Supporting Information

Quantum-Chemical Insights into the Phosphorescence Efficiencies of Blue-Emitting Platinum (II) Complexes with Phenylene-Bridged Pincer Ligands

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Table S1. Calculated absorption wavelengths (nm) by using **TD-DFT** with different functionals in a dichloromethane solution in comparison to the available experimental absorption spectra for **2.**

	B3LYP	**PBE0**	**MPW1K**	**Cam-B3LYP**	**wb97xd**	**EXP**
HF_{exc}	**20%**	**25%**	**42.8%**	**19-65%**	**22-100%**	
S_1	342	330	304	313	311	323
S_2	330	320	293	300	298	309
T_1	416	419	448	415	398	418
T_2	367	360	343	342	337	365
T_3	338	336	324	320	314	

Exp: from ref **19**

Figure S1. Contour plots of the frontier orbitals for platinum complexes in the **S_0** states. (Saturated H atoms are not shown.)

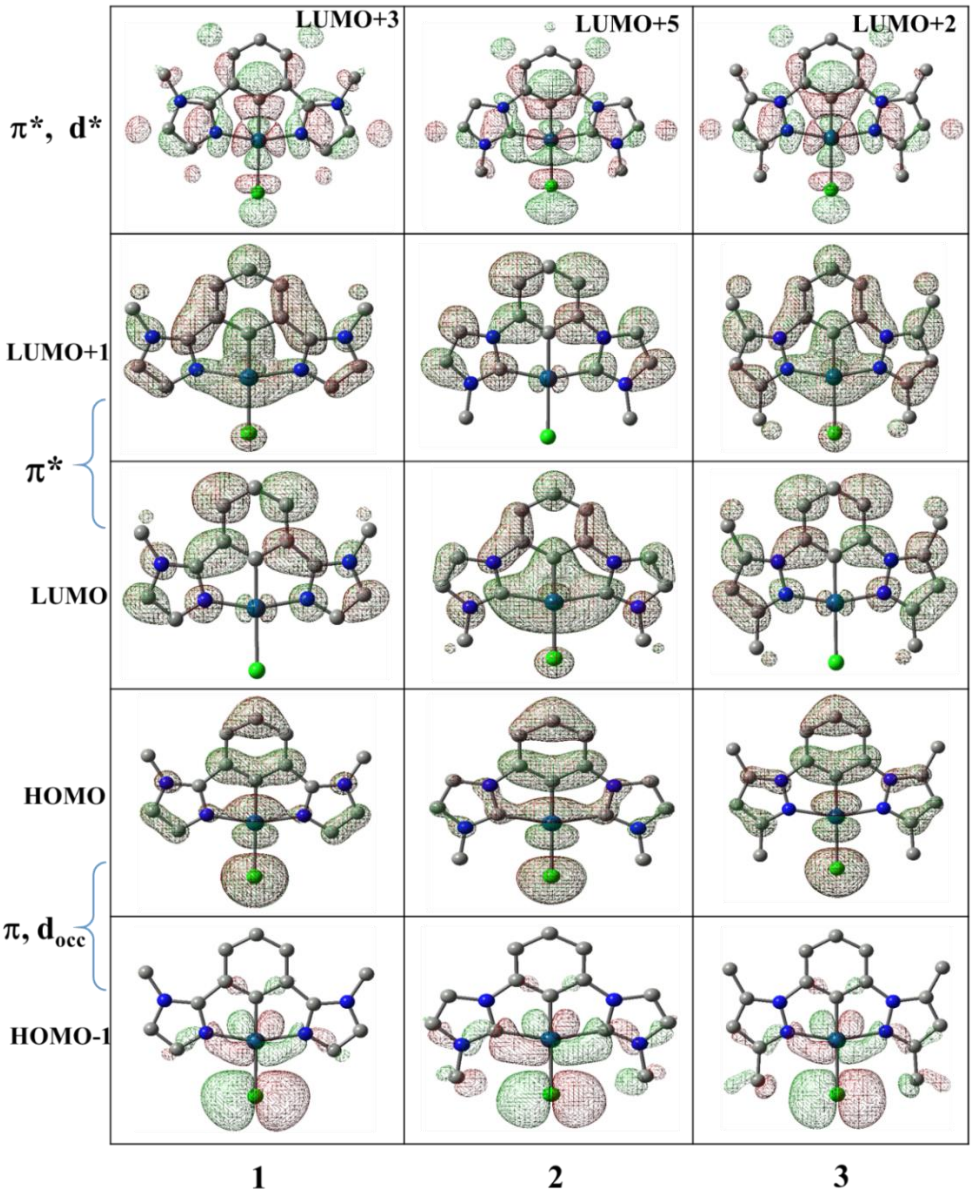
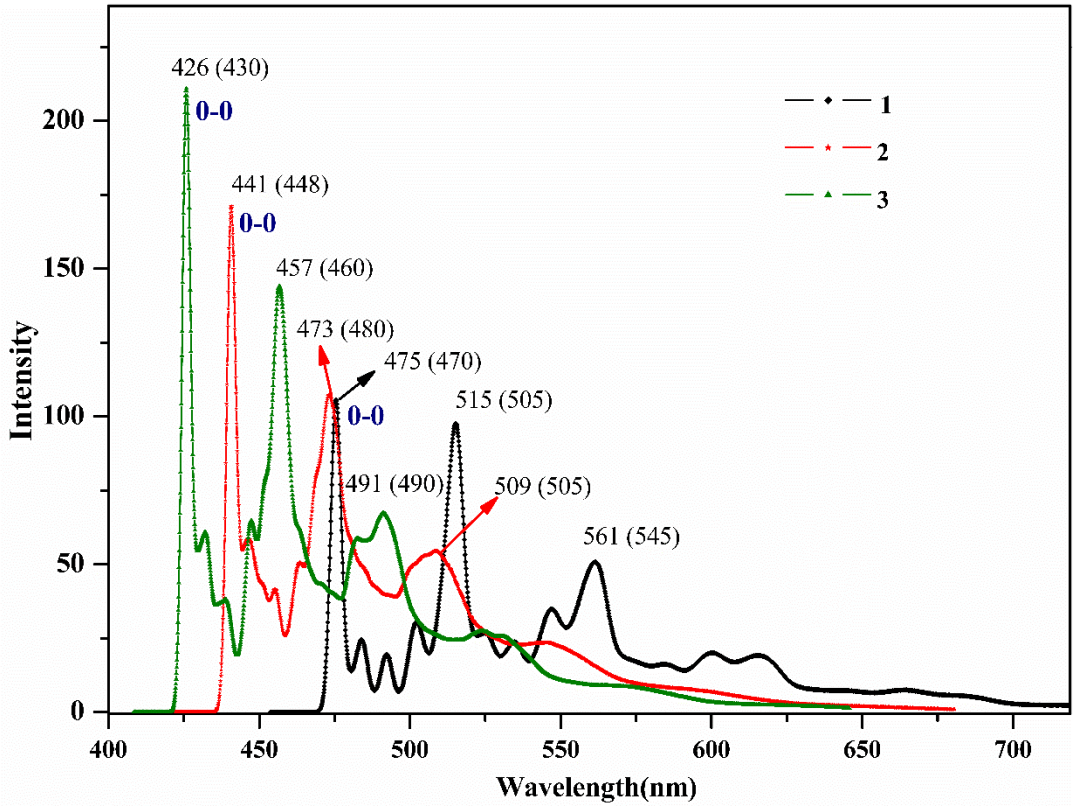


Table S2. Calculated absorption excited energies, dominant orbital excitations, oscillator strength, and transition characters from **TD-DFT** calculations for the complexes **1-3**

	State	Excitation	Ecal (eV)	λcal (nm)	*f*	Character[a]
1	S1	HOMO→LUMO (96%)	3.69	336.4	0.2080	Pt/Ph/I/Cl→Ph/I(MLCT/LLCT)
	S5	HOMO-1→LUMO (60%) HOMO→LUMO+1 (32%)	4.23	293.2	0.2224	Pt/Ph/I→Ph/I(MLCT/LLCT/ILCT) Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT)
	S6	HOMO-2→LUMO+1 (99%)	4.28	289.4	0.0227	Pt→Ph/I/Cl(MLCT)
	S9	HOMO-4→LUMO (95%)	4.73	262.4	0.0645	Pt/I/Cl→Ph/I(MLCT/LLCT)
	S12	HOMO-5→LUMO+1 (88%)	4.95	250.1	0.4547	Pt/Ph→Ph//I(MLCT/LLCT/ILCT)
	S48	HOMO-11→LUMO+1(39.6%) HOMO-5→LUMO+3(18.1%)	6.81	180.1	0.3021	Ph/I→Ph//I(LLCT/ILCT) Pt/Ph→Pt/Ph//I(MLCT/LLCT/ILCT)
	T1	HOMO-1→LUMO (53%) HOMO→LUMO+1(32%)	2.71	457.0	0.0000	Pt/Ph/I→Ph/I(MLCT/LLCT/ILCT) Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT)
	T2	HOMO→LUMO (83%) HOMO-1→LUMO+1(10%)	3.08	403.0	0.0000	Pt/Ph/I/Cl→Ph/I(MLCT/LLCT) Pt/Ph/I→Ph/I/Cl(MLCT/LLCT)
	T3	HOMO→LUMO+1 (59%) HOMO-1→LUMO (36%)	3.35	370.1	0.0000	Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT) Pt/Ph/I→Ph/I(MLCT/LLCT/ILCT)
2	S1	HOMO→LUMO (96%)	3.76	329.6	0.0336	Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT)
	S2	HOMO-1→LUMO (97%)	3.88	319.7	0.0664	Pt/Ph/I→Ph/I/Cl(MLCT/LLCT)
	S6	HOMO-1→LUMO+1 (91%)	4.78	259.1	0.1442	Pt/Ph/I→Ph/I(MLCT/LLCT/ILCT)
	S9	HOMO-5→LUMO (83%)	5.00	248.2	0.3544	Pt/Ph/I→Ph/I/Cl(MLCT/LLCT)
	S22	HOMO→LUMO+3(47.5%) HOMO-5→LUMO+2(20.9%)	5.99	206.9	0.4393	Pt/Ph/I/Cl→Ph/I(MLCT/LLCT/ILCT) Pt/Ph/I→I(MLCT/LLCT/ILCT)
	T1	HOMO→LUMO (73%)	2.96	419.2	0.0000	Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT)
	T2	HOMO-1→LUMO (86%)	3.44	360.0	0.0000	Pt/Ph/I→Ph/I/Cl(MLCT/LLCT)
	T3	HOMO-1→LUMO+1(60%) HOMO→LUMO (18%)	3.69	336.4	0.0000	Pt/Ph/I→Ph/I(MLCT/LLCT/ILCT) Pt/Ph/I/Cl→Ph/I/Cl(MLCT/LLCT/ILCT)
3	S1	HOMO→LUMO+1 (86%) HOMO-1→LUMO (11%)	3.94	314.4	0.0722	Pt/Ph/P/Cl→Ph/P(MLCT/LLCT) Pt/P→Ph/P/Cl(MLCT/LLCT)
	S2	HOMO→LUMO (92%)	3.95	314.1	0.0150	Pt/Ph/P/Cl→Ph/P/Cl(MLCT/LLCT/ILCT)
	S3	HOMO-1→LUMO (80%) HOMO-2→LUMO (9%)	4.22	293.6	0.1608	Pt/P→Ph/P/Cl(MLCT/LLCT) Ph/P→Pt/Ph/P/Cl(LMCT/LLCT)
	S9	HOMO-2→LUMO (85%)	4.66	266.2	0.4484	Ph/P→Pt/Ph/P/Cl(LMCT/LLCT)
	S18	HOMO→LUMO+3(87.7%)	5.70	217.6	0.3356	Pt/Ph/P/Cl→Ph/P(MLCT/LLCT/ILCT)
	T1	HOMO→LUMO (60%) HOMO-2→LUMO+1(26%)	2.98	416.0	0.0000	Pt/Ph/P/Cl→Ph/P/Cl(MLCT/LLCT/ILCT) Ph/P→Pt/Ph/P(LMCT/LLCT/ILCT)
	T2	HOMO→LUMO+1 (62%) HOMO-1→LUMO (19%) HOMO-2→LUMO (11%)	3.39	365.6	0.0000	Pt/Ph/P/Cl→Ph/P(MLCT/LLCT) Pt/P→Ph/P/Cl(MLCT/LLCT) Ph/P→Pt/Ph/P/Cl(LMCT/LLCT)
	T3	HOMO-1→LUMO (58%) HOMO→LUMO+1(25%)	3.59	345.4	0.0000	Pt/P→Ph/P/Cl(MLCT/LLCT) Pt/Ph/P/Cl→Ph/P(MLCT/LLCT)

[a]I and P denote the imidazolyl and pyrazolyl moieties, respectively，Ph denotes the phenyl ring in the pincer ligand

Figure S2. Simulated vibronically-resolved emission spectrum by Franck-Condon calculations for **1-3**



Note: the wavelengths in parentheses are from the experimental measurement (Ref. 32).

Figure S3. Electron difference density maps as obtained from **TD-DFT** calculations at their respective optimized $\mathbf{T_1}$ excited state geometries with respect to the $\mathbf{S_0}$ state for **1-3** (isovalue = 0.001 a.u, electron density increase and decrease region are in color purple and cyan, respectively).

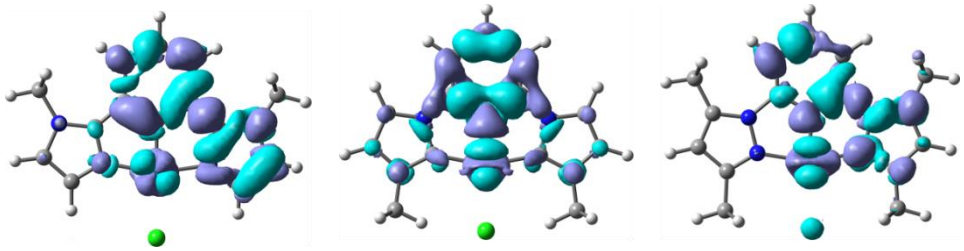


Figure S4. The structures of the $\mathbf{T_1/\ S_0}$ **MECP** for all the studied complexes.

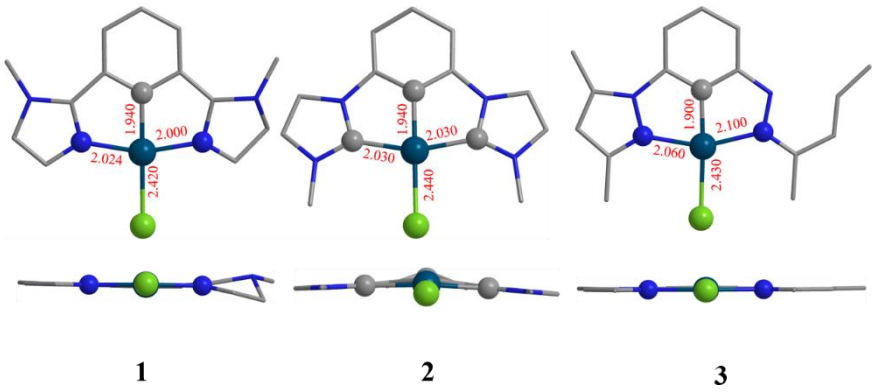


Figure S5. The optimized structures of the **^{3}TS [T_1-^{3}MC]** for **1-2**.

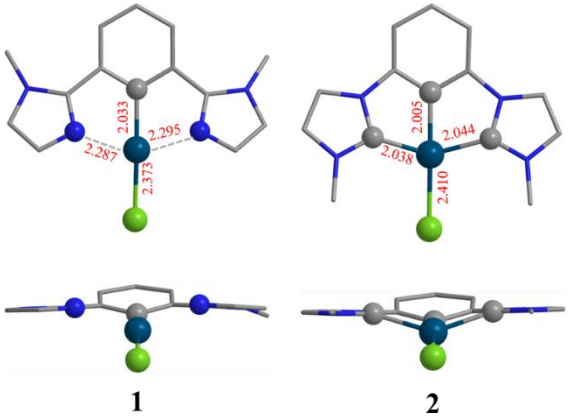


Figure S6. The curve of intrinsic reaction coordinate of **^{3}TS [T_1/^{3}MC]** for **1** and **2**.

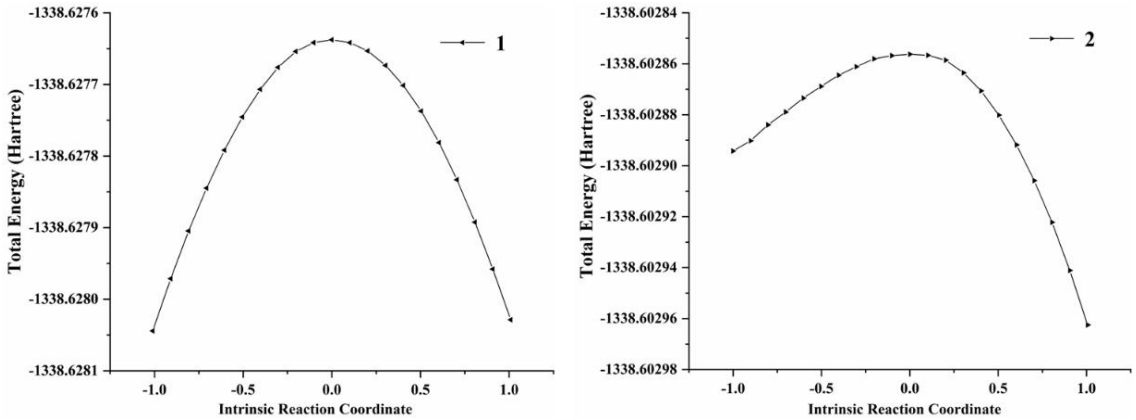


Figure S7. The structures of the**^{3}MC/ S_0 MECP** for all the studied complexes.

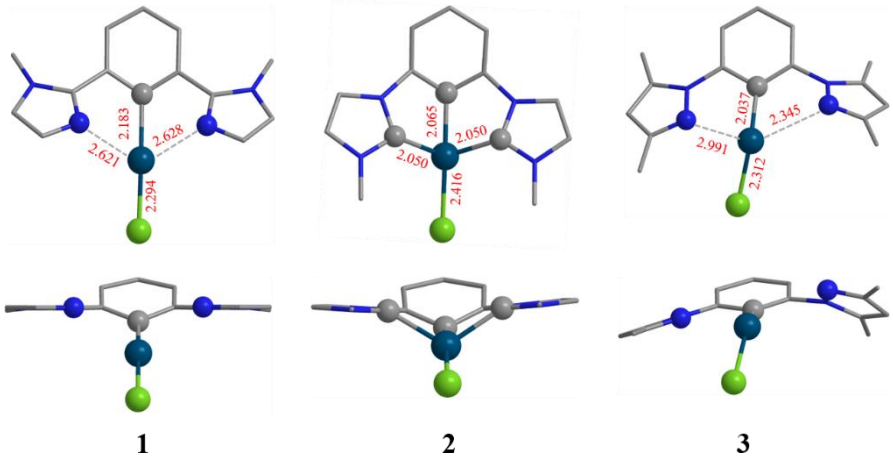


Figure S8. Schematic representation of the energy landscape of complexes **1-3** in a CH_2Cl_2 solution. Energies (kcal/mol) of the respective states are given relative to the **S_0** state.

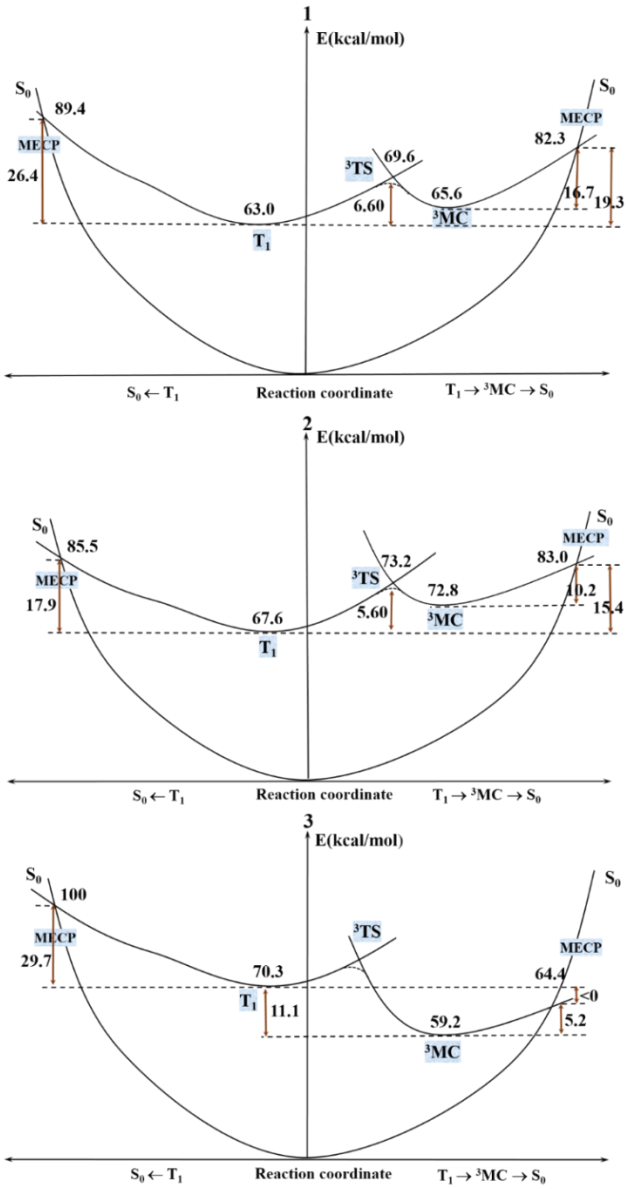


Table S3. Vibrational frequencies (cm^{-1}) at the respective optimized **S_0** and **T_1** states, dimensionless displacement **ΔQ_i**, huang-rhys factors **S_i** and reorganization energy **λ_i** (cm^{-1}) of **1**.

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)
41.93	-1.00E-03	5.00E-07	0.00	40.98		932.03	0.00E+00	0.00E+00	0.00	914.88
60.99	-6.00E-03	1.80E-05	0.00	58.13		938.71	2.40E-02	2.88E-04	0.30	932.99
78.15	2.00E-03	2.00E-06	0.00	70.52		1003.51	-4.13E-01	8.53E-02	84.90	951.09
81.96	-5.49E-01	1.51E-01	12.70	81.01		1017.80	2.83E-01	4.00E-02	41.10	981.59
104.83	-3.00E-03	4.50E-06	0.00	87.68		1030.19	2.36E-01	2.78E-02	29.40	1006.37
104.83	0.00E+00	0.00E+00	0.00	99.11		1037.82	1.67E-01	1.39E-02	14.80	1016.85
126.75	-2.00E-03	2.00E-06	0.00	104.83		1063.55	-2.68E-01	3.59E-02	38.90	1033.05
134.37	0.00E+00	0.00E+00	0.00	122.94		1063.55	1.03E-01	5.30E-03	5.90	1053.07
138.19	3.23E-01	5.22E-02	7.40	134.37		1094.04	3.60E-02	6.48E-04	0.70	1064.50
199.18	-2.00E-03	2.00E-06	0.00	177.26		1096.90	-1.00E-03	5.00E-07	0.00	1092.14
202.99	-2.71E-01	3.67E-02	7.80	202.04		1096.90	6.65E-01	2.21E-01	253.50	1094.04

227.77	0.00E+00	0.00E+00	0.00	207.75		1117.87	0.00E+00	0.00E+00	0.00	1096.90
237.30	1.00E-03	5.00E-07	0.00	221.10		1155.04	-8.20E-02	3.36E-03	3.90	1108.34
250.64	-8.60E-02	3.70E-03	0.90	234.44		1170.28	3.29E-01	5.41E-02	64.90	1139.79
271.61	1.23E-01	7.56E-03	2.00	249.69		1170.28	5.60E-02	1.57E-03	1.90	1166.47
275.42	-1.65E-01	1.36E-02	3.70	258.26		1233.18	3.72E-01	6.92E-02	85.30	1176.96
280.18	0.00E+00	0.00E+00	0.00	260.17		1242.71	1.10E-02	6.05E-05	0.10	1218.89
308.77	5.10E-02	1.30E-03	0.40	303.05		1297.99	-1.69E-01	1.43E-02	18.30	1225.56
327.83	1.00E-03	5.00E-07	0.00	303.05		1303.70	-2.61E-01	3.41E-02	45.80	1284.64
352.61	4.70E-01	1.10E-01	40.00	344.99		1322.76	3.00E-03	4.50E-06	0.00	1297.03
379.29	-2.95E-01	4.35E-02	17.10	373.58		1347.54	-7.00E-03	2.45E-05	0.00	1340.87
441.24	0.00E+00	0.00E+00	0.00	425.99		1352.31	-8.60E-02	3.70E-03	5.20	1346.59
498.42	-9.40E-02	4.42E-03	2.00	440.29		1366.60	7.00E-02	2.45E-03	3.50	1360.88
506.04	3.80E-02	7.22E-04	0.40	484.12		1393.29	1.08E-01	5.83E-03	8.40	1363.74
528.92	0.00E+00	0.00E+00	0.00	494.61		1394.24	1.20E-01	7.20E-03	10.40	1385.66
546.07	-5.90E-02	1.74E-03	1.00	540.35		1402.82	5.90E-02	1.74E-03	2.60	1394.24
604.20	0.00E+00	0.00E+00	0.00	540.35		1423.78	4.00E-02	8.00E-04	1.20	1401.86
606.11	0.00E+00	0.00E+00	0.00	598.48		1423.78	0.00E+00	0.00E+00	0.00	1418.06
684.25	0.00E+00	0.00E+00	0.00	605.16		1438.08	0.00E+00	0.00E+00	0.00	1422.83
687.11	0.00E+00	0.00E+00	0.00	629.93		1449.51	5.40E-02	1.46E-03	2.20	1438.08
687.11	4.05E-01	8.20E-02	55.20	642.32		1460.00	-2.92E-01	4.26E-02	64.40	1442.84
690.93	0.00E+00	0.00E+00	0.00	655.66		1476.20	-2.78E-01	3.86E-02	58.90	1450.47
698.55	0.00E+00	0.00E+00	0.00	669.01		1492.40	7.70E-02	2.96E-03	4.60	1466.67
702.36	-4.28E-01	9.16E-02	65.20	678.54		1493.35	2.33E-01	2.71E-02	42.00	1475.24
718.56	0.00E+00	0.00E+00	0.00	688.07		1527.66	2.40E-02	2.88E-04	0.40	1488.59
730.95	2.36E-01	2.78E-02	20.20	689.02		1537.19	1.35E-01	9.11E-03	14.20	1496.21
758.59	0.00E+00	0.00E+00	0.00	717.61		1558.16	-1.24E-01	7.69E-03	12.40	1528.61
785.27	0.00E+00	0.00E+00	0.00	742.39		1589.60	-1.34E+00	9.02E-01	1501.60	1586.75
844.36	1.72E-01	1.48E-02	11.60	745.25		2937.15	1.30E-02	8.45E-05	0.20	2919.99
844.36	0.00E+00	0.00E+00	0.00	837.69		2937.15	-3.00E-03	4.50E-06	0.00	2939.05
867.23	0.00E+00	0.00E+00	0.00	850.08		3014.34	0.00E+00	0.00E+00	0.00	2989.56
919.65	-2.55E-01	3.25E-02	30.80	901.54		3014.34	0.00E+00	0.00E+00	0.00	3016.25
3045.79	-2.00E-03	2.00E-06	0.00	3035.31		3158.24	3.00E-03	4.50E-06	0.00	3150.62
3045.79	1.00E-03	5.00E-07	0.00	3045.79		3158.24	4.00E-03	8.00E-06	0.00	3159.20
3063.90	-3.00E-02	4.50E-04	1.40	3056.27		3176.35	-3.00E-03	4.50E-06	0.00	3167.77
3074.38	-9.00E-03	4.05E-05	0.10	3085.81		3177.30	4.00E-03	8.00E-06	0.00	3178.26
3086.77	-4.10E-02	8.41E-04	2.80	3100.11						

Table S4. 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)
40.98	-3.00E-03	4.50E-06	0.00	42.89		922.50	0.00E+00	0.00E+00	0.00	845.31
62.90	2.00E-03	2.00E-06	0.00	58.13		988.26	-3.89E-01	7.57E-02	72.00	905.35
70.52	0.00E+00	0.00E+00	0.00	65.76		1003.51	-3.19E-01	5.09E-02	49.60	929.18
98.16	3.00E-03	4.50E-06	0.00	76.24		1004.46	0.00E+00	0.00E+00	0.00	978.73
129.61	0.00E+00	0.00E+00	0.00	115.31		1026.38	-1.81E-01	1.64E-02	17.20	994.93

133.42	0.00E+00	0.00E+00	0.00	115.31		1056.88	0.00E+00	0.00E+00	0.00	1000.65
135.33	1.00E-03	5.00E-07	0.00	138.19		1060.69	0.00E+00	6.05E-05	0.00	1057.83
146.76	4.35E-01	9.46E-02	15.20	152.48		1078.80	1.76E-01	1.29E-01	17.20	1059.74
153.43	0.00E+00	0.00E+00	0.00	154.39		1089.28	1.10E-02	0.00E+00	0.10	1061.64
189.65	3.00E-03	4.50E-06	0.00	164.87		1097.86	5.07E-01	1.83E-01	145.10	1077.84
211.57	1.00E-03	5.00E-07	0.00	194.41		1110.25	0.00E+00	0.00E+00	0.00	1089.28
231.58	0.00E+00	0.00E+00	0.00	220.14		1111.20	0.00E+00	6.27E-02	0.00	1107.39
233.49	0.00E+00	0.00E+00	0.00	224.91		1129.31	0.00E+00	2.49E-01	0.00	1108.34
278.28	-5.65E-01	1.60E-01	38.20	227.77		1130.26	-6.05E-01	0.00E+00	214.50	1115.96
278.28	-1.00E-03	5.00E-07	0.00	259.22		1159.80	0.00E+00	3.28E-03	0.00	1139.79
279.23	0.00E+00	0.00E+00	0.00	266.84		1211.26	0.00E+00	0.00E+00	0.00	1188.39
283.99	2.00E-03	2.00E-06	0.00	279.23		1220.79	3.54E-01	0.00E+00	79.60	1208.40
316.40	4.13E-01	8.53E-02	25.00	279.23		1277.02	0.00E+00	6.05E-03	0.00	1215.08
319.26	0.00E+00	0.00E+00	0.00	317.35		1277.97	7.05E-01	0.00E+00	321.10	1230.32
363.09	6.68E-01	2.23E-01	84.70	362.14		1342.78	0.00E+00	6.92E-02	0.00	1274.16
396.45	0.00E+00	0.00E+00	0.00	393.59		1349.45	-8.10E-02	0.00E+00	4.60	1338.97
419.32	7.30E-02	2.67E-03	1.10	398.35		1352.31	0.00E+00	1.75E-01	0.00	1339.92
510.81	0.00E+00	0.00E+00	0.00	419.32		1371.37	0.00E+00	0.00E+00	0.00	1351.35
512.71	-5.15E-01	1.33E-01	71.70	514.62		1375.18	1.10E-01	0.00E+00	8.50	1351.35
562.27	0.00E+00	0.00E+00	0.00	532.73		1397.10	0.00E+00	8.82E-02	0.00	1366.60
566.08	0.00E+00	0.00E+00	0.00	537.49		1398.05	3.72E-01	2.00E-06	100.80	1390.43
601.34	2.00E-03	2.00E-06	0.00	581.33		1433.31	0.00E+00	7.92E-02	0.00	1399.96
607.06	1.00E-03	5.00E-07	0.00	588.00		1434.27	5.92E-01	0.00E+00	259.00	1408.53
665.19	0.00E+00	0.00E+00	0.00	636.60		1437.12	0.00E+00	1.86E-02	0.00	1432.36
674.72	-1.00E-03	5.00E-07	0.00	638.51		1438.08	0.00E+00	0.00E+00	0.00	1436.17
675.68	-1.00E-03	5.00E-07	0.00	648.04		1448.56	0.00E+00	5.00E-07	0.00	1437.12
676.63	3.40E-01	5.78E-02	40.30	663.29		1460.00	3.17E-01	0.00E+00	75.80	1439.03
689.97	0.00E+00	0.00E+00	0.00	667.10		1479.06	0.00E+00	0.00E+00	0.00	1462.86
700.46	0.00E+00	0.00E+00	0.00	674.72		1484.77	4.20E-01	0.00E+00	135.90	1471.43
705.22	-1.00E-03	5.00E-07	0.00	675.68		1554.34	-2.00E-03	2.21E-04	0.00	1517.18
709.03	5.06E-01	1.28E-01	93.50	697.60		1557.20	-3.98E-01	5.00E-07	126.40	1517.18
749.06	0.00E+00	0.00E+00	0.00	701.41		1598.18	0.00E+00	0.00E+00	0.00	1566.73
764.31	0.00E+00	0.00E+00	0.00	745.25		1601.04	-1.93E-01	2.21E-04	30.70	1567.69
779.55	0.00E+00	0.00E+00	0.00	772.88		2922.85	0.00E+00	0.00E+00	0.00	2920.95
780.51	0.00E+00	0.00E+00	0.00	780.51		3024.82	2.10E-02	1.13E+00	0.70	3026.73
840.55	0.00E+00	0.00E+00	0.00	780.51		3063.90	-1.00E-03	1.08E+00	0.00	3069.61
907.26	0.00E+00	0.00E+00	0.00	823.39		3070.57	0.00E+00	1.08E+00	0.00	3075.33
1601.04	-1.93E-01	2.21E-04	30.70	1567.69		3086.77	2.10E-02	1.06E+00	0.70	3090.58
2922.85	0.00E+00	0.00E+00	0.00	2920.95		3159.20	0.00E+00	1.06E+00	0.00	3156.34
2924.76	1.00E-03	4.05E-05	0.00	2922.85		3159.20	-9.00E-03	1.06E+00	0.10	3156.34
3016.25	0.00E+00	0.00E+00	0.00	3006.72		3180.16	0.00E+00	9.34E-01	0.00	3181.11
3016.25	0.00E+00	8.00E-06	0.00	3006.72		3180.16	-4.00E-03	9.34E-01	0.00	3181.11
3021.96	0.00E+00	1.21E+00	0.00	3024.82						

Table S5. 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)
35.26	0.00E+00	0.00E+00	0.00	32.40		769.07	0.00E+00	0.00E+00	0.00	738.58
49.56	0.00E+00	0.00E+00	0.00	39.07		769.07	-1.88E-01	1.77E-02	13.80	744.29
57.18	0.00E+00	0.00E+00	0.00	47.65		770.02	0.00E+00	0.00E+00	0.00	766.21
74.33	0.00E+00	0.00E+00	0.00	68.62		801.47	0.00E+00	0.00E+00	0.00	770.98
102.92	0.00E+00	0.00E+00	0.00	96.25		845.31	-1.97E-01	1.94E-02	16.10	790.04
121.03	0.00E+00	0.00E+00	0.00	121.03		912.97	2.97E-01	4.41E-02	41.20	892.01
121.03	-2.30E-01	2.65E-02	3.60	129.61		959.67	0.00E+00	0.00E+00	0.00	896.77
128.66	1.54E-01	1.19E-02	1.70	138.19		959.67	4.60E-02	1.06E-03	1.10	941.56
139.14	1.00E-03	5.00E-07	0.00	138.19		971.11	1.15E-01	6.61E-03	6.60	954.91
176.31	0.00E+00	0.00E+00	0.00	160.10		972.06	7.00E-02	2.45E-03	2.50	967.30
182.02	0.00E+00	0.00E+00	0.00	177.26		1003.51	6.70E-02	2.25E-03	2.30	970.15
193.46	0.00E+00	0.00E+00	0.00	183.93		1009.23	-1.91E-01	1.82E-02	18.90	985.40
215.38	5.20E-02	1.35E-03	0.30	195.37		1009.23	0.00E+00	0.00E+00	0.00	997.79
223.00	0.00E+00	0.00E+00	0.00	202.04		1013.99	0.00E+00	0.00E+00	0.00	1004.46
223.96	6.89E-01	2.37E-01	54.90	220.14		1013.99	1.24E-01	7.69E-03	8.10	1008.27
232.53	0.00E+00	0.00E+00	0.00	230.63		1035.91	0.00E+00	0.00E+00	0.00	1009.23
234.44	-1.64E-01	1.34E-02	3.30	233.49		1042.58	0.00E+00	0.00E+00	0.00	1015.90
236.34	-1.19E-01	7.08E-03	1.70	234.44		1062.60	2.98E-01	4.44E-02	48.10	1031.15
259.22	0.00E+00	0.00E+00	0.00	245.87		1105.48	3.74E-01	6.99E-02	78.40	1071.17
283.99	0.00E+00	0.00E+00	0.00	257.31		1120.73	-5.13E-01	1.32E-01	148.70	1076.89
285.90	-2.10E-02	2.21E-04	0.10	282.09		1133.12	-9.90E-02	4.90E-03	5.70	1107.39
1135.98	-2.43E-01	2.95E-02	34.90	1123.59		1473.34	-1.08E-01	5.83E-03	8.90	1466.67
1139.79	-2.40E-02	2.88E-04	0.30	1135.02		1487.63	-2.21E-01	2.44E-02	37.70	1473.34
1151.22	-7.40E-02	2.74E-03	3.30	1140.74		1492.40	3.80E-01	7.22E-02	111.80	1474.29
1162.66	-1.10E-01	6.05E-03	7.30	1153.13		1557.20	9.83E-01	4.83E-01	752.80	1484.77
1265.58	-6.30E-02	1.99E-03	2.50	1183.63		1559.11	3.12E-01	4.87E-02	76.60	1504.79
1277.02	2.60E-02	3.38E-04	0.50	1265.58		1590.56	8.70E-02	3.79E-03	6.10	1527.66
1349.45	1.68E-01	1.41E-02	19.10	1286.55		1598.18	-4.50E-02	1.01E-03	1.70	1569.59
1351.35	7.20E-01	2.59E-01	358.60	1317.05		2926.66	2.70E-02	3.65E-04	1.10	2899.03
1354.21	-1.85E-01	1.71E-02	24.10	1337.06		2926.66	3.00E-03	4.50E-06	0.00	2924.76
1357.07	3.90E-02	7.61E-04	1.10	1352.31		2944.77	1.10E-02	6.05E-05	0.20	2935.24
1358.03	1.23E-01	7.57E-03	10.80	1353.26		2944.77	-3.00E-03	4.50E-06	0.00	2946.68
1371.37	-1.90E-02	1.81E-04	0.20	1357.07		2995.28	0.00E+00	0.00E+00	0.00	2956.21
1372.32	1.59E-01	1.26E-02	18.00	1358.98		2995.28	0.00E+00	0.00E+00	0.00	2993.37
1399.00	-3.90E-02	7.61E-04	1.10	1370.41		3022.92	0.00E+00	0.00E+00	0.00	3005.76
1405.68	-1.84E-01	1.69E-02	24.70	1392.33		3022.92	6.00E-03	1.80E-05	0.10	3021.01
1409.49	-8.20E-02	3.36E-03	5.00	1403.77		3031.49	0.00E+00	0.00E+00	0.00	3025.78
1409.49	0.00E+00	0.00E+00	0.00	1405.68		3031.49	8.00E-03	3.20E-05	0.10	3028.63
1419.02	0.00E+00	0.00E+00	0.00	1410.44		3036.26	2.00E-03	2.00E-06	0.00	3033.40
1419.97	0.00E+00	0.00E+00	0.00	1413.30		3036.26	-2.00E-03	2.00E-06	0.00	3037.21
3078.19	2.00E-03	2.00E-06	0.00	3073.43		3148.71	3.10E-02	4.81E-04	1.60	3143.95
3120.12	5.00E-03	1.25E-05	0.00	3120.12		3148.71	0.00E+00	0.00E+00	0.00	3149.67

3122.98	1.00E-03	5.00E-07	0.00	3142.04	

Table S6. Cartesian coordinates of **1** at the S_0 optimized geometry by **DFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.221614	-3.121857	-0.000065
2	6	0	1.226501	-1.723063	-0.000042
3	6	0	-0.000003	-1.035885	-0.000031
4	6	0	-1.226510	-1.723059	-0.000049
5	6	0	-1.221628	-3.121852	-0.000088
6	6	0	-0.000008	-3.799843	-0.000091
7	78	0	0.000001	0.898421	0.000006
8	6	0	2.314063	-0.754438	-0.000004
9	6	0	-2.314069	-0.754429	-0.000017
10	7	0	3.663026	-0.867799	0.000003
11	6	0	4.195633	0.404717	0.000041
12	6	0	3.143467	1.277907	0.000010
13	7	0	1.992172	0.551737	0.000040
14	7	0	-1.992172	0.551744	0.000005
15	6	0	-3.143465	1.277919	0.000047
16	6	0	-4.195634	0.404733	0.000012
17	7	0	-3.663032	-0.867785	0.000005
18	17	0	0.000020	3.319308	0.000023
19	6	0	4.423061	-2.097713	-0.000008
20	6	0	-4.423071	-2.097696	0.000065
21	1	0	2.141933	-3.698198	-0.000051
22	1	0	-2.141949	-3.698190	-0.000110
23	1	0	-0.000010	-4.885466	-0.000113
24	1	0	5.262019	0.567895	0.000070
25	1	0	3.119343	2.356806	-0.000012
26	1	0	-3.119339	2.356818	0.000074
27	1	0	-5.262019	0.567916	0.000004
28	1	0	5.485194	-1.851707	-0.000171
29	1	0	4.200003	-2.689371	-0.891986
30	1	0	4.200241	-2.689256	0.892108
31	1	0	-4.200249	-2.689274	-0.892027
32	1	0	-5.485204	-1.851686	0.000209
33	1	0	-4.200020	-2.689321	0.892067

Table S7. Cartesian coordinates of **2** at the S_0 optimized geometry by **DFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224449	-3.455490	-0.000027
2	6	0	-1.199940	-2.064843	0.000006
3	6	0	-0.000009	-1.367984	-0.000014
4	6	0	1.199910	-2.064865	-0.000006
5	6	0	1.224397	-3.455513	-0.000028
6	6	0	-0.000032	-4.132074	-0.000049
7	7	0	-2.292359	-1.166158	0.000108
8	7	0	2.292340	-1.166197	0.000096
9	78	0	0.000003	0.574582	-0.000091
10	17	0	0.000085	3.013559	-0.000295
11	6	0	-3.651564	-1.372658	0.000165
12	6	0	-4.220196	-0.140741	0.000337
13	7	0	-3.193650	0.786281	0.000146
14	6	0	-1.992120	0.178030	0.000155
15	6	0	1.992110	0.177989	0.000136

16	7	0	3.193638	0.786232	0.000138
17	6	0	4.220185	-0.140790	0.000243
18	6	0	3.651545	-1.372705	0.000217
19	6	0	-3.389634	2.224383	0.000075
20	6	0	3.389601	2.224336	0.000035
21	1	0	-2.155001	-4.015489	-0.000004
22	1	0	2.154940	-4.015529	-0.000005
23	1	0	-0.000042	-5.217479	-0.000046
24	1	0	-4.098163	-2.353878	0.000127
25	1	0	-5.257749	0.154490	0.000445
26	1	0	5.257739	0.154436	0.000284
27	1	0	4.098139	-2.353927	0.000243
28	1	0	-3.946752	2.521606	-0.892337
29	1	0	-2.408245	2.704674	-0.000178
30	1	0	-3.946332	2.521737	0.892705
31	1	0	3.946518	2.521688	0.892528
32	1	0	2.408201	2.704606	0.000023
33	1	0	3.946486	2.521582	-0.892515

Table S8. Cartesian coordinates of **3** at the S_0 optimized geometry by **DFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.226090	3.256194	0.000002
2	6	0	1.210527	1.861506	-0.000003
3	6	0	0.000001	1.179866	-0.000001
4	6	0	-1.210525	1.861508	0.000012
5	6	0	-1.226086	3.256196	0.000019
6	6	0	0.000002	3.925108	0.000013
7	78	0	0.000000	-0.737730	-0.000012
8	6	0	3.657917	1.148837	0.000018
9	6	0	4.218326	-0.111687	-0.000015
10	6	0	3.159796	-1.036085	-0.000020
11	7	0	2.006049	-0.368539	-0.000029
12	7	0	2.310504	0.973964	-0.000009
13	7	0	-2.310502	0.973967	0.000018
14	7	0	-2.006049	-0.368537	0.000013
15	6	0	-3.159796	-1.036082	0.000015
16	6	0	-4.218326	-0.111684	0.000034
17	6	0	-3.657916	1.148840	0.000030
18	6	0	-4.337750	2.471125	0.000037
19	6	0	-3.241984	-2.518550	0.000002
20	17	0	-0.000005	-3.168633	-0.000020
21	6	0	4.337750	2.471123	0.000048
22	6	0	3.241985	-2.518553	-0.000025
23	1	0	2.142834	3.831056	-0.000003
24	1	0	-2.142829	3.831060	0.000030
25	1	0	0.000002	5.010442	0.000019
26	1	0	5.273414	-0.341808	-0.000022
27	1	0	-5.273413	-0.341806	0.000043
28	1	0	-4.084563	3.061604	0.886802
29	1	0	-5.417568	2.312739	0.000041
30	1	0	-4.084570	3.061609	-0.886727
31	1	0	-2.734665	-2.939624	0.871466
32	1	0	-2.734713	-2.939606	-0.871497
33	1	0	-4.289529	-2.827312	0.000027
34	1	0	5.417568	2.312738	0.000056
35	1	0	4.084558	3.061591	0.886819
36	1	0	4.084576	3.061618	-0.886711
37	1	0	2.734858	-2.939608	0.871560
38	1	0	4.289531	-2.827314	-0.000210
39	1	0	2.734524	-2.939628	-0.871402

Table S9. Cartesian coordinates of **1** at the T_1 optimized geometry by **TDDFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.231650	-3.169281	-0.000163
2	6	0	1.259592	-1.712739	-0.000150
3	6	0	-0.026556	-1.028261	-0.000031
4	6	0	-1.234663	-1.704251	0.000045
5	6	0	-1.238796	-3.130181	0.000120
6	6	0	0.019193	-3.811846	-0.000014
7	78	0	-0.001884	0.899263	0.000027
8	6	0	2.296066	-0.794686	-0.000130
9	6	0	-2.321744	-0.741127	0.000125
10	7	0	3.682300	-0.880550	-0.000093
11	6	0	4.179076	0.402175	-0.000094
12	6	0	3.102978	1.278134	0.000127
13	7	0	1.969494	0.574793	-0.000093
14	7	0	-2.005068	0.569400	0.000166
15	6	0	-3.158159	1.292270	0.000222
16	6	0	-4.208233	0.418056	-0.000052
17	7	0	-3.669837	-0.856317	0.000091
18	17	0	0.058958	3.324191	0.000045
19	6	0	4.458390	-2.093565	-0.000200
20	6	0	-4.427900	-2.087165	0.000082
21	1	0	2.148525	-3.749303	-0.000304
22	1	0	-2.153431	-3.711349	0.000262
23	1	0	0.007463	-4.898494	-0.000020
24	1	0	5.240518	0.598098	-0.000146
25	1	0	3.089549	2.358636	0.000308
26	1	0	-3.139376	2.371229	0.000357
27	1	0	-5.274943	0.577689	-0.000159
28	1	0	5.517644	-1.832618	-0.000176
29	1	0	4.249538	-2.693528	-0.891989
30	1	0	4.249539	-2.693705	0.891469
31	1	0	-4.204070	-2.678927	-0.891636
32	1	0	-5.490469	-1.842775	-0.000061
33	1	0	-4.204291	-2.678831	0.891919

Table S10. Cartesian coordinates of **2** at the T_1 optimized geometry by **TDDFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.260638	-3.448326	-0.000024
2	6	0	1.251654	-2.077680	-0.000093
3	6	0	0.000016	-1.348836	-0.000111
4	6	0	-1.251614	-2.077695	-0.000082
5	6	0	-1.260582	-3.448340	-0.000013
6	6	0	0.000032	-4.127008	0.000016
7	7	0	2.313975	-1.185937	-0.000146
8	7	0	-2.313945	-1.185964	-0.000126
9	78	0	0.000005	0.550624	-0.000274
10	17	0	-0.000014	2.997269	0.000160
11	6	0	3.683194	-1.371252	-0.000159
12	6	0	4.229032	-0.132650	-0.000166
13	7	0	3.195428	0.788289	-0.000127
14	6	0	1.993537	0.170948	-0.000195
15	6	0	-1.993523	0.170924	-0.000182
16	7	0	-3.195419	0.788253	-0.000110
17	6	0	-4.229014	-0.132697	-0.000144
18	6	0	-3.683163	-1.371293	-0.000121
19	6	0	3.385955	2.225372	-0.000075

20	6	0	-3.385954	2.225335	-0.000027
21	1	0	2.178660	-4.027496	-0.000003
22	1	0	-2.178597	-4.027522	0.000017
23	1	0	0.000038	-5.211939	0.000069
24	1	0	4.144758	-2.345268	-0.000139
25	1	0	5.263573	0.174130	-0.000153
26	1	0	-5.263558	0.174072	-0.000132
27	1	0	-4.144716	-2.345314	-0.000094
28	1	0	3.941193	2.527113	0.892524
29	1	0	2.403448	2.702670	0.000115
30	1	0	3.940908	2.527222	-0.892814
31	1	0	-3.941101	2.527170	-0.892650
32	1	0	-2.403446	2.702632	-0.000046
33	1	0	-3.940998	2.527087	0.892689

Table S11. Cartesian coordinates of **3** at the T_1 optimized geometry by **TDDFT** with **PBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.254487	-3.237147	0.000295
2	6	0	-1.237229	-1.854079	0.000080
3	6	0	-0.017776	-1.159263	-0.000002
4	6	0	1.262124	-1.857792	0.000152
5	6	0	1.250958	-3.268947	0.000416
6	6	0	0.026668	-3.915488	0.000452
7	78	0	-0.001998	0.731057	0.000166
8	6	0	-3.680785	-1.143387	-0.000147
9	6	0	-4.238027	0.116739	-0.000209
10	6	0	-3.177549	1.041205	0.000000
11	7	0	-2.023589	0.373435	0.000141
12	7	0	-2.330261	-0.968563	0.000035
13	7	0	2.307593	-0.990226	0.000138
14	7	0	1.998339	0.363438	0.000234
15	6	0	3.176309	1.034469	0.000077
16	6	0	4.229260	0.111804	-0.000084
17	6	0	3.691544	-1.157771	-0.000071
18	6	0	4.362443	-2.479400	-0.000334
19	6	0	3.255196	2.513745	0.000100
20	17	0	-0.017112	3.154780	0.000073
21	6	0	-4.352341	-2.468139	-0.000317
22	6	0	-3.264110	2.523369	0.000023
23	1	0	-2.159230	-3.827310	0.000455
24	1	0	2.160667	-3.854850	0.000626
25	1	0	0.017899	-5.000963	0.000664
26	1	0	-5.292528	0.349562	-0.000366
27	1	0	5.282452	0.352413	-0.000200
28	1	0	4.113582	-3.075717	0.886376
29	1	0	5.443079	-2.323228	-0.000788
30	1	0	4.112827	-3.075709	-0.886834
31	1	0	2.749790	2.936884	0.872857
32	1	0	2.749710	2.936903	-0.872604
33	1	0	4.302075	2.825197	0.000051
34	1	0	-5.433375	-2.319065	-0.000813
35	1	0	-4.091027	-3.056205	0.886130
36	1	0	-4.090226	-3.056363	-0.886419
37	1	0	-2.760232	2.946232	0.872514
38	1	0	-4.312692	2.828424	0.000057
39	1	0	-2.760307	2.946242	-0.872510

Table S12. Cartesian coordinates of **1** at the T_1 optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.238108	-3.162963	0.010047
2	6	0	1.268307	-1.709077	-0.000382
3	6	0	-0.023833	-1.029780	-0.000005
4	6	0	-1.233951	-1.711275	0.009123
5	6	0	-1.235413	-3.125262	0.018662
6	6	0	0.028603	-3.800031	0.018823
7	78	0	-0.005802	0.889923	-0.013571
8	6	0	2.297984	-0.787918	-0.010892
9	6	0	-2.325821	-0.747692	0.006659
10	7	0	3.681504	-0.869777	-0.016632
11	6	0	4.177258	0.413919	-0.026841
12	6	0	3.103158	1.285455	-0.028109
13	7	0	1.968512	0.575826	-0.018655
14	7	0	-2.014913	0.560901	-0.003897
15	6	0	-3.170687	1.280501	-0.003741
16	6	0	-4.216992	0.402287	0.006955
17	7	0	-3.671766	-0.869324	0.013366
18	17	0	0.048996	3.307903	-0.031079
19	6	0	4.459132	-2.081547	-0.009618
20	6	0	-4.423443	-2.104586	0.025014
21	1	0	2.153610	-3.744624	0.011273
22	1	0	-2.146185	-3.711867	0.025491
23	1	0	0.018191	-4.887122	0.026597
24	1	0	5.238592	0.610016	-0.032747
25	1	0	3.088040	2.365613	-0.035108
26	1	0	-3.156915	2.359454	-0.011169
27	1	0	-5.284361	0.556901	0.010358
28	1	0	5.518114	-1.819748	-0.020829
29	1	0	4.242703	-2.690927	-0.893125
30	1	0	4.256729	-2.672382	0.889767
31	1	0	-4.200198	-2.699843	-0.864322
32	1	0	-5.487219	-1.865792	0.029658
33	1	0	-4.190132	-2.689131	0.918856

Table S13. Cartesian coordinates of **2** at the $\mathbf{T_1}$ optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.253882	-3.442392	-0.000040
2	6	0	1.250712	-2.073701	-0.000096
3	6	0	0.000015	-1.343905	-0.000109
4	6	0	-1.250672	-2.073716	-0.000094
5	6	0	-1.253827	-3.442407	-0.000043
6	6	0	0.000032	-4.116055	-0.000015
7	7	0	2.312797	-1.187885	-0.000130
8	7	0	-2.312769	-1.187913	-0.000122
9	78	0	0.000004	0.546763	-0.000245
10	17	0	-0.000024	2.987872	0.000144
11	6	0	3.683438	-1.373918	-0.000094
12	6	0	4.229365	-0.136090	-0.000173
13	7	0	3.197772	0.787507	-0.000111
14	6	0	1.993360	0.171423	-0.000172
15	6	0	-1.993347	0.171398	-0.000159
16	7	0	-3.197764	0.787470	-0.000096
17	6	0	-4.229348	-0.136137	-0.000120
18	6	0	-3.683408	-1.373960	-0.000108
19	6	0	3.391249	2.223426	-0.000088
20	6	0	-3.391244	2.223389	-0.000032
21	1	0	2.171857	-4.021911	-0.000017
22	1	0	-2.171795	-4.021937	-0.000022

23	1	0	0.000039	-5.201166	0.000028
24	1	0	4.144672	-2.348039	-0.000043
25	1	0	5.264439	0.169072	-0.000189
26	1	0	-5.264425	0.169014	-0.000104
27	1	0	-4.144632	-2.348086	-0.000085
28	1	0	3.946649	2.525482	0.892491
29	1	0	2.409746	2.701908	0.000105
30	1	0	3.946333	2.525555	-0.892839
31	1	0	-3.946540	2.525512	-0.892654
32	1	0	-2.409736	2.701863	-0.000063
33	1	0	-3.946431	2.525452	0.892677

Table S14. Cartesian coordinates of **3** at the $\mathbf{T_1}$ optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.250224	-3.271084	-0.024669
2	6	0	-1.269142	-1.856426	-0.023615
3	6	0	0.015156	-1.161813	-0.000666
4	6	0	1.232659	-1.858479	0.019597
5	6	0	1.252695	-3.236317	0.018084
6	6	0	-0.032698	-3.909865	-0.004641
7	78	0	0.000761	0.723051	0.001961
8	6	0	-3.690988	-1.155301	-0.065361
9	6	0	-4.224795	0.119190	-0.073963
10	6	0	-3.172189	1.038871	-0.054585
11	7	0	-1.997024	0.365462	-0.033852
12	7	0	-2.309340	-0.993190	-0.040660
13	7	0	2.329608	-0.973088	0.040141
14	7	0	2.026908	0.368252	0.037167
15	6	0	3.180393	1.033222	0.058867
16	6	0	4.239083	0.106029	0.075752
17	6	0	3.677755	-1.152162	0.063647
18	6	0	4.346320	-2.478428	0.073327
19	6	0	3.272157	2.515325	0.064040
20	17	0	0.024065	3.140883	0.006858
21	6	0	-4.365438	-2.475001	-0.078343
22	6	0	-3.250567	2.518611	-0.056050
23	1	0	-2.158929	-3.858552	-0.040640
24	1	0	2.155453	-3.828194	0.032735
25	1	0	-0.023966	-4.995745	-0.005653
26	1	0	-5.277232	0.362768	-0.092658
27	1	0	5.293979	0.335981	0.094925
28	1	0	4.065905	-3.066351	0.953750
29	1	0	5.427500	-2.332203	0.092474
30	1	0	4.096893	-3.063704	-0.818118
31	1	0	2.757755	2.937340	0.930667
32	1	0	2.783364	2.942167	-0.814898
33	1	0	4.321686	2.816402	0.080444
34	1	0	-5.445582	-2.315585	-0.096665
35	1	0	-4.134574	-3.074252	0.811639
36	1	0	-4.104288	-3.072426	-0.961163
37	1	0	-2.761116	2.943688	0.824943
38	1	0	-4.297744	2.828833	-0.072682
39	1	0	-2.733872	2.943092	-0.921714

Table S15. Cartesian coordinates of **1** at the ^{3}**TS** optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.247472	3.095476	-0.013661
2	6	0	-1.224206	1.697233	-0.052571
3	6	0	-0.003216	1.002306	-0.137967
4	6	0	1.196422	1.730064	-0.028951
5	6	0	1.170834	3.128624	0.021695
6	6	0	-0.047362	3.801895	-0.010581
7	78	0	0.015942	-1.030402	-0.108383
8	6	0	-2.352527	0.795197	0.146819
9	6	0	2.342910	0.849767	0.193196
10	7	0	-3.692808	0.984025	0.043416
11	6	0	-4.306616	-0.211054	0.355702
12	6	0	-3.308780	-1.101685	0.636894
13	7	0	-2.110456	-0.464506	0.511931
14	7	0	2.102142	-0.396482	0.608151
15	6	0	3.300092	-1.034918	0.736287
16	6	0	4.296190	-0.160428	0.408740
17	7	0	3.684994	1.029416	0.070423
18	17	0	0.001055	-3.377881	-0.457486
19	6	0	-4.381990	2.188049	-0.365774
20	6	0	4.395699	2.138543	-0.531907
21	1	0	-2.180375	3.645459	0.062181
22	1	0	2.078558	3.711904	0.140188
23	1	0	-0.062031	4.886613	0.031644
24	1	0	-5.381309	-0.312123	0.344803
25	1	0	-3.371761	-2.144046	0.909992
26	1	0	3.363343	-2.063771	1.056663
27	1	0	5.370474	-0.265846	0.387556
28	1	0	-5.390246	1.923054	-0.686881
29	1	0	-3.859711	2.649539	-1.206292
30	1	0	-4.451174	2.906549	0.456869
31	1	0	4.564911	1.955627	-1.597418
32	1	0	5.358945	2.259835	-0.032258
33	1	0	3.831996	3.060949	-0.420867

Table S16. Cartesian coordinates of **2** at the ^{3}**TS** optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.249766	3.466638	0.011118
2	6	0	1.211577	2.082551	0.127154
3	6	0	0.010318	1.394039	0.308646
4	6	0	-1.177886	2.104334	0.117061
5	6	0	-1.188908	3.489247	0.000079
6	6	0	0.036504	4.163102	-0.000036
7	7	0	2.273323	1.182671	-0.062493
8	7	0	-2.251406	1.222755	-0.080808
9	78	0	-0.007794	-0.609113	0.225943
10	17	0	-0.050481	-2.996146	0.552022
11	6	0	3.642436	1.319020	-0.072966
12	6	0	4.148606	0.080347	-0.308268
13	7	0	3.086557	-0.791090	-0.440060
14	6	0	1.912524	-0.127818	-0.284235
15	6	0	-1.903093	-0.090427	-0.315758
16	7	0	-3.084408	-0.741705	-0.475837
17	6	0	-4.137468	0.135273	-0.319193
18	6	0	-3.619707	1.368937	-0.078796
19	6	0	3.197229	-2.197633	-0.766516
20	6	0	-3.195030	-2.163888	-0.720759
21	1	0	2.187124	4.003096	-0.106277
22	1	0	-2.115224	4.042283	-0.127530
23	1	0	0.046965	5.244888	-0.086111
24	1	0	4.140417	2.258228	0.106739
25	1	0	5.172522	-0.251705	-0.385669

26	1	0	-5.164968	-0.186195	-0.393053
27	1	0	-4.109734	2.312173	0.101264
28	1	0	2.285077	-2.703539	-0.441858
29	1	0	4.055461	-2.624364	-0.242930
30	1	0	3.325069	-2.331381	-1.845229
31	1	0	-2.454322	-2.458678	-1.465439
32	1	0	-4.199334	-2.383571	-1.086870
33	1	0	-2.992644	-2.726720	0.194234

Table S17. Cartesian coordinates of **1** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.209627	-2.999506	0.141267
2	6	0	1.208798	-1.611876	-0.042826
3	6	0	0.000014	-0.913405	-0.215048
4	6	0	-1.208758	-1.611899	-0.042854
5	6	0	-1.209562	-2.999535	0.141213
6	6	0	0.000039	-3.687926	0.194592
7	78	0	-0.000002	1.108038	-0.428956
8	6	0	2.347893	-0.708120	0.069210
9	6	0	-2.347876	-0.708162	0.069153
10	7	0	3.685870	-0.924794	-0.006240
11	6	0	4.314663	0.288951	0.177460
12	6	0	3.327544	1.217435	0.355394
13	7	0	2.120672	0.586753	0.294961
14	7	0	-2.120697	0.586644	0.295311
15	6	0	-3.327570	1.217317	0.355773
16	6	0	-4.314662	0.288878	0.177471
17	7	0	-3.685849	-0.924829	-0.006424
18	17	0	-0.000449	3.394929	-1.058984
19	6	0	4.359830	-2.174369	-0.282920
20	6	0	-4.359804	-2.174332	-0.283442
21	1	0	2.133512	-3.550508	0.287573
22	1	0	-2.133431	-3.550556	0.287539
23	1	0	0.000049	-4.763636	0.341250
24	1	0	5.390686	0.374269	0.161876
25	1	0	3.404687	2.282124	0.515504
26	1	0	-3.404729	2.281964	0.516150
27	1	0	-5.390684	0.374200	0.161795
28	1	0	5.371413	-1.958045	-0.629087
29	1	0	3.831801	-2.716649	-1.069916
30	1	0	4.419896	-2.801548	0.611996
31	1	0	-3.831522	-2.716578	-1.070287
32	1	0	-5.371239	-1.957907	-0.629982
33	1	0	-4.420249	-2.801584	0.611400

Table S18. Cartesian coordinates of **2** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.219150	-3.473898	-0.047536
2	6	0	1.193982	-2.110695	0.221407
3	6	0	0.000027	-1.436784	0.487970
4	6	0	-1.193914	-2.110724	0.221424
5	6	0	-1.219053	-3.473928	-0.047518
6	6	0	0.000056	-4.154805	-0.127842
7	7	0	2.261226	-1.203933	0.118286
8	7	0	-2.261182	-1.203988	0.118317
9	78	0	0.000004	0.564434	0.621240

10	17	0	-0.000018	2.906333	1.206283
11	6	0	3.629180	-1.349111	0.088540
12	6	0	4.144494	-0.097034	-0.023056
13	7	0	3.089390	0.791545	-0.062281
14	6	0	1.909622	0.125433	0.030481
15	6	0	-1.909610	0.125386	0.030504
16	7	0	-3.089396	0.791470	-0.062233
17	6	0	-4.144479	-0.097133	-0.022986
18	6	0	-3.629133	-1.349198	0.088608
19	6	0	3.212027	2.222177	-0.249988
20	6	0	-3.212072	2.222099	-0.249936
21	1	0	2.151028	-4.001080	-0.231657
22	1	0	-2.150921	-4.001132	-0.231625
23	1	0	0.000068	-5.220447	-0.333173
24	1	0	4.120068	-2.305376	0.172163
25	1	0	5.170881	0.233109	-0.070564
26	1	0	-5.170875	0.232986	-0.070474
27	1	0	-4.119997	-2.305473	0.172244
28	1	0	4.078104	2.587232	0.306293
29	1	0	2.307836	2.702613	0.130294
30	1	0	3.333898	2.460246	-1.311297
31	1	0	-3.334075	2.460157	-1.311233
32	1	0	-2.307838	2.702541	0.130234
33	1	0	-4.078084	2.587153	0.306448

Table S19. Cartesian coordinates of **3** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in the gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213732	-3.136925	-0.396052
2	6	0	-1.192727	-1.784488	-0.056038
3	6	0	-0.000002	-1.106551	0.191016
4	6	0	1.192738	-1.784383	-0.056257
5	6	0	1.213811	-3.136798	-0.396337
6	6	0	0.000059	-3.808070	-0.524996
7	78	0	-0.000004	0.880975	0.555283
8	6	0	-3.662952	-1.184164	0.163945
9	6	0	-4.287948	0.048305	0.095771
10	6	0	-3.278626	0.998422	-0.138941
11	7	0	-2.105230	0.373169	-0.222270
12	7	0	-2.338716	-0.952142	-0.037682
13	7	0	2.338672	-0.951963	-0.038074
14	7	0	2.105132	0.373327	-0.222805
15	6	0	3.278544	0.998598	-0.139717
16	6	0	4.287891	0.048535	0.095109
17	6	0	3.662954	-1.183968	0.163235
18	6	0	4.252382	-2.522401	0.437702
19	6	0	3.383079	2.473233	-0.307301
20	17	0	0.000301	3.131710	1.315605
21	6	0	-4.252352	-2.522593	0.438483
22	6	0	-3.383188	2.473079	-0.306327
23	1	0	-2.140333	-3.659294	-0.601048
24	1	0	2.140429	-3.659045	-0.601584
25	1	0	0.000079	-4.859690	-0.793579
26	1	0	-5.345872	0.235593	0.211796
27	1	0	5.345809	0.235867	0.211115
28	1	0	3.653649	-3.087181	1.158401
29	1	0	5.253708	-2.392575	0.852898
30	1	0	4.347550	-3.126742	-0.471456
31	1	0	2.502647	2.969679	0.111194
32	1	0	3.451454	2.740382	-1.367451
33	1	0	4.276847	2.851615	0.193896
34	1	0	-5.253875	-2.392766	0.853204

35	1	0	-3.653885	-3.087147	1.159587
36	1	0	-4.347058	-3.127157	-0.470571
37	1	0	-2.503094	2.969556	0.112851
38	1	0	-4.277354	2.851275	0.194294
39	1	0	-3.450810	2.740411	-1.366478

Table S20. Cartesian coordinates of **1** at the **S_0** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.221817	-3.119759	-0.000056
2	6	0	1.225821	-1.720085	-0.000045
3	6	0	0.000001	-1.036091	-0.000032
4	6	0	-1.225819	-1.720086	-0.000037
5	6	0	-1.221814	-3.119760	-0.000050
6	6	0	0.000002	-3.796834	-0.000060
7	78	0	0.000000	0.900546	-0.000007
8	6	0	2.319485	-0.758390	-0.000014
9	6	0	-2.319485	-0.758392	0.000002
10	7	0	3.664218	-0.882587	-0.000011
11	6	0	4.207672	0.381746	0.000133
12	6	0	3.164062	1.265589	-0.000100
13	7	0	2.002459	0.551042	0.000018
14	7	0	-2.002459	0.551041	0.000026
15	6	0	-3.164062	1.265587	0.000141
16	6	0	-4.207672	0.381743	-0.000035
17	7	0	-3.664217	-0.882590	0.000037
18	17	0	-0.000003	3.372968	0.000055
19	6	0	4.420792	-2.120496	-0.000046
20	6	0	-4.420790	-2.120500	0.000050
21	1	0	2.142585	-3.693625	-0.000048
22	1	0	-2.142582	-3.693626	-0.000050
23	1	0	0.000002	-4.882249	-0.000064
24	1	0	5.275220	0.536431	0.000222
25	1	0	3.167987	2.344153	-0.000203
26	1	0	-3.167988	2.344151	0.000237
27	1	0	-5.275220	0.536427	-0.000086
28	1	0	5.482450	-1.876873	-0.000083
29	1	0	4.193112	-2.706241	-0.893325
30	1	0	4.193169	-2.706242	0.893246
31	1	0	-4.193167	-2.706229	-0.893254
32	1	0	-5.482448	-1.876877	0.000090
33	1	0	-4.193109	-2.706261	0.893318

Table S21. Cartesian coordinates of **2** at the **S_0** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224967	-3.453572	-0.000087
2	6	0	-1.200324	-2.062319	-0.000018
3	6	0	0.000003	-1.366043	-0.000008
4	6	0	1.200331	-2.062316	-0.000032
5	6	0	1.224978	-3.453570	-0.000098
6	6	0	0.000006	-4.129550	-0.000134
7	7	0	-2.295192	-1.168523	0.000069
8	7	0	2.295197	-1.168518	0.000045
9	78	0	-0.000001	0.577558	0.000073

10	17	0	-0.000007	3.051807	-0.000548
11	6	0	-3.653086	-1.387106	0.000121
12	6	0	-4.230189	-0.159581	0.000150
13	7	0	-3.210135	0.774923	0.000090
14	6	0	-2.003859	0.176361	0.000112
15	6	0	2.003860	0.176366	0.000092
16	7	0	3.210133	0.774931	0.000066
17	6	0	4.230191	-0.159569	0.000096
18	6	0	3.653092	-1.387096	0.000099
19	6	0	-3.432298	2.209520	0.000022
20	6	0	3.432288	2.209529	-0.000018
21	1	0	-2.156334	-4.011219	-0.000099
22	1	0	2.156345	-4.011214	-0.000118
23	1	0	0.000007	-5.214875	-0.000186
24	1	0	-4.092326	-2.371770	0.000116
25	1	0	-5.269431	0.129437	0.000169
26	1	0	5.269432	0.129452	0.000095
27	1	0	4.092334	-2.371759	0.000102
28	1	0	-3.996065	2.495494	-0.891016
29	1	0	-2.461842	2.706686	-0.000227
30	1	0	-3.995711	2.495643	0.891237
31	1	0	3.995859	2.495636	0.891102
32	1	0	2.461828	2.706687	-0.000088
33	1	0	3.995892	2.495527	-0.891152

Table S22. Cartesian coordinates of **3** at the **S_0** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.226273	3.254580	0.000038
2	6	0	1.210726	1.859540	0.000006
3	6	0	0.000001	1.178095	-0.000014
4	6	0	-1.210725	1.859540	0.000015
5	6	0	-1.226271	3.254581	0.000048
6	6	0	0.000001	3.922818	0.000054
7	78	0	0.000000	-0.740301	-0.000040
8	6	0	3.659562	1.160860	0.000006
9	6	0	4.226787	-0.097692	-0.000019
10	6	0	3.174826	-1.026347	-0.000003
11	7	0	2.013326	-0.367248	-0.000018
12	7	0	2.313292	0.976888	0.000008
13	7	0	-2.313292	0.976889	0.000025
14	7	0	-2.013327	-0.367248	0.000008
15	6	0	-3.174828	-1.026346	0.000023
16	6	0	-4.226787	-0.097690	0.000030
17	6	0	-3.659561	1.160862	0.000023
18	6	0	-4.334703	2.484765	0.000019
19	6	0	-3.278940	-2.508105	0.000011
20	17	0	0.000000	-3.208662	0.000071
21	6	0	4.334705	2.484763	0.000013
22	6	0	3.278934	-2.508106	-0.000006
23	1	0	2.142908	3.828724	0.000057
24	1	0	-2.142906	3.828724	0.000076
25	1	0	0.000001	5.007933	0.000083
26	1	0	5.283169	-0.321544	-0.000036
27	1	0	-5.283169	-0.321540	0.000034
28	1	0	-4.078778	3.072805	0.887007
29	1	0	-5.414322	2.328106	0.000025
30	1	0	-4.078788	3.072794	-0.886979
31	1	0	-2.787059	-2.938640	0.875358
32	1	0	-2.787106	-2.938616	-0.875376
33	1	0	-4.331326	-2.798071	0.000031
34	1	0	5.414324	2.328102	0.000013

35	1	0	4.078785	3.072794	0.887008
36	1	0	4.078787	3.072801	-0.886978
37	1	0	2.787203	-2.938622	0.875437
38	1	0	4.331319	-2.798076	-0.000151
39	1	0	2.786948	-2.938635	-0.875297

Table S23. Cartesian coordinates of **1** at the $\mathbf{T_1}$ optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.261265	3.155833	-0.000024
2	6	0	1.282810	1.699548	-0.000087
3	6	0	-0.011883	1.025220	-0.000256
4	6	0	-1.214320	1.713129	-0.000020
5	6	0	-1.207345	3.129833	0.000021
6	6	0	0.057359	3.802361	0.000006
7	78	0	-0.008927	-0.898826	-0.000240
8	6	0	2.307905	0.782515	-0.000110
9	6	0	-2.320437	0.764933	0.000039
10	7	0	3.693258	0.865137	0.000072
11	6	0	4.187047	-0.411400	0.000093
12	6	0	3.114492	-1.290631	0.000001
13	7	0	1.973142	-0.591871	-0.000133
14	7	0	-2.020701	-0.548161	-0.000129
15	6	0	-3.190138	-1.250293	0.000158
16	6	0	-4.223325	-0.355757	0.000392
17	7	0	-3.662262	0.904665	0.000106
18	17	0	-0.006029	-3.374338	0.000812
19	6	0	4.473973	2.080611	0.000226
20	6	0	-4.404763	2.150899	0.000067
21	1	0	2.182687	3.727142	0.000169
22	1	0	-2.117657	3.716522	0.000155
23	1	0	0.050975	4.888953	0.000163
24	1	0	5.248115	-0.610236	0.000194
25	1	0	3.126796	-2.370271	-0.000013
26	1	0	-3.206063	-2.328845	0.000147
27	1	0	-5.292649	-0.496355	0.000587
28	1	0	5.531101	1.815591	0.000437
29	1	0	4.262310	2.676039	0.892891
30	1	0	4.262665	2.676072	-0.892502
31	1	0	-4.169932	2.734541	0.892864
32	1	0	-5.469208	1.919471	0.000259
33	1	0	-4.170229	2.734379	-0.892913

Table S24. Cartesian coordinates of **2** at the $\mathbf{T_1}$ optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.254583	-3.430043	0.000074
2	6	0	-1.253860	-2.061948	0.000034
3	6	0	0.000000	-1.328660	0.000017
4	6	0	1.253861	-2.061948	0.000033
5	6	0	1.254584	-3.430042	0.000084
6	6	0	0.000000	-4.102326	0.000104
7	7	0	-2.314829	-1.179247	0.000004
8	7	0	2.314830	-1.179246	-0.000005
9	78	0	0.000000	0.559951	-0.000077
10	17	0	-0.000001	3.041356	0.000162
11	6	0	-3.685102	-1.374794	-0.000031
12	6	0	-4.237102	-0.140407	0.000057

13	7	0	-3.209698	0.789499	0.000021
14	6	0	-2.002061	0.181483	-0.000013
15	6	0	2.002061	0.181484	-0.000039
16	7	0	3.209698	0.789500	-0.000010
17	6	0	4.237103	-0.140407	-0.000030
18	6	0	3.685102	-1.374794	-0.000013
19	6	0	-3.426202	2.222636	0.000090
20	6	0	3.426205	2.222636	0.000032
21	1	0	-2.172003	-4.009504	0.000089
22	1	0	2.172004	-4.009503	0.000101
23	1	0	0.000001	-5.187190	0.000140
24	1	0	-4.140403	-2.351817	-0.000056
25	1	0	-5.273411	0.160300	0.000110
26	1	0	5.273411	0.160300	-0.000026
27	1	0	4.140403	-2.351817	0.000004
28	1	0	-3.988402	2.514034	-0.890919
29	1	0	-2.454374	2.716590	-0.000006
30	1	0	-3.988170	2.513983	0.891263
31	1	0	3.988283	2.513983	0.891135
32	1	0	2.454379	2.716593	0.000049
33	1	0	3.988296	2.514031	-0.891046

Table S25. Cartesian coordinates of **3** at the $\mathbf{T_1}$ optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.281841	3.251943	-0.000247
2	6	0	-1.288071	1.842017	-0.000100
3	6	0	0.003652	1.150231	-0.000015
4	6	0	1.222210	1.862320	-0.000111
5	6	0	1.224286	3.234392	-0.000261
6	6	0	-0.067387	3.901914	-0.000315
7	78	0	0.005768	-0.731612	0.000040
8	6	0	-3.705893	1.131196	0.000076
9	6	0	-4.234138	-0.143719	0.000214
10	6	0	-3.177693	-1.061031	0.000189
11	7	0	-2.002100	-0.385638	0.000022
12	7	0	-2.322911	0.972892	-0.000004
13	7	0	2.323962	0.989509	-0.000006
14	7	0	2.032605	-0.356806	0.000103
15	6	0	3.197445	-1.006553	0.000141
16	6	0	4.245149	-0.068627	0.000374
17	6	0	3.671978	1.184216	0.000161
18	6	0	4.325929	2.516690	0.000192
19	6	0	3.315580	-2.486875	-0.000019
20	17	0	0.039132	-3.194477	-0.000556
21	6	0	-4.385495	2.448236	0.000051
22	6	0	-3.261606	-2.540517	0.000362
23	1	0	-2.195016	3.831975	-0.000329
24	1	0	2.121430	3.835293	-0.000331
25	1	0	-0.064553	4.987205	-0.000453
26	1	0	-5.286189	-0.390370	0.000328
27	1	0	5.302525	-0.287573	0.000593
28	1	0	4.054984	3.099391	-0.886348
29	1	0	5.408159	2.380651	0.000378
30	1	0	4.054702	3.099505	0.886570
31	1	0	2.830009	-2.921099	-0.877098
32	1	0	2.826336	-2.921697	0.874683
33	1	0	4.370478	-2.767033	0.001966
34	1	0	-5.464618	2.283728	0.000242
35	1	0	-4.139509	3.045360	-0.886425
36	1	0	-4.139222	3.045550	0.886319
37	1	0	-2.764468	-2.969508	-0.874729

38	1	0	-4.310175	-2.845010	-0.000196
39	1	0	-2.765540	-2.969264	0.876199

Table S26. Cartesian coordinates of **1** at the **^{3}TS** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.218018	3.032640	0.247319
2	6	0	-1.212751	1.640040	0.089140
3	6	0	0.011714	0.938075	0.085117
4	6	0	1.219393	1.648885	0.210167
5	6	0	1.192816	3.035215	0.420098
6	6	0	-0.019157	3.714871	0.429438
7	78	0	-0.004088	-1.083646	0.032096
8	6	0	-2.404845	0.798357	-0.069319
9	6	0	2.443579	0.836493	0.160863
10	7	0	-3.722175	1.136843	-0.145574
11	6	0	-4.443264	-0.025015	-0.290940
12	6	0	-3.537531	-1.049002	-0.300425
13	7	0	-2.288700	-0.525562	-0.165474
14	7	0	2.421658	-0.456954	0.477426
15	6	0	3.678847	-0.943029	0.267177
16	6	0	4.484610	0.067513	-0.176986
17	7	0	3.697855	1.193950	-0.242565
18	17	0	0.002064	-3.571321	0.024853
19	6	0	-4.331414	2.453081	-0.096069
20	6	0	4.145076	2.406114	-0.908736
21	1	0	-2.139556	3.600757	0.252808
22	1	0	2.103229	3.590245	0.618616
23	1	0	-0.032841	4.788365	0.590389
24	1	0	-5.519478	-0.011648	-0.373648
25	1	0	-3.707621	-2.111274	-0.394922
26	1	0	3.932100	-1.975243	0.461894
27	1	0	5.528951	0.096031	-0.449790
28	1	0	-5.405875	2.336141	-0.233886
29	1	0	-3.945537	3.088050	-0.896213
30	1	0	-4.154663	2.927569	0.871785
31	1	0	3.590069	3.273070	-0.564894
32	1	0	4.018675	2.311688	-1.990854
33	1	0	5.201541	2.559749	-0.685011

Table S27. Cartesian coordinates of **2** at the **^{3}TS** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.197024	3.483160	-0.017890
2	6	0	1.182458	2.097592	-0.137592
3	6	0	-0.007384	1.392969	-0.341174
4	6	0	-1.208190	2.080589	-0.148764
5	6	0	-1.243886	3.465354	-0.029829
6	6	0	-0.028095	4.158701	-0.019702
7	7	0	2.253011	1.214756	0.077676
8	7	0	-2.270581	1.183696	0.058194
9	78	0	0.006900	-0.610575	-0.243488
10	17	0	0.032998	-3.035893	-0.640345
11	6	0	3.620226	1.371979	0.099357
12	6	0	4.140658	0.146299	0.373039
13	7	0	3.089339	-0.734051	0.524720
14	6	0	1.908836	-0.095019	0.331610
15	6	0	-1.917583	-0.124491	0.298799

16	7	0	-3.091296	-0.772641	0.491679
17	6	0	-4.149493	0.104315	0.365932
18	6	0	-3.638362	1.334151	0.095698
19	6	0	3.215346	-2.147824	0.814449
20	6	0	-3.212738	-2.169808	0.858992
21	1	0	2.124344	4.032650	0.114559
22	1	0	-2.179973	4.002159	0.092246
23	1	0	-0.036473	5.240318	0.068207
24	1	0	4.107440	2.315419	-0.087898
25	1	0	5.168125	-0.168241	0.472198
26	1	0	-5.173791	-0.218638	0.471357
27	1	0	-4.132351	2.274622	-0.089146
28	1	0	4.215930	-2.341985	1.201150
29	1	0	3.043380	-2.738744	-0.088187
30	1	0	2.472103	-2.430075	1.561232
31	1	0	-3.312335	-2.270674	1.943419
32	1	0	-2.319066	-2.696834	0.521419
33	1	0	-4.092747	-2.595071	0.373906

Table S28. Cartesian coordinates of **1** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210999	-2.979939	0.157504
2	6	0	1.211357	-1.593679	-0.043772
3	6	0	-0.000005	-0.903409	-0.223500
4	6	0	-1.211338	-1.593726	-0.043751
5	6	0	-1.210913	-2.979988	0.157514
6	6	0	0.000057	-3.665655	0.219848
7	78	0	-0.000019	1.108616	-0.454198
8	6	0	2.359272	-0.697145	0.058333
9	6	0	-2.359292	-0.697238	0.058360
10	7	0	3.691407	-0.933729	-0.022285
11	6	0	4.340724	0.265731	0.163582
12	6	0	3.371310	1.212020	0.349188
13	7	0	2.150768	0.603351	0.289627
14	7	0	-2.150851	0.603279	0.289605
15	6	0	-3.371424	1.211873	0.349268
16	6	0	-4.340796	0.265517	0.163775
17	7	0	-3.691421	-0.933905	-0.022125
18	17	0	-0.000004	3.513405	-0.978758
19	6	0	4.353035	-2.196084	-0.293076
20	6	0	-4.353009	-2.196307	-0.292794
21	1	0	2.134360	-3.529058	0.307709
22	1	0	-2.134243	-3.529157	0.307729
23	1	0	0.000078	-4.739395	0.379166
24	1	0	5.417975	0.331434	0.145582
25	1	0	3.476816	2.272449	0.522237
26	1	0	-3.476981	2.272300	0.522300
27	1	0	-5.418052	0.331153	0.145855
28	1	0	5.371448	-1.989768	-0.621762
29	1	0	3.829816	-2.728415	-1.088986
30	1	0	4.389782	-2.819953	0.603776
31	1	0	-3.829847	-2.728647	-1.088734
32	1	0	-5.371466	-1.990059	-0.621388
33	1	0	-4.389633	-2.820138	0.604090

Table S29. Cartesian coordinates of **2** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.220183	-3.471662	-0.028168
2	6	0	1.193893	-2.112509	0.264710
3	6	0	0.000028	-1.450798	0.561199
4	6	0	-1.193825	-2.112538	0.264731
5	6	0	-1.220086	-3.471692	-0.028146
6	6	0	0.000056	-4.151420	-0.114025
7	7	0	2.255910	-1.198680	0.146425
8	7	0	-2.255867	-1.198735	0.146467
9	78	0	0.000007	0.549321	0.741712
10	17	0	-0.000007	2.890919	1.506987
11	6	0	3.621907	-1.347358	0.058320
12	6	0	4.132953	-0.095940	-0.078842
13	7	0	3.075966	0.792094	-0.075366
14	6	0	1.903539	0.129293	0.065766
15	6	0	-1.903529	0.129247	0.065802
16	7	0	-3.075974	0.792021	-0.075310
17	6	0	-4.132939	-0.096039	-0.078764
18	6	0	-3.621861	-1.347444	0.058391
19	6	0	3.194866	2.222413	-0.279357
20	6	0	-3.194910	2.222336	-0.279302
21	1	0	2.151960	-3.992923	-0.226575
22	1	0	-2.151855	-3.992976	-0.226537
23	1	0	0.000067	-5.214075	-0.334117
24	1	0	4.114527	-2.304631	0.118864
25	1	0	5.155985	0.234468	-0.172523
26	1	0	-5.155981	0.234346	-0.172426
27	1	0	-4.114458	-2.304729	0.118946
28	1	0	4.071807	2.592557	0.254345
29	1	0	2.298972	2.704207	0.114526
30	1	0	3.297418	2.447285	-1.344717
31	1	0	-3.297490	2.447205	-1.344659
32	1	0	-2.299020	2.704152	0.114562
33	1	0	-4.071848	2.592461	0.254419

Table S30. Cartesian coordinates of **3** at the ^{3}**MC** optimized geometry by **DFT** with **UPBE0** method in a CH_2Cl_2 solvent.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213905	-3.106560	-0.439877
2	6	0	-1.194656	-1.757648	-0.084085
3	6	0	0.000021	-1.080710	0.164616
4	6	0	1.194676	-1.757592	-0.084334
5	6	0	1.213905	-3.106513	-0.440098
6	6	0	0.000000	-3.775353	-0.578889
7	78	0	-0.000005	0.904942	0.524153
8	6	0	-3.665308	-1.198004	0.188667
9	6	0	-4.316102	0.022240	0.133310
10	6	0	-3.332089	0.989851	-0.131023
11	7	0	-2.146248	0.390447	-0.242780
12	7	0	-2.350492	-0.939667	-0.046707
13	7	0	2.350487	-0.939563	-0.047187
14	7	0	2.146137	0.390555	-0.243126
15	6	0	3.331984	0.989996	-0.131657
16	6	0	4.316118	0.022405	0.132297
17	6	0	3.665382	-1.197859	0.187812
18	6	0	4.226388	-2.545241	0.475355
19	6	0	3.476275	2.460592	-0.308336
20	17	0	0.000020	3.265733	1.231476
21	6	0	-4.226171	-2.545400	0.476429
22	6	0	-3.476496	2.460432	-0.307753
23	1	0	-2.140397	-3.626998	-0.648688
24	1	0	2.140371	-3.626928	-0.649071

25	1	0	-0.000003	-4.823058	-0.861634
26	1	0	-5.374488	0.187728	0.275345
27	1	0	5.374544	0.187919	0.273999
28	1	0	3.599415	-3.104931	1.175115
29	1	0	5.217099	-2.429499	0.918352
30	1	0	4.338854	-3.144914	-0.434292
31	1	0	2.555775	2.973322	-0.016866
32	1	0	3.691753	2.708501	-1.353352
33	1	0	4.301377	2.838978	0.299593
34	1	0	-5.216688	-2.429682	0.919865
35	1	0	-3.598881	-3.105101	1.175895
36	1	0	-4.339025	-3.145050	-0.433186
37	1	0	-2.556027	2.973241	-0.016326
38	1	0	-4.301609	2.838778	0.300184
39	1	0	-3.692013	2.708296	-1.352773