Electronic Supplementary Information

Insights into the Effects of Substitution Position on the Photophysics of Mono-*o*-Carborane-Substituted Pyrenes

Seonah Kim,[a]‡, Ji Hye Lee,[a]‡ Hyunhee So,[a]‡ Mingi Kim,[a] Min Sik Mun,[a] Hyonseok Hwang,[a] Myung Hwan Park,*[b] and Kang Mun Lee*[a]

[a] Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon, Gangwon 24341, Republic of Korea
[b] Department of Chemistry Education, Chungbuk National University, Cheongju, Chungbuk 28644, Republic of Korea

Contents

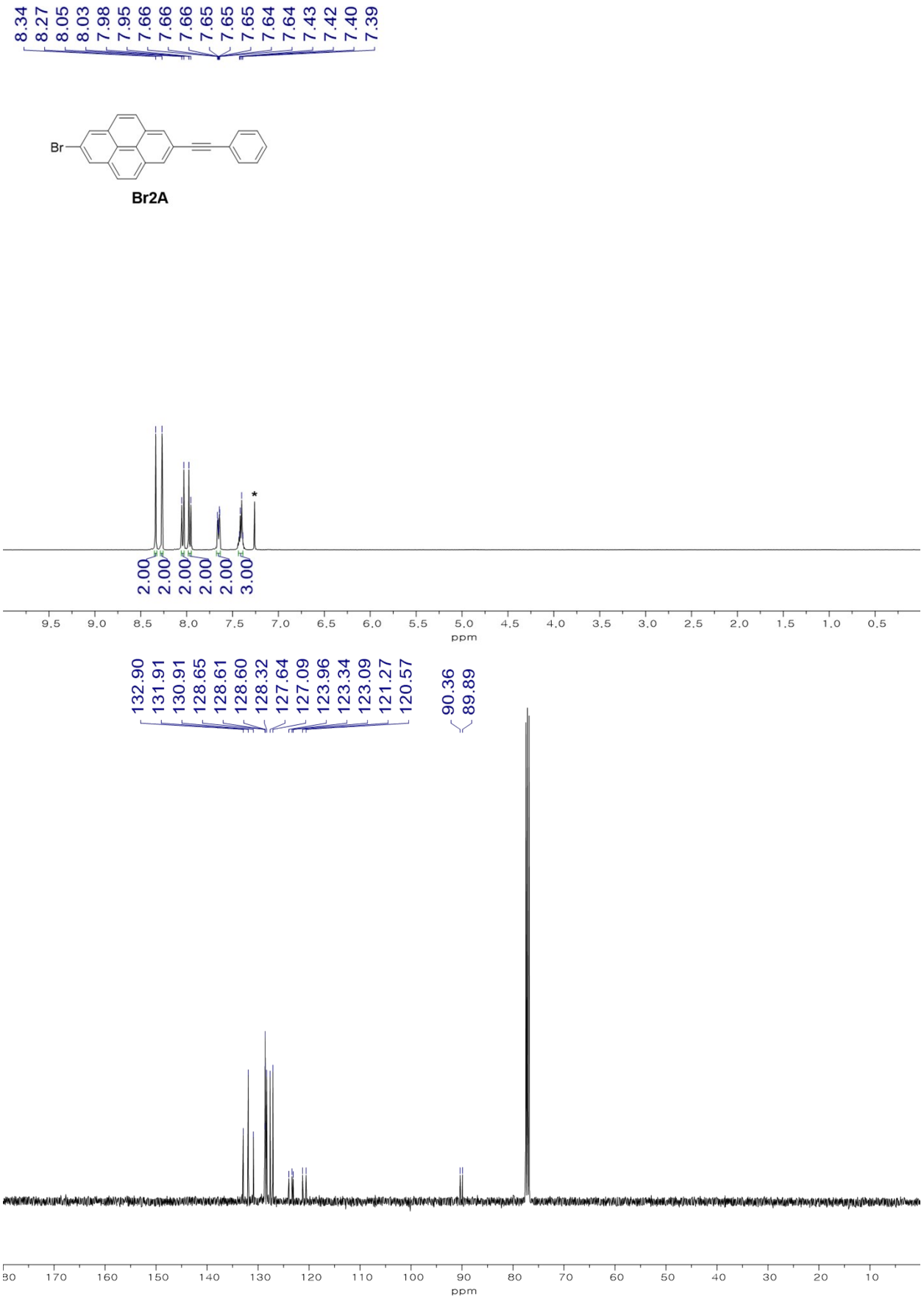
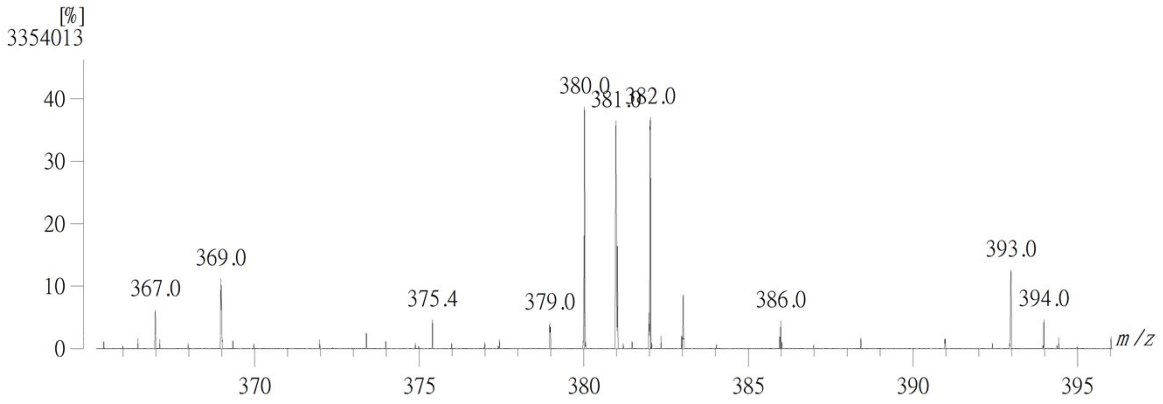


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **Br2A** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

[Mass Spectrum]

RT : 0.96 min Scan# : 26
Elements : C 24/0, H 49/0, 79Br 1/0, 81Br 1/0
Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 10mmu if m/z > 10
Unsaturation (U.S.) : -0.5 - 20.0



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	380.0202	38.73	+0.4 / +0.1	18.0	C24 H13 79Br
2	382.0219	37.06	+10.2 / +3.9	18.0	C24 H13 81Br

Fig. S2 HRMS spectra of **Br2A**.

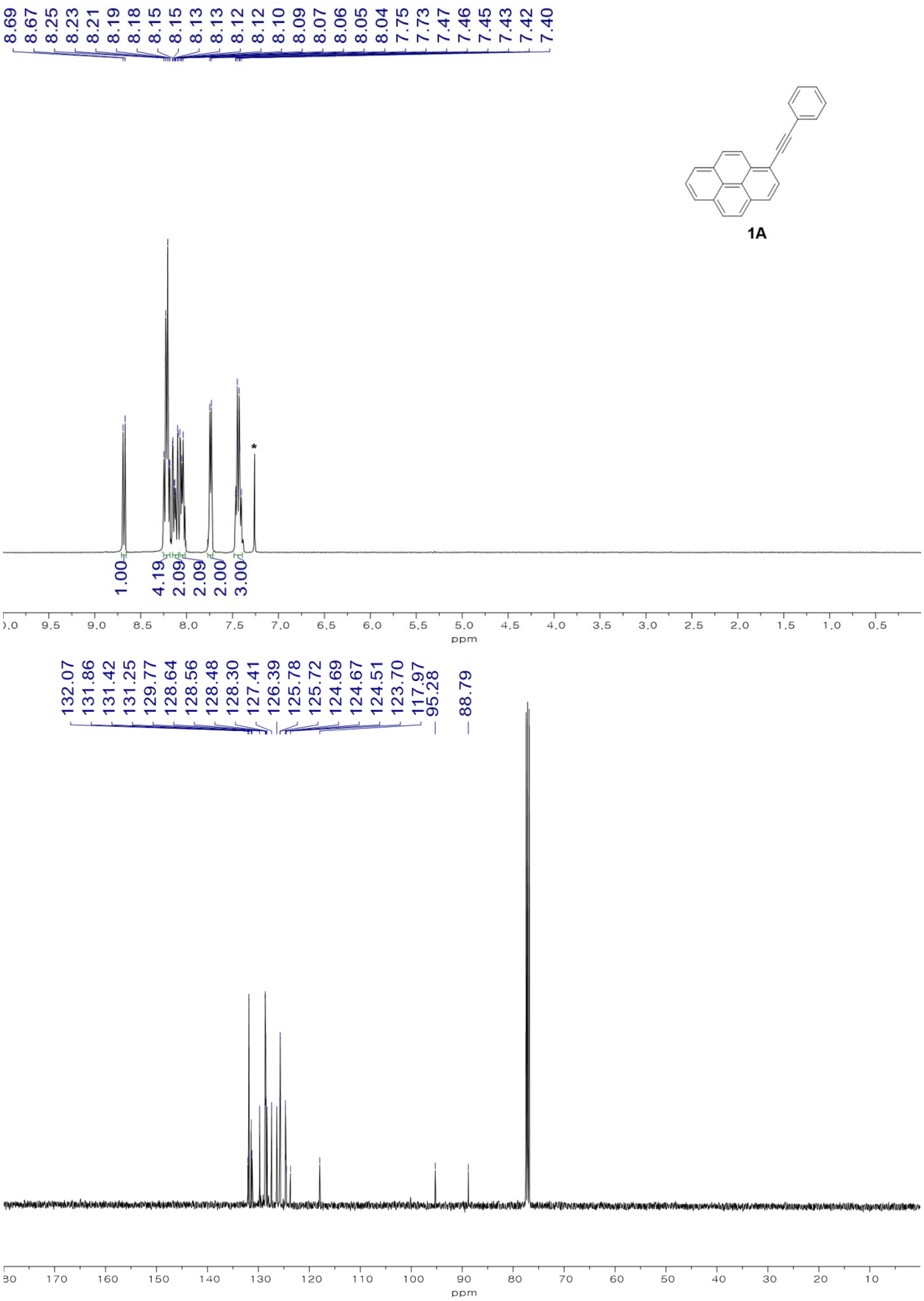


Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1A** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

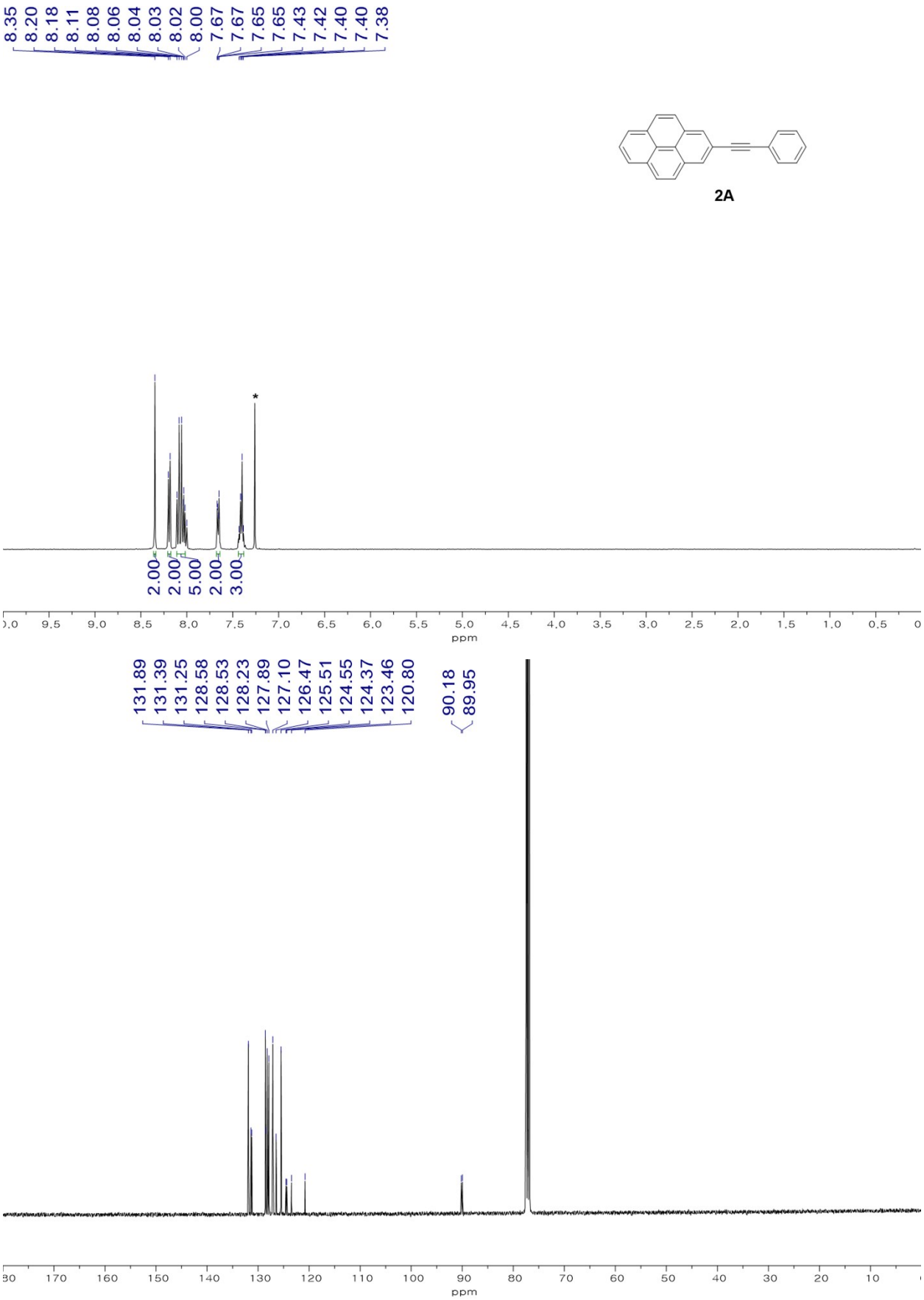


Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2A** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

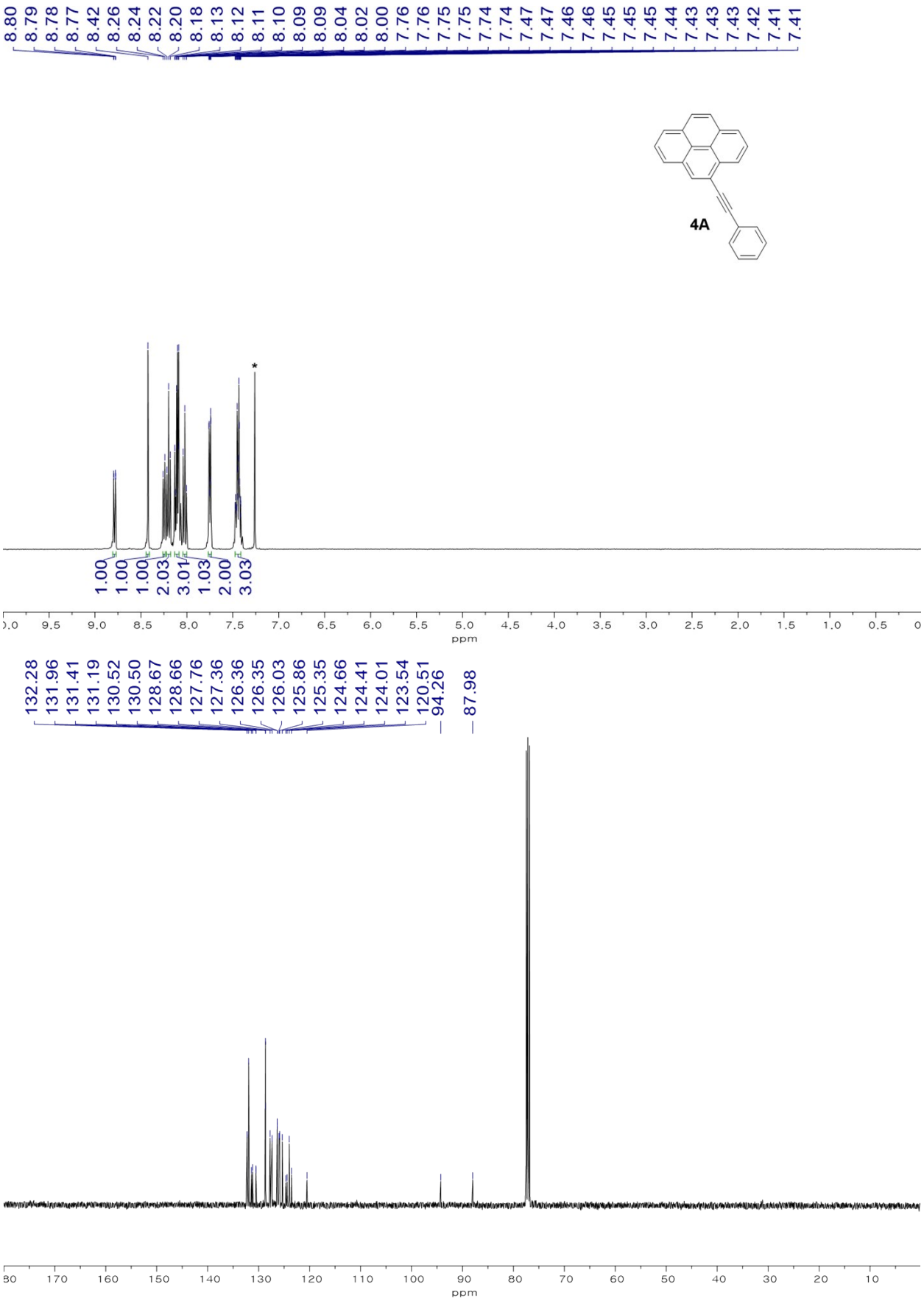


Fig. S5 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4A** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

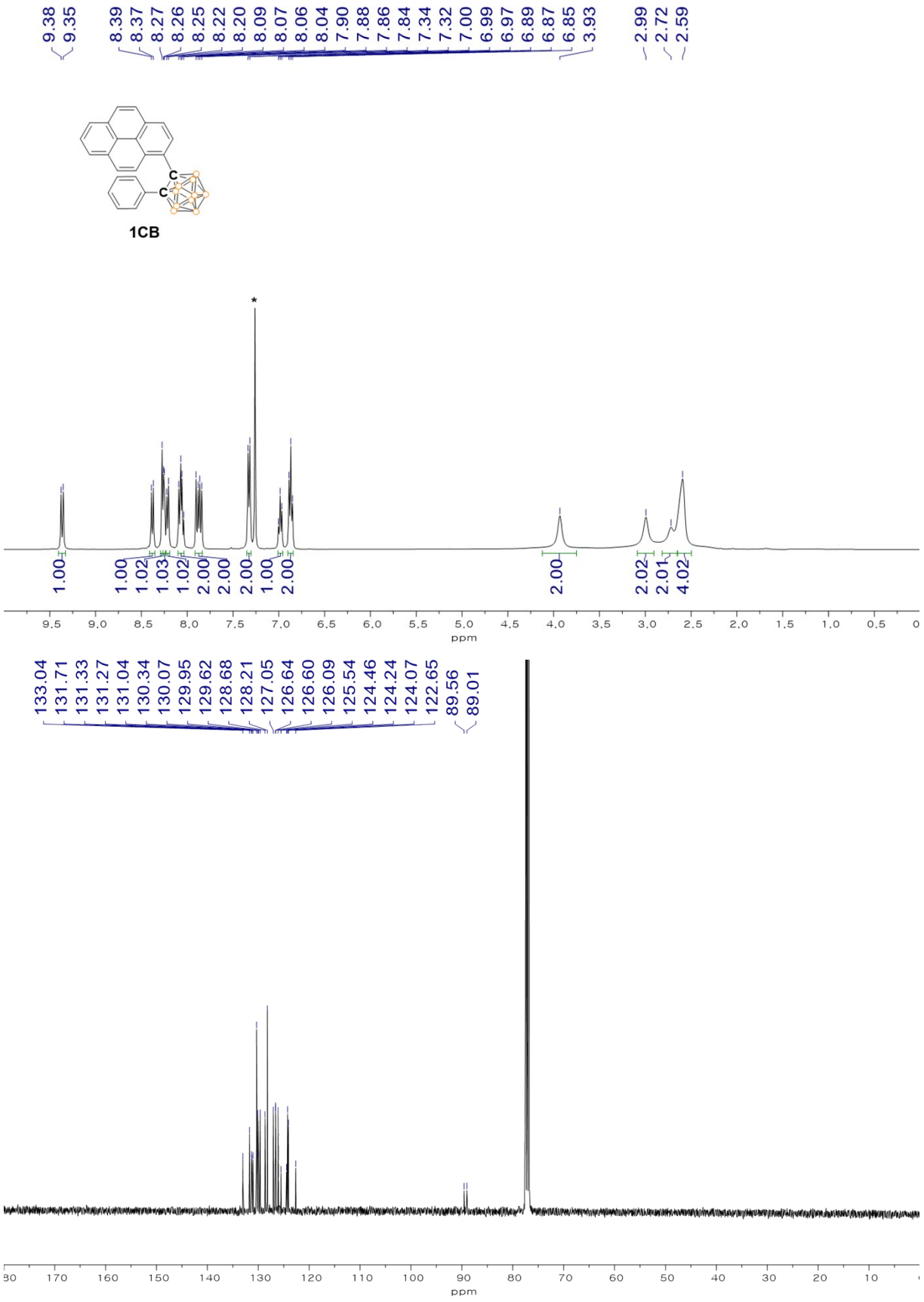


Fig. S6 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **1CB** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

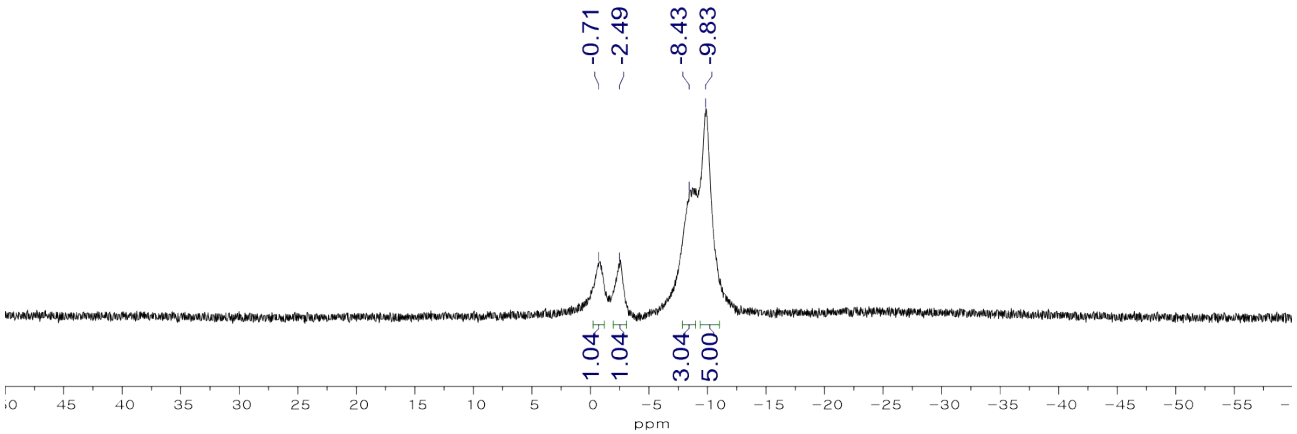


Fig. S7 $^{11}B\{^{1}H\}$ NMR spectra of **1CB** in $CDCl_3$.

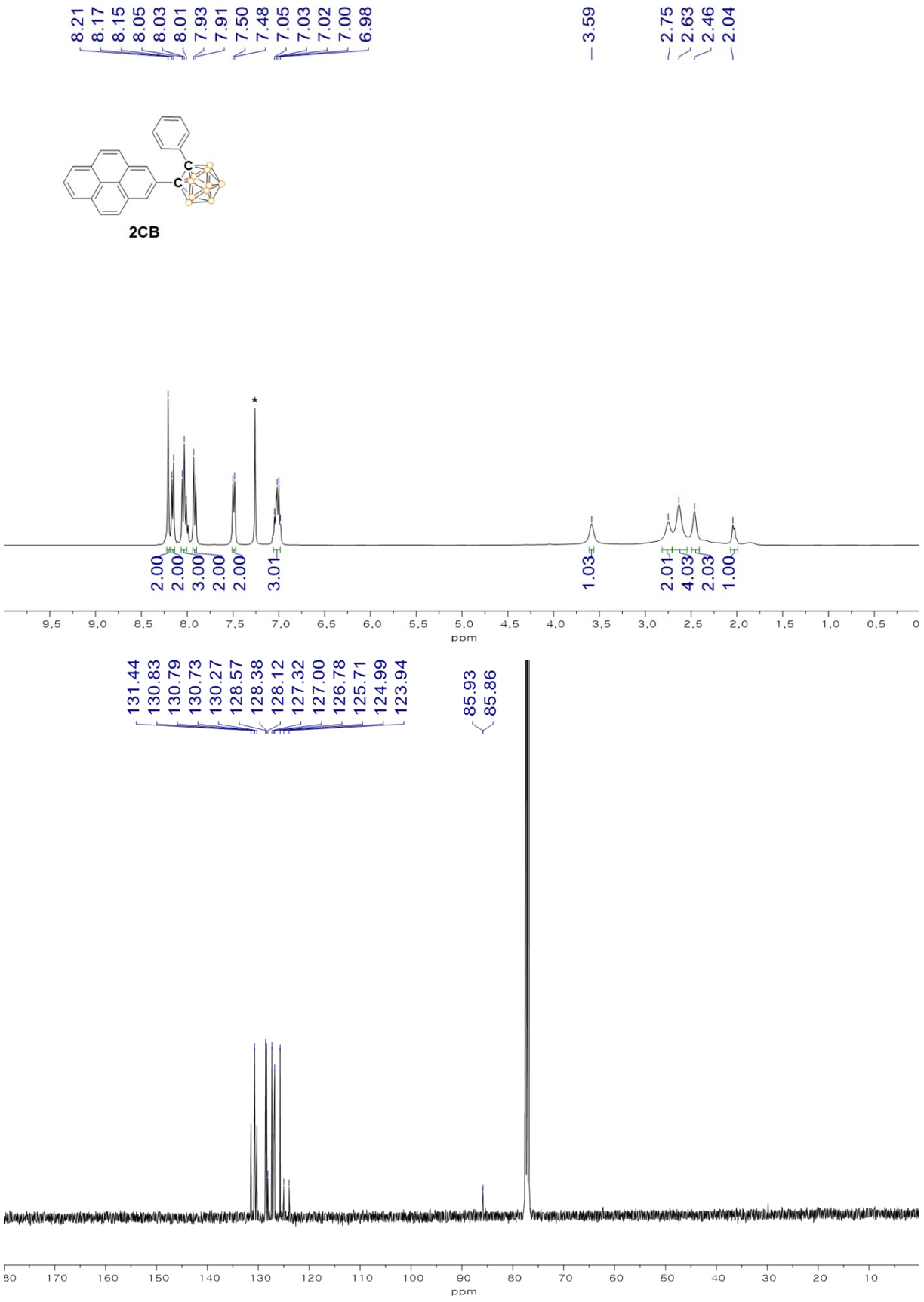


Fig. S8 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **2CB** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

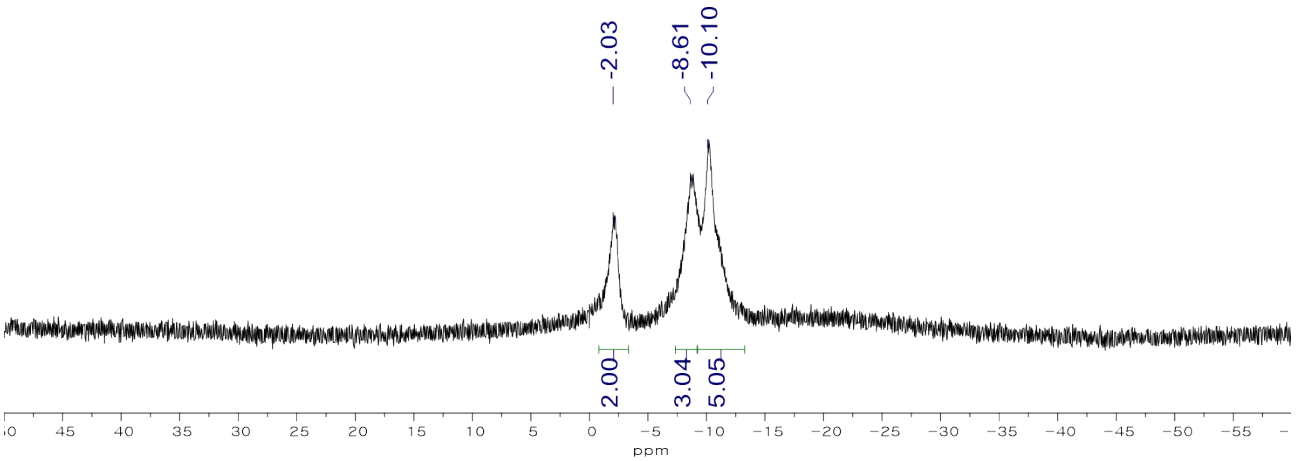


Fig. S9 $^{11}B\{^{1}H\}$ NMR spectra of **2CB** in $CDCl_3$.

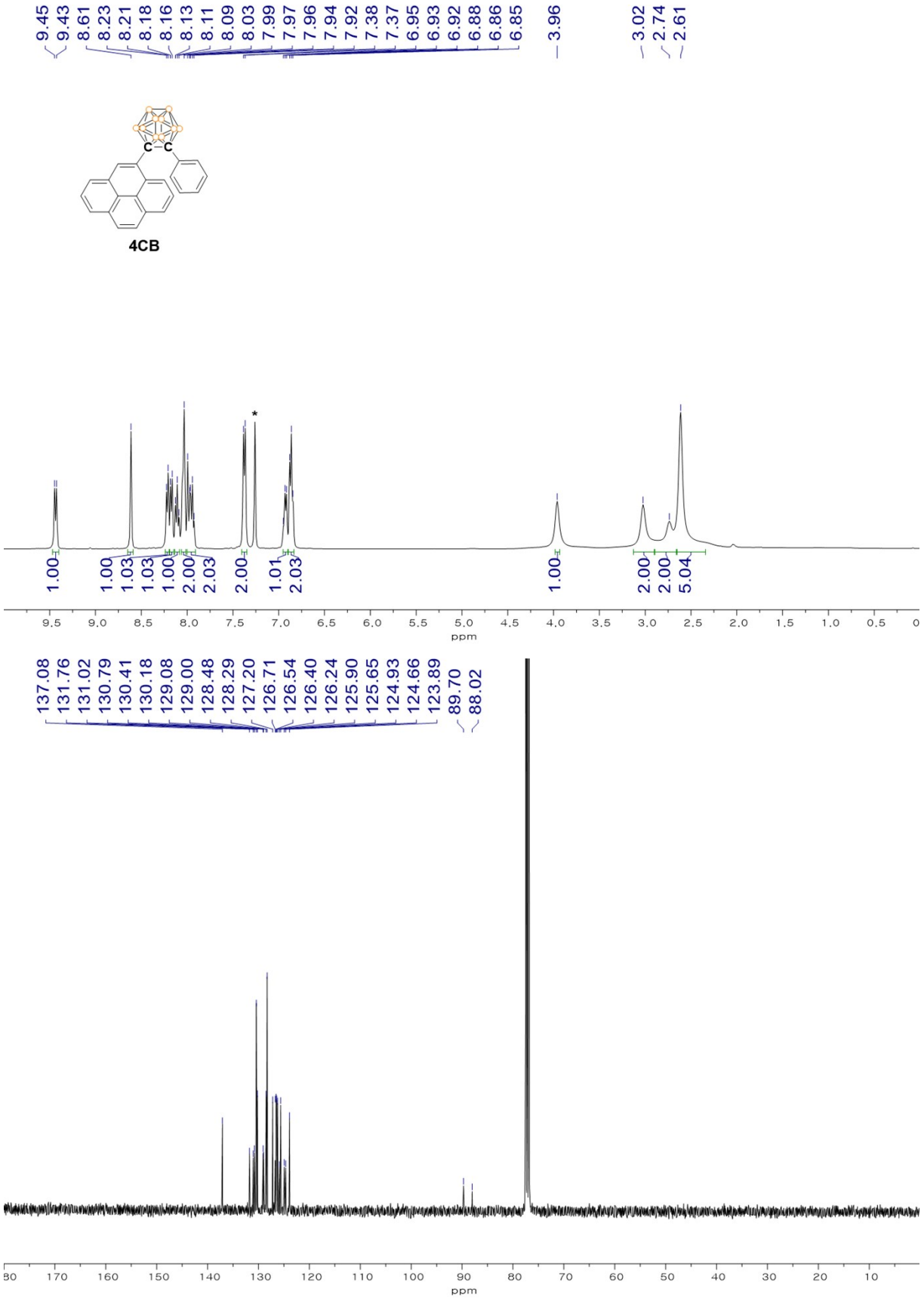


Fig. S10 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **4CB** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

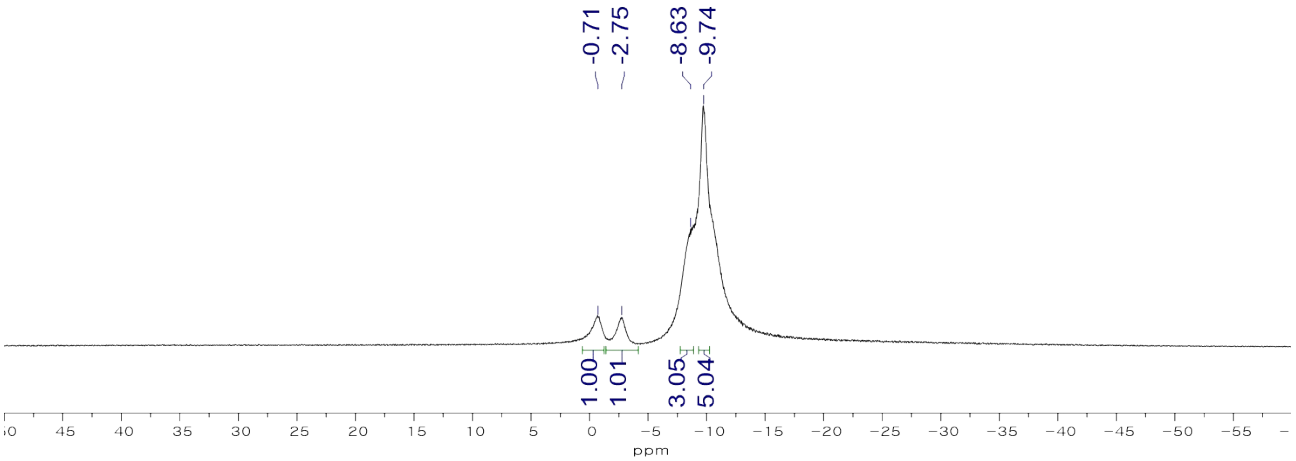


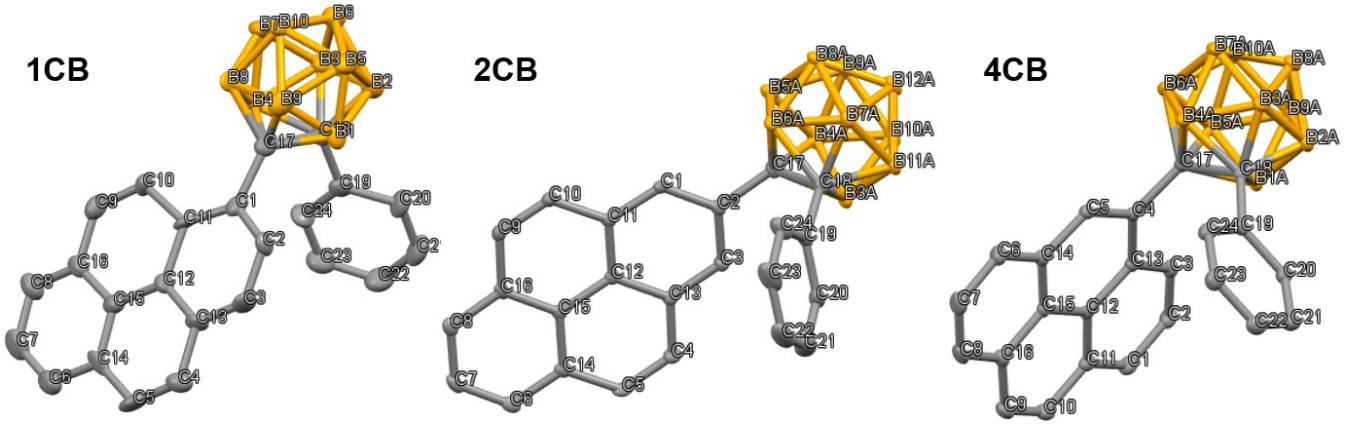
Fig. S11 $^{11}B\{^{1}H\}$ NMR spectra of **4CB** in $CDCl_3$.

Table S1 Crystallographic data and parameters for the pyrene based *o*-carboranyl complexes **1CB**, **2CB** and **4CB**.

Compound	**1CB**	**2CB**	**4CB**
Formula	$C_{24}H_{24}B_{10}$	$C_{24}H_{24}B_{10}$	$C_{24}H_{24}B_{10}$
Formula weight	420.53	420.53	420.53
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P_1	P_{-1}	$P2_1/n$
a (Å)	12.839(3)	10.7108(7)	16.2276(9)
b (Å)	13.981(3)	25.1022(16)	12.7661(7)
c (Å)	13.619(3)	25.7908(17)	21.7252(13)
α (°)	90.00(3)	89.113(2)	90
β (°)	114.47(3)	88.861(2)	90.3316(19)
γ (°)	90.00(3)	89.861(2)	90
V (Å^3)	2225.1(9)	6932.0(8)	4500.6(4)
Z	4	12	8
ρ_{calc}(g cm^{-3})	1.255	1.209	1.241
μ (mm^{-1})	0.064	0.062	0.063
F(000)	872	2616	1744
T (K)	293(2)	153(2)	153(2)
Scan mode	*multi-scan*	*multi-scan*	*multi-scan*
hkl range	$-16 < h < 16$, $-18 < k < 17$, $-17 < l < 17$	$-13 < h < 13$, $-31 < k < 31$, $-32 < l < 32$	$-20 < h < 19$, $-16 < k < 16$, $-27 < l < 27$
Measd reflns	22702	246745	64075
Unique reflns [R_{int}]	16955 [0.0856]	28543 [0.0978]	9745 [0.1287]
Reflns used for refinement	16955	28543	9745
Refined parameters	1225	1838	674
R_1[a] (I > 2σ(I))	0.0834	0.0899	0.0687
wR_2[b] all data	0.2342	0.2121	0.1477
GOF on F^2	1.005	1.089	1.087
ρ_{fin} (max/min) (e Å^{-3})	0.242, −0.234	0.653, −0.296	0.292, −0.240

[a]$R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b]$wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for **1CB**, **2CB** and **4CB**.



1CB		**2CB**		**4CB**	
lengths (Å)					
C1–C17	1.514(18)	C2–C17	1.496(5)	C4–C17	1.516(3)
C17–C18	1.762(18)	C17–C18	1.736(5)	C17–C18	1.783(3)
C18–C19	1.517(19)	C18–C19	1.502(5)	C18–C19	1.500(3)
angles (°)					
C1–C17–C18	120.4(10)	C2–C17–C18	119.1(3)	C4–C17–C18	118.18(17)
C17–C18–C19	117.4(11)	C17–C18–C19	119.3(3)	C17–C18–C19	120.61(17)

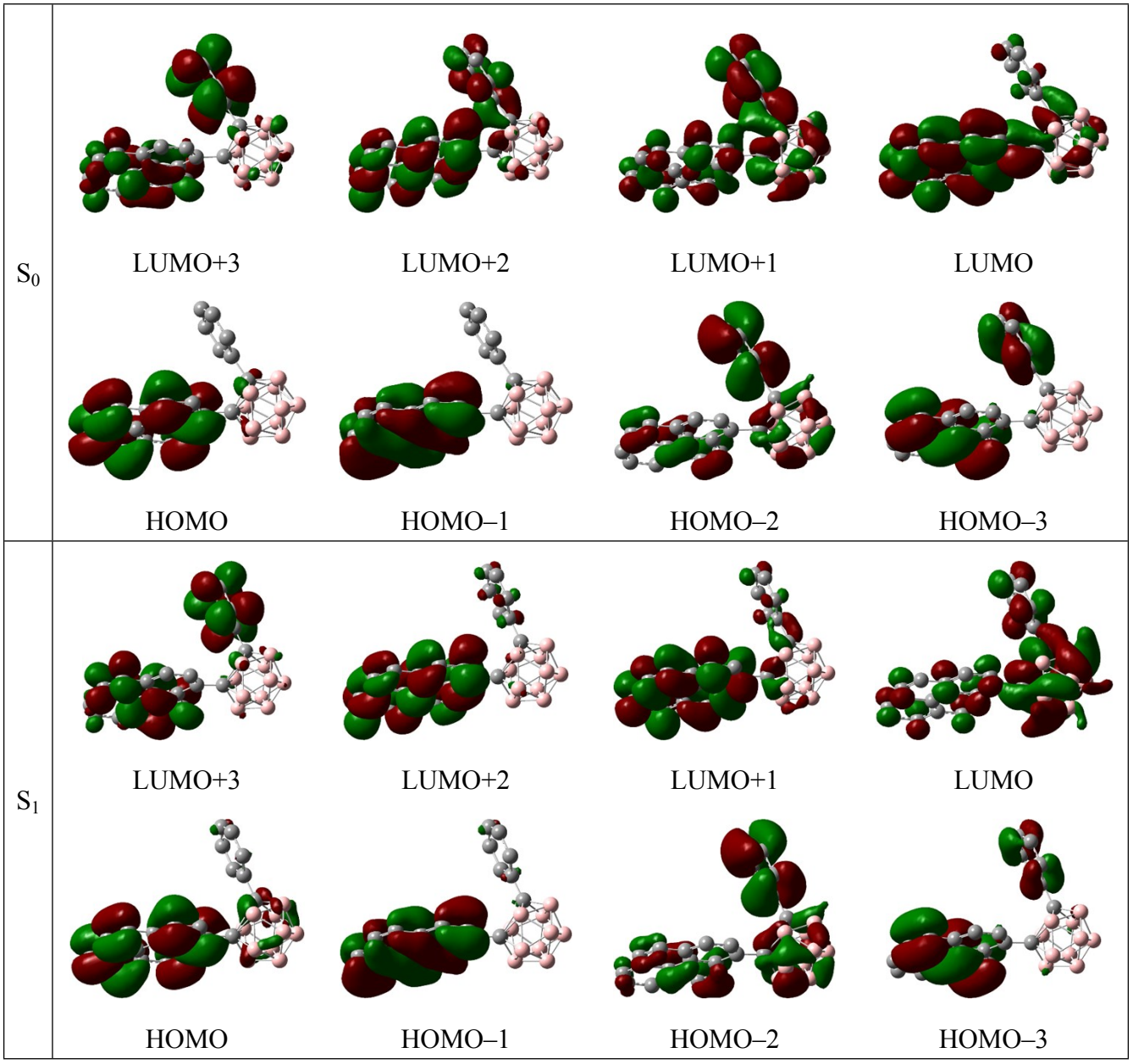


Fig. S12 The selected frontier orbitals of **1CB** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S3 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **1CB** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	383.99	0.5213	HOMO → LUMO (92.8%)
2	340.17	0.0347	HOMO−1 → LUMO (59.0%)
			HOMO → LUMO+1 (11.9%)
			HOMO → LUMO+2 (25.7%)
3	316.51	0.0635	HOMO → LUMO+1 (79.6%)
			HOMO → LUMO+2 (8.7%)
4	293.92	0.0266	HOMO−3 → LUMO (50.6%)
			HOMO−2 → LUMO (11.1%)
			HOMO → LUMO+2 (21.0%)
5	284.80	0.1973	HOMO−3 → LUMO (18.4%)
			HOMO−2 → LUMO (13.0%)
			HOMO−1 → LUMO (22.5%)
			HOMO → LUMO+2 (33.4%)
			S_1
1	624.71	0.3977	HOMO → LUMO (99.6%)
2	429.10	0.1773	HOMO → LUMO+1 (97.9%)
3	390.45	0.0185	HOMO−2 → LUMO (29.6%)
			HOMO−1 → LUMO (61.9%)
4	387.95	0.0146	HOMO−3 → LUMO (92.7%)
5	380.06	0.1158	HOMO−4 → LUMO (67.7%)
			HOMO−1 → LUMO +1(28.1%)

Table S4 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **1CB** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

	E (eV)	carborane	pyrene	Car-phenyl
		S_0		
LUMO+3	−0.48	7.1	31.2	61.7
LUMO+2	−1.01	6.2	79.9	13.9
LUMO+1	−1.36	33.0	31.0	35.9
LUMO	−2.17	22.1	74.7	3.2
HOMO	−5.69	3.2	96.6	0.2
HOMO−1	−6.57	1.3	98.1	0.5
HOMO−2	−7.15	10.7	16.6	72.8
HOMO−3	−7.16	2.4	75.9	21.7
		S_1		
LUMO+3	−0.49	5.6	48.6	45.8
LUMO+2	−0.97	2.7	94.8	2.5
LUMO+1	−1.87	5.6	91.7	2.6
LUMO	−3.43	76.7	10.6	12.7
HOMO	−5.62	5.6	92.9	1.5
HOMO−1	−6.64	2.4	96.2	1.4
HOMO−2	−7.11	16.5	17.5	66.0
HOMO−3	−7.18	3.2	86.1	10.8

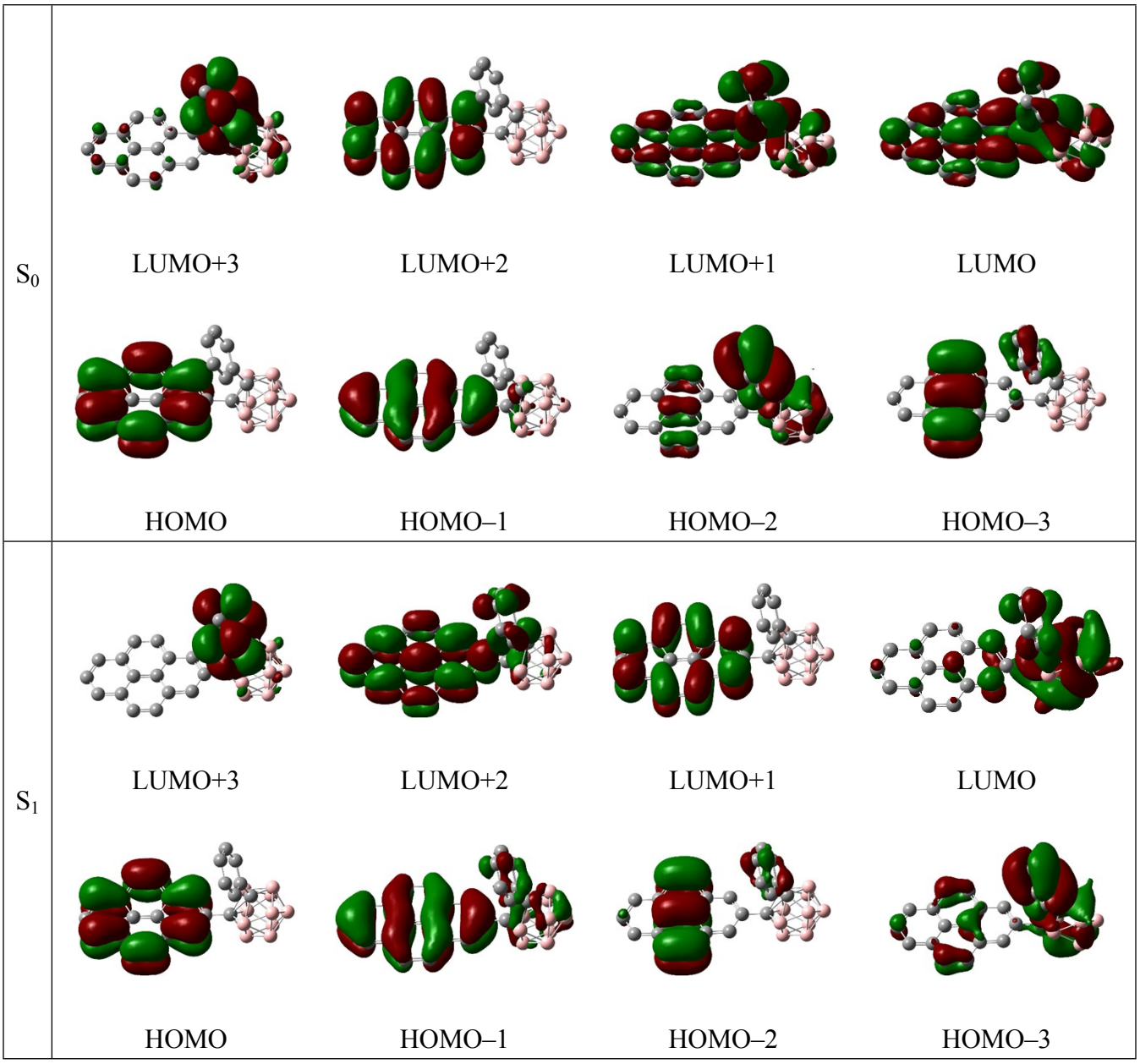


Fig. S13 The selected frontier orbitals of **2CB** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S5 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **2CB** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	344.82	0.4191	HOMO → LUMO (91.6%)
2	307.08	0.0095	HOMO−1 → LUMO (22.8%)
			HOMO → LUMO (13.6%)
			HOMO → LUMO+1 (62.2%)
3	282.13	0.0983	HOMO−3 → LUMO (9.7%)
			HOMO−1 → LUMO (30.1%)
			HOMO → LUMO+1 (22.9%)
			HOMO → LUMO+2 (31.5%)
4	274.18	0.1330	HOMO−1 → LUMO (25.2%)
			HOMO → LUMO+2 (11.2%)
			HOMO → LUMO+4 (47.1%)
5	269.00	0.2621	HOMO−1 → LUMO+1 (86.7%)
			S_1
1	624.67	0.1029	HOMO → LUMO (99.7%)
2	417.36	0.4173	HOMO → LUMO+1 (98.9%)
3	398.45	0.0033	HOMO−1 → LUMO (97.3%)
4	393.85	0.0495	HOMO−2 → LUMO (96.9%)
5	384.21	0.2714	HOMO−3 → LUMO (90.7%)
			HOMO → LUMO+1 (7.6%)

Table S6 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **2CB** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

	E (eV)	carborane	pyrene	Car-phenyl
		S_0		
LUMO+3	−0.50	8.9	4.6	86.5
LUMO+2	−0.99	1.6	97.8	0.7
LUMO+1	−1.52	27.1	32.7	40.2
LUMO	−1.38	23.8	61.1	15.0
HOMO	−5.66	0.4	99.5	0.1
HOMO−1	−6.56	4.4	95.4	0.2
HOMO−2	−7.17	10.3	9.2	80.5
HOMO−3	−7.18	1.1	90.8	8.0
		S_1		
LUMO+3	−0.52	7.1	0.6	92.4
LUMO+2	−0.93	5.2	79.0	15.8
LUMO+1	−1.94	1.2	98.8	0.0
LUMO	−3.52	75.8	10.7	13.4
HOMO	−5.51	0.4	99.6	0.0
HOMO−1	−6.60	7.3	87.7	5.0
HOMO−2	−7.13	1.3	93.2	5.5
HOMO−3	−7.20	17.6	12.3	70.1

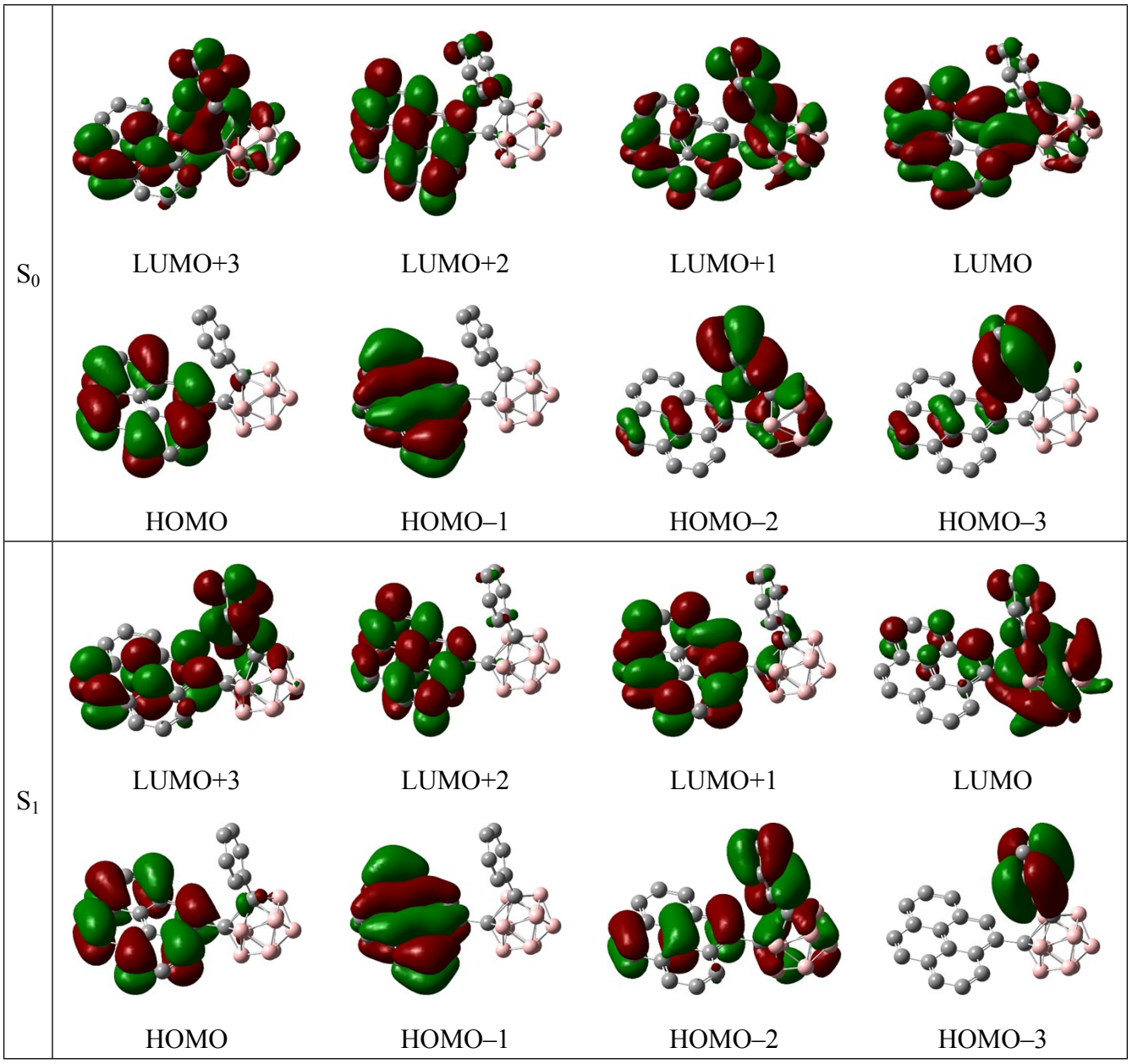


Fig. S14 The selected frontier orbitals of **4CB** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S7 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **4CB** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	377.51	0.2133	HOMO → LUMO (88.8%)
			HOMO → LUMO+1 (7.3%)
2	336.59	0.0173	HOMO−1 → LUMO (58.8%)
			HOMO → LUMO+2 (31.0%)
3	322.62	0.1194	HOMO → LUMO+1 (82.5%)
4	290.82	0.1904	HOMO−1 → LUMO (33.3%)
			HOMO−1 → LUMO+1 (14.7%)
			HOMO → LUMO+2 (46.4%)
5	286.74	0.0147	HOMO → LUMO+3 (86.7%)
			S_1
1	646.41	0.1453	HOMO → LUMO (99.6%)
2	476.65	0.0514	HOMO−1 → LUMO (99.3%)
3	408.09	0.2582	HOMO → LUMO+1 (96.1%)
4	397.72	0.0026	HOMO−2 → LUMO (97.8%)
5	377.76	0.1931	HOMO−4 → LUMO (7.5%)
			HOMO−3 → LUMO (82.3%)

Table S8 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **4CB** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

	E (eV)	carborane	pyrene	Car-phenyl
		S_0		
LUMO+3	−0.69	13.0	50.2	36.8
LUMO+2	−0.99	3.8	89.9	6.3
LUMO+1	−1.38	33.9	33.7	32.4
LUMO	−2.05	20.6	75.5	3.9
HOMO	−5.68	2.1	97.8	0.1
HOMO−1	−6.52	0.4	99.3	0.2
HOMO−2	−7.15	11.8	9.7	78.5
HOMO−3	−7.18	1.8	10.2	87.9
		S_1		
LUMO+3	−0.61	6.6	59.0	34.4
LUMO+2	−0.91	1.9	96.3	1.8
LUMO+1	−1.90	4.4	93.7	1.9
LUMO	−3.50	75.5	12.0	12.5
HOMO	−5.57	4.2	95.0	0.8
HOMO−1	−6.61	0.7	98.7	0.5
HOMO−2	−7.03	12.7	41.8	45.5
HOMO−3	−7.23	1.5	0.1	98.3

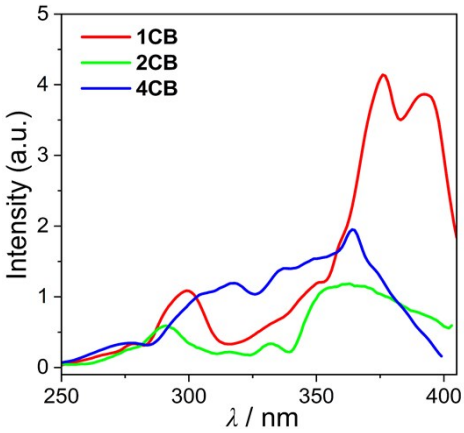


Fig. S15 Excitation graphs in THF (3.0×10^{-5} M) of **of 1CB**, **2CB** and **4CB**.

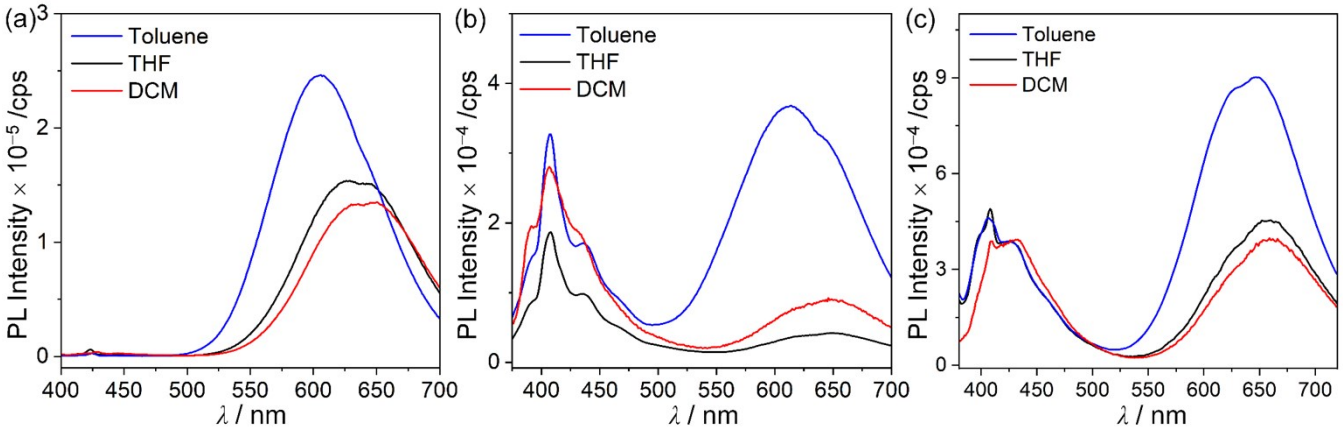


Fig. S16 PL spectra of (a) **1CB**, (b) **2CB**, and (c) **4CB** in various organic solvents (3.0×10^{-5} M, λ_{ex} = 376 nm for **1CB**, 362 nm for **2CB** and 364 nm for **4CB**, respectively).

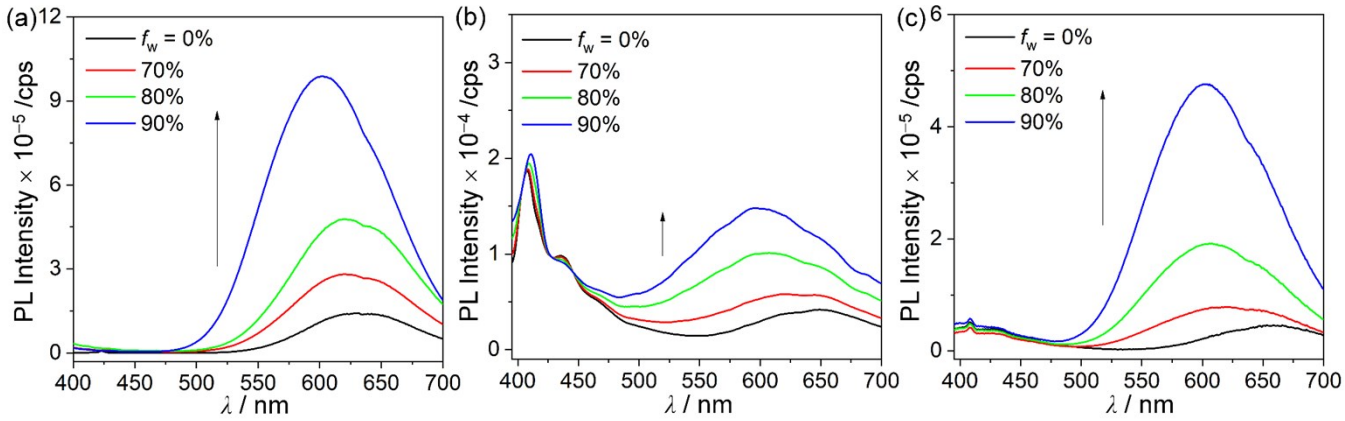


Fig. S17 PL spectra of (a) **1CB**, (b) **2CB**, and (c) **4CB** in THF/distilled water mixtures (3.0×10^{-5} M).

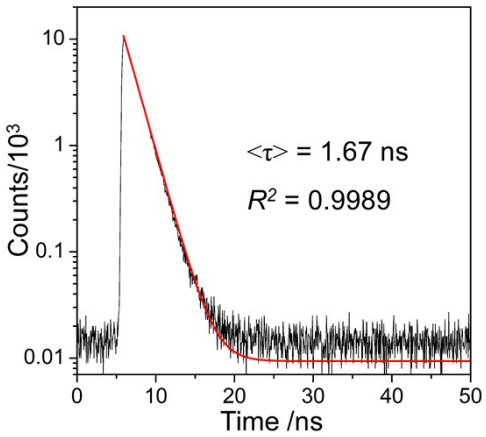


Fig. S18 Emission decay curve for **1CB** in THF (3.0×10^{-5} M) detected at 628 nm. The red-line is its single exponential fitting curve.

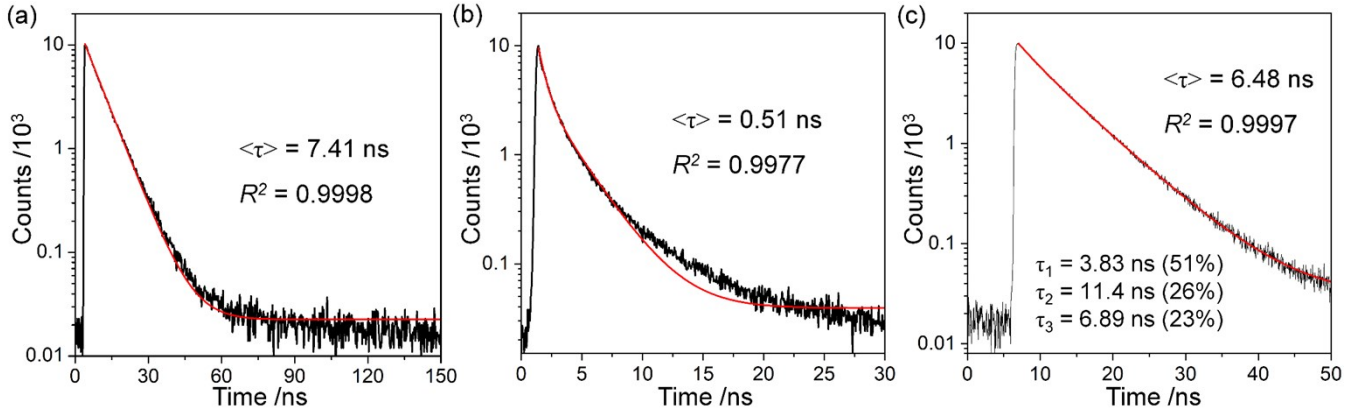


Fig. S19 Emission decay curves for (a) **1CB**, (b) **2CB**, and (c) **4CB** in the film state (5 wt% doped in PMMA) detected at 574 nm for **1CB**, 579 nm for **2CB** and 580 nm for **4CB** at 298 K. Each red-line is its single (for **1CB** and **2CB**) or triple (for **4CB**) exponential fitting curve.

Table S9 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **1CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	2.745334	0.209231	-0.321139
C	1.596661	-0.913473	0.582223
C	0.212971	-0.415526	0.946224
C	0.112870	0.409056	2.081044
H	0.997012	0.618059	2.663733
C	-1.078677	0.976466	2.497320
H	-1.092396	1.611919	3.377583
C	-2.263355	0.748450	1.789523
C	-3.499522	1.362485	2.184971
H	-3.489524	2.025846	3.044862
C	-4.652457	1.125305	1.504446
H	-5.582276	1.597421	1.808811
C	-4.670249	0.240171	0.374812
C	-5.854155	-0.025132	-0.332568
H	-6.773688	0.460645	-0.018499
C	-5.860497	-0.898373	-1.419232
H	-6.786496	-1.091647	-1.951829
C	-4.684349	-1.526828	-1.819600
H	-4.688924	-2.213901	-2.661015
C	-3.477203	-1.284834	-1.142358
C	-2.253024	-1.925214	-1.508411
H	-2.265525	-2.642000	-2.324773
C	-1.084329	-1.670948	-0.856880
H	-0.211985	-2.214779	-1.172566
C	-0.991717	-0.739731	0.239298
C	-2.227301	-0.128023	0.661977
C	-3.452157	-0.389218	-0.034323
C	2.271586	1.581627	-0.712339
C	2.538369	2.686744	0.112357
H	3.068603	2.552272	1.047024
C	2.140130	3.967873	-0.264895
H	2.357571	4.808005	0.387074
C	1.470073	4.169405	-1.472225
H	1.158803	5.167457	-1.764686
C	1.210154	3.080148	-2.304647
H	0.698256	3.224734	-3.250783
C	1.608698	1.797802	-1.930955
H	1.408401	0.968266	-2.597036
B	2.967639	-0.138226	1.345971
H	2.812615	0.717023	2.134352
B	2.550083	-1.837197	1.653627
H	2.051921	-2.125225	2.687043
B	1.972654	-2.500647	0.116057
H	1.087793	-3.281098	0.077567
B	2.045334	-1.161120	-1.071512
H	1.249147	-0.993075	-1.916368
B	4.245910	-1.352678	1.434870
H	4.996122	-1.364633	2.353970
B	3.635130	-2.825845	0.643056
H	3.946006	-3.918542	0.987125
B	3.294361	-2.420170	-1.063776
H	3.359009	-3.208261	-1.948234
B	3.750974	-0.725797	-1.323184
H	4.052855	-0.252464	-2.364302
B	4.334615	-0.071799	0.213588
H	5.050031	0.868704	0.263070
B	4.725986	-1.745313	-0.239907
H	5.836109	-2.045529	-0.533814

Table S10 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **1CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	3.072169	0.207803	-0.260016
C	1.278811	-1.238658	0.419047
C	-0.080949	-0.785144	0.890603
C	-0.208051	-0.421123	2.236273
H	0.653854	-0.497625	2.884585
C	-1.398346	0.058146	2.775642
H	-1.435319	0.340337	3.823530
C	-2.554376	0.194357	1.983154
C	-3.773371	0.702210	2.518224
H	-3.800025	0.999115	3.562093
C	-4.897432	0.816989	1.735447
H	-5.820567	1.207988	2.151345
C	-4.866690	0.419457	0.368933
C	-6.016801	0.520475	-0.457272
H	-6.933118	0.914685	-0.028623
C	-5.984734	0.121711	-1.789303
H	-6.875247	0.206478	-2.402456
C	-4.809250	-0.389844	-2.334631
H	-4.780389	-0.706512	-3.372766
C	-3.635465	-0.507368	-1.549686
C	-2.428711	-1.034225	-2.075154
H	-2.403094	-1.368571	-3.107528
C	-1.291357	-1.131950	-1.299994
H	-0.406475	-1.550215	-1.749526
C	-1.260952	-0.712356	0.062517
C	-2.483355	-0.204667	0.617327
C	-3.656590	-0.097557	-0.185092
C	2.932572	1.665251	-0.360671
C	3.214846	2.501312	0.741483
H	3.529737	2.057470	1.679427
C	3.104192	3.884450	0.636304
H	3.331690	4.506841	1.496857
C	2.704595	4.473049	-0.567562
H	2.616253	5.552262	-0.646862
C	2.422052	3.659221	-1.669021
H	2.115911	4.105546	-2.610702
C	2.531380	2.275566	-1.568960
H	2.312823	1.655747	-2.431508
B	2.690255	-0.640389	1.221628
H	2.549922	0.023764	2.191726
B	2.108074	-2.396461	1.237072
H	1.577324	-2.873580	2.185985
B	1.581041	-2.588957	-0.461738
H	0.659544	-3.241199	-0.824704
B	1.960669	-0.868041	-1.096344
H	1.281379	-0.368155	-1.926312
B	3.843698	-2.064139	1.227775
H	4.489575	-2.406646	2.166447
B	3.150092	-3.235290	0.060284
H	3.311254	-4.412644	0.129516
B	2.996081	-2.338147	-1.488581
H	3.032418	-2.877340	-2.548672
B	3.787193	-0.766208	-1.340275
H	4.272784	-0.247647	-2.291951
B	4.328762	-0.596351	0.380846
H	5.234109	0.060871	0.779208
B	4.449942	-2.174270	-0.454113
H	5.521503	-2.602328	-0.747441

Table S11 Cartesian coordinates of **1CB** at Ψ = 0° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.957728	-0.335707	-0.000043
C	-1.107342	-1.016140	-0.000422
C	0.074403	-0.056693	-0.000497
C	-0.192216	1.318210	-0.000300
H	-1.211596	1.664225	-0.000410
C	0.806568	2.278530	-0.000064
H	0.537330	3.330525	0.000058
C	2.153828	1.908964	0.000045
C	3.199529	2.893872	0.000391
H	2.914702	3.942094	0.000575
C	4.509058	2.530347	0.000506
H	5.293227	3.282201	0.000779
C	4.886427	1.145242	0.000276
C	6.234438	0.751372	0.000395
H	7.005148	1.516986	0.000675
C	6.588381	-0.596883	0.000157
H	7.636348	-0.880512	0.000252
C	5.602451	-1.579972	-0.000207
H	5.876267	-2.631222	-0.000402
C	4.242074	-1.228972	-0.000328
C	3.200019	-2.207588	-0.000721
H	3.474817	-3.258747	-0.000978
C	1.884193	-1.858889	-0.000793
H	1.161485	-2.655302	-0.001148
C	1.441924	-0.485905	-0.000498
C	2.478541	0.517980	-0.000193
C	3.862731	0.144835	-0.000088
C	-3.355017	1.112037	-0.000134
C	-3.591175	1.786528	-1.209790
H	-3.427746	1.280900	-2.153912
C	-4.036248	3.106786	-1.207266
H	-4.212868	3.612710	-2.151062
C	-4.256805	3.772903	-0.000221
H	-4.602550	4.801852	-0.000247
C	-4.035712	3.107029	1.206861
H	-4.211915	3.613148	2.150631
C	-3.590626	1.786778	1.209477
H	-3.426731	1.281361	2.153638
B	-2.184394	-1.040665	-1.371741
H	-1.909127	-0.363505	-2.297298
B	-1.165136	-2.424274	-0.896443
H	-0.236112	-2.666623	-1.582349
B	-1.164676	-2.423739	0.896563
H	-0.234934	-2.665691	1.581641
B	-2.183960	-1.040134	1.371882
H	-1.907484	-0.362164	2.296488
B	-2.818177	-2.721079	-1.438930
H	-3.010695	-3.260306	-2.477745
B	-2.188616	-3.574927	0.000630
H	-1.927324	-4.732708	0.000619
B	-2.817476	-2.720493	1.440054
H	-3.009326	-3.259171	2.479277
B	-3.869642	-1.421159	0.892211
H	-4.751038	-0.958755	1.530392
B	-3.870082	-1.421439	-0.891159
H	-4.751774	-0.959652	-1.529365
B	-3.842170	-2.965787	0.000821
H	-4.796641	-3.671149	0.001205

Table S12 Cartesian coordinates of **1CB** at Ψ = 22.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.899215	-0.266122	0.119223
C	1.185654	-1.046338	-0.220840
C	-0.022606	-0.134987	-0.373601
C	0.205758	1.200404	-0.737361
H	1.204459	1.527549	-0.973805
C	-0.803071	2.149788	-0.781669
H	-0.561406	3.175643	-1.042892
C	-2.122821	1.804202	-0.476941
C	-3.171026	2.785661	-0.445580
H	-2.908237	3.822155	-0.636604
C	-4.457154	2.433229	-0.180578
H	-5.242020	3.183807	-0.151226
C	-4.811628	1.060945	0.049663
C	-6.138249	0.674962	0.301814
H	-6.909736	1.438854	0.340240
C	-6.471121	-0.665028	0.494656
H	-7.503112	-0.943094	0.685304
C	-5.486996	-1.648293	0.433108
H	-5.748071	-2.694240	0.567045
C	-4.146031	-1.304469	0.193188
C	-3.111371	-2.285220	0.078683
H	-3.383112	-3.335835	0.131546
C	-1.809796	-1.936780	-0.118066
H	-1.092312	-2.728632	-0.246407
C	-1.379710	-0.564170	-0.212967
C	-2.422128	0.431167	-0.222144
C	-3.787152	0.062784	0.009790
C	3.152645	1.211652	0.236341
C	2.938297	1.891556	1.444854
H	2.534327	1.366306	2.301013
C	3.245499	3.246814	1.558408
H	3.071931	3.755451	2.501352
C	3.773936	3.943510	0.471230
H	4.011605	4.998781	0.561804
C	4.000855	3.273334	-0.732791
H	4.419084	3.802572	-1.583065
C	3.695929	1.919329	-0.850318
H	3.880175	1.412531	-1.790329
B	2.022689	-1.093923	1.330437
H	1.545279	-0.498858	2.228424
B	1.202543	-2.502245	0.633811
H	0.223802	-2.859036	1.178538
B	1.452915	-2.431369	-1.133377
H	0.619263	-2.700276	-1.928354
B	2.432613	-0.960566	-1.407373
H	2.264774	-0.249789	-2.333365
B	2.768812	-2.717798	1.415948
H	2.833182	-3.298469	2.448294
B	2.425179	-3.539181	-0.134722
H	2.256399	-4.711434	-0.212929
B	3.192589	-2.577602	-1.429556
H	3.592352	-3.044784	-2.443993
B	4.038181	-1.225654	-0.667161
H	4.969253	-0.670288	-1.137810
B	3.784043	-1.322991	1.091213
H	4.523757	-0.816970	1.862750
B	4.010405	-2.811414	0.139274
H	5.006950	-3.445792	0.253385

Table S13 Cartesian coordinates of **1CB** at Ψ = 45° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.827751	-0.103707	0.158837
C	1.382131	-0.946014	-0.419677
C	0.092931	-0.150585	-0.602808
C	0.174710	1.098802	-1.241299
H	1.128976	1.469235	-1.578237
C	-0.939264	1.869781	-1.530570
H	-0.815819	2.810488	-2.058452
C	-2.220072	1.439132	-1.172002
C	-3.393715	2.183725	-1.533228
H	-3.266086	3.087818	-2.121481
C	-4.632795	1.768832	-1.157134
H	-5.516046	2.333295	-1.442450
C	-4.802390	0.586695	-0.360292
C	-6.071872	0.157581	0.060205
H	-6.946011	0.727196	-0.242479
C	-6.217880	-0.975329	0.859449
H	-7.207762	-1.289018	1.176225
C	-5.098091	-1.698788	1.261813
H	-5.209224	-2.572053	1.898304
C	-3.810785	-1.309124	0.855783
C	-2.631088	-1.995931	1.281400
H	-2.733962	-2.821406	1.980327
C	-1.391495	-1.628681	0.853081
H	-0.547139	-2.162840	1.250660
C	-1.176742	-0.536999	-0.062539
C	-2.341540	0.238504	-0.409300
C	-3.646331	-0.163491	0.024209
C	2.754528	1.342785	0.582420
C	2.171945	1.728030	1.798464
H	1.728926	0.987769	2.451918
C	2.157543	3.068257	2.183992
H	1.699490	3.345227	3.128218
C	2.729628	4.043959	1.367632
H	2.718858	5.086106	1.671222
C	3.319875	3.669624	0.159553
H	3.773676	4.417311	-0.483192
C	3.332149	2.332028	-0.230625
H	3.798407	2.059036	-1.170074
B	2.033169	-1.319229	1.118975
H	1.414178	-1.008280	2.070562
B	1.517524	-2.607788	-0.008744
H	0.547357	-3.240814	0.185336
B	1.909736	-2.067523	-1.638647
H	1.170277	-2.253366	-2.542810
B	2.702369	-0.496114	-1.507429
H	2.545808	0.360854	-2.295244
B	3.012184	-2.784098	0.919784
H	3.085416	-3.568135	1.806992
B	2.953664	-3.249000	-0.808197
H	2.971227	-4.384016	-1.154878
B	3.682683	-1.937412	-1.752316
H	4.236397	-2.100706	-2.788750
B	4.225770	-0.693011	-0.620665
H	5.094581	0.084667	-0.812440
B	3.809729	-1.205380	1.025751
H	4.389490	-0.779219	1.964314
B	4.370255	-2.400131	-0.168021
H	5.438787	-2.905236	-0.060228

Table S14 Cartesian coordinates of **1CB** at Ψ = 67.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.786994	0.069361	0.275332
C	1.517161	-0.904935	-0.568612
C	0.166349	-0.264709	-0.844811
C	0.129174	0.788780	-1.774095
H	1.038117	1.096427	-2.265729
C	-1.036138	1.451772	-2.117961
H	-1.000513	2.253560	-2.849254
C	-2.257716	1.097647	-1.538156
C	-3.475634	1.769232	-1.895638
H	-3.423885	2.563912	-2.634169
C	-4.662271	1.422741	-1.330293
H	-5.579060	1.935103	-1.608076
C	-4.731311	0.374221	-0.352658
C	-5.948013	0.005707	0.244002
H	-6.854843	0.528329	-0.046850
C	-6.002078	-1.011828	1.195367
H	-6.952721	-1.281691	1.644794
C	-4.840602	-1.681101	1.571175
H	-4.879829	-2.473018	2.313768
C	-3.602958	-1.343689	0.997768
C	-2.387674	-2.002006	1.360078
H	-2.425705	-2.787300	2.109934
C	-1.193137	-1.671989	0.795516
H	-0.325968	-2.215344	1.123704
C	-1.060826	-0.642017	-0.204247
C	-2.275009	0.044553	-0.573219
C	-3.530404	-0.308114	0.021798
C	2.467171	1.474696	0.709817
C	1.801072	1.731887	1.918015
H	1.482551	0.913678	2.551041
C	1.548293	3.041539	2.323685
H	1.030303	3.218184	3.261020
C	1.960953	4.116154	1.535329
H	1.763917	5.135133	1.853673
C	2.635153	3.871782	0.338238
H	2.969797	4.698623	-0.280230
C	2.886432	2.563788	-0.071688
H	3.421229	2.393828	-0.998302
B	2.005941	-1.254518	1.047413
H	1.252428	-1.042594	1.923111
B	1.767376	-2.543936	-0.174049
H	0.829247	-3.255296	-0.125997
B	2.326856	-1.895180	-1.718360
H	1.751501	-2.110966	-2.728966
B	2.917546	-0.256164	-1.406694
H	2.814507	0.622573	-2.177016
B	3.138063	-2.613966	0.948372
H	3.170013	-3.427302	1.811433
B	3.363769	-3.003641	-0.782512
H	3.554280	-4.112254	-1.161462
B	4.071408	-1.577097	-1.570354
H	4.775951	-1.632651	-2.523311
B	4.325581	-0.338513	-0.329750
H	5.120846	0.534704	-0.386122
B	3.752970	-0.972464	1.220562
H	4.145797	-0.546040	2.251486
B	4.585626	-2.048209	0.073969
H	5.676470	-2.451984	0.310091

Table S15 Cartesian coordinates of **1CB** at Ψ = 90° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.711852	0.325750	-0.320304
C	-1.650954	-0.955508	0.507083
C	-0.247231	-0.590796	0.934893
C	-0.110295	-0.076181	2.237942
H	-0.983287	0.003599	2.869556
C	1.097778	0.365143	2.748356
H	1.140721	0.773061	3.753607
C	2.261707	0.308331	1.972990
C	3.510273	0.826500	2.456399
H	3.526376	1.291675	3.437688
C	4.643287	0.743934	1.708646
H	5.581739	1.145783	2.080073
C	4.630206	0.111292	0.420366
C	5.795129	-0.003359	-0.355882
H	6.723544	0.412789	0.024908
C	5.772183	-0.644720	-1.593432
H	6.684018	-0.725694	-2.176950
C	4.586248	-1.190103	-2.078532
H	4.570424	-1.703320	-3.035830
C	3.396538	-1.089394	-1.337886
C	2.166760	-1.668642	-1.781149
H	2.165475	-2.241977	-2.704014
C	1.012775	-1.538596	-1.069319
H	0.137153	-2.042166	-1.439929
C	0.943869	-0.803740	0.168260
C	2.193420	-0.303533	0.683997
C	3.400604	-0.424123	-0.077561
C	-2.138269	1.688283	-0.591969
C	-1.472237	1.962902	-1.797286
H	-1.342475	1.183760	-2.537667
C	-0.980389	3.239868	-2.062014
H	-0.468271	3.430143	-2.999917
C	-1.147564	4.266068	-1.131414
H	-0.763214	5.259963	-1.338702
C	-1.819166	4.007621	0.064174
H	-1.964857	4.799546	0.792038
C	-2.311456	2.731682	0.332132
H	-2.841058	2.553997	1.259794
B	-2.102730	-1.018733	-1.172412
H	-1.302252	-0.830305	-2.006669
B	-2.124345	-2.459067	-0.111537
H	-1.283275	-3.281673	-0.225986
B	-2.675978	-1.896624	1.479122
H	-2.213707	-2.309597	2.486305
B	-2.964888	-0.146596	1.315522
H	-2.738697	0.625001	2.171578
B	-3.432630	-2.186399	-1.279715
H	-3.543168	-2.888667	-2.229580
B	-3.814122	-2.714435	0.382231
H	-4.204864	-3.807324	0.631179
B	-4.328056	-1.272952	1.299033
H	-5.085778	-1.313045	2.211217
B	-4.318305	0.111561	0.192339
H	-4.968535	1.090859	0.323789
B	-3.772235	-0.449491	-1.393696
H	-4.030260	0.128261	-2.393085
B	-4.821973	-1.487717	-0.402944
H	-5.947623	-1.684472	-0.724070

Table S16 Cartesian coordinates of **1CB** at Ψ = 112.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.695576	0.430280	0.075514
C	-1.710273	-1.001668	-0.242697
C	-0.257644	-1.110468	0.229505
C	-0.044644	-2.079640	1.229574
H	-0.891243	-2.587556	1.665953
C	1.211255	-2.441144	1.682511
H	1.305423	-3.205284	2.448060
C	2.359561	-1.846473	1.151170
C	3.672214	-2.244945	1.574577
H	3.753114	-3.035322	2.315066
C	4.785092	-1.655281	1.062795
H	5.774912	-1.966323	1.384723
C	4.678111	-0.604062	0.091695
C	5.816955	0.022754	-0.440014
H	6.798784	-0.306239	-0.111520
C	5.700478	1.052773	-1.372038
H	6.593207	1.525347	-1.769841
C	4.442836	1.480230	-1.789205
H	4.348968	2.288843	-2.508547
C	3.278411	0.876214	-1.285856
C	1.969080	1.303182	-1.666117
H	1.873580	2.144543	-2.346893
C	0.848144	0.697920	-1.185596
H	-0.101472	1.101434	-1.480260
C	0.888584	-0.414945	-0.274696
C	2.200662	-0.815160	0.177017
C	3.379524	-0.183945	-0.338982
C	-2.038955	1.658473	0.654815
C	-1.902979	2.810650	-0.137150
H	-2.251101	2.808329	-1.163366
C	-1.328830	3.968207	0.384177
H	-1.237074	4.848292	-0.244434
C	-0.874597	3.994734	1.703528
H	-0.425466	4.895902	2.109219
C	-1.003636	2.855292	2.497466
H	-0.656005	2.863076	3.525670
C	-1.583401	1.696702	1.980783
H	-1.679059	0.827198	2.617740
B	-2.299171	-0.018171	-1.548909
H	-1.598205	0.655451	-2.198078
B	-2.336275	-1.782681	-1.653041
H	-1.551941	-2.329055	-2.349559
B	-2.725412	-2.387662	-0.040406
H	-2.241243	-3.385424	0.359021
B	-2.888193	-0.979856	1.039036
H	-2.498206	-0.984851	2.148380
B	-3.725429	-0.816733	-2.201888
H	-3.973189	-0.712552	-3.357421
B	-4.001609	-2.291581	-1.254144
H	-4.449233	-3.285397	-1.724043
B	-4.328943	-1.804549	0.432128
H	-5.002616	-2.436522	1.176714
B	-4.292931	-0.035831	0.508225
H	-4.842275	0.642918	1.306011
B	-3.918162	0.568706	-1.110296
H	-4.227183	1.658636	-1.445780
B	-4.970866	-0.843281	-0.923836
H	-6.129770	-0.765327	-1.167802

Table S17 Cartesian coordinates of **1CB** at Ψ = 135° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.611876	0.477285	0.059732
C	-1.772826	-1.041634	-0.133747
C	-0.290706	-1.234162	0.224253
C	-0.025360	-2.413411	0.944264
H	-0.848865	-3.013831	1.296166
C	1.250867	-2.850961	1.249886
H	1.380615	-3.770147	1.813051
C	2.371399	-2.129414	0.831758
C	3.701962	-2.583258	1.123980
H	3.815743	-3.509540	1.679594
C	4.790238	-1.878058	0.717587
H	5.793858	-2.228711	0.941028
C	4.638017	-0.653638	-0.015162
C	5.752104	0.086828	-0.442983
H	6.747379	-0.283034	-0.213313
C	5.594718	1.277075	-1.151058
H	6.468896	1.834843	-1.472448
C	4.319663	1.752107	-1.445339
H	4.193298	2.680878	-1.994425
C	3.179152	1.040234	-1.037470
C	1.854039	1.498584	-1.309284
H	1.726358	2.439142	-1.837932
C	0.755672	0.797714	-0.915820
H	-0.202734	1.225150	-1.136228
C	0.832531	-0.451872	-0.204903
C	2.165210	-0.917938	0.104898
C	3.320970	-0.179407	-0.314711
C	-1.894962	1.698176	0.593290
C	-1.929124	2.898556	-0.135010
H	-2.440162	2.942185	-1.088536
C	-1.304524	4.044553	0.353654
H	-1.347101	4.961918	-0.224984
C	-0.628888	4.012431	1.574128
H	-0.140692	4.904661	1.953486
C	-0.585191	2.823468	2.301739
H	-0.061117	2.782303	3.251339
C	-1.214952	1.676349	1.819622
H	-1.162495	0.766159	2.402166
B	-2.274533	-0.134569	-1.532649
H	-1.483666	0.392596	-2.218310
B	-2.481715	-1.889702	-1.472587
H	-1.752030	-2.564116	-2.113802
B	-2.911581	-2.317623	0.186872
H	-2.554437	-3.328255	0.672431
B	-2.924204	-0.828643	1.150129
H	-2.516924	-0.778743	2.253106
B	-3.779449	-0.852077	-2.103983
H	-4.031375	-0.823406	-3.262888
B	-4.179455	-2.208569	-1.033129
H	-4.717457	-3.195051	-1.415352
B	-4.445503	-1.555541	0.608277
H	-5.167072	-2.059515	1.403715
B	-4.241223	0.198267	0.534958
H	-4.716831	0.995333	1.267752
B	-3.829608	0.627421	-1.133780
H	-4.061015	1.702352	-1.562461
B	-5.007538	-0.655342	-0.821543
H	-6.156922	-0.488920	-1.065798

Table S18 Cartesian coordinates of **1CB** at Ψ = 157.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.545913	0.521464	0.076847
C	-1.790354	-1.097072	-0.085451
C	-0.288016	-1.407219	0.033633
C	-0.004885	-2.747018	0.362550
H	-0.815249	-3.445868	0.493641
C	1.278250	-3.221510	0.574631
H	1.423201	-4.260627	0.854266
C	2.383359	-2.375670	0.448384
C	3.715260	-2.827704	0.737031
H	3.845145	-3.846436	1.090683
C	4.785925	-2.005163	0.577729
H	5.789863	-2.351809	0.805980
C	4.617128	-0.666724	0.087076
C	5.714543	0.187414	-0.110774
H	6.710571	-0.172368	0.131448
C	5.539837	1.474468	-0.616633
H	6.401376	2.118164	-0.765279
C	4.265681	1.932790	-0.941822
H	4.129570	2.929809	-1.351159
C	3.140297	1.114062	-0.750524
C	1.819561	1.529097	-1.106507
H	1.685993	2.498369	-1.578451
C	0.735377	0.737247	-0.883223
H	-0.219736	1.097762	-1.211890
C	0.824847	-0.560754	-0.271178
C	2.160364	-1.042219	-0.007169
C	3.299660	-0.198795	-0.218982
C	-1.790419	1.786428	0.422363
C	-1.805548	2.868238	-0.474356
H	-2.303218	2.775074	-1.431757
C	-1.175660	4.068195	-0.151740
H	-1.202212	4.890716	-0.859543
C	-0.517117	4.211485	1.070746
H	-0.026345	5.146524	1.322046
C	-0.496861	3.143250	1.966834
H	0.011351	3.239488	2.921049
C	-1.130217	1.942074	1.649280
H	-1.098055	1.129031	2.362082
B	-2.414548	-0.253084	-1.470463
H	-1.663327	0.166481	-2.272953
B	-2.707673	-1.991430	-1.231448
H	-2.101278	-2.753943	-1.901367
B	-2.937272	-2.243066	0.509179
H	-2.562888	-3.197902	1.087094
B	-2.750652	-0.674638	1.304869
H	-2.207071	-0.562370	2.342407
B	-4.018340	-0.940625	-1.797360
H	-4.413031	-1.005104	-2.914175
B	-4.343565	-2.177179	-0.559787
H	-4.969464	-3.161043	-0.780839
B	-4.369170	-1.363475	1.031204
H	-5.004072	-1.754664	1.953686
B	-4.103424	0.356966	0.766237
H	-4.449892	1.236340	1.476595
B	-3.888534	0.615461	-0.975386
H	-4.124588	1.659592	-1.471903
B	-5.069795	-0.571118	-0.400667
H	-6.232362	-0.362462	-0.516023

Table S19 Cartesian coordinates of **1CB** at Ψ = 180° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.770425	0.422860	0.001710
C	1.491554	-1.372288	-0.001878
C	-0.026569	-1.555158	-0.005723
C	-0.445900	-2.901744	-0.007061
H	0.292575	-3.690710	-0.008070
C	-1.780658	-3.272875	-0.004473
H	-2.039513	-4.327583	-0.004524
C	-2.795729	-2.310211	-0.000378
C	-4.185463	-2.672187	0.005840
H	-4.441321	-3.727875	0.008057
C	-5.158996	-1.722345	0.009221
H	-6.207807	-2.005562	0.014312
C	-4.826830	-0.325211	0.005575
C	-5.818176	0.669899	0.008218
H	-6.862851	0.371723	0.013807
C	-5.476806	2.021433	0.003536
H	-6.258025	2.775405	0.005585
C	-4.138800	2.408751	-0.004220
H	-3.873898	3.462326	-0.008594
C	-3.114936	1.446909	-0.006788
C	-1.728254	1.801592	-0.017066
H	-1.457885	2.853727	-0.025518
C	-0.750376	0.854429	-0.017895
H	0.272953	1.178275	-0.030029
C	-1.031603	-0.551011	-0.008158
C	-2.419592	-0.934856	-0.003136
C	-3.448799	0.059996	-0.001317
C	2.320974	1.840966	0.002907
C	2.148722	2.533300	1.215221
H	2.272701	2.012057	2.157267
C	1.821197	3.886524	1.213656
H	1.693457	4.408134	2.156686
C	1.660121	4.569230	0.005275
H	1.404243	5.624157	0.006226
C	1.831754	3.891268	-1.204345
H	1.712316	4.416544	-2.146428
C	2.159541	2.538110	-1.208243
H	2.291830	2.020456	-2.151169
B	2.393999	-0.667831	1.313657
H	1.796463	-0.259827	2.247298
B	2.389548	-2.420556	0.898421
H	1.790331	-3.155477	1.603284
B	2.393433	-2.418940	-0.900181
H	1.797428	-3.152698	-1.608970
B	2.400252	-0.665734	-1.313163
H	1.806782	-0.256190	-2.248768
B	3.901955	-1.706708	1.435435
H	4.360258	-2.029646	2.480810
B	3.900085	-2.767982	0.002098
H	4.341628	-3.870051	0.002166
B	3.908485	-1.704485	-1.429508
H	4.371383	-2.026088	-2.473270
B	4.053012	-0.037526	-0.900352
H	4.537031	0.800839	-1.579699
B	4.048610	-0.038863	0.909259
H	4.529288	0.798602	1.592084
B	4.899360	-1.335915	0.005581
H	6.086128	-1.362120	0.008342

Table S20 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **2CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	2.982443	0.343837	-0.008269
C	1.893592	-1.045859	0.008994
C	0.402520	-0.822009	0.007952
C	-0.300904	-0.728581	1.216333
H	0.224243	-0.797022	2.161042
C	-1.692399	-0.558709	1.238575
C	-2.429518	-0.456198	2.470067
H	-1.882386	-0.515043	3.406630
C	-3.780863	-0.287452	2.469805
H	-4.323371	-0.210193	3.407931
C	-4.526799	-0.208057	1.242052
C	-5.920299	-0.035748	1.215752
H	-6.462658	0.043399	2.153675
C	-6.605837	0.032778	0.003136
H	-7.683358	0.166304	0.002343
C	-5.922801	-0.069837	-1.208481
H	-6.467107	-0.017020	-2.147134
C	-4.529382	-0.243032	-1.232783
C	-3.786050	-0.357232	-2.459367
H	-4.330518	-0.306351	-3.398152
C	-2.434763	-0.526280	-2.457691
H	-1.889600	-0.611741	-3.393361
C	-1.695090	-0.593950	-1.225312
C	-2.406121	-0.484733	0.006093
C	-3.820537	-0.311359	0.005115
C	2.408814	1.737405	-0.019234
C	2.194456	2.430498	1.182529
H	2.421064	1.959654	2.130980
C	1.701415	3.734264	1.172238
H	1.542910	4.251804	2.113064
C	1.417974	4.370281	-0.036879
H	1.033318	5.385385	-0.043700
C	1.641060	3.695246	-1.237363
H	1.435095	4.182221	-2.185291
C	2.134466	2.391471	-1.230439
H	2.313832	1.890452	-2.173392
B	2.796280	-0.614023	1.413518
H	2.231638	-0.158143	2.338280
B	2.609086	-2.307094	0.909016
H	1.879432	-2.999119	1.531298
B	2.606406	-2.326584	-0.864839
H	1.875080	-3.032194	-1.469607
B	2.792283	-0.645164	-1.407430
H	2.225158	-0.212529	-2.341639
B	4.186145	-1.702679	1.455125
H	4.641579	-2.046507	2.495186
B	4.081316	-2.765959	0.024663
H	4.465281	-3.888952	0.036518
B	4.181968	-1.734674	-1.429304
H	4.633808	-2.101771	-2.462951
B	4.386407	-0.054872	-0.893000
H	4.888166	0.815432	-1.516987
B	4.388888	-0.035488	0.880529
H	4.893377	0.847863	1.483541
B	5.176456	-1.368303	0.007502
H	6.358754	-1.472551	0.007085
C	-0.303610	-0.763389	-1.201105
H	0.219495	-0.859317	-2.144556

Table S21 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **2CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	3.329259	0.286220	0.000606
C	1.559371	-1.337551	-0.001980
C	0.105376	-1.013824	-0.001719
C	-0.603544	-0.864126	1.196131
H	-0.085664	-0.990611	2.140556
C	-1.987448	-0.548266	1.225352
C	-2.696231	-0.390843	2.445255
H	-2.166840	-0.516737	3.384006
C	-4.044967	-0.079468	2.449217
H	-4.571003	0.037516	3.391069
C	-4.759439	0.091070	1.233887
C	-6.143120	0.411312	1.207618
H	-6.671828	0.531030	2.147961
C	-6.820087	0.571337	0.000786
H	-7.876091	0.815391	0.001172
C	-6.142501	0.417909	-1.206551
H	-6.670779	0.542620	-2.146481
C	-4.758761	0.097993	-1.233867
C	-4.043601	-0.065639	-2.449675
H	-4.569139	0.056605	-3.391137
C	-2.694841	-0.376901	-2.446663
H	-2.164875	-0.497400	-3.385807
C	-1.986740	-0.541214	-1.227304
C	-2.687221	-0.382283	-0.000750
C	-4.066608	-0.064580	-0.000241
C	3.127443	1.744196	0.002495
C	3.031832	2.465239	1.210762
H	3.107427	1.933730	2.153322
C	2.850508	3.846222	1.210637
H	2.784439	4.377224	2.156132
C	2.756384	4.548309	0.005746
H	2.614206	5.624749	0.006922
C	2.851437	3.849063	-1.200725
H	2.786057	4.382373	-2.144972
C	3.032704	2.468104	-1.204078
H	3.108878	1.938672	-2.147756
B	2.602930	-0.744167	1.209274
H	2.112320	-0.214861	2.153391
B	2.206326	-2.544302	0.891291
H	1.464950	-3.169036	1.580679
B	2.207129	-2.541410	-0.898663
H	1.465875	-3.163544	-1.590558
B	2.603675	-0.740610	-1.210947
H	2.113742	-0.208495	-2.153882
B	3.825389	-2.099081	1.429661
H	4.209967	-2.514162	2.477863
B	3.606880	-3.165003	-0.003954
H	3.853511	-4.330744	-0.005279
B	3.826558	-2.094998	-1.434340
H	4.211908	-2.507198	-2.483396
B	4.418439	-0.518757	-0.901729
H	5.124316	0.132853	-1.601768
B	4.417321	-0.521370	0.902029
H	5.122594	0.128271	1.604482
B	4.904623	-1.977974	-0.001802
H	6.045356	-2.322678	-0.002003
C	-0.602771	-0.857138	-1.199061
H	-0.084267	-0.978056	-2.143884

Table S22 Cartesian coordinates of **2CB** at Ψ = 0° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.995769	0.127289	0.000003
C	1.742617	-1.104988	-0.000006
C	0.260139	-0.778179	-0.000011
C	-0.244055	0.526927	-0.000010
H	0.419103	1.377785	0.000011
C	-1.625679	0.775889	-0.000010
C	-2.155855	2.113568	-0.000003
H	-1.457901	2.946051	0.000000
C	-3.499359	2.338732	-0.000006
H	-3.884468	3.354707	-0.000002
C	-4.442405	1.252136	-0.000008
C	-5.832017	1.456952	-0.000003
H	-6.218420	2.472288	-0.000001
C	-6.710477	0.373833	-0.000003
H	-7.781669	0.551356	0.000001
C	-6.228443	-0.935185	-0.000005
H	-6.921973	-1.771400	-0.000004
C	-4.847456	-1.189784	-0.000009
C	-4.305683	-2.523065	-0.000008
H	-4.998418	-3.360057	-0.000004
C	-2.961867	-2.744495	-0.000008
H	-2.571162	-3.758075	-0.000006
C	-2.027714	-1.649557	-0.000014
C	-2.536837	-0.318430	-0.000017
C	-3.942488	-0.085318	-0.000012
C	2.727460	1.614337	-0.000003
C	2.643817	2.324038	1.208032
H	2.727545	1.802251	2.153350
C	2.449763	3.704493	1.205964
H	2.383463	4.234867	2.150556
C	2.345970	4.399478	0.000014
H	2.194073	5.474272	0.000021
C	2.449998	3.704544	-1.205943
H	2.383887	4.234962	-2.150525
C	2.644051	2.324090	-1.208028
H	2.727972	1.802348	-2.153351
B	2.681193	-0.805579	1.420500
H	2.137832	-0.296212	2.333397
B	2.299415	-2.455799	0.887343
H	1.496376	-3.058032	1.510601
B	2.299464	-2.455825	-0.887370
H	1.496401	-3.058015	-1.510635
B	2.681217	-0.805645	-1.420551
H	2.137959	-0.296189	-2.333457
B	3.933020	-2.065273	1.444709
H	4.336601	-2.479354	2.480426
B	3.697472	-3.091001	0.000020
H	3.931440	-4.254510	0.000023
B	3.933083	-2.065277	-1.444671
H	4.336759	-2.479359	-2.480349
B	4.340192	-0.438933	-0.889370
H	4.952984	0.373406	-1.491097
B	4.340230	-0.438956	0.889441
H	4.952950	0.373426	1.491183
B	4.959608	-1.845687	0.000042
H	6.120509	-2.092209	0.000050
C	-0.641189	-1.854208	-0.000017
H	-0.274668	-2.873008	0.000006

Table S23 Cartesian coordinates of **2CB** at Ψ = 22.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.978694	0.183221	0.063273
C	1.794916	-1.100857	-0.111882
C	0.305458	-0.814188	-0.108468
C	-0.218032	0.444707	-0.426302
H	0.432189	1.258953	-0.710177
C	-1.600417	0.685481	-0.413029
C	-2.150516	1.976028	-0.733041
H	-1.466647	2.780694	-0.987842
C	-3.495172	2.192728	-0.714233
H	-3.895042	3.173490	-0.956520
C	-4.419978	1.143191	-0.377350
C	-5.810446	1.340103	-0.351908
H	-6.212079	2.320194	-0.593495
C	-6.671039	0.293507	-0.021733
H	-7.743220	0.464325	-0.007333
C	-6.169949	-0.970581	0.289063
H	-6.849826	-1.778858	0.543334
C	-4.787222	-1.215657	0.277116
C	-4.226401	-2.503864	0.588438
H	-4.905347	-3.313425	0.841592
C	-2.881364	-2.717038	0.569253
H	-2.476204	-3.696503	0.806976
C	-1.964971	-1.657827	0.238217
C	-2.493203	-0.371834	-0.075363
C	-3.900322	-0.147966	-0.058171
C	2.605586	1.633690	0.263520
C	2.243045	2.128097	1.524700
H	2.188185	1.463513	2.377273
C	1.949547	3.480516	1.697280
H	1.667632	3.842637	2.680840
C	2.020247	4.361392	0.617903
H	1.791226	5.413567	0.754794
C	2.396018	3.881372	-0.638030
H	2.465431	4.557430	-1.484294
C	2.689543	2.530423	-0.814479
H	2.982588	2.175503	-1.795269
B	2.723145	-0.953093	1.340227
H	2.160390	-0.618344	2.318649
B	2.429612	-2.528993	0.580123
H	1.689834	-3.271549	1.121827
B	2.414794	-2.289772	-1.177185
H	1.627821	-2.840773	-1.866697
B	2.711560	-0.562552	-1.473918
H	2.142721	0.050354	-2.304408
B	4.040483	-2.131959	1.191718
H	4.467275	-2.666186	2.160946
B	3.853482	-2.960495	-0.382737
H	4.149797	-4.099205	-0.537622
B	4.026621	-1.736168	-1.669698
H	4.451115	-1.976166	-2.751059
B	4.347714	-0.181780	-0.890076
H	4.919864	0.731752	-1.374315
B	4.357938	-0.424158	0.871123
H	4.926264	0.331286	1.581355
B	5.046615	-1.660777	-0.204484
H	6.218923	-1.842898	-0.236045
C	-0.576826	-1.853503	0.220641
H	-0.195877	-2.837894	0.459541

Table S24 Cartesian coordinates of **2CB** at Ψ = 45° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.951550	0.274275	0.135173
C	1.885903	-1.049842	-0.264272
C	0.389246	-0.827656	-0.251652
C	-0.190419	0.307446	-0.832613
H	0.422713	1.046192	-1.330662
C	-1.577312	0.515134	-0.801513
C	-2.188112	1.671765	-1.401149
H	-1.546969	2.401599	-1.887114
C	-3.537270	1.854597	-1.364332
H	-3.983745	2.732683	-1.822654
C	-4.406314	0.902944	-0.724675
C	-5.799925	1.069125	-0.672170
H	-6.246940	1.946648	-1.130784
C	-6.605740	0.122576	-0.039947
H	-7.681358	0.267686	-0.009388
C	-6.045252	-1.008094	0.554066
H	-6.682376	-1.738740	1.044364
C	-4.656869	-1.217460	0.527355
C	-4.036314	-2.367925	1.128965
H	-4.673040	-3.098231	1.620529
C	-2.687059	-2.548870	1.090395
H	-2.235720	-3.423486	1.550092
C	-1.826628	-1.593938	0.443264
C	-2.414313	-0.443822	-0.160289
C	-3.825893	-0.252964	-0.119583
C	2.403869	1.637966	0.481129
C	1.854686	1.912252	1.742019
H	1.783418	1.132414	2.489072
C	1.395730	3.192289	2.051634
H	0.971894	3.382680	3.032527
C	1.483129	4.219871	1.112436
H	1.126205	5.215581	1.356425
C	2.037853	3.959529	-0.141599
H	2.118965	4.751247	-0.879651
C	2.495112	2.681058	-0.455114
H	2.928369	2.498653	-1.431359
B	2.736382	-1.041265	1.238152
H	2.108964	-0.884574	2.221579
B	2.593573	-2.515913	0.257959
H	1.889306	-3.383508	0.636984
B	2.637452	-2.042669	-1.448118
H	1.925352	-2.551404	-2.243574
B	2.818878	-0.279647	-1.497993
H	2.263817	0.399069	-2.283349
B	4.141079	-2.091101	1.007248
H	4.565428	-2.719236	1.919637
B	4.089734	-2.709252	-0.670361
H	4.481234	-3.792646	-0.955760
B	4.224536	-1.314829	-1.772345
H	4.714586	-1.372761	-2.851081
B	4.387854	0.142243	-0.777332
H	4.909761	1.149344	-1.108822
B	4.339821	-0.333177	0.933459
H	4.816019	0.356588	1.767715
B	5.168756	-1.362641	-0.256292
H	6.351836	-1.456422	-0.249292
C	-0.435251	-1.758253	0.395965
H	-0.004495	-2.630151	0.871722

Table S25 Cartesian coordinates of **2CB** at Ψ = 67.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.960582	0.313447	0.152918
C	1.909670	-1.001014	-0.336084
C	0.414630	-0.794946	-0.297825
C	-0.227745	0.097568	-1.164805
H	0.340694	0.662506	-1.891892
C	-1.618275	0.277734	-1.124567
C	-2.294888	1.187151	-2.010737
H	-1.702020	1.747564	-2.727930
C	-3.646457	1.346506	-1.959043
H	-4.142778	2.036757	-2.635493
C	-4.452646	0.614799	-1.018587
C	-5.847557	0.761238	-0.945799
H	-6.344446	1.451027	-1.622153
C	-6.591820	0.032382	-0.018597
H	-7.669457	0.158415	0.022965
C	-5.967218	-0.856635	0.855948
H	-6.556896	-1.419274	1.574188
C	-4.574941	-1.036732	0.820880
C	-3.890150	-1.942518	1.704666
H	-4.479555	-2.504772	2.423570
C	-2.538616	-2.100693	1.651762
H	-2.038286	-2.789552	2.326361
C	-1.740215	-1.365979	0.706484
C	-2.392218	-0.460420	-0.181752
C	-3.806492	-0.294134	-0.126548
C	2.364495	1.640682	0.549223
C	1.881707	1.864450	1.847403
H	1.908063	1.072005	2.584239
C	1.370246	3.110249	2.208696
H	1.000200	3.261613	3.217776
C	1.338030	4.154455	1.284163
H	0.940003	5.123764	1.567818
C	1.828139	3.945997	-0.005632
H	1.818026	4.752413	-0.732091
C	2.337791	2.701257	-0.370643
H	2.724628	2.561680	-1.372849
B	2.737165	-1.057377	1.178061
H	2.097388	-0.948642	2.159416
B	2.614249	-2.485945	0.127459
H	1.888552	-3.362288	0.445561
B	2.686892	-1.926769	-1.551810
H	1.994469	-2.398687	-2.386402
B	2.858301	-0.162516	-1.505440
H	2.332186	0.553589	-2.275000
B	4.148794	-2.087919	0.924088
H	4.563092	-2.755956	1.812553
B	4.131062	-2.622302	-0.781250
H	4.537604	-3.686217	-1.115036
B	4.273624	-1.172544	-1.809660
H	4.781546	-1.172968	-2.881690
B	4.411293	0.237505	-0.740499
H	4.925506	1.265525	-1.016970
B	4.338385	-0.324700	0.941509
H	4.794985	0.321175	1.820760
B	5.193559	-1.289608	-0.283185
H	6.376925	-1.377853	-0.261355
C	-0.348045	-1.510487	0.636138
H	0.134916	-2.197086	1.321303

Table S26 Cartesian coordinates of **2CB** at Ψ = 90° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.982179	0.343660	0.022353
C	1.893929	-1.044985	-0.044521
C	0.402751	-0.822007	-0.037735
C	-0.297514	-0.661024	-1.240711
H	0.229880	-0.676570	-2.186500
C	-1.689025	-0.489879	-1.256698
C	-2.423132	-0.318619	-2.482309
H	-1.873728	-0.325169	-3.419356
C	-3.774483	-0.149956	-2.475992
H	-4.314636	-0.020405	-3.409713
C	-4.523460	-0.139006	-1.247579
C	-5.917004	0.031999	-1.215071
H	-6.457086	0.163460	-2.148422
C	-6.605488	0.033092	-0.002195
H	-7.682988	0.166670	0.003413
C	-5.925427	-0.137049	1.203482
H	-6.471974	-0.136384	2.142333
C	-4.532118	-0.311848	1.221438
C	-3.791835	-0.494458	2.441559
H	-4.338569	-0.495733	3.380393
C	-2.440595	-0.663682	2.433805
H	-1.897805	-0.801181	3.364648
C	-1.697899	-0.662838	1.201375
C	-2.405834	-0.484824	-0.023801
C	-3.820240	-0.311318	-0.016617
C	2.408039	1.736064	0.075627
C	2.121687	2.348768	1.305488
H	2.292079	1.816281	2.232671
C	1.627774	3.651565	1.351702
H	1.412365	4.106124	2.313528
C	1.416240	4.366890	0.172667
H	1.031185	5.381179	0.210075
C	1.711792	3.772219	-1.054461
H	1.562443	4.321369	-1.978724
C	2.205229	2.469521	-1.104005
H	2.441534	2.031118	-2.065522
B	2.787358	-0.690647	1.387817
H	2.215025	-0.289711	2.332996
B	2.604036	-2.353325	0.789078
H	1.871195	-3.079009	1.367598
B	2.612868	-2.276028	-0.983148
H	1.885137	-2.946919	-1.630358
B	2.801319	-0.567399	-1.430755
H	2.241486	-0.080985	-2.342806
B	4.177213	-1.780089	1.378799
H	4.625317	-2.181176	2.401388
B	4.082140	-2.763320	-0.108664
H	4.466541	-3.885248	-0.155534
B	4.191828	-1.653708	-1.502992
H	4.651372	-1.962715	-2.552130
B	4.391781	-0.006260	-0.873139
H	4.898392	0.896250	-1.445196
B	4.383131	-0.083556	0.898835
H	4.882400	0.766032	1.552669
B	5.176744	-1.366690	-0.041572
H	6.359068	-1.470654	-0.040475
C	-0.306452	-0.830941	1.171016
H	0.214600	-0.979576	2.108823

Table S27 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **4CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	2.535330	0.414958	0.195682
C	1.450587	-0.772861	-0.669326
C	-2.848845	-2.694710	1.909961
H	-3.558301	-3.210206	2.550763
C	-3.295525	-1.650785	1.087997
C	-4.681033	-1.264870	1.074500
H	-5.360687	-1.791817	1.738278
C	-5.141302	-0.280507	0.257236
H	-6.192206	-0.005718	0.256414
C	-4.248356	0.407499	-0.630957
C	-4.690978	1.406942	-1.513397
H	-5.743928	1.674323	-1.519121
C	-3.803883	2.048046	-2.377339
H	-4.168559	2.815077	-3.053366
C	-2.453123	1.709035	-2.376816
H	-1.761402	2.209469	-3.048218
C	-1.969774	0.719170	-1.504193
C	-0.585594	0.372544	-1.463157
H	0.058493	0.911177	-2.142836
C	-0.054072	-0.570266	-0.620181
C	-0.968686	-1.327374	0.248115
C	-2.364975	-0.967721	0.239073
C	-2.863642	0.054411	-0.622425
C	1.915257	1.548705	0.965911
C	1.543863	1.392119	2.310716
H	1.678307	0.439080	2.806230
C	1.008024	2.460372	3.028022
H	0.726683	2.317304	4.066518
C	0.838279	3.704095	2.418591
H	0.420582	4.534886	2.978747
C	1.216754	3.874457	1.086441
H	1.099527	4.839357	0.603383
C	1.751361	2.807865	0.366011
H	2.051605	2.963470	-0.662805
B	2.332958	-1.189340	0.760277
H	1.754113	-1.361850	1.765513
B	2.228133	-2.283492	-0.653466
H	1.549627	-3.247985	-0.607798
B	2.263486	-1.253900	-2.093527
H	1.587162	-1.477907	-3.037373
B	2.405731	0.419861	-1.518393
H	1.894422	1.331304	-2.052274
B	3.761014	-2.087645	0.217611
H	4.196819	-2.973757	0.875041
B	3.737124	-2.106919	-1.569219
H	4.159340	-3.019528	-2.199870
B	3.832901	-0.419542	-2.127806
H	4.317978	-0.095986	-3.161037
B	3.968483	0.622211	-0.700728
H	4.449925	1.702274	-0.685749
B	3.925376	-0.400750	0.742283
H	4.378406	-0.046707	1.775845
B	4.780594	-0.958755	-0.713713
H	5.965454	-1.026719	-0.726651
C	-0.597142	-2.406715	1.070575
H	0.418235	-2.761153	1.083068
C	-1.514337	-3.072581	1.882753
H	-1.169729	-3.898000	2.497954

Table S28 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **4CB** from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.901930	0.247914	0.017183
C	-1.025548	-1.184240	0.501375
C	3.062869	-1.431077	-2.866748
H	3.737682	-1.583683	-3.702887
C	3.529436	-0.737098	-1.721205
C	4.859396	-0.249012	-1.662361
H	5.512311	-0.405969	-2.514908
C	5.331917	0.414125	-0.543978
H	6.355268	0.774649	-0.518653
C	4.494014	0.625607	0.579514
C	4.954563	1.286565	1.744435
H	5.977351	1.648794	1.776231
C	4.109629	1.466989	2.835256
H	4.472389	1.972635	3.723476
C	2.796144	1.001716	2.791179
H	2.140511	1.146937	3.644369
C	2.291219	0.338861	1.644580
C	0.953580	-0.134862	1.576660
H	0.325225	0.021159	2.444334
C	0.419888	-0.765845	0.463923
C	1.300567	-1.000096	-0.660129
C	2.651422	-0.529132	-0.611592
C	3.147316	0.149133	0.532734
C	-2.769803	1.628748	-0.474439
C	-2.717550	1.907033	-1.856226
H	-2.767008	1.088623	-2.566092
C	-2.612548	3.215788	-2.320029
H	-2.578610	3.403625	-3.389371
C	-2.552360	4.283052	-1.419538
H	-2.468416	5.302889	-1.782562
C	-2.604332	4.024334	-0.046639
H	-2.564430	4.845319	0.663516
C	-2.709785	2.717280	0.420857
H	-2.753935	2.530992	1.488359
B	-2.119672	-1.084377	-0.799759
H	-1.704284	-0.858237	-1.885550
B	-1.620999	-2.657461	0.106687
H	-0.873601	-3.476648	-0.315959
B	-1.626406	-2.021487	1.778373
H	-0.855184	-2.313465	2.634033
B	-2.135708	-0.268516	1.486061
H	-1.689890	0.579171	2.183944
B	-3.266589	-2.498078	-0.520579
H	-3.627348	-3.259000	-1.362028
B	-2.989328	-3.001632	1.181261
H	-3.158699	-4.110531	1.580991
B	-3.274494	-1.530913	2.169613
H	-3.622628	-1.586501	3.306435
B	-3.951536	-0.257867	1.152399
H	-4.683803	0.559299	1.607364
B	-3.940602	-0.867744	-0.546678
H	-4.670009	-0.530638	-1.421670
B	-4.352253	-1.961641	0.804638
H	-5.472714	-2.343166	0.936915
C	0.902130	-1.708293	-1.835410
H	-0.094461	-2.110528	-1.897849
C	1.763295	-1.915395	-2.908594
H	1.411035	-2.459722	-3.777370

Table S29 Cartesian coordinates of **4CB** at Ψ = 0° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.661553	-0.021476	0.000004
C	1.085572	-1.179331	-0.000258
C	-3.985269	-2.876800	-0.000551
H	-4.913956	-3.440026	-0.000672
C	-4.029563	-1.475914	-0.000315
C	-5.288318	-0.779895	-0.000231
H	-6.196974	-1.375425	-0.000381
C	-5.355037	0.578094	0.000037
H	-6.314935	1.086625	0.000098
C	-4.156884	1.367796	0.000253
C	-4.184613	2.772229	0.000565
H	-5.145326	3.279508	0.000641
C	-3.003532	3.513152	0.000784
H	-3.047389	4.597913	0.001023
C	-1.768158	2.869409	0.000697
H	-0.848178	3.446906	0.000860
C	-1.698869	1.465996	0.000386
C	-0.444864	0.780579	0.000252
H	0.431665	1.406816	0.000419
C	-0.316113	-0.580174	-0.000084
C	-1.535686	-1.404485	-0.000247
C	-2.808573	-0.725406	-0.000140
C	-2.893633	0.698952	0.000158
C	2.635066	1.480318	-0.000275
C	2.667848	2.194381	1.209172
H	2.657855	1.663536	2.153460
C	2.710757	3.587058	1.206471
H	2.734030	4.122542	2.150161
C	2.727167	4.288510	-0.000865
H	2.759573	5.373509	-0.001094
C	2.710240	3.586558	-1.207902
H	2.733091	4.121646	-2.151826
C	2.667370	2.193878	-1.210011
H	2.657020	1.662633	-2.154077
B	2.122037	-0.912129	1.375876
H	1.667468	-0.337658	2.299829
B	1.525494	-2.521422	0.896454
H	0.698614	-3.012885	1.579331
B	1.525830	-2.521979	-0.895947
H	0.699503	-3.013665	-1.579321
B	2.122151	-0.912681	-1.375682
H	1.668569	-0.338483	-2.300292
B	3.196317	-2.348434	1.440342
H	3.530694	-2.813365	2.479069
B	2.828409	-3.342888	0.000668
H	2.899157	-4.527629	0.000745
B	3.196718	-2.348901	-1.439312
H	3.531693	-2.814166	-2.477698
B	3.845064	-0.807449	-0.890921
H	4.562754	-0.115817	-1.526946
B	3.844966	-0.807285	0.891628
H	4.562263	-0.115065	1.527455
B	4.248013	-2.298228	0.000594
H	5.360783	-2.710784	0.000807
C	-1.566409	-2.811534	-0.000443
H	-0.653165	-3.379776	-0.000487
C	-2.761250	-3.529482	-0.000598
H	-2.722606	-4.614394	-0.000750

Table S30 Cartesian coordinates of **4CB** at Ψ = 22.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.604858	0.108347	0.103782
C	1.199469	-1.140344	-0.204712
C	-3.764753	-3.033686	0.409302
H	-4.654442	-3.622944	0.611644
C	-3.868589	-1.638388	0.317427
C	-5.139177	-0.978751	0.457495
H	-6.006285	-1.590904	0.689347
C	-5.269406	0.364829	0.291047
H	-6.239013	0.844329	0.390772
C	-4.132463	1.173398	-0.046829
C	-4.237366	2.552243	-0.295446
H	-5.209689	3.029761	-0.212463
C	-3.119158	3.303134	-0.655529
H	-3.223120	4.366589	-0.847556
C	-1.869501	2.697451	-0.770255
H	-0.997810	3.285126	-1.043199
C	-1.721080	1.323362	-0.517921
C	-0.441969	0.686039	-0.573865
H	0.389863	1.323467	-0.826756
C	-0.234642	-0.632385	-0.270462
C	-1.409345	-1.491469	-0.059535
C	-2.698528	-0.857249	0.048292
C	-2.853449	0.546121	-0.155441
C	2.398394	1.588333	0.274262
C	2.035912	2.133757	1.515260
H	1.851568	1.485237	2.362285
C	1.910686	3.513446	1.672278
H	1.627687	3.916314	2.639493
C	2.149223	4.370143	0.597050
H	2.050951	5.443940	0.721766
C	2.522668	3.837860	-0.639138
H	2.720958	4.494538	-1.480227
C	2.648710	2.459887	-0.800207
H	2.941364	2.062079	-1.764781
B	2.081866	-0.984471	1.310994
H	1.491075	-0.591103	2.251445
B	1.694338	-2.552592	0.581450
H	0.896634	-3.208423	1.142536
B	1.824551	-2.351835	-1.188135
H	1.073304	-2.836210	-1.962743
B	2.300578	-0.646105	-1.434574
H	1.878566	0.008253	-2.320096
B	3.288106	-2.304469	1.295277
H	3.576341	-2.869678	2.297501
B	3.134601	-3.142243	-0.277003
H	3.325260	-4.307117	-0.401140
B	3.511204	-1.953124	-1.555109
H	3.983642	-2.244767	-2.603354
B	3.943605	-0.432214	-0.764675
H	4.638522	0.395802	-1.242418
B	3.815310	-0.656442	0.995623
H	4.403382	0.027233	1.760621
B	4.436101	-1.975106	-0.028907
H	5.582267	-2.278993	0.020651
C	-1.389230	-2.897674	-0.035381
H	-0.474392	-3.432705	-0.223781
C	-2.539820	-3.650596	0.197733
H	-2.466614	-4.733669	0.210510

Table S31 Cartesian coordinates of **4CB** at Ψ = 45° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.561675	0.255083	0.102119
C	1.357163	-0.928401	-0.432645
C	-3.262781	-2.967046	1.355726
H	-4.062600	-3.584723	1.753753
C	-3.580435	-1.793773	0.656949
C	-4.947673	-1.380768	0.486131
H	-5.726827	-2.034907	0.867383
C	-5.269418	-0.204188	-0.115456
H	-6.307330	0.096542	-0.226232
C	-4.241938	0.676998	-0.592971
C	-4.528745	1.930940	-1.157701
H	-5.565725	2.240604	-1.252799
C	-3.505676	2.778235	-1.581664
H	-3.749384	3.745589	-2.009800
C	-2.173255	2.390036	-1.460146
H	-1.377309	3.049379	-1.793926
C	-1.845640	1.137733	-0.913711
C	-0.490503	0.690309	-0.831452
H	0.247784	1.365957	-1.234016
C	-0.120979	-0.547864	-0.373932
C	-1.152401	-1.382281	0.261644
C	-2.528797	-0.974858	0.132494
C	-2.878065	0.269962	-0.468809
C	2.131190	1.564852	0.714546
C	1.646824	1.642059	2.028417
H	1.539368	0.745751	2.625355
C	1.299834	2.872956	2.584494
H	0.924823	2.910070	3.602342
C	1.436615	4.046451	1.842794
H	1.167601	5.003436	2.278862
C	1.926063	3.981402	0.537390
H	2.043606	4.886992	-0.049281
C	2.269943	2.752582	-0.022604
H	2.653695	2.721490	-1.035627
B	2.288886	-1.228923	0.971218
H	1.742554	-1.209983	2.013511
B	2.019906	-2.502060	-0.255870
H	1.309570	-3.413613	-0.046755
B	2.013146	-1.717737	-1.832832
H	1.243091	-2.032263	-2.673575
B	2.328808	0.001233	-1.579249
H	1.823372	0.839530	-2.228754
B	3.613609	-2.303027	0.484393
H	4.030842	-3.107300	1.249988
B	3.457122	-2.599927	-1.274143
H	3.754980	-3.638380	-1.765631
B	3.640225	-1.046527	-2.109230
H	4.070492	-0.936907	-3.209312
B	3.950194	0.192068	-0.886932
H	4.521948	1.211040	-1.063575
B	3.927279	-0.574182	0.713093
H	4.481935	-0.083809	1.635246
B	4.641233	-1.426081	-0.676909
H	5.814339	-1.592194	-0.745217
C	-0.903492	-2.529685	1.035684
H	0.105504	-2.829869	1.255472
C	-1.933848	-3.304712	1.567743
H	-1.682332	-4.182745	2.154642

Table S32 Cartesian coordinates of **4CB** at Ψ = 67.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.544537	0.373422	0.181308
C	1.434024	-0.804781	-0.614804
C	-2.965909	-2.877346	1.657813
H	-3.704425	-3.456146	2.204851
C	-3.379216	-1.771706	0.902000
C	-4.766400	-1.395509	0.847641
H	-5.477300	-1.998622	1.405399
C	-5.188990	-0.322329	0.127809
H	-6.240673	-0.052064	0.099128
C	-4.251545	0.477391	-0.607505
C	-4.647823	1.596404	-1.358516
H	-5.700066	1.865300	-1.385595
C	-3.714764	2.357607	-2.061506
H	-4.043135	3.218506	-2.635440
C	-2.364482	2.018118	-2.031208
H	-1.637450	2.610375	-2.579233
C	-1.928438	0.904914	-1.292642
C	-0.550731	0.532850	-1.250125
H	0.121373	1.151775	-1.824747
C	-0.065872	-0.548149	-0.559916
C	-1.014179	-1.364335	0.215738
C	-2.410401	-1.003696	0.177199
C	-2.867832	0.121463	-0.571233
C	1.964331	1.559655	0.903784
C	1.525826	1.460079	2.233265
H	1.575784	0.513017	2.755002
C	1.028893	2.577892	2.901716
H	0.693578	2.478722	3.929234
C	0.966854	3.814442	2.258335
H	0.580062	4.683754	2.780951
C	1.412402	3.927260	0.940843
H	1.378506	4.885233	0.431698
C	1.907189	2.811033	0.268867
H	2.260278	2.920750	-0.749363
B	2.302370	-1.206979	0.818839
H	1.707336	-1.332012	1.823470
B	2.170088	-2.342137	-0.561188
H	1.476388	-3.292070	-0.495564
B	2.226427	-1.368879	-2.033539
H	1.537694	-1.609855	-2.964165
B	2.421671	0.317651	-1.531925
H	1.940935	1.218976	-2.109224
B	3.706011	-2.158796	0.305459
H	4.118228	-3.031604	0.995022
B	3.678581	-2.242691	-1.480640
H	4.071723	-3.192133	-2.074605
B	3.822433	-0.584792	-2.102935
H	4.314246	-0.313610	-3.147932
B	3.986208	0.506247	-0.717165
H	4.499789	1.571045	-0.738529
B	3.914164	-0.458081	0.766286
H	4.379353	-0.071868	1.782754
B	4.754543	-1.093997	-0.666906
H	5.937114	-1.194172	-0.676742
C	-0.671062	-2.481449	0.999411
H	0.351745	-2.803196	1.076679
C	-1.622515	-3.219189	1.702627
H	-1.296930	-4.072081	2.290112

Table S33 Cartesian coordinates of **4CB** at Ψ = 90° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	2.532939	0.443799	0.149998
C	1.451158	-0.823062	-0.626263
C	-2.774289	-2.222237	2.387550
H	-3.461858	-2.588070	3.144580
C	-3.242317	-1.347478	1.396874
C	-4.624045	-0.950226	1.353254
H	-5.281254	-1.311512	2.139241
C	-5.109897	-0.161682	0.357512
H	-6.158592	0.120548	0.334998
C	-4.250837	0.294512	-0.698036
C	-4.727197	1.058594	-1.776484
H	-5.779499	1.326929	-1.806350
C	-3.875154	1.462356	-2.803878
H	-4.266264	2.047492	-3.630295
C	-2.525665	1.118955	-2.774828
H	-1.861109	1.436702	-3.573030
C	-2.007611	0.366152	-1.707240
C	-0.619389	0.043708	-1.623962
H	0.005267	0.413318	-2.425557
C	-0.054432	-0.645178	-0.579499
C	-0.945214	-1.225325	0.434952
C	-2.339742	-0.863898	0.395126
C	-2.867047	-0.058740	-0.657930
C	1.904669	1.614309	0.855522
C	1.595492	1.549412	2.223619
H	1.784765	0.641861	2.782688
C	1.052723	2.651505	2.881953
H	0.820745	2.579476	3.939826
C	0.812510	3.838393	2.188630
H	0.388815	4.695555	2.702687
C	1.128277	3.918171	0.831848
H	0.955853	4.838648	0.283098
C	1.670813	2.817795	0.170575
H	1.921649	2.904018	-0.879297
B	2.373629	-1.115409	0.819603
H	1.833637	-1.221576	1.853301
B	2.254344	-2.312118	-0.503506
H	1.585295	-3.275601	-0.359884
B	2.247544	-1.388299	-2.018617
H	1.561556	-1.692891	-2.932187
B	2.361648	0.328177	-1.560055
H	1.804226	1.186900	-2.135240
B	3.805437	-2.027178	0.312354
H	4.271604	-2.856597	1.020976
B	3.744331	-2.174213	-1.465544
H	4.172785	-3.119203	-2.042005
B	3.794212	-0.525488	-2.144239
H	4.252325	-0.268048	-3.207966
B	3.939324	0.616113	-0.796157
H	4.399336	1.703262	-0.869277
B	3.950549	-0.305397	0.713319
H	4.416966	0.125761	1.711035
B	4.782995	-0.948050	-0.719473
H	5.968415	-0.995771	-0.754401
C	-0.558935	-2.158543	1.413923
H	0.444985	-2.545362	1.433421
C	-1.451940	-2.642501	2.369566
H	-1.098923	-3.359293	3.104527

Table S34 Cartesian coordinates of **4CB** at Ψ = 112.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.592047	0.023185	0.247857
C	-1.316703	-0.977043	-0.432240
C	2.578030	2.470019	-1.978719
H	3.195255	3.237090	-2.437254
C	3.189292	1.424082	-1.273230
C	4.619745	1.368841	-1.132915
H	5.206793	2.143506	-1.618261
C	5.231025	0.392306	-0.410664
H	6.312319	0.370215	-0.309815
C	4.456543	-0.621837	0.245461
C	5.045426	-1.624839	1.033347
H	6.126073	-1.639606	1.144026
C	4.265412	-2.587777	1.672735
H	4.741519	-3.352226	2.278768
C	2.879398	-2.574614	1.536203
H	2.272092	-3.327773	2.029772
C	2.253188	-1.590940	0.751750
C	0.839065	-1.578771	0.559897
H	0.295120	-2.377735	1.043041
C	0.168829	-0.662633	-0.213405
C	0.945343	0.433294	-0.810464
C	2.381455	0.407996	-0.666486
C	3.035180	-0.601109	0.099936
C	-2.228833	1.329703	0.909702
C	-2.596418	2.540890	0.300742
H	-3.121177	2.534697	-0.647316
C	-2.299212	3.760068	0.906271
H	-2.595565	4.683913	0.419656
C	-1.625129	3.792349	2.127907
H	-1.391922	4.742199	2.598845
C	-1.255180	2.595031	2.740030
H	-0.732278	2.605921	3.691118
C	-1.556260	1.372506	2.139654
H	-1.265250	0.456635	2.637005
B	-2.404292	-0.104377	-1.468368
H	-2.067597	0.819934	-2.099546
B	-1.937227	-1.768710	-1.838490
H	-1.173211	-1.962717	-2.720227
B	-1.815264	-2.629421	-0.300939
H	-0.988510	-3.454586	-0.141871
B	-2.176481	-1.467319	0.998854
H	-1.597231	-1.461066	2.021932
B	-3.627798	-1.244264	-2.015441
H	-4.111373	-1.107079	-3.090004
B	-3.269946	-2.819782	-1.279840
H	-3.485341	-3.850139	-1.828186
B	-3.398233	-2.638303	0.491575
H	-3.700544	-3.524349	1.220340
B	-3.870192	-0.967170	0.837792
H	-4.431472	-0.581776	1.804890
B	-4.007670	-0.111867	-0.703114
H	-4.682421	0.851954	-0.810916
B	-4.541467	-1.795869	-0.585100
H	-5.696107	-2.065436	-0.636884
C	0.400827	1.539834	-1.482815
H	-0.663763	1.661281	-1.545473
C	1.194898	2.531490	-2.057315
H	0.714199	3.360365	-2.567721

Table S35 Cartesian coordinates of **4CB** at Ψ = 135° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.570764	-0.027321	0.163160
C	-1.266810	-1.104780	-0.253874
C	2.370417	2.710058	-1.607585
H	2.922919	3.562450	-1.992043
C	3.067838	1.638474	-1.033930
C	4.503177	1.664180	-0.943534
H	5.019797	2.531823	-1.344242
C	5.203811	0.647335	-0.375005
H	6.287610	0.685359	-0.313467
C	4.521829	-0.496266	0.159027
C	5.205964	-1.562016	0.766756
H	6.289498	-1.520872	0.833890
C	4.516165	-2.659557	1.280620
H	5.065060	-3.471901	1.746670
C	3.127267	-2.718852	1.197539
H	2.589496	-3.574969	1.594451
C	2.407463	-1.672143	0.596342
C	0.986085	-1.717796	0.478777
H	0.513378	-2.602311	0.877971
C	0.217659	-0.732320	-0.088165
C	0.905505	0.459979	-0.611552
C	2.346781	0.508870	-0.524499
C	3.096166	-0.548154	0.071367
C	-2.293058	1.353471	0.716659
C	-2.865630	2.477987	0.100355
H	-3.477860	2.360955	-0.785003
C	-2.650641	3.755995	0.613136
H	-3.105523	4.610193	0.121578
C	-1.856505	3.936072	1.746258
H	-1.688155	4.931786	2.144386
C	-1.279992	2.825487	2.362045
H	-0.657337	2.949846	3.242342
C	-1.497701	1.544448	1.855661
H	-1.034930	0.700504	2.349967
B	-2.255820	-0.403156	-1.504227
H	-1.820315	0.411611	-2.224937
B	-1.785603	-2.106270	-1.574143
H	-0.952668	-2.427367	-2.349620
B	-1.790956	-2.728959	0.079854
H	-1.016856	-3.543259	0.430720
B	-2.223129	-1.394703	1.165529
H	-1.715378	-1.235466	2.214972
B	-3.449587	-1.616596	-1.960513
H	-3.852322	-1.642399	-3.076043
B	-3.164190	-3.063316	-0.973878
H	-3.344097	-4.164740	-1.377717
B	-3.423732	-2.623607	0.738175
H	-3.789298	-3.393526	1.563338
B	-3.898236	-0.921927	0.795497
H	-4.529172	-0.393221	1.644524
B	-3.911593	-0.305506	-0.864960
H	-4.582615	0.616933	-1.167550
B	-4.472290	-1.950233	-0.534192
H	-5.622989	-2.224087	-0.630427
C	0.275362	1.582222	-1.175815
H	-0.794751	1.635068	-1.228138
C	0.985575	2.677399	-1.664248
H	0.436400	3.512319	-2.088299

Table S36 Cartesian coordinates of **4CB** at Ψ = 157.5° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.544431	-0.115413	0.123689
C	-1.164921	-1.226862	-0.155053
C	2.179070	2.964485	-1.064537
H	2.649222	3.924079	-1.259223
C	2.955109	1.901491	-0.581653
C	4.369302	2.056473	-0.368510
H	4.803929	3.036742	-0.543271
C	5.153017	1.015769	0.021847
H	6.221111	1.149516	0.167522
C	4.587353	-0.287750	0.222874
C	5.369728	-1.405527	0.557139
H	6.440994	-1.278817	0.686249
C	4.792218	-2.665618	0.710233
H	5.416100	-3.517434	0.962600
C	3.420118	-2.837989	0.541680
H	2.971449	-3.819362	0.665621
C	2.601502	-1.741441	0.221762
C	1.184535	-1.878335	0.098557
H	0.795630	-2.870038	0.271832
C	0.325752	-0.836051	-0.147759
C	0.918674	0.461327	-0.499310
C	2.340694	0.632757	-0.325223
C	3.178591	-0.455793	0.053807
C	-2.409248	1.352804	0.466142
C	-2.968073	2.316564	-0.390112
H	-3.435857	2.013899	-1.318867
C	-2.920624	3.670351	-0.064591
H	-3.360530	4.396498	-0.740893
C	-2.313453	4.088746	1.120640
H	-2.276723	5.143520	1.374370
C	-1.755460	3.139345	1.976202
H	-1.279212	3.449283	2.900972
C	-1.805064	1.782976	1.655710
H	-1.363134	1.067698	2.336415
B	-2.203953	-0.739800	-1.459562
H	-1.783969	-0.023234	-2.292654
B	-1.675670	-2.428482	-1.273558
H	-0.848374	-2.835345	-2.013480
B	-1.630974	-2.767256	0.466822
H	-0.825089	-3.457407	0.977462
B	-2.098570	-1.285033	1.312435
H	-1.580960	-0.948472	2.314180
B	-3.356373	-2.068757	-1.705541
H	-3.768319	-2.294793	-2.794761
B	-2.999449	-3.328828	-0.500610
H	-3.137932	-4.487186	-0.718818
B	-3.258239	-2.622567	1.120591
H	-3.578224	-3.261957	2.067069
B	-3.806596	-0.962681	0.909421
H	-4.450166	-0.335084	1.677414
B	-3.867166	-0.624180	-0.830959
H	-4.580840	0.208166	-1.267090
B	-4.348533	-2.216377	-0.226866
H	-5.487770	-2.547574	-0.254595
C	0.220518	1.546100	-1.051741
H	-0.819873	1.449570	-1.294108
C	0.830674	2.769130	-1.325237
H	0.232666	3.572315	-1.744148

Table S37 Cartesian coordinates of **4CB** at Ψ = 180° in THF from B3LYP calculations (in Å).

Atom	x	y	z
C	-2.769478	-0.358912	0.002366
C	-0.802983	-1.352305	-0.002709
C	1.918803	3.303228	-0.005241
H	2.250937	4.337489	-0.002892
C	2.872769	2.274326	0.000937
C	4.281676	2.564056	0.008645
H	4.586412	3.606865	0.011723
C	5.215255	1.574238	0.011268
H	6.275007	1.813202	0.016616
C	4.821117	0.193726	0.006023
C	5.752373	-0.857718	0.005875
H	6.813135	-0.623142	0.010426
C	5.331089	-2.187270	-0.000417
H	6.067090	-2.985368	-0.000580
C	3.973108	-2.499026	-0.006400
H	3.648822	-3.535701	-0.010987
C	3.009187	-1.476211	-0.006148
C	1.608920	-1.766085	-0.009567
H	1.342270	-2.814329	-0.010662
C	0.627220	-0.804501	-0.007427
C	1.036836	0.594285	-0.008597
C	2.441331	0.909354	-0.001895
C	3.426906	-0.118412	-0.000091
C	-3.033221	1.105077	0.002938
C	-3.218082	1.795811	-1.208495
H	-3.096364	1.275040	-2.151119
C	-3.557607	3.146061	-1.205070
H	-3.698831	3.665656	-2.147284
C	-3.717713	3.827287	0.004290
H	-3.981116	4.880354	0.004821
C	-3.540011	3.149192	1.212954
H	-3.667444	3.671298	2.155746
C	-3.200554	1.798917	1.215049
H	-3.065381	1.280619	2.157170
B	-1.934193	-1.150570	-1.313244
H	-1.601707	-0.512783	-2.250205
B	-1.112975	-2.700278	-0.900098
H	-0.244402	-3.071498	-1.609628
B	-1.107337	-2.699435	0.897823
H	-0.234338	-3.070074	1.602190
B	-1.925368	-1.148712	1.313759
H	-1.586776	-0.510289	2.248045
B	-2.786653	-2.772692	-1.428097
H	-3.047923	-3.272424	-2.471714
B	-2.283450	-3.709666	0.003143
H	-2.161249	-4.890598	0.003513
B	-2.777463	-2.770905	1.436458
H	-3.032152	-3.269184	2.482390
B	-3.683506	-1.362753	0.911233
H	-4.497864	-0.845199	1.595013
B	-3.689505	-1.364116	-0.898977
H	-4.508618	-0.847886	-1.578034
B	-3.834204	-2.906445	0.007749
H	-4.872683	-3.481561	0.011490
C	0.138089	1.667538	-0.018431
H	-0.917463	1.474739	-0.030938
C	0.565026	2.994844	-0.016481
H	-0.176420	3.787624	-0.024103