.032	5.12E-04	0.7	1327
404	-0.04	8.00E-04	0.3	401		1345	-0.084	3.53E-03	4.8	1348
414	0.007	2.45E-05	0	403		1346	-0.045	1.01E-03	1.3	1349
461	0.136	9.25E-03	4.2	406		1357	0.082	3.36E-03	4.5	1357
461	-0.08	3.20E-03	1.5	415		1357	-0.094	4.42E-03	6	1357
467	-0.022	2.42E-04	0.1	464		1357	-0.089	3.96E-03	5.3	1359
505	0.166	1.38E-02	7	465		1377	-0.217	2.35E-02	32.4	1379
507	0.168	1.41E-02	7.1	470		1378	-0.202	2.04E-02	28	1379
507	-0.201	2.02E-02	10.3	503		1378	0.22	2.42E-02	33.5	1383
541	-0.058	1.68E-03	0.9	506		1438	0.212	2.25E-02	32.3	1402
541	0.066	2.18E-03	1.2	507		1438	-0.335	5.61E-02	80.8	1440
541	-0.094	4.42E-03	2.4	539		1441	0.268	3.59E-02	51.6	1442
574	-0.054	1.46E-03	0.8	541		1484	0.16	1.28E-02	19	1448

574	-0.03	4.50E-04	0.3	578		1484	0.3	4.50E-02	66.9	1452
575	0.032	5.12E-04	0.3	580		1486	0.221	2.44E-02	36.1	1485
669	-0.504	1.27E-01	85.1	612		1499	0.148	1.10E-02	16.4	1487
669	0.141	9.94E-03	6.6	637		1499	-0.192	1.84E-02	27.5	1493
671	0.444	9.86E-02	66.3	665		1499	0.057	1.62E-03	2.5	1496
689	0.005	1.25E-05	0	669		1581	0.193	1.86E-02	29.5	1498
689	-0.025	3.13E-04	0.2	670		1581	-0.128	8.19E-03	12.9	1500
689	0.039	7.61E-04	0.5	680		1581	-0.117	6.84E-03	10.7	1579
718	0.015	1.13E-04	0.1	687		1609	0.125	7.81E-03	12.6	1580
718	-0.027	3.65E-04	0.3	688		1609	-0.736	2.71E-01	435.2	1587
718	0.024	2.88E-04	0.2	689		1610	0.542	1.47E-01	236.2	1611
740	-0.035	6.13E-04	0.4	720		1636	-0.166	1.38E-02	22.7	1612
741	0.022	2.42E-04	0.2	721		1636	-0.032	5.12E-04	0.9	1637
741	-0.003	4.50E-06	0	733		1636	-0.106	5.62E-03	9.2	1638
764	0.008	3.20E-05	0	740		1681	0.537	1.44E-01	242.6	1652
765	0.007	2.45E-05	0	742		1681	0.282	3.98E-02	67	1680
765	-0.05	1.25E-03	1	763		1684	-0.439	9.64E-02	162.5	1682
808	0.032	5.12E-04	0.4	764		3181	-0.013	8.45E-05	0.3	3184
808	-0.006	1.80E-05	0	765		3181	-0.025	3.13E-04	1	3185
811	-0.035	6.13E-04	0.5	808		3181	0.023	2.65E-04	0.8	3193
890	0.005	1.25E-05	0	811		3201	0.03	4.50E-04	1.4	3202
890	0.01	5.00E-05	0	892		3201	0.001	5.00E-07	0	3204
893	-0.014	9.80E-05	0.1	894		3201	0.023	2.65E-04	0.9	3212
896	-0.003	4.50E-06	0	896		3229	0.001	5.00E-07	0	3219
896	-0.005	1.25E-05	0	898		3229	0.004	8.00E-06	0	3224
899	0.018	1.62E-04	0.1	901		3229	0	0.00E+00	0	3224
951	-0.011	6.05E-05	0.1	937		3235	0.006	1.80E-05	0.1	3233
951	0.012	7.20E-05	0.1	938		3235	0.008	3.20E-05	0.1	3234
951	-0.02	2.00E-04	0.2	954		3235	0.008	3.20E-05	0.1	3240
993	0.311	4.84E-02	48.2	954		3315	0.001	5.00E-07	0	3302
993	0.115	6.61E-03	6.5	963		3315	0.002	2.00E-06	0	3316
994	-0.265	3.51E-02	34.9	990		3315	-0.001	5.00E-07	0	3318
1010	-0.02	2.00E-04	0.2	993		3725	0.014	9.80E-05	0.4	3724
1010	-0.014	9.80E-05	0.1	994		3725	0.032	5.12E-04	1.9	3724
1011	0.021	2.21E-04	0.2	995		3725	0.022	2.42E-04	0.9	3751

Table S7. Vibrational frequencies (cm^{-1}) at the respective optimized S_0 and T_1 states, dimensionless displacement ΔQ_i, huang-rhys factors S_i and reorganization energy λ_i (cm^{-1}) of **2**.

ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)		ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)
31	0.485	1.18E-01	3.7	30		1006	0.03	4.50E-04	0.5	1000
31	-0.203	2.06E-02	0.6	33		1006	-0.057	1.62E-03	1.6	1001
34	0.766	2.93E-01	10	37		1006	0.006	1.80E-05	0	1006
45	-0.721	2.60E-01	11.8	46		1058	0.391	7.64E-02	80.7	1008
45	0.68	2.31E-01	10.5	47		1058	0.567	1.61E-01	169.8	1012
52	0.26	3.38E-02	1.7	52		1066	-0.298	4.44E-02	47.5	1059
93	-0.152	1.16E-02	1.1	72		1074	-0.173	1.50E-02	16	1062
93	0.022	2.42E-04	0	93		1074	0.116	6.73E-03	7.2	1067
94	0.258	3.33E-02	3.1	99		1076	-0.237	2.81E-02	30.2	1074
160	-0.35	6.13E-02	9.8	145		1125	-0.084	3.53E-03	4	1078
163	-0.454	1.03E-01	16.7	157		1126	0.153	1.17E-02	13.2	1111
163	-0.327	5.35E-02	8.7	163		1126	0.127	8.06E-03	9.1	1128
174	0.2	2.00E-02	3.5	165		1130	-0.105	5.51E-03	6.3	1129
178	0.198	1.96E-02	3.5	174		1130	0.244	2.98E-02	33.7	1131
178	-0.789	3.11E-01	55.3	179		1134	-0.195	1.90E-02	21.5	1133
188	0.03	4.50E-04	0.1	183		1169	-0.112	6.27E-03	7.3	1146
215	-0.187	1.75E-02	3.8	195		1169	0.166	1.38E-02	16.1	1169
215	0.013	8.45E-05	0	213		1173	0.158	1.25E-02	14.6	1171
234	0.338	5.71E-02	13.4	220		1186	0.058	1.68E-03	2	1173
234	0.072	2.59E-03	0.6	227		1186	0.005	1.25E-05	0	1187
265	0.202	2.04E-02	5.4	230		1187	-0.082	3.36E-03	4	1188
288	-0.259	3.35E-02	9.7	256		1189	-0.101	5.10E-03	6	1189
318	-0.205	2.10E-02	6.7	269		1189	-0.157	1.23E-02	14.7	1190
318	-0.11	6.05E-03	1.9	284		1191	-0.098	4.80E-03	5.7	1200
324	-0.268	3.59E-02	11.6	305		1275	0.085	3.61E-03	4.6	1233
324	-0.158	1.25E-02	4.1	317		1275	0.048	1.15E-03	1.5	1254
326	-0.209	2.18E-02	7.1	321		1275	0.089	3.96E-03	5.1	1276
403	0.01	5.00E-05	0	324		1301	-0.058	1.68E-03	2.2	1280
403	0.165	1.36E-02	5.5	400		1301	0.027	3.65E-04	0.5	1302
412	0.034	5.78E-04	0.2	402		1302	-0.052	1.35E-03	1.8	1303
459	0.004	8.00E-06	0	405		1358	-0.15	1.13E-02	15.2	1332
459	-0.08	3.20E-03	1.5	415		1358	0.031	4.81E-04	0.7	1356
463	0.019	1.81E-04	0.1	458		1358	-0.112	6.27E-03	8.5	1360
508	-0.039	7.61E-04	0.4	464		1402	0.313	4.90E-02	68.8	1362
508	-0.029	4.21E-04	0.2	484		1402	0.327	5.35E-02	74.9	1402
508	-0.082	3.36E-03	1.7	500		1402	0.315	4.96E-02	69.5	1403
542	0.047	1.10E-03	0.6	507		1460	-0.337	5.68E-02	82.9	1414
543	0.006	1.80E-05	0	511		1460	0.203	2.06E-02	30.1	1428
543	-0.04	8.00E-04	0.4	540		1463	0.257	3.30E-02	48.3	1442
558	-0.186	1.73E-02	9.7	542		1481	0.025	3.13E-04	0.5	1460

559	0.216	2.33E-02	13.1	559		1481	0.194	1.88E-02	27.9	1462
559	-0.122	7.44E-03	4.2	561		1481	0.136	9.25E-03	13.7	1481
668	-0.083	3.44E-03	2.3	606		1521	0.041	8.41E-04	1.3	1482
668	0.434	9.42E-02	63	637		1521	0.094	4.42E-03	6.8	1506
670	-0.402	8.08E-02	54.2	655		1521	-0.034	5.78E-04	0.9	1520
680	-0.001	5.00E-07	0	667		1561	0.329	5.41E-02	84.5	1522
680	-0.035	6.13E-04	0.4	670		1561	0.114	6.50E-03	10.1	1542
681	-0.041	8.41E-04	0.6	679		1561	-0.45	1.01E-01	157.8	1561
717	-0.001	5.00E-07	0	680		1607	0.581	1.69E-01	271.4	1562
717	0.065	2.11E-03	1.5	682		1607	-0.386	7.45E-02	119.6	1593
717	-0.005	1.25E-05	0	691		1609	0.504	1.27E-01	204.3	1610
737	0.045	1.01E-03	0.7	718		1634	-0.107	5.72E-03	9.4	1611
738	-0.017	1.45E-04	0.1	720		1634	-0.007	2.45E-05	0	1636
738	-0.008	3.20E-05	0	732		1635	0.059	1.74E-03	2.8	1636
760	-0.033	5.45E-04	0.4	738		1681	-0.703	2.47E-01	414.8	1678
762	-0.032	5.12E-04	0.4	739		1681	-0.355	6.30E-02	105.9	1680
762	-0.028	3.92E-04	0.3	759		1683	0.573	1.64E-01	275.9	1684
793	0.009	4.05E-05	0	760		3174	-0.012	7.20E-05	0.2	3177
793	0.016	1.28E-04	0.1	762		3174	0.024	2.88E-04	0.9	3178
794	-0.047	1.10E-03	0.9	782		3174	0.023	2.65E-04	0.8	3187
815	-0.002	2.00E-06	0	796		3197	-0.013	8.45E-05	0.3	3198
815	-0.02	2.00E-04	0.2	797		3197	0.021	2.21E-04	0.7	3201
816	0.039	7.61E-04	0.6	818		3197	0.02	2.00E-04	0.6	3206
887	0.004	8.00E-06	0	819		3222	0.009	4.05E-05	0.1	3214
887	-0.004	8.00E-06	0	887		3222	0.004	8.00E-06	0	3220
889	-0.023	2.65E-04	0.2	891		3223	0.007	2.45E-05	0.1	3222
945	-0.002	2.00E-06	0	911		3229	0.001	5.00E-07	0	3230
945	0.023	2.65E-04	0.2	932		3229	-0.009	4.05E-05	0.1	3230
945	0.035	6.13E-04	0.6	947		3230	-0.01	5.00E-05	0.1	3233
985	-0.098	4.80E-03	4.7	951		3318	-0.003	4.50E-06	0	3310
985	0.083	3.44E-03	3.4	952		3318	-0.003	4.50E-06	0	3318
985	-0.186	1.73E-02	17.1	959		3318	-0.004	8.00E-06	0	3318
999	0.296	4.38E-02	43.8	985		3727	0.028	3.92E-04	1.4	3726
999	-0.425	9.03E-02	90.4	985		3727	-0.016	1.28E-04	0.5	3726
1001	0.304	4.62E-02	46.3	989		3728	0.02	2.00E-04	0.7	3754

Table S8. Vibrational frequencies (cm^{-1}) at the respective optimized S_0 and T_1 states, dimensionless displacement ΔQ_i, huang-rhys factors S_i and reorganization energy λ_i (cm^{-1}) of **3**.

ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)		ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)
32	0.186	1.73E-02	0.6	29		1013	0.115	6.61E-03	6.7	1003
32	0.748	2.80E-01	9	34		1013	-0.085	3.61E-03	3.7	1004
34	-0.095	4.51E-03	0.2	35		1014	0.03	4.50E-04	0.5	1007
47	-0.41	8.41E-02	3.9	45		1061	-0.844	3.56E-01	378.2	1015
47	0.43	9.25E-02	4.3	47		1061	0	0.00E+00	0	1015
54	0.072	2.59E-03	0.1	52		1068	0.452	1.02E-01	109.1	1057
94	-0.013	8.45E-05	0	67		1080	-0.005	1.25E-05	0	1061
94	0.182	1.66E-02	1.6	95		1080	0.266	3.54E-02	38.2	1067
98	0.287	4.12E-02	4	100		1084	0.313	4.90E-02	53.1	1078
160	0.14	9.80E-03	1.6	148		1109	0.073	2.66E-03	2.9	1082
164	-0.088	3.87E-03	0.6	158		1109	0.076	2.89E-03	3.2	1083
164	0.171	1.46E-02	2.4	162		1109	0.044	9.68E-04	1.1	1109
176	0.013	8.45E-05	0	167		1141	0.381	7.26E-02	82.7	1109
180	-0.274	3.75E-02	6.8	175		1141	0.128	8.19E-03	9.3	1119
180	0.112	6.27E-03	1.1	175		1142	0.294	4.32E-02	49.5	1143
196	-0.001	5.00E-07	0	193		1171	-0.079	3.12E-03	3.7	1144
220	-0.025	3.13E-04	0.1	216		1171	-0.017	1.45E-04	0.2	1160
220	0.083	3.44E-03	0.8	217		1173	0.101	5.10E-03	6	1172
237	0.204	2.08E-02	4.9	232		1187	-0.272	3.70E-02	44	1173
237	0.068	2.31E-03	0.6	234		1187	0.037	6.85E-04	0.8	1187
268	0.263	3.46E-02	9.3	259		1187	0.183	1.67E-02	19.8	1187
287	0.387	7.49E-02	21.5	270		1197	-0.075	2.81E-03	3.4	1194
320	-0.137	9.38E-03	3	283		1197	0.033	5.45E-04	0.6	1199
320	0.025	3.13E-04	0.1	308		1202	0.062	1.92E-03	2.3	1200
332	0.159	1.26E-02	4.2	318		1275	0.013	8.45E-05	0.1	1207
332	-0.03	4.50E-04	0.2	331		1275	-0.106	5.62E-03	7.1	1277
338	-0.179	1.60E-02	5.4	335		1280	-0.092	4.23E-03	5.4	1282
402	0.13	8.45E-03	3.4	373		1344	0.202	2.04E-02	27.6	1299
402	0.03	4.50E-04	0.2	400		1344	-0.144	1.04E-02	13.9	1341
411	0.052	1.35E-03	0.6	401		1345	0.167	1.39E-02	18.7	1345
471	-0.109	5.94E-03	2.8	411		1346	0.047	1.10E-03	1.5	1345
471	0.009	4.05E-05	0	457		1346	-0.403	8.12E-02	109.2	1349
479	-0.041	8.41E-04	0.4	469		1347	-0.282	3.98E-02	53.6	1349
511	-0.166	1.38E-02	7.1	477		1384	-0.014	9.80E-05	0.1	1350
513	-0.185	1.71E-02	8.8	496		1384	-0.042	8.82E-04	1.2	1385
513	-0.145	1.05E-02	5.4	498		1386	0.034	5.78E-04	0.8	1387
547	0.052	1.35E-03	0.7	511		1402	-0.004	8.00E-06	0	1396
547	0.049	1.20E-03	0.7	512		1402	0.08	3.20E-03	4.5	1402
547	-0.046	1.06E-03	0.6	519		1403	-0.054	1.46E-03	2	1403
576	-0.034	5.78E-04	0.3	546		1486	-0.05	1.25E-03	1.8	1431

576	0.007	2.45E-05	0	547		1487	-0.141	9.94E-03	14.7	1459
576	0.027	3.65E-04	0.2	581		1487	-0.048	1.15E-03	1.7	1483
670	0.597	1.78E-01	119.5	587		1490	-0.168	1.41E-02	21	1486
670	-0.167	1.39E-02	9.4	614		1490	-0.459	1.05E-01	156.7	1487
672	0.489	1.20E-01	80.2	633		1491	0.346	5.99E-02	89.2	1490
686	-0.001	5.00E-07	0	637		1531	-0.158	1.25E-02	19.1	1491
686	0.019	1.81E-04	0.1	668		1532	0.211	2.23E-02	34	1510
686	-0.007	2.45E-05	0	670		1532	-0.037	6.85E-04	1	1532
715	-0.129	8.32E-03	6	673		1627	-0.519	1.35E-01	219.3	1533
715	0.069	2.38E-03	1.7	686		1627	0.594	1.76E-01	286.7	1573
715	0.19	1.81E-02	12.9	687		1628	-0.562	1.58E-01	256.6	1628
738	-0.048	1.15E-03	0.8	689		1641	-0.178	1.58E-02	26	1629
738	0.015	1.13E-04	0.1	716		1642	-0.149	1.11E-02	18.2	1642
738	-0.009	4.05E-05	0	717		1642	-0.154	1.19E-02	19.4	1642
763	-0.013	8.45E-05	0.1	729		1678	-0.763	2.91E-01	487.9	1663
764	-0.012	7.20E-05	0.1	737		1678	-0.269	3.62E-02	60.5	1677
764	-0.021	2.21E-04	0.2	738		1680	0.571	1.63E-01	273.6	1679
766	-0.023	2.65E-04	0.2	748		3185	-0.028	3.92E-04	1.2	3186
766	-0.01	5.00E-05	0	764		3185	0.017	1.45E-04	0.4	3187
766	0.011	6.05E-05	0	765		3185	-0.024	2.88E-04	0.9	3191
813	-0.029	4.21E-04	0.3	767		3197	-0.026	3.38E-04	1.1	3197
813	0.011	6.05E-05	0	768		3197	0.003	4.50E-06	0	3199
816	0.024	2.88E-04	0.2	813		3197	-0.021	2.21E-04	0.7	3211
892	0.003	4.50E-06	0	815		3223	-0.007	2.45E-05	0.1	3217
892	0.005	1.25E-05	0	893		3223	-0.001	5.00E-07	0	3219
894	-0.021	2.21E-04	0.2	895		3223	0.008	3.20E-05	0.1	3221
950	0.011	6.05E-05	0.1	921		3232	0.022	2.42E-04	0.7	3227
950	-0.006	1.80E-05	0	931		3232	-0.001	5.00E-07	0	3228
951	-0.025	3.13E-04	0.3	952		3233	0.013	8.45E-05	0.3	3237
987	-0.254	3.23E-02	31.8	953		3333	-0.024	2.88E-04	0.9	3334
987	-0.396	7.84E-02	77.3	960		3333	0.001	5.00E-07	0	3334
989	0.29	4.21E-02	41.6	963		3333	-0.034	5.78E-04	1.9	3344
1002	0.033	5.45E-04	0.5	977		3718	-0.006	1.80E-05	0.1	3714
1002	-0.007	2.45E-05	0	987		3718	-0.008	3.20E-05	0.1	3716
1004	0.01	5.00E-05	0.1	989		3718	0.003	4.50E-06	0	3722

Table S9. Vibrational frequencies (cm^{-1}) at the respective optimized S_0 and T_1 states, dimensionless displacement ΔQ_i, huang-rhys factors S_i and reorganization energy λ_i (cm^{-1}) of **4**.

ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)		ω_i (S_0)	ΔQ_i	S_i	λ_i	ω_i (T_1)
33	-0.844	3.56E-01	11.6	30		1009	-0.128	8.19E-03	8.3	1004
33	0.192	1.84E-02	0.6	33		1009	0.6	1.80E-01	181.3	1008
35	0.527	1.39E-01	4.8	35		1013	-0.288	4.15E-02	41.9	1008
45	-0.03	4.50E-04	0	44		1061	0.298	4.44E-02	47	1011
45	0.244	2.98E-02	1.3	46		1061	-0.551	1.52E-01	161.2	1025
53	0.236	2.78E-02	1.5	54		1065	0.158	1.25E-02	13.3	1051
98	0.171	1.46E-02	1.4	80		1068	-0.127	8.06E-03	8.6	1061
98	-0.03	4.50E-04	0	98		1068	-0.014	9.80E-05	0.1	1065
101	0.025	3.13E-04	0	100		1069	0.312	4.87E-02	52.2	1067
162	0.117	6.84E-03	1.1	146		1104	-0.555	1.54E-01	170.2	1068
162	-0.239	2.86E-02	4.6	159		1104	0.001	5.00E-07	0	1095
166	0.261	3.41E-02	5.7	163		1112	-0.407	8.28E-02	92	1104
172	0.045	1.01E-03	0.2	166		1141	-0.092	4.23E-03	4.8	1109
184	0.122	7.44E-03	1.4	177		1142	-0.12	7.20E-03	8.2	1126
184	-0.044	9.68E-04	0.2	181		1142	0.078	3.04E-03	3.5	1142
193	0.309	4.77E-02	9.2	185		1169	0.182	1.66E-02	19.3	1143
217	-0.153	1.17E-02	2.5	208		1169	0.21	2.21E-02	25.7	1154
217	0.447	9.99E-02	21.7	214		1170	-0.245	3.00E-02	35.1	1170
240	-0.113	6.38E-03	1.5	233		1187	0.123	7.56E-03	9	1172
240	0.05	1.25E-03	0.3	238		1187	-0.158	1.25E-02	14.8	1182
275	-0.249	3.10E-02	8.5	258		1187	-0.127	8.06E-03	9.6	1187
285	0.605	1.83E-01	52.2	270		1200	-0.008	3.20E-05	0	1187
312	-0.022	2.42E-04	0.1	278		1200	-0.146	1.07E-02	12.7	1195
312	0.274	3.75E-02	11.7	310		1201	-0.094	4.42E-03	5.3	1198
322	0.202	2.04E-02	6.6	312		1283	-0.024	2.88E-04	0.4	1201
325	-0.1	5.00E-03	1.6	321		1283	0.011	6.05E-05	0.1	1261
325	0.332	5.51E-02	17.9	321		1285	-0.012	7.20E-05	0.1	1285
416	-0.395	7.80E-02	32.5	410		1348	-0.021	2.21E-04	0.3	1287
416	0.259	3.35E-02	14	415		1348	-0.312	4.87E-02	65.6	1341
425	-0.28	3.92E-02	16.7	418		1349	-0.199	1.98E-02	26.8	1344
470	-0.108	5.83E-03	2.8	428		1365	0.142	1.01E-02	13.7	1349
470	0.046	1.06E-03	0.5	471		1365	-0.075	2.81E-03	3.8	1365
475	0.032	5.12E-04	0.2	473		1365	0.121	7.32E-03	10	1368
533	0.093	4.32E-03	2.3	479		1386	-0.099	4.90E-03	6.9	1369
534	-0.126	7.94E-03	4.2	527		1387	-0.115	6.61E-03	9.1	1388
534	0.01	5.00E-05	0	532		1387	-0.034	5.78E-04	0.8	1389
556	0.143	1.02E-02	5.7	536		1446	0.466	1.09E-01	157.3	1410
556	-0.033	5.45E-04	0.3	555		1446	-0.102	5.20E-03	7.5	1445
557	0.113	6.38E-03	3.5	556		1447	-0.353	6.23E-02	90.1	1447
670	0.311	4.84E-02	32.5	561		1491	-0.238	2.83E-02	42.3	1454

670	0.235	2.76E-02	18.4	597		1491	0.582	1.69E-01	252.9	1473
671	0.279	3.89E-02	26.2	646		1492	0.349	6.09E-02	90.7	1490
673	0.046	1.06E-03	0.7	669		1499	-0.328	5.38E-02	80.8	1492
673	0.031	4.81E-04	0.3	671		1499	0.14	9.80E-03	14.6	1498
674	-0.14	9.80E-03	6.6	672		1501	-0.38	7.22E-02	108.5	1499
717	-0.169	1.43E-02	10.2	672		1506	-0.81	3.28E-01	494	1501
718	-0.107	5.72E-03	4.1	704		1506	-0.107	5.72E-03	8.6	1504
718	-0.14	9.80E-03	7	715		1506	0.565	1.60E-01	240.4	1508
728	-0.048	1.15E-03	0.8	718		1539	-0.165	1.36E-02	20.8	1514
728	0.049	1.20E-03	0.9	722		1543	-0.045	1.01E-03	1.5	1540
729	0.032	5.12E-04	0.4	728		1543	0.24	2.88E-02	44.6	1543
764	0.017	1.45E-04	0.1	730		1639	-0.599	1.79E-01	294	1596
764	-0.007	2.45E-05	0	734		1639	-0.039	7.61E-04	1.3	1641
764	0.006	1.80E-05	0	741		1640	0.419	8.78E-02	143.8	1641
781	-0.006	1.80E-05	0	763		1671	0.102	5.20E-03	8.6	1651
781	-0.005	1.25E-05	0	765		1671	-0.176	1.55E-02	26	1672
783	0.013	8.45E-05	0.1	780		1674	0.139	9.66E-03	16.1	1674
821	0.002	2.00E-06	0	784		3207	-0.015	1.13E-04	0.3	3206
821	-0.028	3.92E-04	0.3	814		3207	-0.015	1.13E-04	0.3	3207
824	-0.041	8.41E-04	0.7	822		3207	0.015	1.13E-04	0.3	3215
882	-0.002	2.00E-06	0	829		3227	0.003	4.50E-06	0	3224
882	-0.012	7.20E-05	0.1	838		3227	0.011	6.05E-05	0.2	3224
883	0.02	2.00E-04	0.2	850		3227	0.008	3.20E-05	0.1	3228
896	-0.005	1.25E-05	0	883		3233	0.001	5.00E-07	0	3231
896	0.002	2.00E-06	0	889		3233	-0.007	2.45E-05	0.1	3232
899	0.021	2.21E-04	0.2	895		3233	0.006	1.80E-05	0.1	3241
967	-0.014	9.80E-05	0.1	899		3245	0.022	2.42E-04	0.8	3246
967	0.005	1.25E-05	0	955		3245	-0.007	2.45E-05	0.1	3246
968	-0.025	3.13E-04	0.3	957		3246	0.017	1.45E-04	0.5	3263
980	-0.335	5.61E-02	55	967		3312	0.006	1.80E-05	0.1	3296
980	0.593	1.76E-01	172.3	969		3312	-0.002	2.00E-06	0	3312
980	-0.474	1.12E-01	110	980		3312	-0.004	8.00E-06	0	3312
1006	0.05	1.25E-03	1.3	981		3332	0.003	4.50E-06	0	3323
1006	-0.023	2.65E-04	0.3	986		3332	0.004	8.00E-06	0	3332
1007	0.035	6.13E-04	0.6	1001		3332	0.001	5.00E-07	0	3332

Table S10. Cartesian coordinates of **1** at the $\mathbf{T_1}$ optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.007344	-0.019979	-0.159707
2	7	0	-0.177156	1.860944	-1.260885
3	6	0	-0.798349	2.479836	-2.293051
4	7	0	-0.458710	3.742628	-2.435414
5	7	0	0.424986	3.922160	-1.427253
6	6	0	0.599771	2.798716	-0.713511
7	6	0	1.408765	2.486080	0.440938
8	6	0	2.260281	3.404831	1.064302
9	6	0	2.995403	3.013450	2.171760
10	6	0	2.868207	1.703793	2.640725
11	6	0	2.019475	0.793947	2.016750
12	6	0	1.256657	1.146961	0.892484
13	7	0	1.621692	-0.734073	-1.329730
14	6	0	2.404887	-0.458622	-2.379870
15	7	0	3.372330	-1.338498	-2.593166
16	7	0	3.185569	-2.242196	-1.598979
17	6	0	2.129807	-1.891115	-0.792729
18	6	0	1.561855	-2.434061	0.347090
19	6	0	1.981835	-3.637512	1.006580
20	6	0	1.290245	-4.070078	2.102137
21	6	0	0.159743	-3.355652	2.619354
22	6	0	-0.256282	-2.175857	1.999159
23	6	0	0.387987	-1.654061	0.877768
24	7	0	-1.537358	-1.027932	-1.308601
25	6	0	-1.750028	-1.811570	-2.392992
26	7	0	-3.010461	-2.145359	-2.562731
27	7	0	-3.618420	-1.535526	-1.518188
28	6	0	-2.742657	-0.862888	-0.755972
29	6	0	-2.887199	-0.068674	0.441663
30	6	0	-4.113284	0.172336	1.070997
31	6	0	-4.149839	0.951405	2.216710
32	6	0	-2.956587	1.479169	2.715592
33	6	0	-1.740268	1.234927	2.082886
34	6	0	-1.653974	0.451029	0.922387
35	1	0	2.351027	4.422222	0.687648
36	1	0	3.659833	3.715405	2.666087
37	1	0	3.440987	1.389305	3.509856
38	1	0	1.932855	-0.212865	2.414992
39	1	0	2.835170	-4.200614	0.637459
40	1	0	1.605215	-4.984192	2.600758
41	1	0	-0.356530	-3.734560	3.494894
42	1	0	-1.103291	-1.633378	2.409784
43	1	0	-5.036123	-0.245658	0.672146
44	1	0	-5.092786	1.147132	2.717911
45	1	0	-2.978158	2.089036	3.615719
46	1	0	-0.831483	1.653918	2.505275
47	1	0	-0.963365	-2.136738	-3.057572
48	1	0	-4.612102	-1.636015	-1.392935
49	1	0	-1.507004	1.990117	-2.944393
50	1	0	0.849043	4.824844	-1.291278
51	1	0	2.271050	0.406845	-3.013363
52	1	0	3.825116	-3.009806	-1.497864

Table S11. Cartesian coordinates of **2** at the $\mathbf{T_1}$ optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.009767	0.007888	-0.153983
2	7	0	-1.365327	1.071469	-1.291581
3	7	0	-2.525107	2.910692	-1.632429
4	6	0	-1.574482	2.344055	-0.798980
5	6	0	-0.911115	2.748000	0.334848
6	6	0	-1.029647	4.029406	0.983146
7	6	0	-0.261425	4.291510	2.080008
8	6	0	0.652167	3.325701	2.604871
9	6	0	0.769769	2.068863	1.994942
10	6	0	0.024709	1.710658	0.878400
11	7	0	1.724066	0.632771	-1.284223
12	7	0	3.863753	0.625119	-1.555847
13	6	0	2.853445	0.174385	-0.770496
14	6	0	2.826909	-0.638298	0.422310
15	6	0	3.968068	-1.166931	1.032807
16	6	0	3.833985	-1.936553	2.178813
17	6	0	2.556973	-2.164577	2.695328
18	6	0	1.425594	-1.634319	2.078953
19	6	0	1.511771	-0.849244	0.919475
20	7	0	-0.301332	-1.836932	-1.230669
21	7	0	-1.438629	-3.653346	-1.480467
22	6	0	-1.300619	-2.536453	-0.722097
23	6	0	-1.991908	-2.055269	0.450217
24	6	0	-3.042690	-2.733683	1.074151
25	6	0	-3.628372	-2.191292	2.208625
26	6	0	-3.151544	-0.975610	2.703314
27	6	0	-2.105351	-0.303860	2.075741
28	6	0	-1.487082	-0.813214	0.923945
29	1	0	-1.722977	4.776382	0.603715
30	1	0	-0.346792	5.258003	2.572122
31	1	0	1.241005	3.569444	3.483397
32	1	0	1.453484	1.339050	2.419825
33	1	0	4.958766	-0.979867	0.620665
34	1	0	4.710279	-2.352967	2.666501
35	1	0	2.444667	-2.763153	3.596497
36	1	0	0.449114	-1.824323	2.515887
37	1	0	-3.404016	-3.682634	0.680472
38	1	0	-4.444349	-2.707989	2.704976
39	1	0	-3.604010	-0.546943	3.594472
40	1	0	-1.746604	0.633850	2.490834
41	1	0	-2.117130	-4.386191	-1.357681
42	1	0	-2.865343	3.854652	-1.604765
43	1	0	4.846968	0.449681	-1.433111
44	6	0	-2.827474	1.948416	-2.555624
45	7	0	-2.149976	0.844723	-2.353575
46	1	0	-3.543661	2.089368	-3.351613
47	7	0	1.971961	1.377333	-2.387280
48	6	0	3.267661	1.363137	-2.540819
49	1	0	3.811156	1.859712	-3.330396
50	7	0	0.223645	-2.472940	-2.304121
51	6	0	-0.474257	-3.567138	-2.445424
52	1	0	-0.324502	-4.311817	-3.212483

Table S12. Cartesian coordinates of **3** at the T_1 optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.008437	-0.020618	-0.161466
2	7	0	-0.479197	1.783000	-1.233281
3	6	0	0.127255	2.891065	-0.709868
4	6	0	0.973114	2.683241	0.451023
5	6	0	1.658281	3.723292	1.085441
6	6	0	2.445122	3.455903	2.196709
7	6	0	2.536637	2.143783	2.662276
8	6	0	1.851280	1.110264	2.027817
9	6	0	1.046809	1.338659	0.901508
10	7	0	1.723202	-0.462229	-1.307117
11	6	0	2.456419	-1.529009	-0.789421
12	6	0	1.956687	-2.143901	0.352154
13	6	0	2.584023	-3.262374	1.020005
14	6	0	1.981756	-3.807367	2.107359
15	6	0	0.730910	-3.294475	2.621746
16	6	0	0.114982	-2.199417	1.998354
17	6	0	0.652580	-1.574340	0.882923
18	7	0	-1.360765	-1.256187	-1.274156
19	6	0	-2.617200	-1.300141	-0.735098
20	6	0	-2.837614	-0.526188	0.473177
21	6	0	-4.072041	-0.478914	1.127161
22	6	0	-4.212431	0.277763	2.281974
23	6	0	-3.109824	0.979643	2.769884
24	6	0	-1.881540	0.928416	2.113911
25	6	0	-1.697317	0.177538	0.943606
26	1	0	1.574688	4.741633	0.710465
27	1	0	2.980052	4.258538	2.696172
28	1	0	3.148734	1.924054	3.534051
29	1	0	1.927699	0.100432	2.421369
30	1	0	3.526462	-3.656352	0.648512
31	1	0	2.448692	-4.650391	2.612416
32	1	0	0.286286	-3.756782	3.496699
33	1	0	-0.812539	-1.814518	2.412201
34	1	0	-4.921123	-1.035962	0.735337
35	1	0	-5.167333	0.319406	2.798035
36	1	0	-3.208425	1.571730	3.676986
37	1	0	-1.039995	1.477981	2.525847
38	7	0	-1.216700	2.074180	-2.257861
39	7	0	2.280687	0.045810	-2.350106
40	7	0	-1.269125	-1.976163	-2.347669
41	6	0	-0.279038	3.950276	-1.490870
42	1	0	-0.067190	5.006733	-1.464206
43	7	0	-1.094662	3.386101	-2.414520
44	7	0	3.384639	-0.665086	-2.561041
45	7	0	-2.474894	-2.500240	-2.519742
46	6	0	3.568702	-1.657405	-1.647524
47	1	0	4.410269	-2.328068	-1.669165
48	6	0	-3.353125	-2.123317	-1.558439
49	1	0	-4.378036	-2.456298	-1.538890
50	1	0	-2.629083	-3.108604	-3.307923
51	1	0	-1.595100	3.831783	-3.166686
52	1	0	3.966734	-0.419988	-3.344722

Table S13. Cartesian coordinates of **4** at the $\mathbf{T_1}$ optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.004799	-0.013506	-0.175035
2	7	0	-1.307414	-1.312074	-1.293450
3	6	0	-2.784449	-0.673117	0.435294
4	6	0	-4.037003	-0.752463	1.033970
5	6	0	-4.250012	-0.023819	2.196865
6	6	0	-3.216799	0.753299	2.720897
7	6	0	-1.973226	0.807589	2.093321
8	6	0	-1.706285	0.091423	0.918633
9	7	0	-0.565052	1.760785	-1.250656
10	6	0	0.819738	2.724274	0.393412
11	6	0	1.412266	3.846550	0.961031
12	6	0	2.222751	3.664751	2.073418
13	6	0	2.413674	2.379631	2.581113
14	6	0	1.802946	1.276943	1.987445
15	6	0	0.977639	1.407030	0.862101
16	7	0	1.722209	-0.424789	-1.343493
17	6	0	2.024271	-2.036901	0.322186
18	6	0	2.747224	-3.106013	0.943096
19	6	0	2.208355	-3.667859	2.061044
20	6	0	0.965724	-3.206887	2.606600
21	6	0	0.271537	-2.159799	2.006007
22	6	0	0.742372	-1.520643	0.857444
23	1	0	-4.811401	-1.372388	0.594249
24	1	0	-5.215960	-0.063770	2.690804
25	1	0	-3.382155	1.322910	3.631787
26	1	0	-1.184279	1.414370	2.528219
27	1	0	1.233259	4.827644	0.533662
28	1	0	2.700795	4.520045	2.540680
29	1	0	3.046690	2.234496	3.452616
30	1	0	1.961148	0.289674	2.411586
31	1	0	3.685919	-3.429602	0.509509
32	1	0	2.730710	-4.483073	2.554623
33	1	0	0.572870	-3.681201	3.500343
34	1	0	-0.659117	-1.815052	2.445754
35	7	0	-0.019973	2.857885	-0.737719
36	7	0	-0.342106	3.966354	-1.361269
37	6	0	-1.153228	3.567134	-2.344928
38	6	0	-1.299729	2.181349	-2.281833
39	1	0	-1.584590	4.278134	-3.033106
40	1	0	-1.866814	1.490389	-2.885542
41	6	0	3.630402	-0.797966	-2.420297
42	6	0	2.484617	-0.005520	-2.372780
43	7	0	3.639018	-1.711370	-1.441108
44	7	0	2.467736	-1.448030	-0.782608
45	1	0	4.448931	-0.747796	-3.124217
46	1	0	2.172245	0.813176	-3.002349
47	7	0	-2.517568	-1.402332	-0.751176
48	7	0	-3.346467	-2.179749	-1.405959
49	6	0	-2.630723	-2.628039	-2.442392
50	6	0	-1.346818	-2.086837	-2.378973
51	1	0	-3.062572	-3.304702	-3.164167
52	1	0	-0.480330	-2.204713	-3.010767

Table S14. Cartesian coordinates of **1** at the ^{3}**MC** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.349163	0.083578	0.016766
2	7	0	3.005588	-0.168927	-0.607193
3	6	0	3.907207	-0.619423	-1.513837
4	7	0	4.367350	-1.839149	-1.301920
5	7	0	3.706975	-2.180794	-0.180761
6	6	0	2.890763	-1.183403	0.237731
7	6	0	2.072262	-1.290866	1.449457
8	6	0	2.645111	-1.942330	2.554958
9	6	0	1.933467	-2.124986	3.730681
10	6	0	0.630043	-1.642269	3.808868
11	6	0	0.065220	-0.980391	2.722537
12	6	0	0.756690	-0.787234	1.514916
13	7	0	-0.841629	-1.860392	-0.805078
14	6	0	-0.288359	-3.007998	-1.265149
15	7	0	-1.172544	-3.913644	-1.625708
16	7	0	-2.346796	-3.294296	-1.371224
17	6	0	-2.158959	-2.060769	-0.877599
18	6	0	-3.067392	-1.019086	-0.451834
19	6	0	-4.458913	-1.134694	-0.471311
20	6	0	-5.237196	-0.068210	-0.040330
21	6	0	-4.617014	1.099681	0.408444
22	6	0	-3.228628	1.207905	0.430547
23	6	0	-2.406006	0.156837	-0.001955
24	7	0	0.501158	0.984598	-1.743058
25	6	0	0.908333	0.731782	-3.011047
26	7	0	1.519616	1.746553	-3.577803
27	7	0	1.495280	2.687258	-2.602605
28	6	0	0.890555	2.240054	-1.493843
29	6	0	0.632641	2.834793	-0.205639
30	6	0	0.949899	4.154750	0.128550
31	6	0	0.654653	4.627704	1.397912
32	6	0	0.047209	3.770349	2.318720
33	6	0	-0.265005	2.456869	1.979246
34	6	0	0.012405	1.937431	0.705632
35	1	0	3.678580	-2.278323	2.496991
36	1	0	2.393263	-2.624743	4.578009
37	1	0	0.051715	-1.772857	4.720014
38	1	0	-0.956670	-0.615980	2.810015
39	1	0	-4.940054	-2.047445	-0.818161
40	1	0	-6.320221	-0.144933	-0.051995
41	1	0	-5.227338	1.935178	0.742345
42	1	0	-2.771286	2.126480	0.786588
43	1	0	1.422945	4.813961	-0.597190
44	1	0	0.894951	5.650280	1.672018
45	1	0	-0.181739	4.134516	3.317359
46	1	0	-0.725890	1.815554	2.725944
47	1	0	0.750776	-0.210677	-3.513581
48	1	0	1.920613	3.584557	-2.766539
49	1	0	4.237901	-0.030369	-2.358788
50	1	0	3.834421	-3.093478	0.226336
51	1	0	0.777285	-3.171275	-1.330426
52	1	0	-3.212637	-3.773373	-1.556399

Table S15. Cartesian coordinates of **2** at the ^{3}**MC** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.488304	0.091270	-0.129397
2	7	0	-2.107602	-0.985526	-1.022532
3	7	0	-4.228004	-1.245932	-1.345791
4	6	0	-3.295672	-0.496369	-0.705649
5	6	0	-3.376936	0.643485	0.174225
6	6	0	-4.572819	1.221560	0.604941
7	6	0	-4.534797	2.329503	1.440749
8	6	0	-3.299068	2.848175	1.835344
9	6	0	-2.109395	2.265967	1.408101
10	6	0	-2.099413	1.140780	0.567417
11	7	0	0.549129	0.595937	-1.869774
12	7	0	2.382605	1.313818	-2.757023
13	6	0	1.661900	1.278757	-1.613921
14	6	0	1.910838	1.748366	-0.273956
15	6	0	2.978752	2.567066	0.102614
16	6	0	3.140168	2.905946	1.439610
17	6	0	2.236952	2.408833	2.383230
18	6	0	1.172106	1.595820	1.998820
19	6	0	0.957886	1.245691	0.656041
20	7	0	2.919988	-1.204623	-0.966034
21	7	0	3.742061	-0.897344	1.033663
22	6	0	2.677803	-1.370591	0.315920
23	6	0	1.534367	-2.028739	0.972261
24	6	0	1.846800	-3.132216	1.780351
25	6	0	0.858888	-3.832393	2.459095
26	6	0	-0.465987	-3.432009	2.316053
27	6	0	-0.781896	-2.347712	1.503958
28	6	0	0.195984	-1.598216	0.824447
29	1	0	-5.533106	0.814106	0.292646
30	1	0	-5.458199	2.788371	1.781090
31	1	0	-3.267337	3.722109	2.481403
32	1	0	-1.165376	2.697467	1.726340
33	1	0	3.678088	2.941290	-0.642397
34	1	0	3.959739	3.548883	1.746842
35	1	0	2.364959	2.664976	3.432740
36	1	0	0.490603	1.218283	2.757650
37	1	0	2.883576	-3.454087	1.853854
38	1	0	1.119084	-4.685730	3.078610
39	1	0	-1.258550	-3.969112	2.831316
40	1	0	-1.825463	-2.057877	1.409872
41	1	0	3.776603	-0.797130	2.035232
42	1	0	-5.226422	-1.121916	-1.320610
43	1	0	3.370372	1.509599	-2.805258
44	6	0	-3.524517	-2.187323	-2.046363
45	7	0	-2.241469	-2.042777	-1.858194
46	1	0	-3.985286	-2.941776	-2.665975
47	7	0	0.537498	0.173520	-3.159814
48	6	0	1.659755	0.593171	-3.669290
49	1	0	1.985657	0.421768	-4.684110
50	7	0	4.138539	-0.587106	-1.090422
51	6	0	4.610108	-0.405865	0.115757
52	1	0	5.550410	0.063132	0.367278

Table S16. Cartesian coordinates of **3** at the ^{3}**MC** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.341714	-0.124383	0.057421
2	7	0	3.047302	0.320836	0.180064
3	6	0	2.712240	1.442243	-0.522414
4	6	0	1.748081	1.470399	-1.631455
5	6	0	2.116781	2.179347	-2.785272
6	6	0	1.265369	2.281821	-3.876550
7	6	0	0.024201	1.655142	-3.823434
8	6	0	-0.344827	0.940270	-2.686828
9	6	0	0.491847	0.835703	-1.564297
10	7	0	-0.960917	1.763626	0.877720
11	6	0	-2.317527	1.898105	0.997787
12	6	0	-3.118166	0.757374	0.593743
13	6	0	-4.512909	0.746344	0.639088
14	6	0	-5.206712	-0.390705	0.242159
15	6	0	-4.499481	-1.510405	-0.198311
16	6	0	-3.108013	-1.497058	-0.246982
17	6	0	-2.372395	-0.366747	0.144583
18	7	0	0.803456	-0.853244	1.670250
19	6	0	1.311385	-2.108672	1.454816
20	6	0	0.950324	-2.746268	0.204986
21	6	0	1.357294	-4.034112	-0.149768
22	6	0	0.969956	-4.568521	-1.371254
23	6	0	0.180220	-3.802934	-2.230025
24	6	0	-0.223178	-2.518954	-1.871462
25	6	0	0.140107	-1.947113	-0.643763
26	1	0	3.103077	2.637071	-2.824491
27	1	0	1.572458	2.832401	-4.761279
28	1	0	-0.658646	1.716056	-4.667406
29	1	0	-1.323720	0.465296	-2.663184
30	1	0	-5.058867	1.622570	0.982958
31	1	0	-6.292313	-0.405154	0.276078
32	1	0	-5.040604	-2.402629	-0.504026
33	1	0	-2.578005	-2.379430	-0.593480
34	1	0	1.976837	-4.618217	0.527783
35	1	0	1.282565	-5.569192	-1.654978
36	1	0	-0.120446	-4.211610	-3.191911
37	1	0	-0.828384	-1.943159	-2.567139
38	7	0	3.940699	0.609727	1.072913
39	7	0	-0.338809	2.831735	1.266589
40	7	0	1.192803	-0.358300	2.808778
41	6	0	3.464598	2.484679	-0.021602
42	1	0	3.505579	3.534923	-0.262598
43	7	0	4.200383	1.917256	0.956633
44	7	0	-1.291530	3.674243	1.647918
45	7	0	1.959868	-1.296750	3.343609
46	6	0	-2.536135	3.158481	1.504991
47	1	0	-3.429898	3.703064	1.763026
48	6	0	2.075222	-2.397162	2.560642
49	1	0	2.673482	-3.250140	2.836351
50	1	0	2.396513	-1.114080	4.232849
51	1	0	4.874143	2.345479	1.570735
52	1	0	-1.024253	4.582770	1.991690

Table S17. Cartesian coordinates of **4** at the ^{3}**MC** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.325362	0.094879	-0.015387
2	7	0	3.899674	-1.460561	0.130278
3	6	0	1.815891	-1.765536	1.282188
4	6	0	2.360779	-2.508636	2.330627
5	6	0	1.659581	-2.644349	3.519152
6	6	0	0.409736	-2.043145	3.642250
7	6	0	-0.112906	-1.295000	2.591041
8	6	0	0.579024	-1.118188	1.381942
9	7	0	-1.336384	-1.578701	-0.882216
10	6	0	-3.217343	-0.301670	-0.288718
11	6	0	-4.593148	-0.137280	-0.206877
12	6	0	-5.076641	1.036678	0.361423
13	6	0	-4.188444	2.005527	0.831286
14	6	0	-2.812561	1.811735	0.738445
15	6	0	-2.277692	0.645496	0.169910
16	7	0	0.669848	0.876482	-1.718411
17	6	0	1.269419	2.529377	-0.155305
18	6	0	1.925847	3.710510	0.171650
19	6	0	1.851204	4.153491	1.485306
20	6	0	1.135564	3.410524	2.426399
21	6	0	0.491141	2.230449	2.063977
22	6	0	0.529267	1.744809	0.749101
23	1	0	3.334959	-2.967458	2.195362
24	1	0	2.080384	-3.222681	4.335883
25	1	0	-0.159983	-2.148460	4.561686
26	1	0	-1.084302	-0.821288	2.716391
27	1	0	-5.256744	-0.911104	-0.578501
28	1	0	-6.148326	1.193260	0.438083
29	1	0	-4.574543	2.921042	1.271190
30	1	0	-2.135944	2.575821	1.108940
31	1	0	2.473480	4.256488	-0.589444
32	1	0	2.352345	5.071788	1.775110
33	1	0	1.084975	3.754936	3.455951
34	1	0	-0.047501	1.663556	2.818620
35	7	0	-2.661807	-1.470009	-0.851771
36	7	0	-3.304116	-2.499906	-1.354733
37	6	0	-2.332890	-3.332412	-1.736911
38	6	0	-1.090737	-2.762647	-1.441425
39	1	0	-2.565858	-4.283208	-2.192082
40	1	0	-0.072239	-3.096909	-1.569797
41	6	0	1.594395	1.713421	-3.522261
42	6	0	0.841517	0.652855	-3.028555
43	7	0	1.870926	2.563143	-2.524961
44	7	0	1.301628	2.025773	-1.473305
45	1	0	1.943741	1.905859	-4.525444
46	1	0	0.428859	-0.222892	-3.502973
47	7	0	2.597370	-1.686639	0.090396
48	7	0	2.094685	-1.913278	-1.114963
49	6	0	3.149463	-1.811529	-1.922675
50	6	0	4.276140	-1.531739	-1.144577
51	1	0	3.051063	-1.946272	-2.989862
52	1	0	5.306127	-1.378775	-1.430888

Table S18. Cartesian coordinates of **1** at the **^{3}TS** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.306271	-0.000282	0.029231
2	7	0	2.711120	0.211746	-0.949672
3	6	0	3.758148	0.113807	-1.803245
4	7	0	4.844716	-0.443365	-1.302597
5	7	0	4.453179	-0.710224	-0.042971
6	6	0	3.175025	-0.316498	0.175513
7	6	0	2.465443	-0.487345	1.442287
8	6	0	3.220284	-0.790765	2.589164
9	6	0	2.615751	-1.035819	3.810433
10	6	0	1.227085	-0.974083	3.896161
11	6	0	0.477848	-0.637751	2.774228
12	6	0	1.059696	-0.374913	1.520998
13	7	0	-0.066585	-1.991097	-0.770067
14	6	0	0.857293	-2.841034	-1.279135
15	7	0	0.365303	-4.015582	-1.612355
16	7	0	-0.941478	-3.889460	-1.289868
17	6	0	-1.211237	-2.676247	-0.784331
18	6	0	-2.427439	-2.052230	-0.309890
19	6	0	-3.667736	-2.691339	-0.256792
20	6	0	-4.773521	-1.994515	0.213584
21	6	0	-4.627427	-0.669497	0.628822
22	6	0	-3.386441	-0.038680	0.577907
23	6	0	-2.245977	-0.703629	0.103727
24	7	0	-0.024425	1.104473	-1.803977
25	6	0	0.321712	0.978025	-3.107932
26	7	0	0.370473	2.122484	-3.750920
27	7	0	0.039607	3.016592	-2.788055
28	6	0	-0.197677	2.415282	-1.612219
29	6	0	-0.561757	2.908198	-0.306943
30	6	0	-0.795386	4.256986	-0.020186
31	6	0	-1.150321	4.631639	1.265969
32	6	0	-1.265558	3.646582	2.249902
33	6	0	-1.030454	2.306463	1.957017
34	6	0	-0.668749	1.877781	0.669453
35	1	0	4.306884	-0.810604	2.534628
36	1	0	3.218331	-1.267001	4.683558
37	1	0	0.726417	-1.174018	4.840023
38	1	0	-0.605145	-0.593282	2.870292
39	1	0	-3.779023	-3.726032	-0.576213
40	1	0	-5.743703	-2.480099	0.258645
41	1	0	-5.494457	-0.124544	0.994023
42	1	0	-3.298416	0.991851	0.910198
43	1	0	-0.704073	5.013533	-0.797705
44	1	0	-1.335140	5.674603	1.503820
45	1	0	-1.541544	3.932004	3.262239
46	1	0	-1.122079	1.575625	2.755049
47	1	0	0.539402	0.031377	-3.578827
48	1	0	0.006884	3.997630	-3.010240
49	1	0	3.722579	0.468117	-2.824857
50	1	0	5.082604	-1.187147	0.580944
51	1	0	1.897714	-2.580941	-1.404460
52	1	0	-1.569347	-4.660795	-1.445498

Table S19. Cartesian coordinates of **2** at the **^{3}TS** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.358278	-0.063980	0.047633
2	7	0	-1.698133	1.087618	1.269421
3	7	0	-3.708899	1.589270	1.881073
4	6	0	-2.972750	0.818970	1.041148
5	6	0	-3.327761	-0.152991	0.032680
6	6	0	-4.638611	-0.483770	-0.316508
7	6	0	-4.861077	-1.433692	-1.305556
8	6	0	-3.771924	-2.037353	-1.937161
9	6	0	-2.466519	-1.699021	-1.587539
10	6	0	-2.196620	-0.750725	-0.589796
11	7	0	0.430242	-1.304448	1.567020
12	7	0	1.812825	-2.857268	2.136642
13	6	0	1.295489	-2.187241	1.079937
14	6	0	1.521051	-2.264886	-0.340186
15	6	0	2.359809	-3.191040	-0.964435
16	6	0	2.503306	-3.160850	-2.344632
17	6	0	1.806294	-2.200377	-3.081713
18	6	0	0.970766	-1.279973	-2.452523
19	6	0	0.792970	-1.278961	-1.061455
20	7	0	2.651789	0.477908	0.846687
21	7	0	4.019618	2.083761	0.311196
22	6	0	2.758440	1.577046	0.133703
23	6	0	1.727998	2.185802	-0.705626
24	6	0	2.057318	3.334253	-1.444879
25	6	0	1.124942	3.986113	-2.235837
26	6	0	-0.174890	3.491556	-2.287136
27	6	0	-0.510712	2.356181	-1.557320
28	6	0	0.418075	1.655885	-0.766514
29	1	0	-5.486412	-0.007718	0.173966
30	1	0	-5.875812	-1.701446	-1.584910
31	1	0	-3.946984	-2.782151	-2.709802
32	1	0	-1.636488	-2.180996	-2.096269
33	1	0	2.900069	-3.935111	-0.381129
34	1	0	3.151364	-3.875001	-2.843770
35	1	0	1.920068	-2.170220	-4.162939
36	1	0	0.448393	-0.538154	-3.052102
37	1	0	3.069290	3.733843	-1.417062
38	1	0	1.408726	4.869467	-2.800231
39	1	0	-0.928745	3.989266	-2.892017
40	1	0	-1.533515	1.988365	-1.613175
41	1	0	4.401152	2.928182	-0.078997
42	1	0	-4.711884	1.610146	1.960713
43	6	0	-2.802296	2.312746	2.605274
44	7	0	-1.582622	2.020523	2.243932
45	1	0	-3.076132	3.025983	3.367986
46	7	0	0.378689	-1.382194	2.918822
47	6	0	1.224914	-2.317298	3.247693
48	1	0	1.440124	-2.641234	4.254805
49	7	0	3.833742	0.252565	1.491135
50	6	0	4.641174	1.225102	1.161073
51	1	0	5.659563	1.350395	1.500326
52	1	0	2.547530	-3.544164	2.109247

Table S20. Cartesian coordinates of **3** at the **^{3}TS** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.324053	0.049620	-0.019661
2	7	0	2.612923	-0.496698	-0.869808
3	6	0	2.823221	-1.583456	-0.076468
4	6	0	1.847428	-2.058268	0.907261
5	6	0	2.235546	-3.099970	1.765855
6	6	0	1.369852	-3.630247	2.708816
7	6	0	0.079590	-3.116009	2.802656
8	6	0	-0.313575	-2.082435	1.958168
9	6	0	0.548145	-1.516500	1.001430
10	7	0	-1.464975	-1.323526	-1.211304
11	6	0	-2.820710	-1.178897	-1.091642
12	6	0	-3.282811	-0.134563	-0.194273
13	6	0	-4.632680	0.115253	0.058345
14	6	0	-4.992211	1.133768	0.933290
15	6	0	-3.999018	1.892611	1.553803
16	6	0	-2.652602	1.638387	1.303433
17	6	0	-2.250366	0.623964	0.421049
18	7	0	0.436129	1.282717	-1.596531
19	6	0	1.143780	2.357620	-1.124617
20	6	0	1.275241	2.477813	0.314690
21	6	0	1.968154	3.518680	0.937490
22	6	0	2.045129	3.566668	2.323078
23	6	0	1.427056	2.566357	3.075520
24	6	0	0.737344	1.529791	2.451492
25	6	0	0.634364	1.449189	1.054601
26	1	0	3.245898	-3.497329	1.698302
27	1	0	1.697919	-4.433395	3.362593
28	1	0	-0.621379	-3.515653	3.531411
29	1	0	-1.326013	-1.692682	2.051222
30	1	0	-5.403295	-0.482588	-0.424317
31	1	0	-6.041109	1.333856	1.132993
32	1	0	-4.279706	2.689717	2.238106
33	1	0	-1.894556	2.236735	1.800939
34	1	0	2.447440	4.291794	0.339880
35	1	0	2.582150	4.373248	2.813859
36	1	0	1.487051	2.595391	4.161084
37	1	0	0.272209	0.757601	3.059564
38	7	0	3.625932	-0.303420	-1.651849
39	7	0	-1.156581	-2.276690	-2.032020
40	7	0	0.374176	1.272139	-2.893188
41	6	0	4.066950	-2.091383	-0.406545
42	1	0	4.639458	-2.935110	-0.056475
43	7	0	4.511475	-1.265048	-1.376197
44	7	0	-2.315873	-2.762499	-2.458491
45	7	0	1.046346	2.348741	-3.279003
46	6	0	-3.382576	-2.129140	-1.913439
47	1	0	-4.401982	-2.392626	-2.144460
48	6	0	1.545888	3.058769	-2.237835
49	1	0	2.122388	3.960019	-2.368563
50	1	0	1.134679	2.535930	-4.265008
51	1	0	5.383310	-1.297147	-1.880154
52	1	0	-2.306121	-3.526564	-3.115292

Table S21. Cartesian coordinates of **4** at the **^{3}TS** optimized geometry**.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.248425	0.019583	0.078607
2	7	0	-4.230888	1.292580	-0.750422
3	6	0	-2.532653	1.192519	0.957483
4	6	0	-3.374616	1.869226	1.842752
5	6	0	-2.887060	2.284781	3.072147
6	6	0	-1.563860	2.013552	3.410353
7	6	0	-0.746692	1.326928	2.516994
8	6	0	-1.197375	0.896050	1.258804
9	7	0	0.638278	1.896426	-0.884007
10	6	0	2.831407	1.400856	-0.180844
11	6	0	4.171523	1.746766	-0.073425
12	6	0	5.018864	0.863901	0.588433
13	6	0	4.515981	-0.323104	1.122801
14	6	0	3.164970	-0.639572	0.999125
15	6	0	2.273441	0.214017	0.332909
16	7	0	0.107929	-1.282121	-1.676209
17	6	0	-0.080999	-2.881397	0.049128
18	6	0	-0.228753	-4.205888	0.446832
19	6	0	-0.274437	-4.479667	1.806891
20	6	0	-0.174050	-3.432348	2.724082
21	6	0	-0.028355	-2.116922	2.291215
22	6	0	0.025668	-1.787422	0.928864
23	1	0	-4.400743	2.059829	1.548489
24	1	0	-3.539126	2.811804	3.761946
25	1	0	-1.165748	2.332171	4.369886
26	1	0	0.286020	1.130115	2.799977
27	1	0	4.530843	2.679624	-0.495260
28	1	0	6.072477	1.106402	0.688902
29	1	0	5.185335	-1.006686	1.638085
30	1	0	2.789015	-1.566402	1.422493
31	1	0	-0.300982	-4.990041	-0.299524
32	1	0	-0.388936	-5.503514	2.149125
33	1	0	-0.213377	-3.644748	3.789281
34	1	0	0.033739	-1.321414	3.028228
35	7	0	1.917659	2.258843	-0.835176
36	7	0	2.180105	3.411228	-1.407681
37	6	0	0.995705	3.828905	-1.859433
38	6	0	0.020494	2.883264	-1.532492
39	1	0	0.900025	4.768534	-2.382161
40	1	0	-1.044043	2.858154	-1.705689
41	6	0	0.093535	-2.618178	-3.414928
42	6	0	0.179763	-1.287535	-3.010969
43	7	0	-0.023947	-3.398135	-2.334447
44	7	0	-0.011308	-2.557852	-1.325759
45	1	0	0.114596	-3.044841	-4.406513
46	1	0	0.284576	-0.370723	-3.569331
47	7	0	-3.085906	0.806309	-0.296377
48	7	0	-2.491284	-0.068322	-1.086637
49	6	0	-3.301913	-0.163869	-2.138239
50	6	0	-4.392088	0.685213	-1.924104
51	1	0	-3.070155	-0.823640	-2.961313
52	1	0	-5.257721	0.884333	-2.538664