Electronic Supplementary Information

Through-space charge transfer and emission color tuning of di-*o*-carborane substituted benzene

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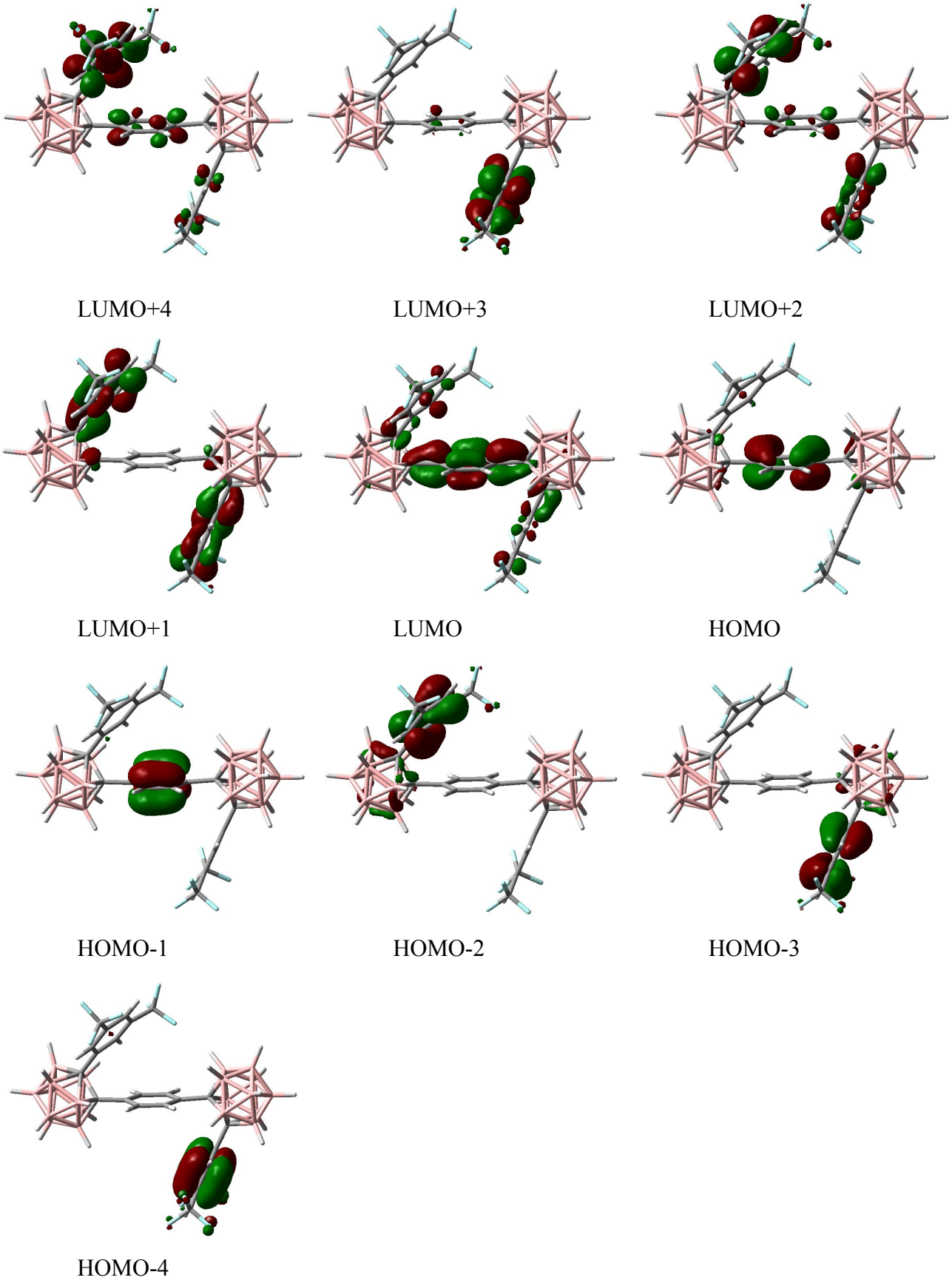

Figure S1. Molecular orbitals of **1** from B3LYP calculations (Isovalue = 0.04) at their lowest singlet ground state (S_0) geometries.

Table S1. Computed absorption wavelengths ($\lambda_{calc.}$ in nm) and oscillator strengths ($f_{calc.}$) for **1** from B3LYP calculations using the B3LYP geometries.

state	$\lambda_{calc.}$(/nm)	$f_{calc.}$	major contribution
1	256.6	0.0661	HOMO-1→ LUMO (60.05%)
			HOMO→ LUMO (19.91%)
2	251.12	0.4204	HOMO→ LUMO (72.44%)
			HOMO-1→ LUMO (18.74%)
3	244.76	0.0246	HOMO-2 → LUMO (32.59%)
			HOMO-5 → LUMO+1 (11.91%)
			HOMO-2 → LUMO+4 (10.07%)
4	242.93	0.0027	HOMO-3→ LUMO+3 (35.65%)
			HOMO-4 → LUMO (23.46%)
			HOMO-4 → LUMO+1 (18.23%)
5	238.37	0.0138	HOMO → LUMO+1 (74.68%)
			HOMO-2 → LUMO (17.05%)
6	236.37	0.0652	HOMO-3 → LUMO (78.40%)
7	235.13	0.0011	HOMO-1 → LUMO+1 (28.85%)
			HOMO-2 → LUMO (24.29%)
			HOMO-5 → LUMO (14.21%)
8	234.61	0.0134	HOMO-1 → LUMO+1 (63.02%)
9	231.32	0.0031	HOMO→ LUMO+2 (38.64%)
			HOMO-1 → LUMO+2 (27.09%)
			HOMO → LUMO+3 (16.10%)
10	230.4	0.0559	HOMO → LUMO+2 (39.30%)
			HOMO-1→ LUMO+2 (32.13%)

Table S2. Molecular orbital distributions (in %) of **1** from B3LYP calculations.

molecular orbital	Aryl1	CF_3-1	Aryl2	CF_3-2	Phenylene	Carborane1	Carborane2
LUMO+4	53.08	6.49	8.26	0.56	12.79	11.53	7.29
LUMO+3	1.34	0.08	69.89	8.08	5.67	1.69	12.95
LUMO+2	42.98	3.58	20.49	0.99	9.81	13.22	8.94
LUMO+1	31.45	1.44	30.25	1.40	2.35	16.41	16.69
LUMO	9.52	0.55	8.54	0.28	31.66	23.12	26.32
HOMO	4.27	0.47	1.29	0.05	66.70	13.22	14.01
HOMO-1	3.47	0.14	2.09	0.21	89.57	2.46	2.05
HOMO-2	74.55	2.71	0.78	0.04	2.51	19.06	0.36
HOMO-3	1.19	0.11	75.63	2.67	1.40	0.40	18.61
HOMO-4	3.72	0.39	82.10	9.08	1.99	0.16	2.57

Table S3. Molecular orbital energies (in eV) of **1** from B3LYP calculations.

MO	$HOMO_{-4}$	$HOMO_{-3}$	$HOMO_{-2}$	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	$LUMO_{+2}$	$LUMO_{+3}$	$LUMO_{+4}$
Energy	-8.03	-7.89	-7.88	-7.66	-7.59	-2.10	-1.78	-1.64	-1.61	-1.48

Table S4. Cartesian coordinates of **1** from B3LYP calculation (in Å).

	S_0		
	X	Y	Z
C	5.823779	-1.72719	-1.87444
C	5.164114	-1.08049	-0.6812
C	-3.65516	2.681903	-1.76819
C	-0.28743	-0.80478	-1.56311
C	4.520512	0.14703	-0.84159
C	0.533872	0.314371	-1.48175
C	-3.72434	0.253476	-1.15943
C	-3.57896	-2.20943	-0.53734
C	-4.13365	1.557914	-0.88278
C	-1.86631	-2.49148	-0.55738
C	5.244542	-1.68113	0.572738
C	-4.05517	-0.79658	-0.29489
C	-0.93933	-1.30837	-0.42843
C	-4.90963	1.83639	0.239893
C	3.940202	0.796645	0.254553
C	0.744604	0.968101	-0.25981
C	-4.82731	-0.50985	0.83867
C	3.279785	2.14309	0.086389
C	1.561476	2.233362	-0.19023
C	4.681577	-1.03145	1.670451
C	-5.26124	0.790622	1.092361
C	4.040049	0.196247	1.516884
C	-0.70839	-0.67164	0.797545
C	0.114507	0.448924	0.878861
C	4.819237	-1.638	3.045434
C	-6.15778	1.057308	2.276506
H	-3.1541	-4.73607	-3.39493
H	-2.66503	-1.76014	-2.83518
H	-5.32436	-2.90541	-2.15919
H	-0.4957	-3.70466	-2.22929
H	-0.42648	-1.28056	-2.52663
H	-4.85403	-5.79194	-1.04323
H	-1.81445	-6.286	-1.09931
H	2.773276	1.792707	-2.34816
H	0.993342	0.687676	-2.38818
H	4.476458	0.591819	-1.82741
H	-3.13911	0.07114	-2.04975
H	2.975497	4.845022	-2.62104
H	5.731327	-2.64199	0.691513
H	0.308354	3.42483	-1.96245
H	5.13739	3.165841	-1.19224
H	-5.34237	-3.35431	0.800061
H	-5.23152	2.849808	0.449286
H	-0.50722	-4.11448	0.732468
H	-3.19992	-5.42823	1.523263
H	-5.09198	-1.29817	1.531744
H	4.167174	5.871476	0.030202
H	1.132406	6.034717	-0.45523
H	-2.72541	-2.39697	1.811468
H	-1.17938	-1.03659	1.701374
H	3.619311	0.679557	2.388402
H	-0.15295	3.579105	0.987785
H	4.672488	3.317113	1.762583
H	0.243799	0.929708	1.840842
H	2.035827	2.033973	2.269041
H	2.204041	5.101318	2.279607
B	-3.0744	-4.31982	-2.2864
B	-2.79452	-2.60086	-2.01935
B	-4.36392	-3.30905	-1.59585
B	-1.516	-3.77151	-1.63188
B	-4.05127	-4.92639	-0.92113
B	-2.2958	-5.21168	-0.94779
B	2.668113	2.571273	-1.46965
B	2.778362	4.326268	-1.57202
B	-4.36724	-3.55718	0.160886
B	-1.52166	-4.02323	0.127649
B	1.215475	3.559336	-1.21347
B	4.062586	3.407045	-0.75664
B	-3.09229	-4.72238	0.575396
B	-2.80642	-2.99727	0.799093
B	3.466176	4.915614	-0.03014
B	1.713013	5.009653	-0.31058
B	0.940381	3.651742	0.538448
B	3.787423	3.497789	0.996392

B	2.226686	2.716018	1.326762
B	2.330791	4.475778	1.278954
F	5.112199	-1.52146	-3.00392
F	5.958721	-3.0585	-1.70871
F	7.057237	-1.22028	-2.08572
F	-4.50561	3.726896	-1.75279
F	-3.51276	2.281463	-3.04923
F	4.791241	-2.98592	2.99452
F	-7.4596	0.921182	1.945126
F	3.828391	-1.23591	3.869769
F	-5.99453	2.310323	2.749518
F	5.987371	-1.28449	3.622789
F	-5.91181	0.198896	3.288875
F	-2.44814	3.140465	-1.36015

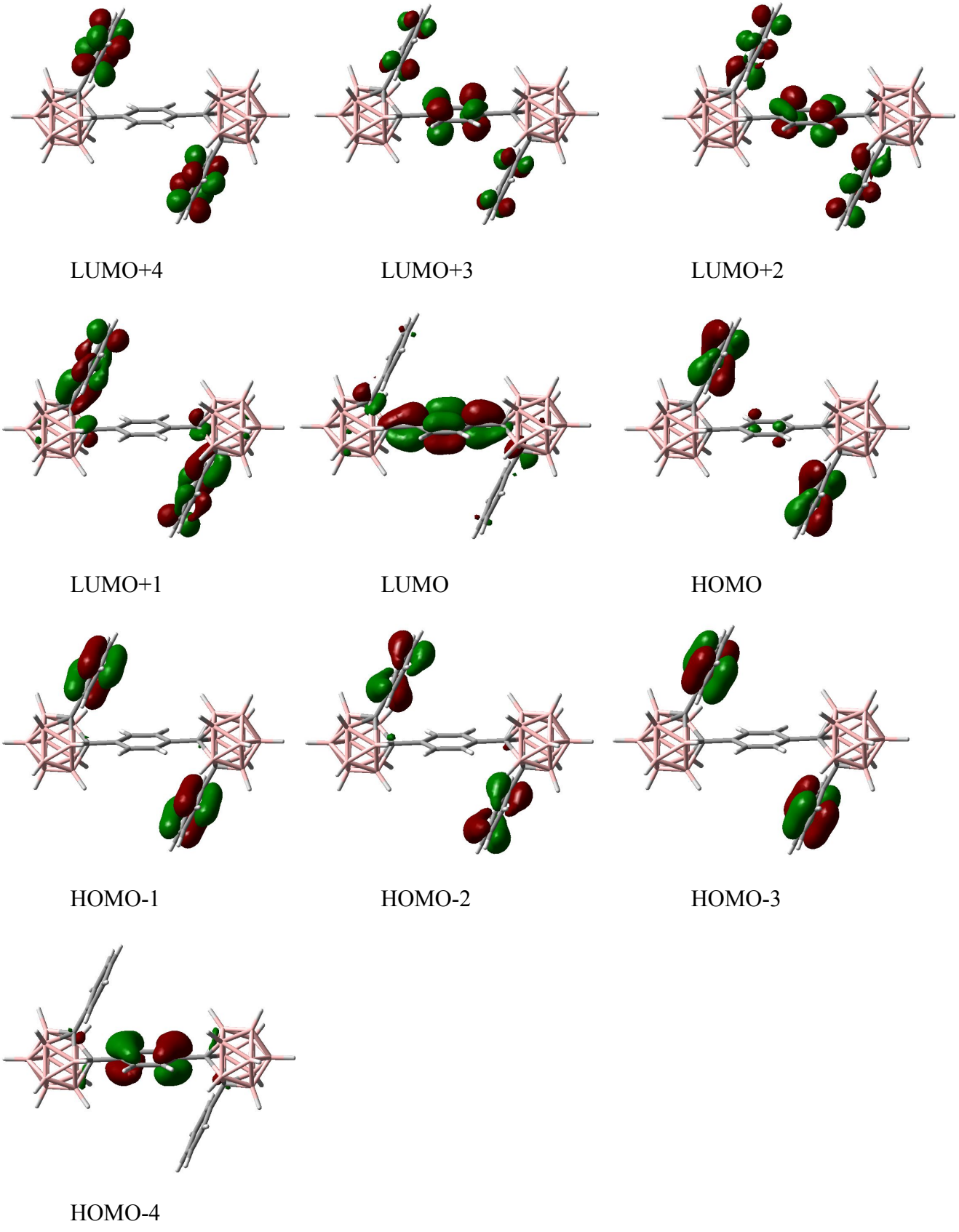

Figure S2. Molecular orbitals of **2** from B3LYP calculations (Isovalue = 0.04) at their lowest singlet ground state (S_0) geometries.

Table S5. Computed absorption wavelengths ($\lambda_{calc.}$ in nm) and oscillator strengths ($f_{calc.}$) for **2** from B3LYP calculations using the B3LYP geometries.

state	$\lambda_{calc.}$(/nm)	$f_{calc.}$	major contribution
1	262.71	0.0979	HOMO→ LUMO (89.96%)
2	261.19	0.0686	HOMO-1→ LUMO (93.09%)
3	260.34	0.0000	HOMO-2 → LUMO (95.59%)
4	260.01	0.0000	HOMO-3→ LUMO (92.93%)
5	252.07	0.0058	HOMO-5 → LUMO (75.08%)
6	244.99	0.6002	HOMO-4 → LUMO (90.11%)
7	237.42	0.0000	HOMO → LUMO+1 (30.38%)
			HOMO-1 → LUMO +1 (14.33%)
			HOMO-3 → LUMO+2 (13.35%)
8	237.16	0.0085	HOMO-3 → LUMO+1 (40.68%)
			HOMO → LUMO+2 (19.68%)
			HOMO-1 → LUMO+3 (13.70%)
			HOMO-2 → LUMO+4 (11.70%)
9	225.07	0.0000	HOMO-1 → LUMO +1 (39.17%)
			HOMO → LUMO+1 (27.65%)
			HOMO-4 → LUMO+1 (20.56%)
10	222.52	0.3059	HOMO-2 → LUMO+1 (73.88%)

Table S6. Molecular orbital distributions (in %) of **2** from B3LYP calculations.

molecular orbital	Aryl1	Aryl2	Phenylene	Carborane1	Carborane2
LUMO+4	39.01	39.01	1.10	10.44	10.44
LUMO+3	14.79	14.79	38.29	16.07	16.07
LUMO+2	17.50	17.49	30.20	17.41	17.40
LUMO+1	22.44	22.44	2.53	26.30	26.30
LUMO	3.01	3.01	38.40	27.79	27.79
HOMO	42.58	42.60	7.40	3.71	3.71
HOMO-1	42.56	42.55	2.39	6.25	6.25
HOMO-2	41.36	41.33	0.63	8.34	8.34
HOMO-3	48.86	48.88	0.11	1.08	1.08
HOMO-4	2.03	2.03	68.18	13.88	13.88

Table S7. Molecular orbital energies (in eV) of **2** from B3LYP calculations.

MO	$HOMO_{-4}$	$HOMO_{-3}$	$HOMO_{-2}$	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	$LUMO_{+2}$	$LUMO_{+3}$	$LUMO_{+4}$
Energy	-7.46	-7.23	-7.22	-7.21	-7.19	-1.88	-1.23	-1.04	-0.96	-0.52

Table S8. Cartesian coordinates of **2** from B3LYP calculation (in Å).

	S_0		
	X	Y	Z
C	4.09808	-0.1718	0.014073
C	3.818168	-1.65297	0.020715
C	3.774759	-2.37632	-1.18121
C	3.558855	-3.75328	-1.17603
C	3.387076	-4.43443	0.029061
C	3.444728	-3.72812	1.230427
C	3.661345	-2.35116	1.22785
H	3.721071	-1.82414	2.172234
H	3.325803	-4.24755	2.176969
H	3.530102	-4.2926	-2.11849
H	3.924995	-1.86782	-2.12596
C	2.761596	0.96891	-0.01582
C	1.346166	0.449492	-0.01173
C	0.695271	0.085967	-1.19813
C	-0.62312	-0.359	-1.18544
C	-1.34618	-0.44952	0.011696
C	-2.76161	-0.96892	0.01578
C	-4.09808	0.17181	-0.01408
C	-3.81815	1.652967	-0.02068
C	-3.66127	2.351192	-1.22779
C	-3.44463	3.728153	-1.23032
C	-3.38702	4.434426	-0.02893
C	-3.55886	3.753246	1.176138
C	-3.77478	2.376291	1.181272
H	-3.92507	1.867769	2.125997
H	-3.53014	4.292539	2.118607
H	-3.32566	4.2476	-2.17684
H	-3.72096	1.8242	-2.17219
B	-3.70626	-0.7607	-1.41146
H	-3.21511	-0.2191	-2.33596
B	-4.84893	-2.10511	-1.44317
H	-5.20637	-2.55515	-2.48224
B	-3.19133	-2.36958	-0.8619
H	-2.32174	-2.91029	-1.45804
B	-4.55496	-3.09703	0.014972
H	-4.70359	-4.27523	0.02422
B	-5.90877	-1.94493	-0.01362
H	-7.04734	-2.28205	-0.023
B	-5.38871	-0.49912	-0.91101
H	-6.04647	0.259596	-1.53926
B	-5.40865	-0.4811	0.864369
H	-6.0828	0.288257	1.461401
B	-4.88373	-2.07598	1.444398
H	-5.2685	-2.50207	2.483742
B	-3.21154	-2.35284	0.912351
H	-2.35477	-2.87771	1.540458
B	-3.73949	-0.73306	1.412713
H	-3.28336	-0.17046	2.342122
C	-0.69528	-0.08599	1.1981
C	0.623109	0.358978	1.185404
H	1.086026	0.64342	2.122519
H	-1.21177	-0.15348	2.147218
H	-1.08604	-0.64345	-2.12255
H	1.211757	0.153454	-2.14725
B	3.739483	0.733025	-1.41274
H	3.283369	0.170399	-2.34214
B	4.883709	2.07596	-1.44445
H	5.268483	2.502031	-2.4838
B	5.408644	0.481098	-0.86438
H	6.082813	-0.28827	-1.46139
B	5.908746	1.944953	0.013577
H	7.047307	2.282094	0.02296
B	4.554919	3.097038	-0.01505
H	4.703532	4.275242	-0.02433
B	3.211516	2.352813	-0.91242
H	2.354743	2.877652	-1.54054
B	3.191293	2.369592	0.861834
H	2.321695	2.910309	1.457951
B	4.848892	2.105155	1.443113
H	5.206327	2.555224	2.482178
B	5.388692	0.499157	0.910998
H	6.046459	-0.25953	1.539267
B	3.706238	0.76073	1.411431
H	3.215096	0.219149	2.335942

H	3.218139	-5.50752	0.03232
H	-3.21807	5.50751	-0.03215

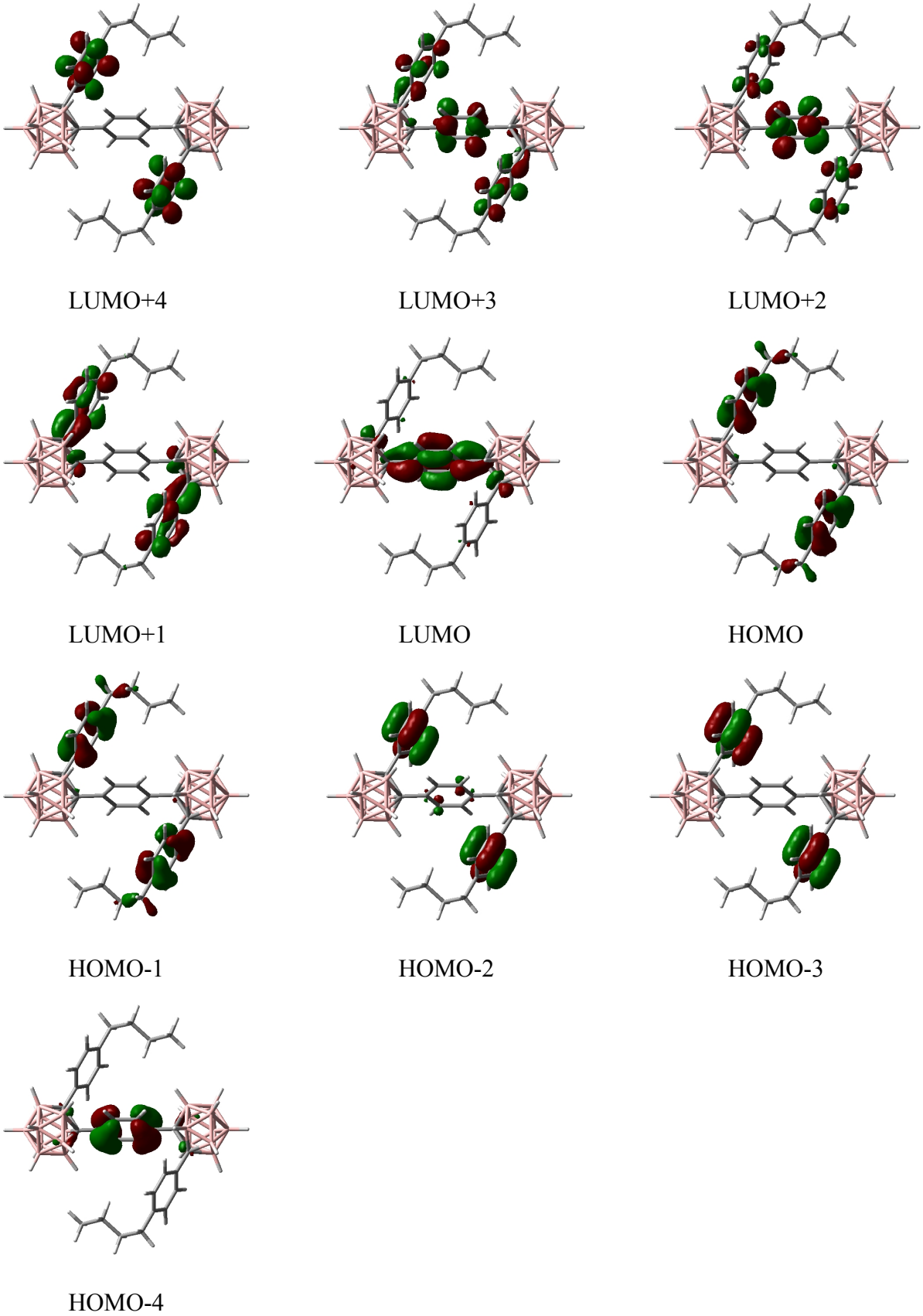

Figure S3. Molecular orbitals of **3** from B3LYP calculations (Isovalue = 0.04) at their lowest singlet ground state (S_0) geometries.

Table S9. Computed absorption wavelengths ($\lambda_{calc.}$ in nm) and oscillator strengths ($f_{calc.}$) for **3** from B3LYP calculations using the B3LYP geometries.

state	$\lambda_{calc.}$(/nm)	$f_{calc.}$	major contribution
1	273.94	0.0903	HOMO → LUMO(97.96%)
2	273.31	0	HOMO-1→ LUMO(98.59%)
3	259.65	0.0212	HOMO-2 → LUMO(91.01%)
4	258.25	0	HOMO-3→ LUMO(93.61%)
5	249.9	0.0126	HOMO-5 → LUMO(67.10%)
			HOMO-4 → LUMO+2(12.98%)
6	243.8	0.4103	HOMO-4 → LUMO(80.20%)
7	239.86	0	HOMO-2 → LUMO+1 (26.84%)
			HOMO-1 → LUMO+2 (15.68%)
			HOMO → LUMO+4 (13.59%)
			HOMO-3 → LUMO+2 (11.73%)
8	239.75	0.0091	HOMO-3 → LUMO+1(25.71%)
			HOMO → LUMO+2(17.72%)
			HOMO-1 → LUMO+4(13.66%)
			HOMO-2 → LUMO+2(11.59%)
9	230.72	0	HOMO → LUMO+1(47.65%)
			HOMO-1 → LUMO+2(30.99%)
10	229.79	0.1363	HOMO → LUMO+2(62.71%)

Table S10. Molecular orbital distributions (in %) of **3** from B3LYP calculations.

molecular orbital	Aryl1	Bu-1	Aryl2	Bu-2	Phenylene	Carborane1	Carborane2
LUMO+4	38.0	2.5	38.0	2.5	1.2	8.8	8.8
LUMO+3	17.0	1.8	17.0	1.8	30.0	16.2	16.2
LUMO+2	13.1	1.7	13.1	1.7	41.0	14.6	14.6
LUMO+1	22.4	3.3	22.4	3.3	2.2	23.1	23.1
LUMO	3.0	0.5	3.0	0.5	42.1	25.5	25.5
HOMO	36.3	6.1	36.2	6.1	0.8	7.3	7.3
HOMO-1	36.5	6.2	36.5	6.2	0.5	7.1	7.1
HOMO-2	44.4	0.5	44.4	0.5	7.1	1.5	1.5
HOMO-3	48.4	0.5	48.4	0.5	0.1	1.0	1.0
HOMO-4	2.5	0.1	2.5	0.1	65.7	14.6	14.6

Table S11. Molecular orbital energies (in eV) of **3** from B3LYP calculations.

MO	$HOMO_{-4}$	$HOMO_{-3}$	$HOMO_{-2}$	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	$LUMO_{+2}$	$LUMO_{+3}$	$LUMO_{+4}$
Energy	-7.50	-7.29	-7.27	-7.01	-7.01	-1.91	-1.22	-1.15	-0.96	-0.60

Table S12. Cartesian coordinates of **3** from B3LYP calculation (in Å).

	S_0		
	X	Y	Z
C	3.49457	-2.15362	-0.06309
C	4.08015	-0.76958	-0.16412
C	4.69758	-0.18509	0.95412
C	5.27026	1.07957	0.87319
C	5.24788	1.81706	-0.31932
C	5.86335	3.19878	-0.38647
C	5.08165	4.27877	0.39409
C	3.68837	4.58415	-0.16915
C	2.95099	5.66766	0.62419
H	2.8114	5.3669	1.66992
H	3.51025	6.61154	0.62403
H	1.96015	5.86662	0.20139
H	3.087	3.66576	-0.18095
H	3.78515	4.89954	-1.21813
H	4.99085	3.97066	1.44549
H	5.6807	5.19995	0.39735
H	6.88567	3.1526	0.01208
H	5.95301	3.5071	-1.43583
C	4.64054	1.22575	-1.43278
C	4.07	-0.04445	-1.36279
H	3.62298	-0.46891	-2.25316
H	4.61663	1.76332	-2.37739
H	5.75008	1.4984	1.75464
H	4.74643	-0.7278	1.89118
C	1.75747	-2.33745	0.08696
C	0.87354	-1.11708	0.04555
C	0.65938	-0.32206	1.17886
C	-0.1948	0.77535	1.13237
C	-0.87354	1.11709	-0.04544
C	-1.75747	2.33746	-0.08686
C	-3.49458	2.15362	0.06311
C	-4.08017	0.76957	0.1641
C	-4.07007	0.04442	1.36276
C	-4.6406	-1.22577	1.4327
C	-5.24789	-1.81707	0.3192
C	-5.86335	-3.1988	0.38631
C	-5.08162	-4.27877	-0.39425
C	-3.68835	-4.58415	0.16902
C	-2.95094	-5.66765	-0.62431
H	-1.96011	-5.8666	-0.20149
H	-3.51019	-6.61153	-0.62418
H	-2.81132	-5.36687	-1.67003
H	-3.78516	-4.89956	1.218
H	-3.08699	-3.66575	0.18086
H	-5.68066	-5.19995	-0.39754
H	-4.99079	-3.97064	-1.44564
H	-5.95304	-3.50714	1.43565
H	-6.88566	-3.15262	-0.01227
C	-5.27021	-1.07957	-0.8733
C	-4.69754	0.1851	-0.95418
H	-4.74635	0.72782	-1.89124
H	-5.74999	-1.49839	-1.75478
H	-4.61673	-1.76336	2.37731
H	-3.62309	0.46888	2.25315
B	-2.56835	2.79403	1.36847
H	-2.40606	2.13636	2.33351
B	-2.75123	4.54839	1.29168
H	-2.72883	5.18969	2.29076
B	-1.27305	3.78902	0.66799
H	-0.21527	3.78635	1.20171
B	-2.03942	5.10004	-0.25279
H	-1.50099	6.15308	-0.36327
B	-3.80077	4.91939	-0.10409
H	-4.55126	5.83962	-0.11246
B	-4.13191	3.49661	0.91393
H	-5.06335	3.28421	1.6143
B	-4.26287	3.37511	-0.85077
H	-5.28941	3.0911	-1.36817
B	-2.97028	4.35099	-1.5811
H	-3.11484	4.85086	-2.64846
B	-1.4033	3.67044	-1.09798
H	-0.43733	3.57687	-1.77803
B	-2.77878	2.603	-1.44684
H	-2.78451	1.81311	-2.32193

C	-0.65938	0.32207	-1.17875
C	0.19479	-0.77535	-1.13226
H	0.32419	-1.37373	-2.0261
H	-1.15502	0.55645	-2.11214
H	-0.3242	1.37373	2.02621
H	1.15502	-0.55644	2.11225
B	2.77884	-2.60298	1.4469
H	2.7846	-1.81308	2.32197
B	2.97034	-4.35097	1.58118
H	3.11495	-4.85082	2.64854
B	4.26289	-3.3751	0.85078
H	5.28946	-3.09108	1.36813
B	3.80076	-4.91938	0.10414
H	4.55125	-5.83962	0.11249
B	2.03942	-5.10003	0.25292
H	1.50099	-6.15307	0.36344
B	1.40334	-3.67042	1.09812
H	0.4374	-3.57683	1.7782
B	1.27301	-3.78902	-0.66785
H	0.21521	-3.78636	-1.20153
B	2.75117	-4.54841	-1.29159
H	2.72872	-5.18973	-2.29066
B	4.13186	-3.49663	-0.91392
H	5.06327	-3.28423	-1.61433
B	2.56828	-2.79405	-1.3684
H	2.40595	-2.13639	-2.33344

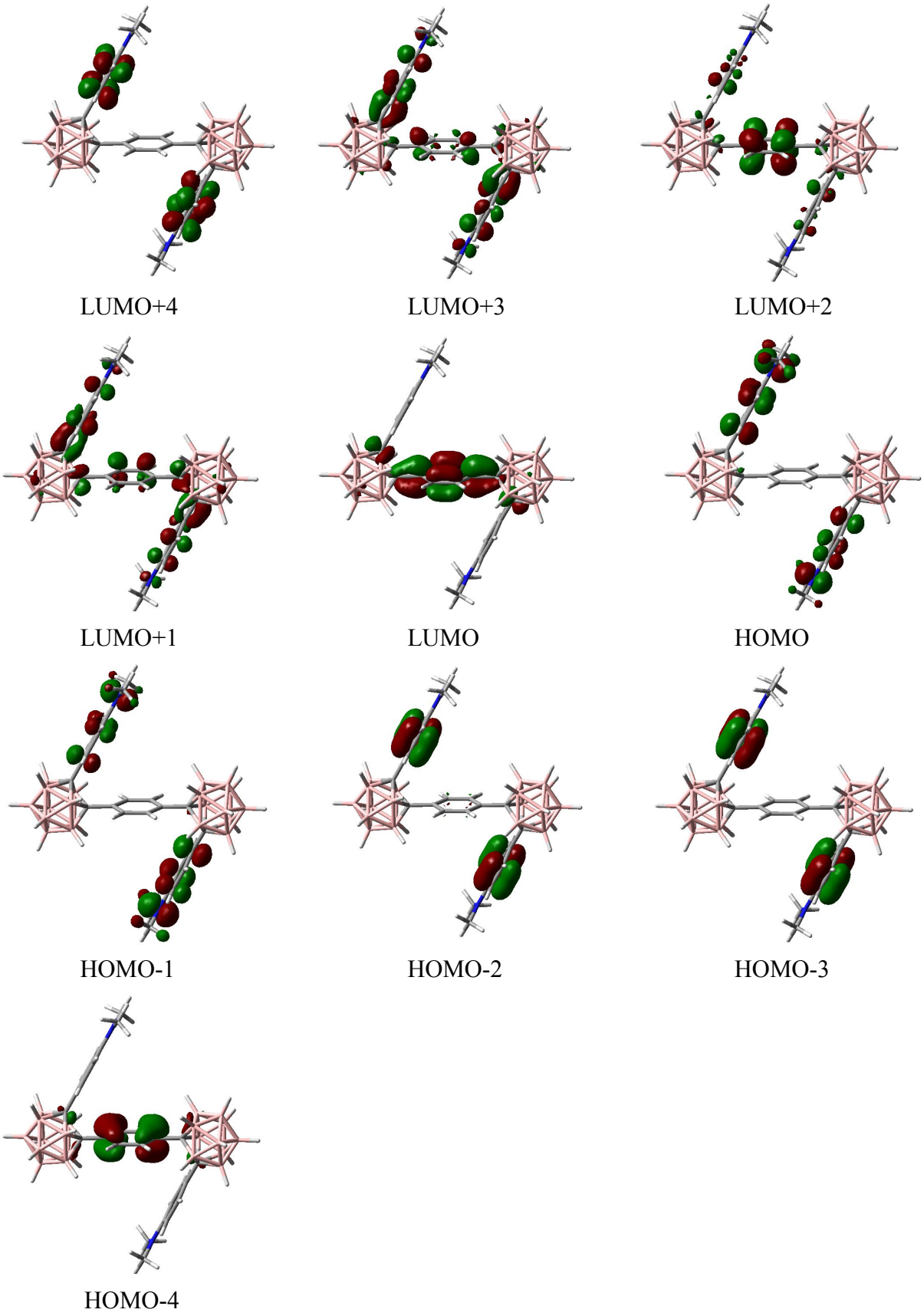

Figure S4. Molecular orbitals of **4** from B3LYP calculations (Isovalue = 0.04) at their lowest singlet ground state (S_0) geometries.

Table S13. Computed absorption wavelengths ($\lambda_{calc.}$ in nm) and oscillator strengths ($f_{calc.}$) for **4** from B3LYP calculations using the B3LYP geometries.

state	$\lambda_{calc.}$(/nm)	$f_{calc.}$	major contribution
1	395.16	0.1218	HOMO→ LUMO (98.80%)
2	393.94	0.0016	HOMO-1→ LUMO (98.87%)
3	306.23	0.0053	HOMO → LUMO+1 (58.15%)
			HOMO → LUMO+2 (38.95%)
4	306.1	0.1071	HOMO-1 → LUMO+1 (58.31%)
			HOMO -1→ LUMO+2 (38.75%)
5	298.2	0.0238	HOMO → LUMO+2 (57.29%)
			HOMO → LUMO+1 (39.78%)
6	297.96	0.5084	HOMO-1 → LUMO+2 (57.23%)
			HOMO-1 → LUMO+1 (38.83%)
7	276.87	0.2933	HOMO → LUMO+3 (78.08%)
8	276.51	0.0187	HOMO-1 → LUMO+3 (72.29%)
			HOMO-1 → LUMO+4 (10.24%)
9	274.85	0.0719	HOMO → LUMO +4 (33.93%)
			HOMO-1 → LUMO+7 (13.35%)
			HOMO → LUMO+3 (10.99%)
10	274.78	0.0410	HOMO-1 → LUMO+4 (30.18%)
			HOMO-1 → LUMO+3 (16.65%)
			HOMO → LUMO+7 (11.80%)
			HOMO-1 → LUMO+7 (10.15%)
			HOMO → LUMO+4 (10.01%)

Table S14. Molecular orbital distributions (in %) of **4** from B3LYP calculations.

molecular orbital	Aryl1	NMe_2-1	Aryl2	NMe_2-2	Phenylene	Carborane1	Carborane2
LUMO+4	37.50	0.97	37.36	0.96	1.07	11.06	11.09
LUMO+3	16.80	4.05	16.74	4.04	13.70	22.40	22.27
LUMO+2	7.92	0.84	8.00	0.85	45.72	18.30	18.37
LUMO+1	11.26	2.81	11.21	2.80	14.69	28.64	28.59
LUMO	1.93	0.54	1.93	0.55	38.35	28.31	28.39
HOMO	14.46	20.46	23.12	32.74	0.28	3.43	5.52
HOMO-1	23.02	32.61	14.37	20.38	0.40	5.65	3.57
HOMO-2	46.39	0.18	47.17	0.18	4.66	0.70	0.71
HOMO-3	49.26	0.19	48.47	0.19	0.11	0.90	0.88
HOMO-4	0.39	0.20	0.39	0.20	69.03	14.89	14.90

Table S15. Molecular orbital energies (in eV) of **4** from B3LYP calculations.

MO	$HOMO_{-4}$	$HOMO_{-3}$	$HOMO_{-2}$	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	$LUMO_{+2}$	$LUMO_{+3}$	$LUMO_{+4}$
Energy	-7.32	-7.05	-7.03	-5.45	-5.45	-1.82	-0.95	-0.84	-0.58	-0.30

Table S16. Cartesian coordinates of **4** from B3LYP calculation (in Å).

	S_0		
	X	Y	Z
C	4.775273	1.410061	1.498695
C	-0.46332	0.51924	0.968636
C	4.326663	0.107426	1.340042
C	0.466597	-0.51636	0.968685
C	-4.32079	-0.10968	1.341759
C	-3.67706	1.877436	-0.08738
C	-4.76875	-1.41259	1.500074
C	-1.92122	2.203526	-0.24348
C	5.076644	2.222673	0.379298
C	-4.14523	0.465828	0.072538
C	-0.95206	1.052497	-0.23093
C	-5.0743	-2.22348	0.380508
C	4.145855	-0.46598	0.070606
C	0.952527	-1.05221	-0.23086
C	-4.47378	-0.32924	-1.03768
C	3.677227	-1.8775	-0.08914
C	1.921542	-2.20339	-0.24344
C	4.919738	1.635021	-0.89913
C	-4.92361	-1.63339	-0.89752
C	4.46942	0.331051	-1.03965
C	-0.46727	0.514896	-1.4317
C	0.46509	-0.51705	-1.43166
H	-3.12383	4.989833	2.100499
H	-2.57654	1.978322	2.175696
H	-5.30088	2.919605	1.457644
H	-0.50588	3.778194	1.030692
H	-0.80182	0.914601	1.918005
H	-4.99086	5.475192	-0.30482
H	-1.97778	6.017838	-0.57491
H	2.578905	-1.97727	2.175026
H	0.807324	-0.90962	1.918117
H	4.122299	-0.47598	2.230596
H	-4.11293	0.472249	2.232448
H	3.125752	-4.98901	2.100515
H	0.506764	-3.77745	1.032276
H	5.302264	-2.91929	1.45497
H	-5.52153	2.657205	-1.53775
H	-0.72724	3.520935	-1.96054
H	-3.48407	4.559089	-2.83625
H	-4.38559	0.077191	-2.03857
H	4.990623	-5.47548	-0.30598
H	1.97722	-6.01786	-0.57373
H	-2.90583	1.563106	-2.46148
H	-0.81161	0.908057	-2.38062
H	4.376643	-0.07348	-2.04087
H	0.726001	-3.52141	-1.95905
H	5.520676	-2.65784	-1.5405
H	0.80725	-0.91227	-2.38052
H	2.903919	-1.56422	-2.46285
H	3.481692	-4.56023	-2.83673
B	-3.09451	4.33872	1.107478
B	-2.77458	2.601886	1.194898
B	-4.39251	3.181517	0.743447
B	-1.55848	3.694259	0.491926
B	-4.17274	4.613916	-0.29027
B	-2.43186	4.927584	-0.44552
B	2.775707	-2.60144	1.194361
B	3.095537	-4.33827	1.107272
B	-4.52255	3.028134	-1.01964
B	-1.68981	3.539718	-1.26924
B	1.559031	-3.69401	0.492784
B	4.393241	-3.18121	0.741618
B	-3.30513	4.087513	-1.76085
B	-2.98004	2.357007	-1.59236
B	4.172609	-4.61412	-0.29127
B	2.431555	-4.92764	-0.44499
B	1.689089	-3.53984	-1.26848
B	4.522092	-3.02875	-1.02162
B	2.979267	-2.35759	-1.59336
B	3.303876	-4.08822	-1.76133
H	-5.16014	-2.19601	-1.79233
H	-4.88317	-1.80022	2.505042
H	5.15179	2.199303	-1.79404
H	4.893447	1.7962	2.503826

N	-5.50483	-3.52288	0.527829
N	5.509364	3.521311	0.527616
C	-5.78754	-4.33431	-0.64485
H	-6.10335	-5.32835	-0.32506
H	-6.5947	-3.90276	-1.25257
H	-4.9025	-4.44962	-1.28626
C	-5.61562	-4.1075	1.854106
H	-5.95244	-5.14114	1.763196
H	-4.65136	-4.11032	2.381552
H	-6.34292	-3.56893	2.477254
C	5.777816	4.33851	-0.64447
H	4.885259	4.45823	-1.27477
H	6.099267	5.330387	-0.32358
H	6.576984	3.908983	-1.26385
C	5.616729	4.105493	1.854383
H	6.339961	3.564013	2.479498
H	5.958126	5.137763	1.764979
H	4.6507	4.111669	2.378832