Supporting Information

Crucial factor regulating intramolecular charge-transfer-based radiative efficiency in *ortho*-carboranyl luminophores : Planarity between substituted biphenyl rings

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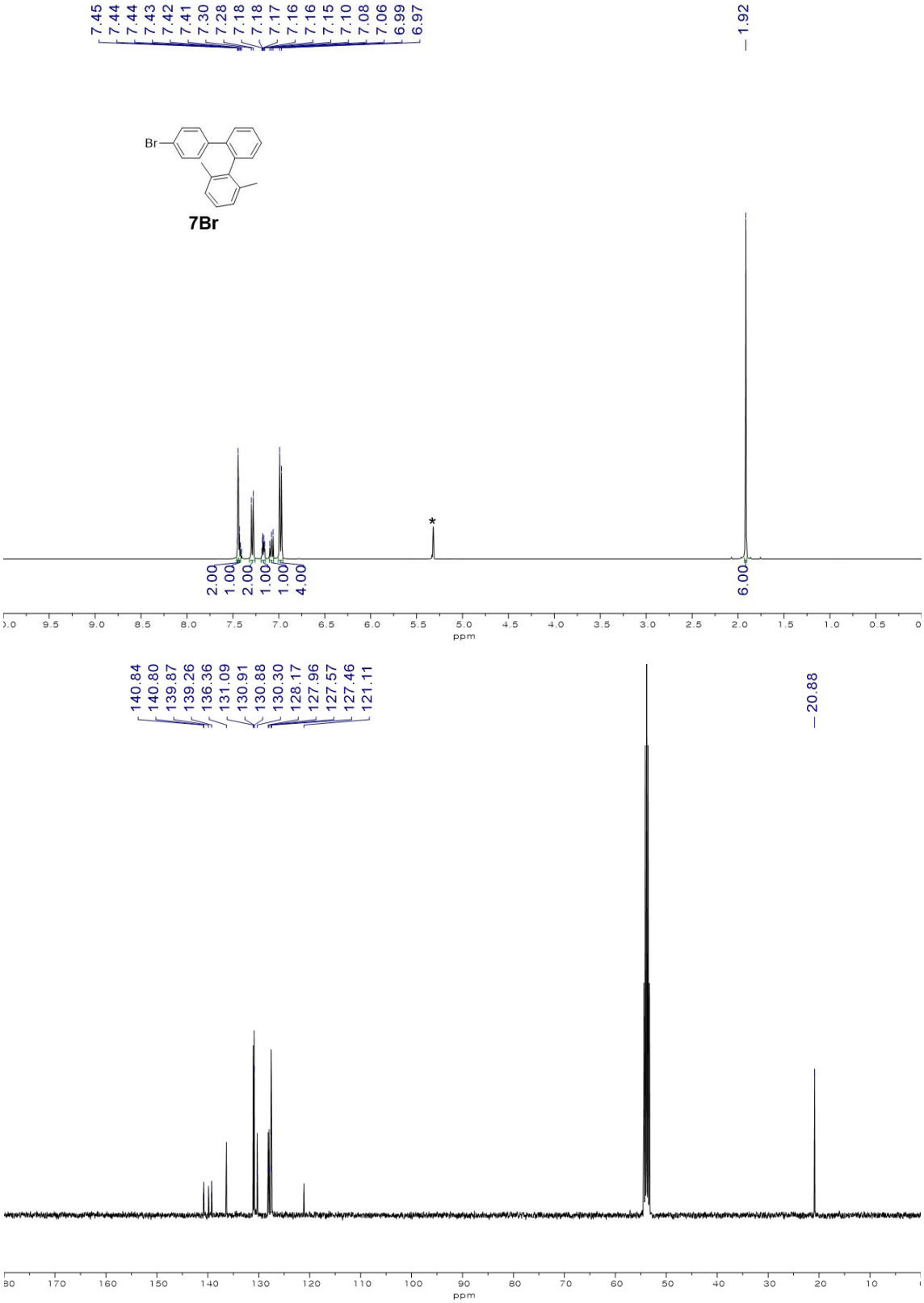


Figure S1. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **7Br** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

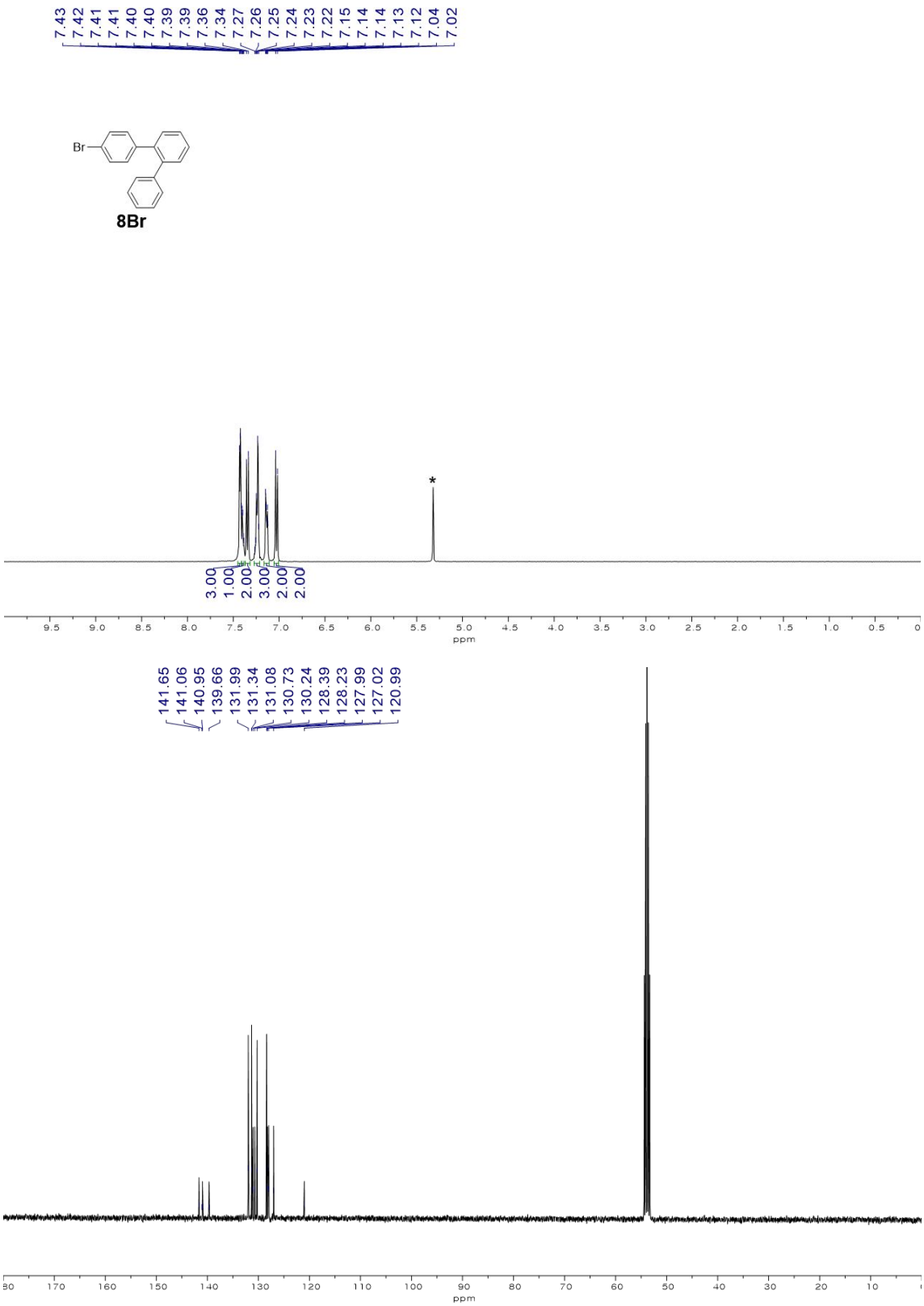


Figure S2. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **8Br** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

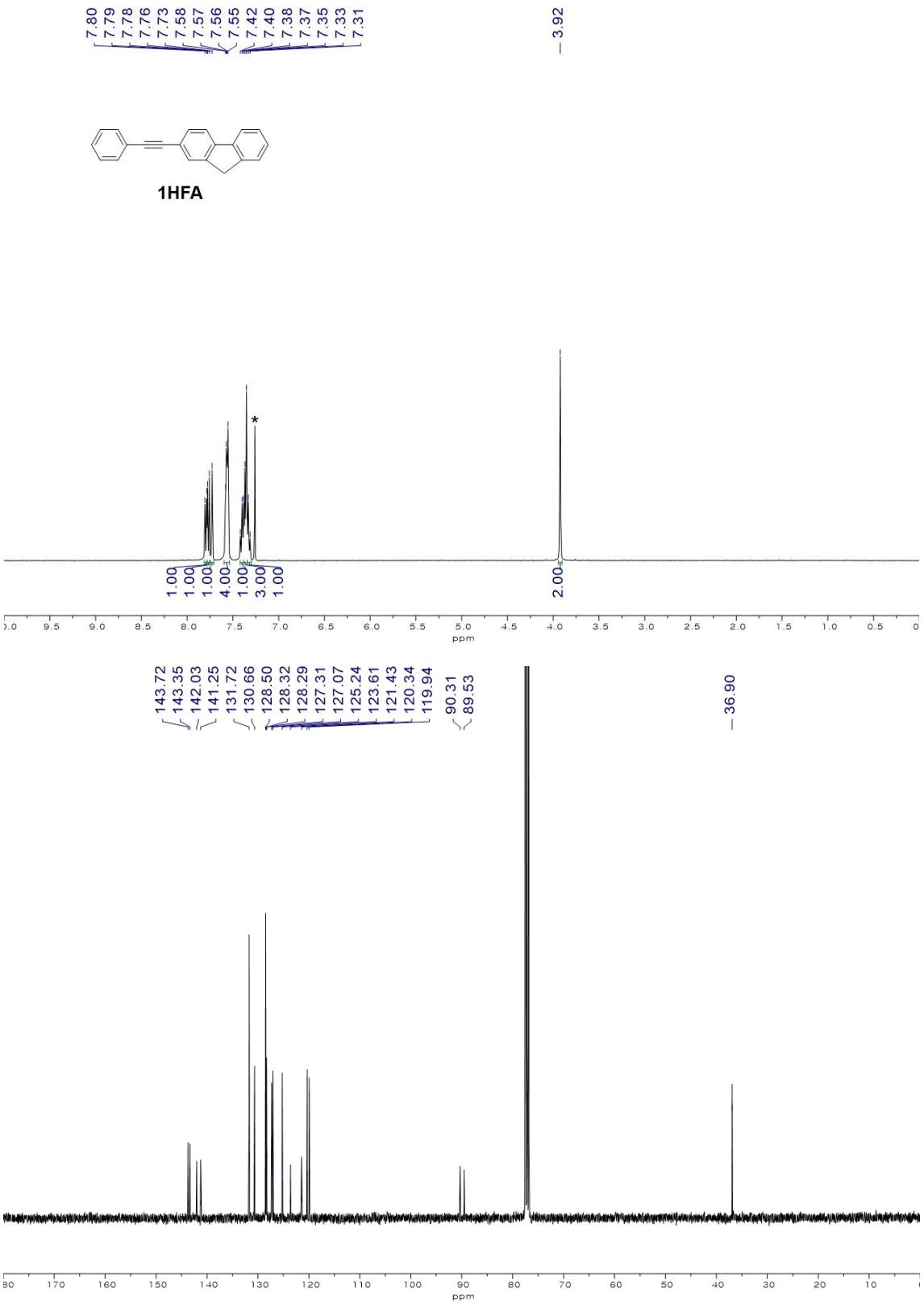


Figure S3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1HFA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

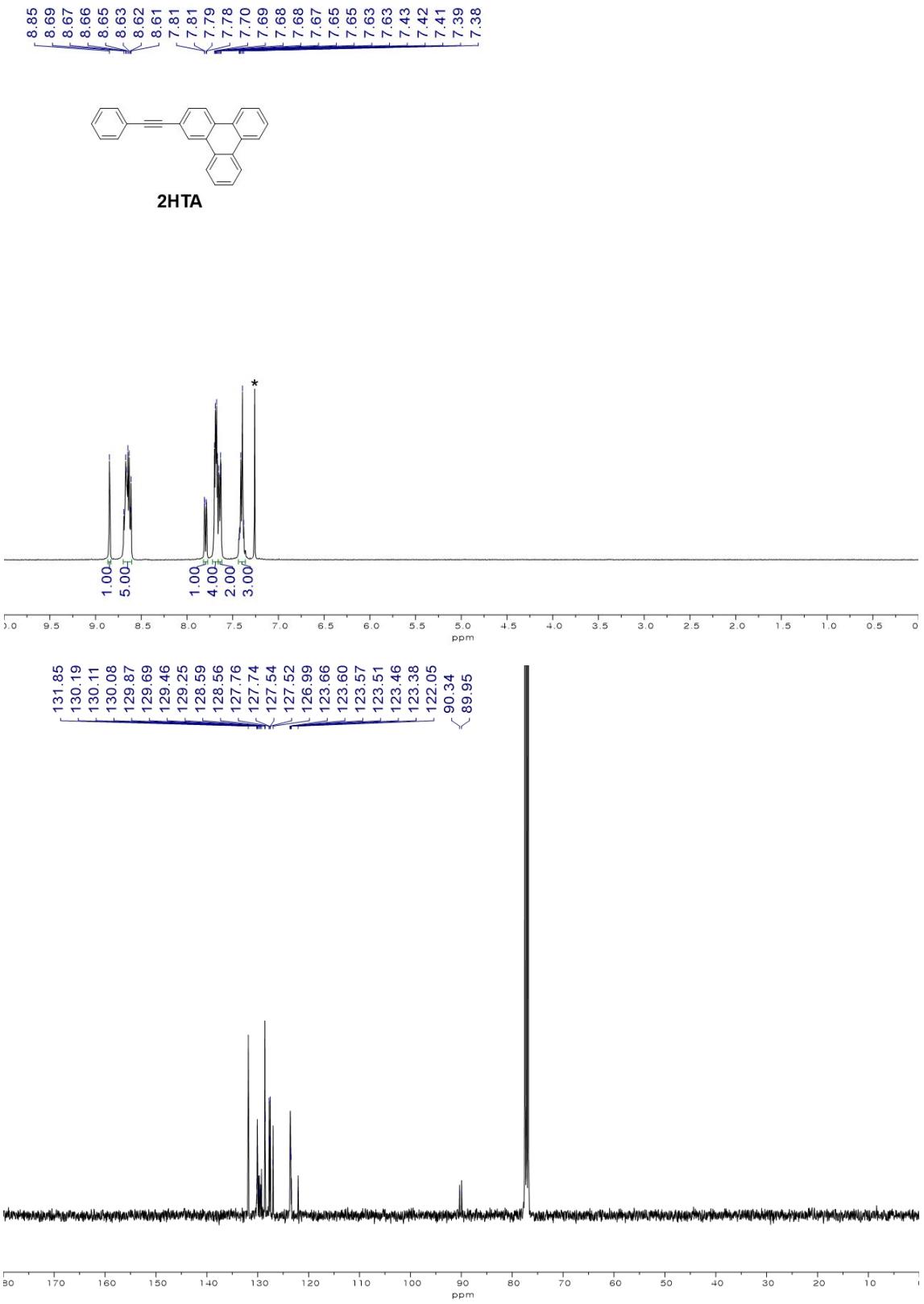


Figure S4. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2HTA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

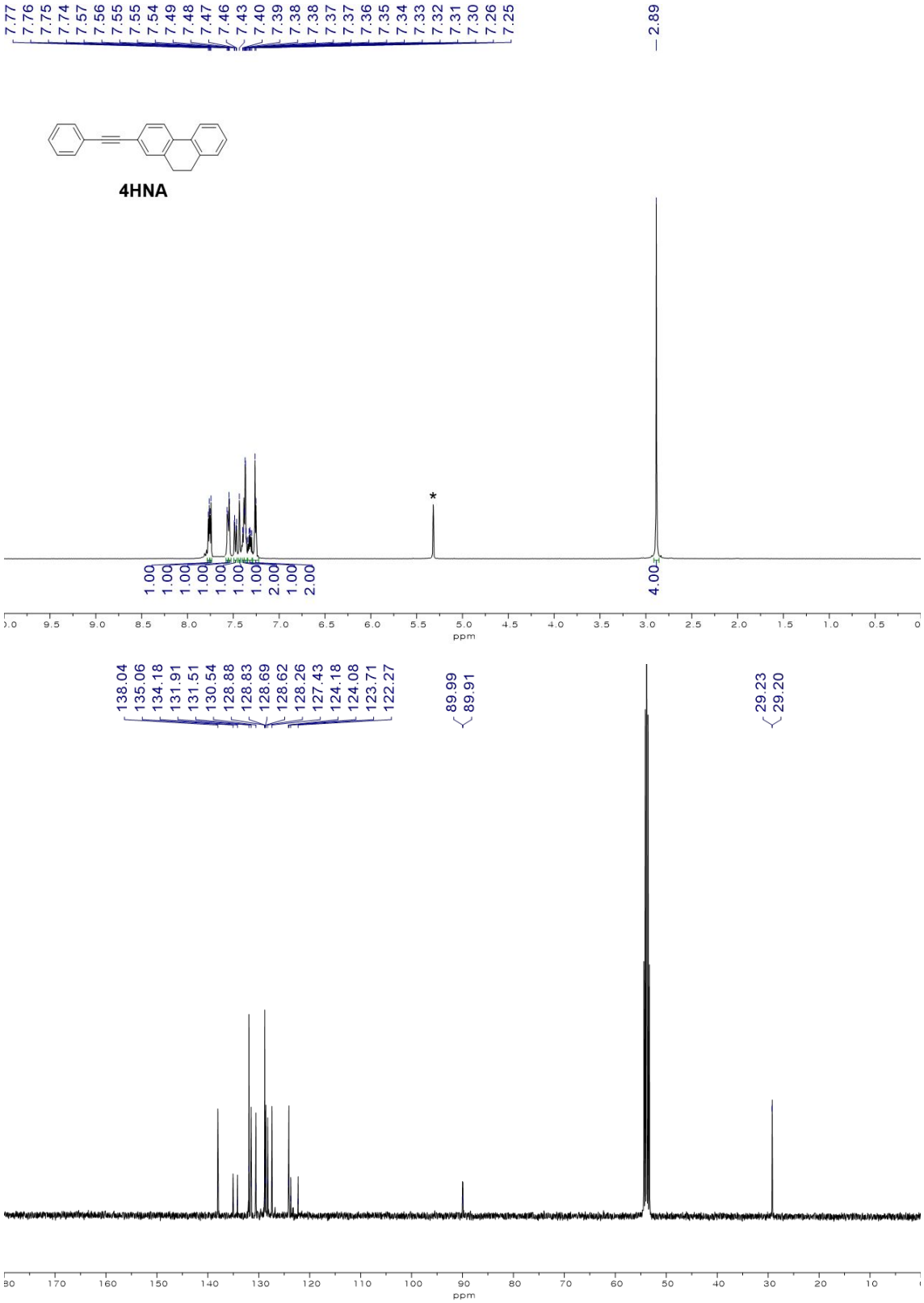


Figure S5. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4HNA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

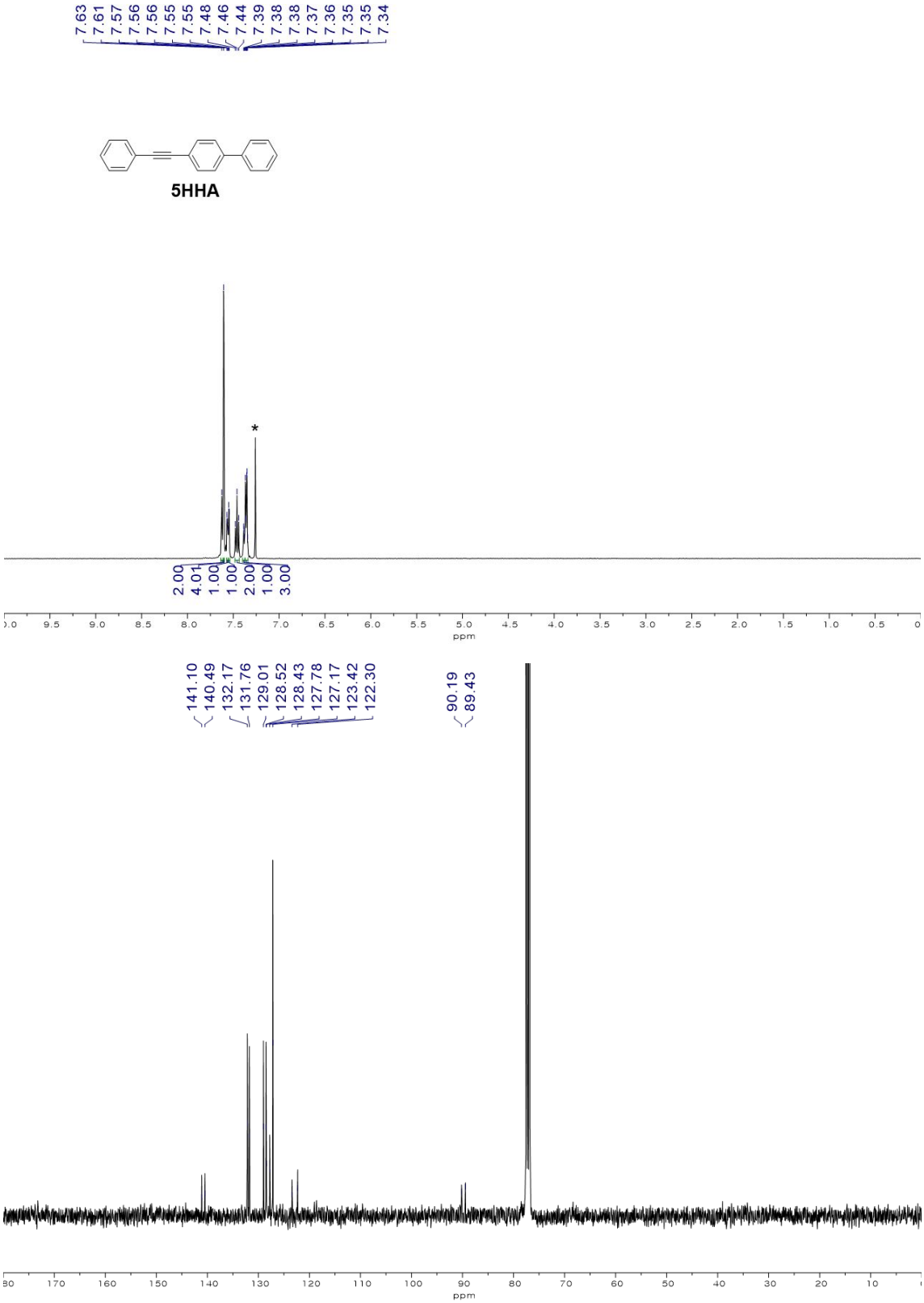


Figure S6. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **5HHA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

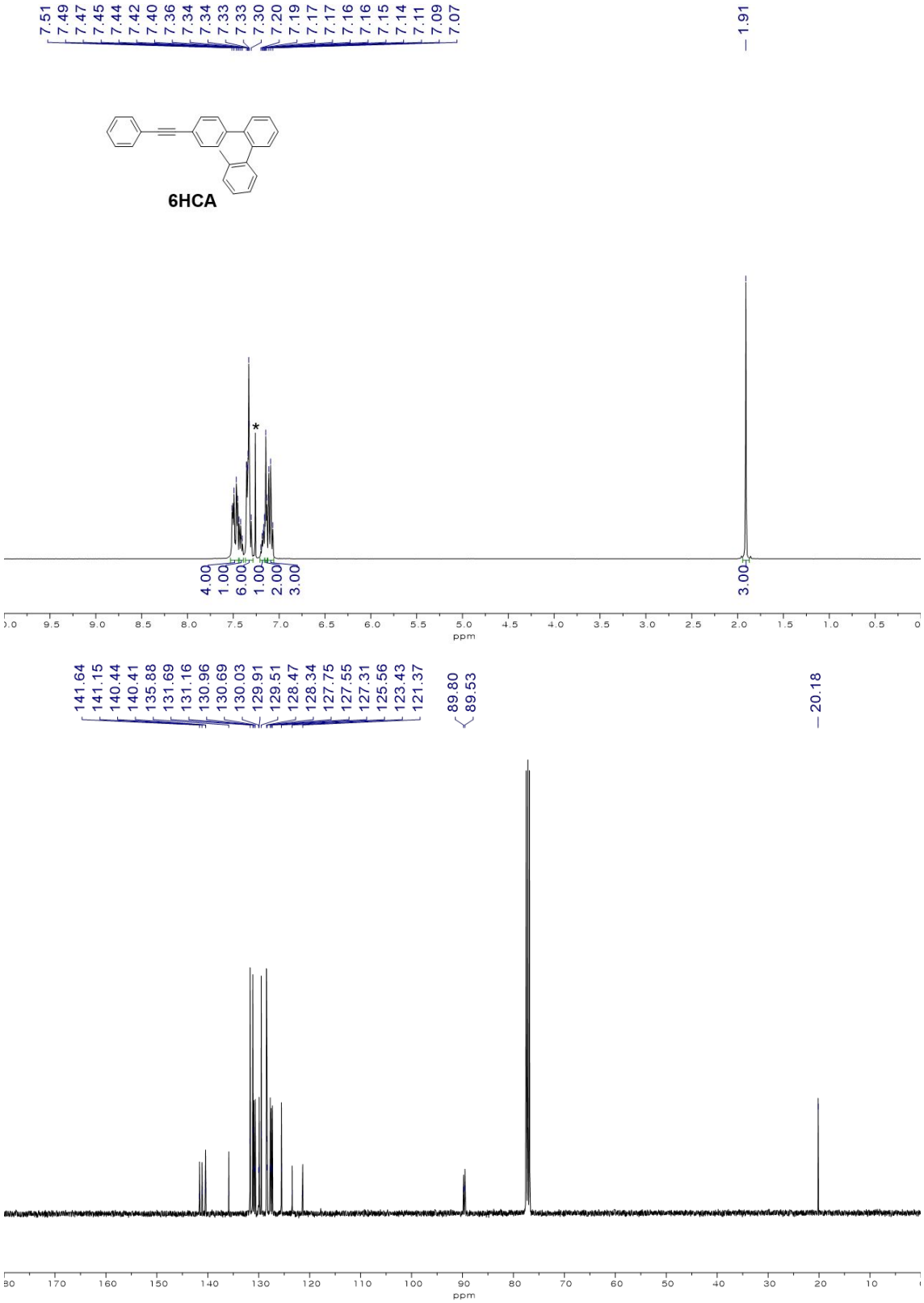


Figure S7. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **6HCA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

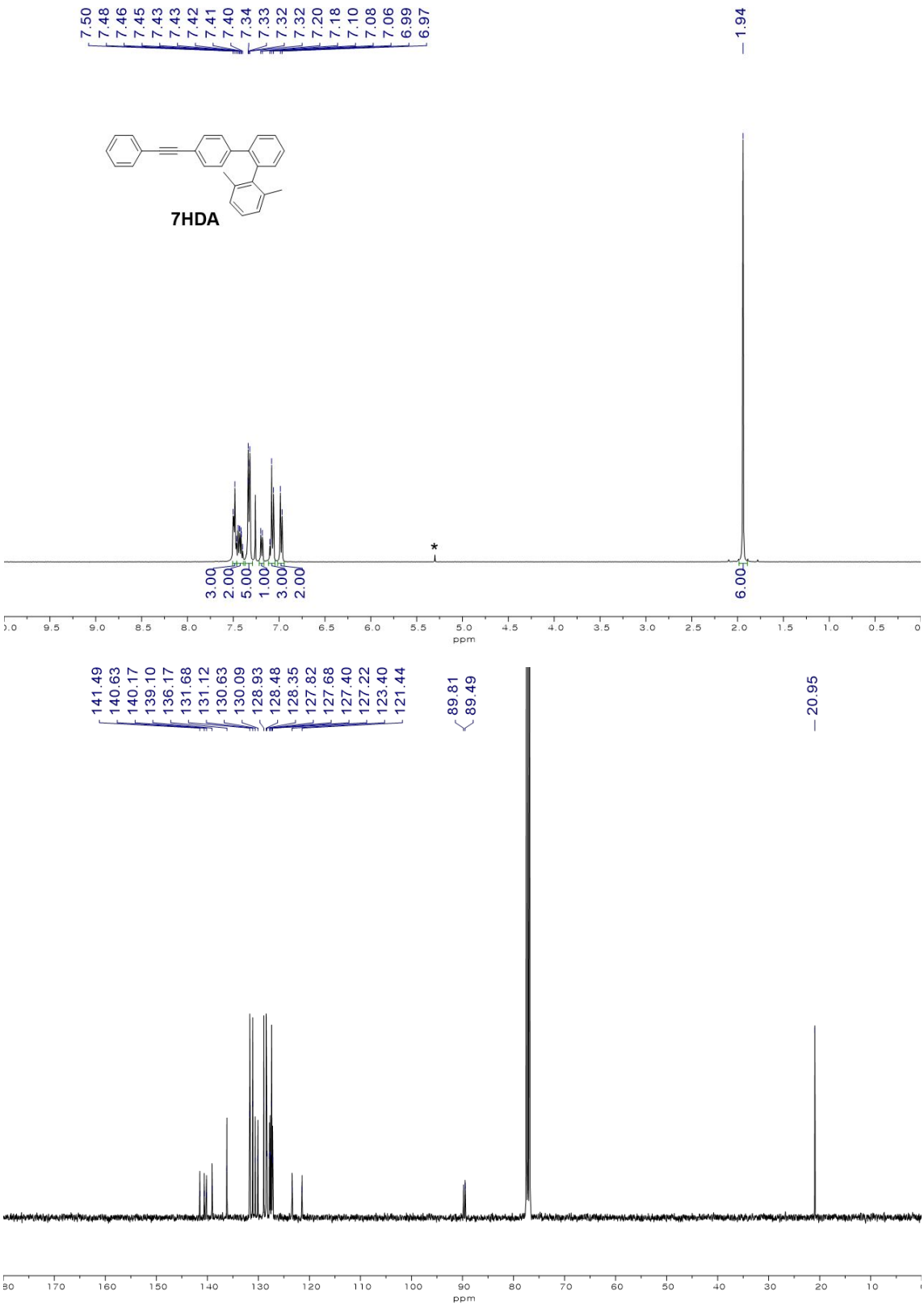


Figure S8. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **7HDA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

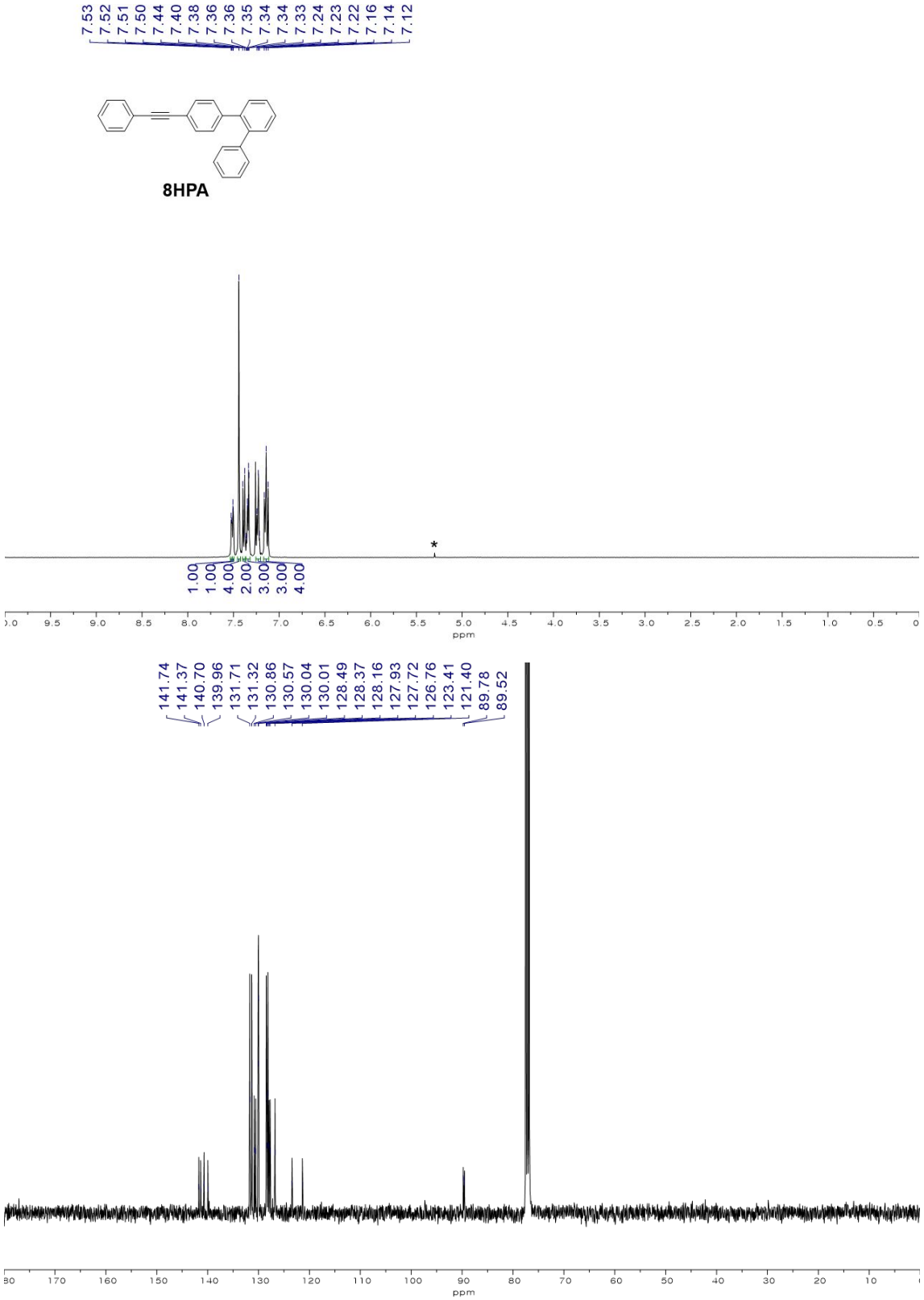


Figure S9. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **8HPA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

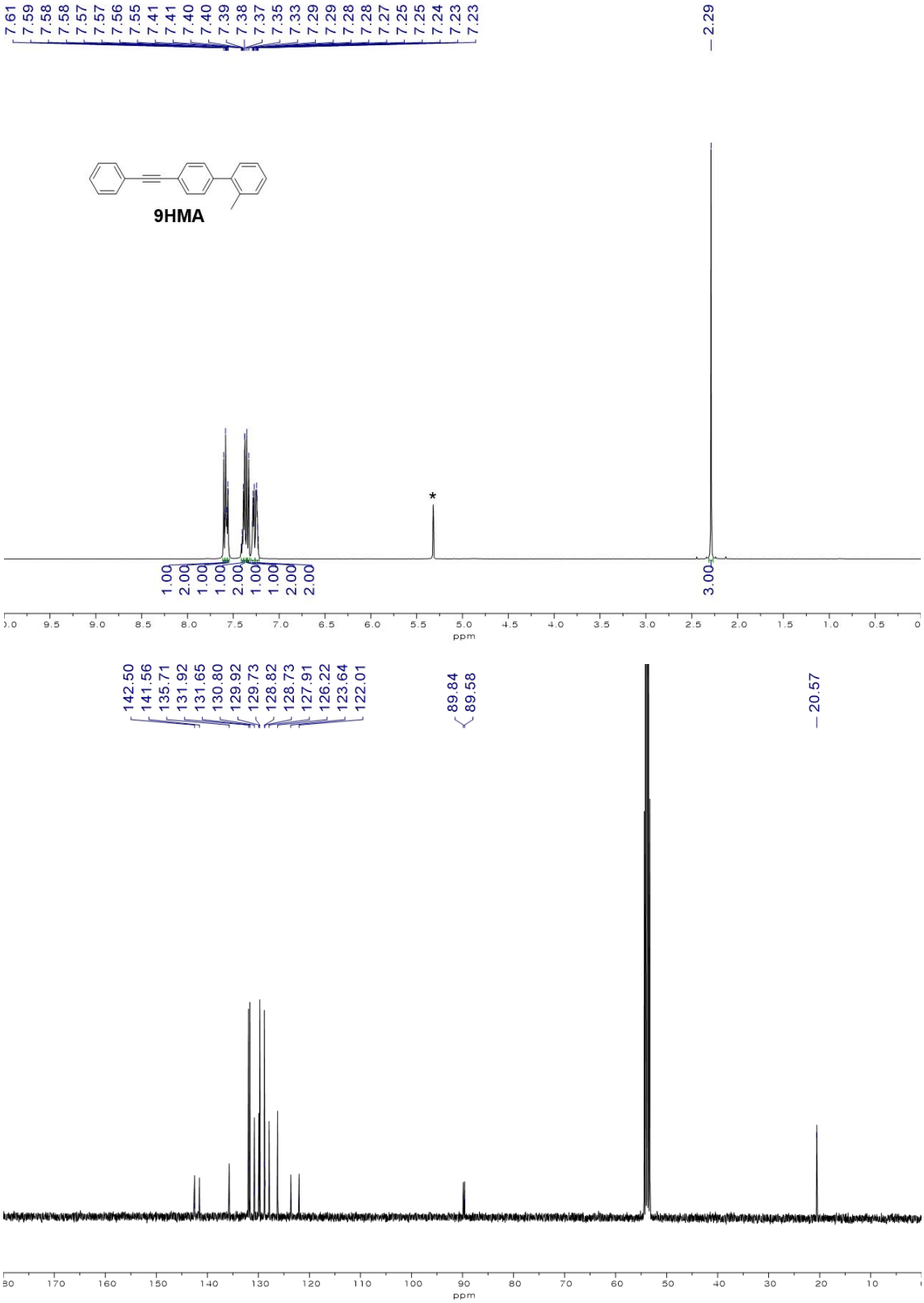


Figure S10. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **9HMA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

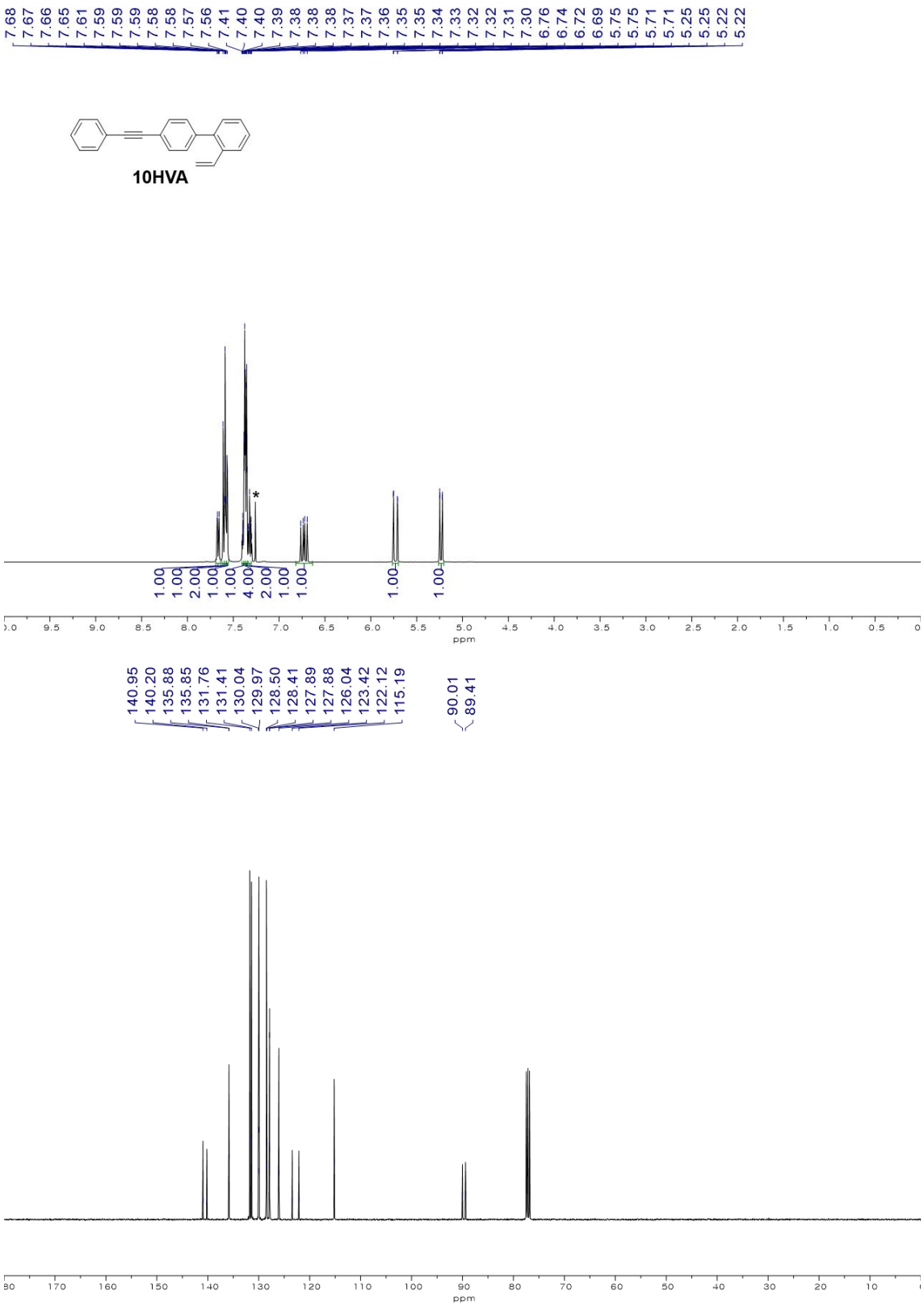


Figure S11. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **10HVA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

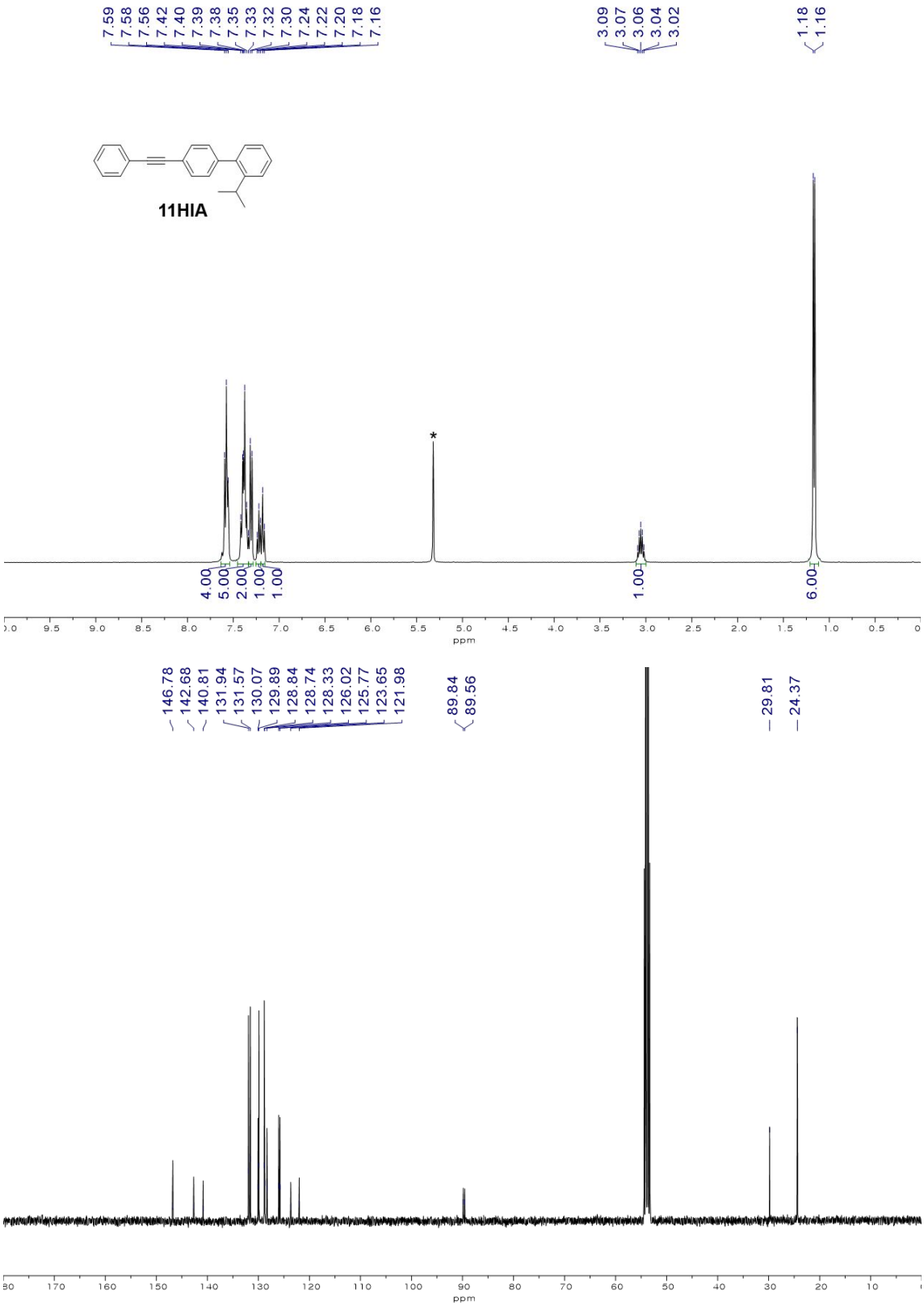


Figure S12. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **11HIA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

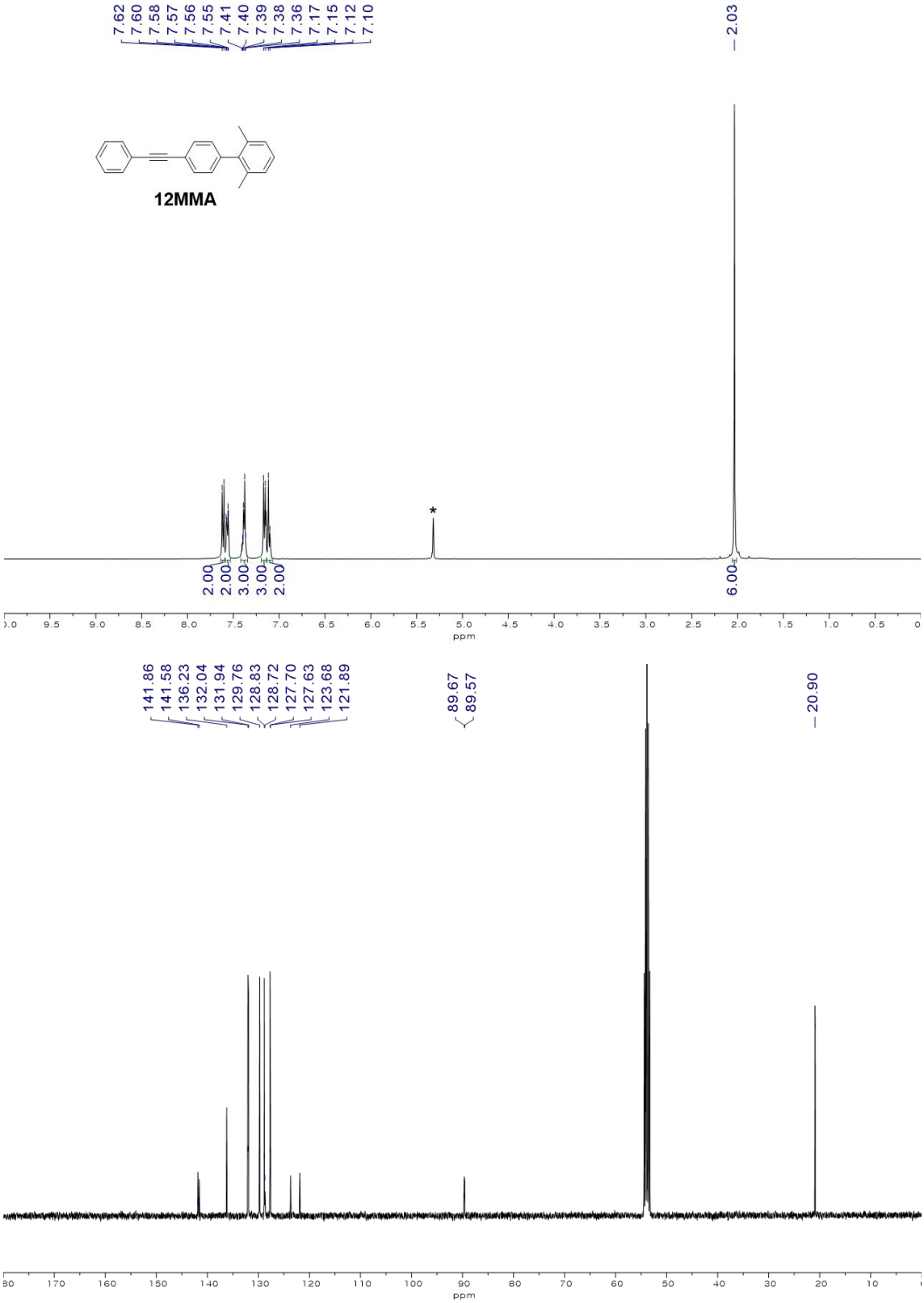


Figure S13. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **12MMA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

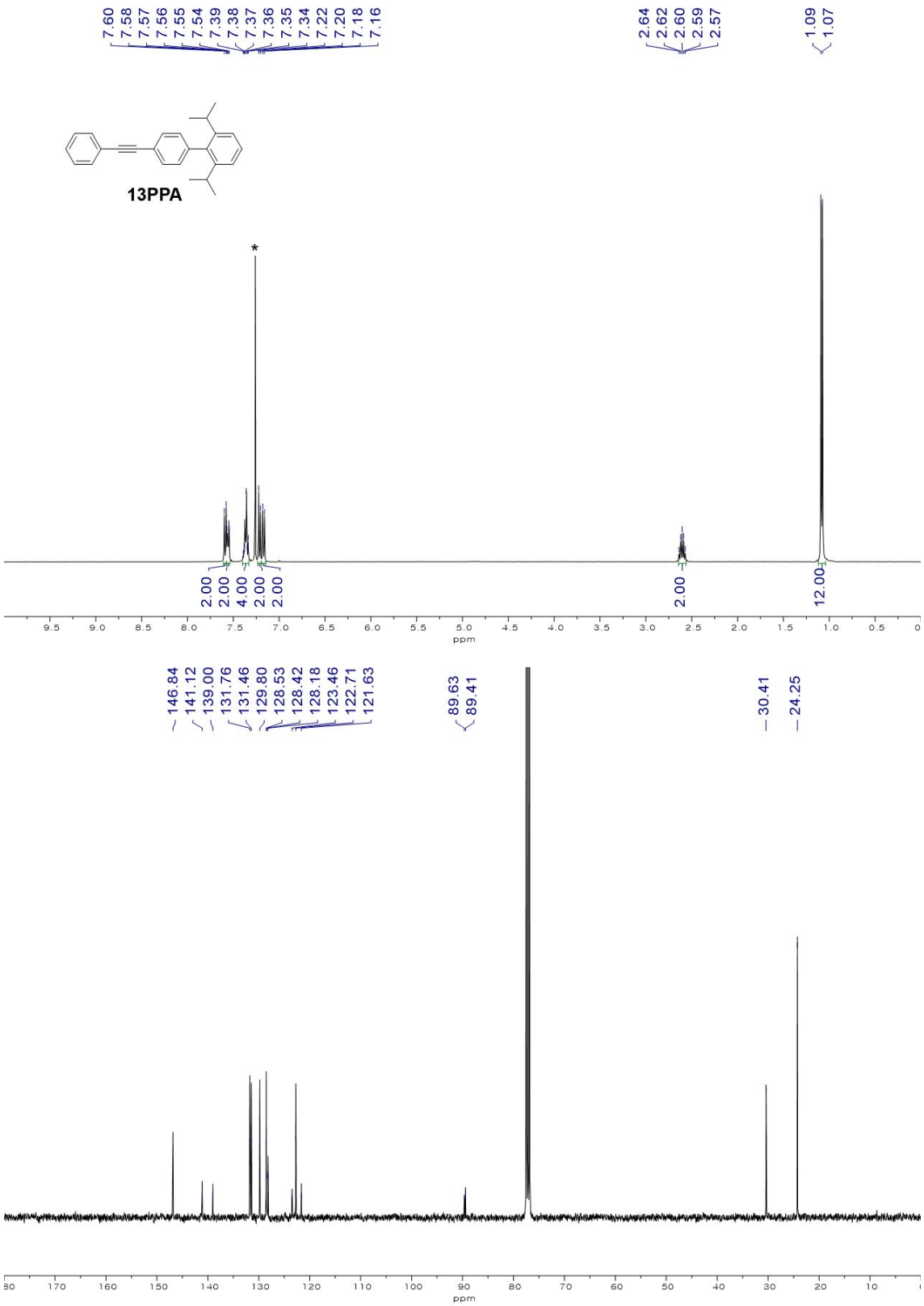


Figure S14. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **13PPA** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

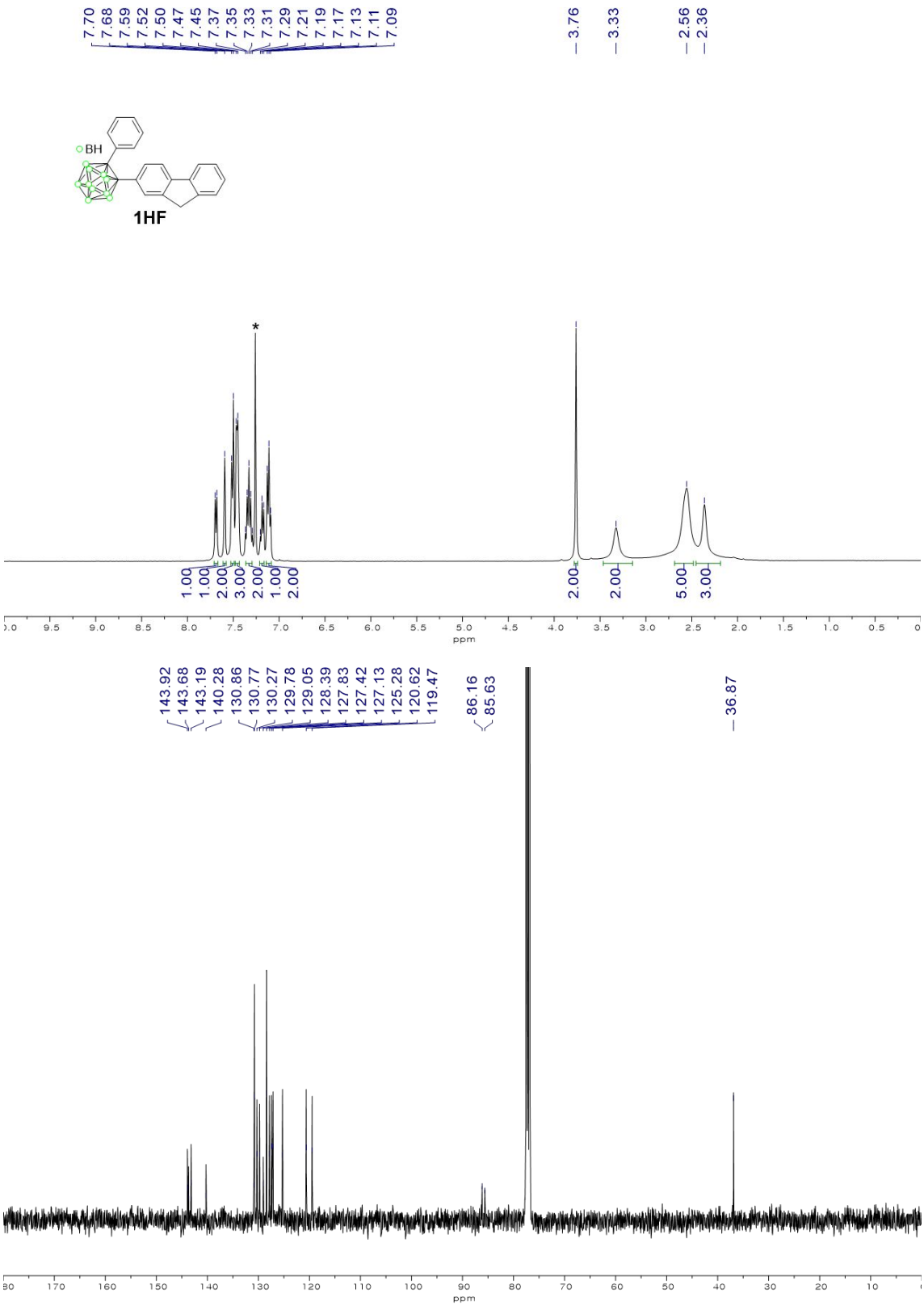


Figure S15. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **1HF** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

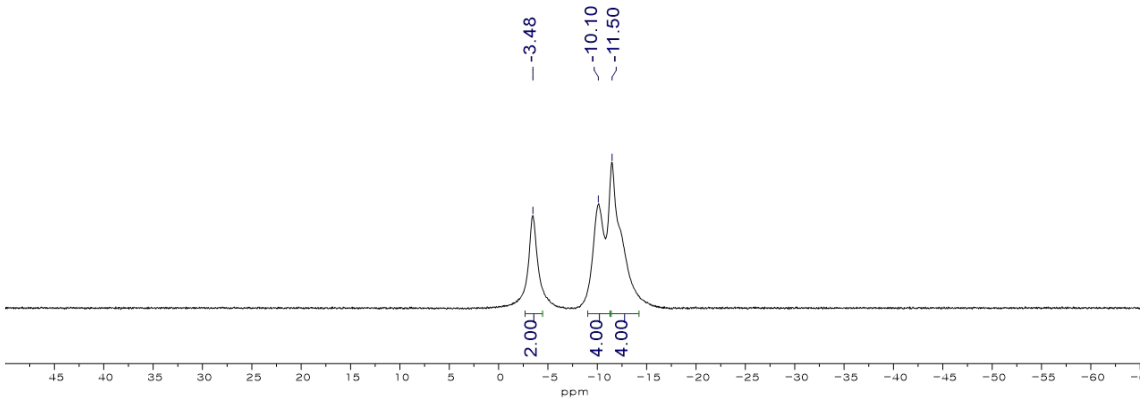


Figure S16. $^{11}B\{^{1}H\}$ NMR spectra of **1HF** in $CDCl_3$.

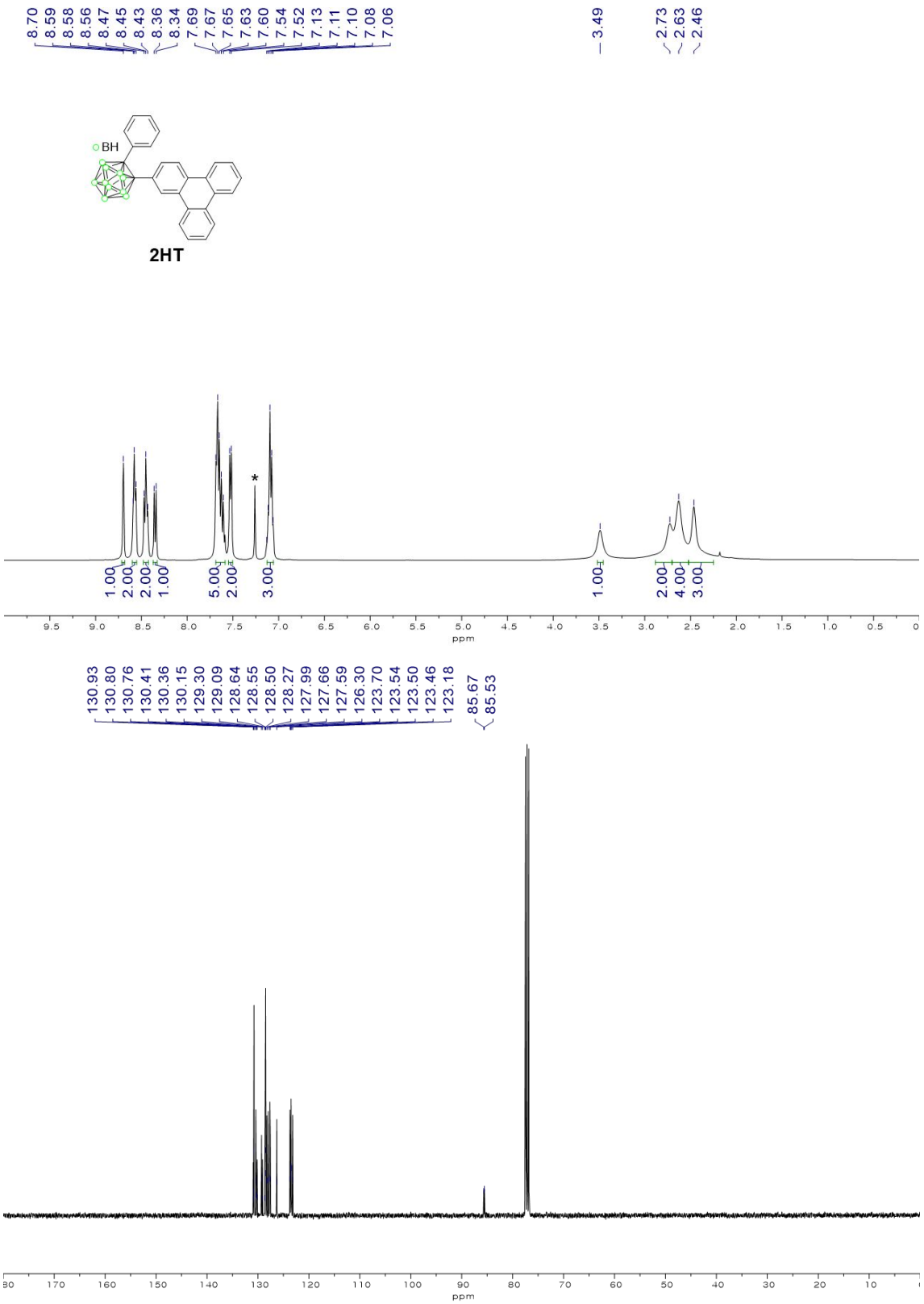


Figure S17. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **2HT** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

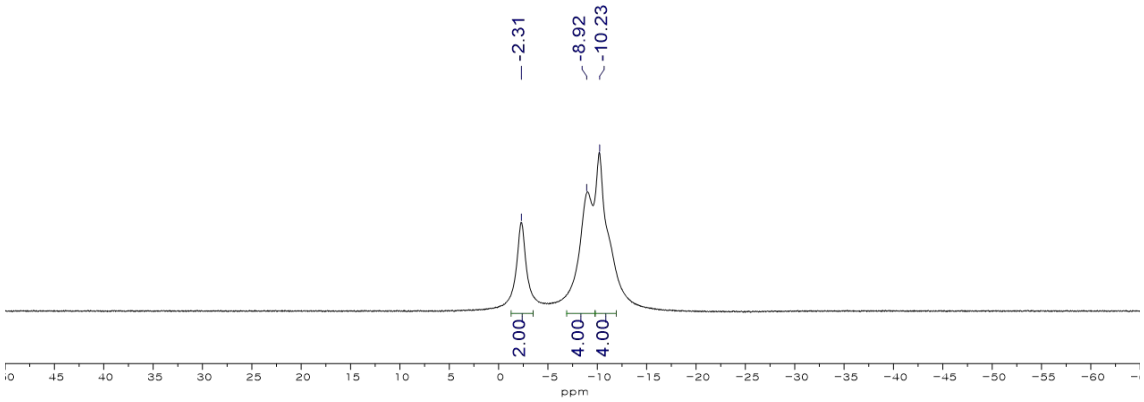


Figure S18. $^{11}B\{^{1}H\}$ NMR spectra of **2HT** in $CDCl_3$.

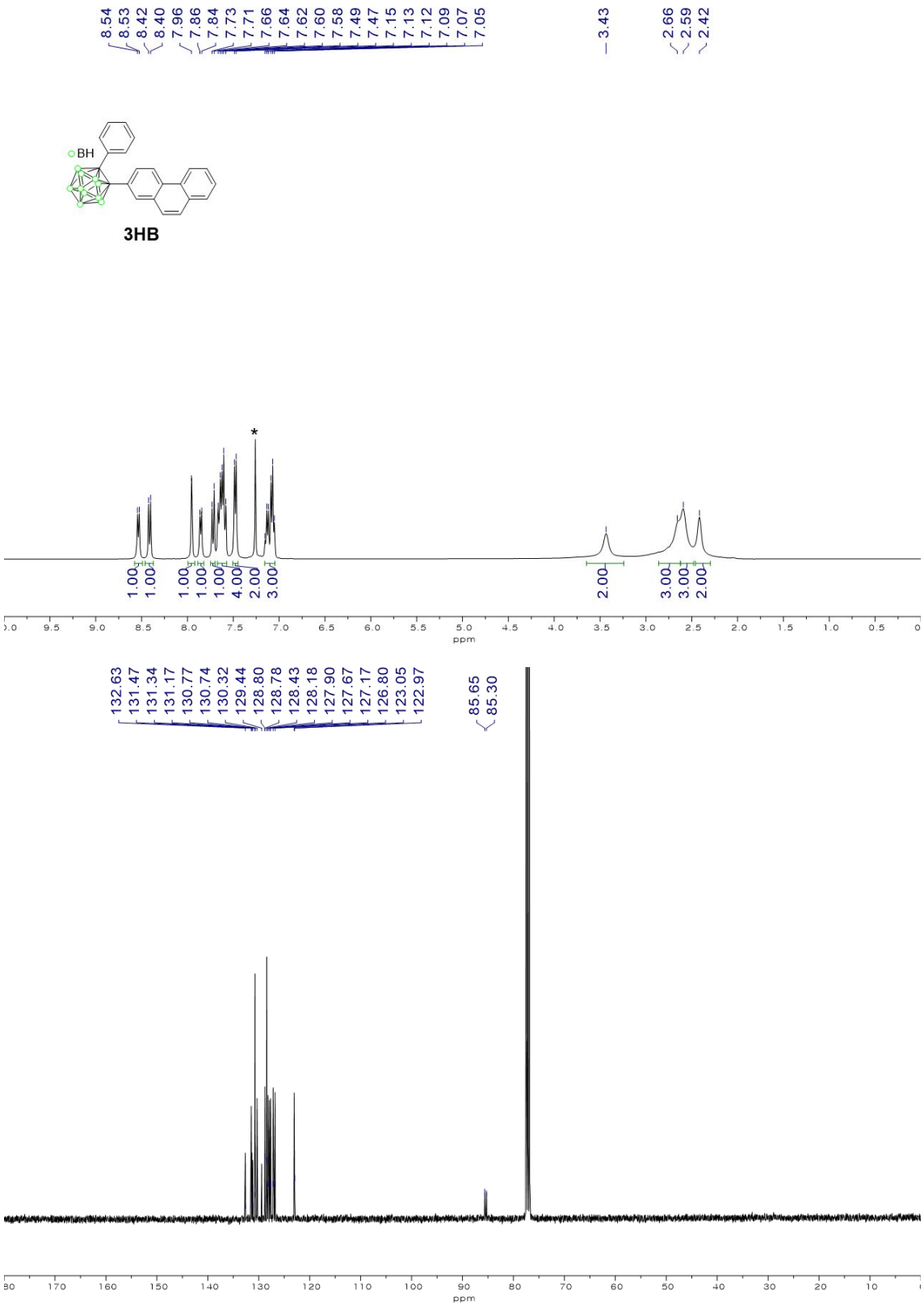


Figure S19. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **3HB** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

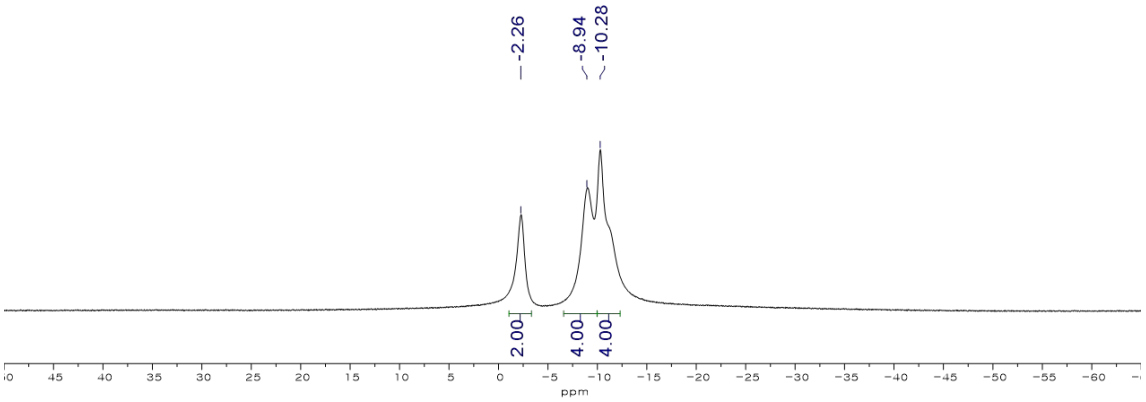


Figure S20. $^{11}B\{^{1}H\}$ NMR spectra of **3HB** in $CDCl_3$.

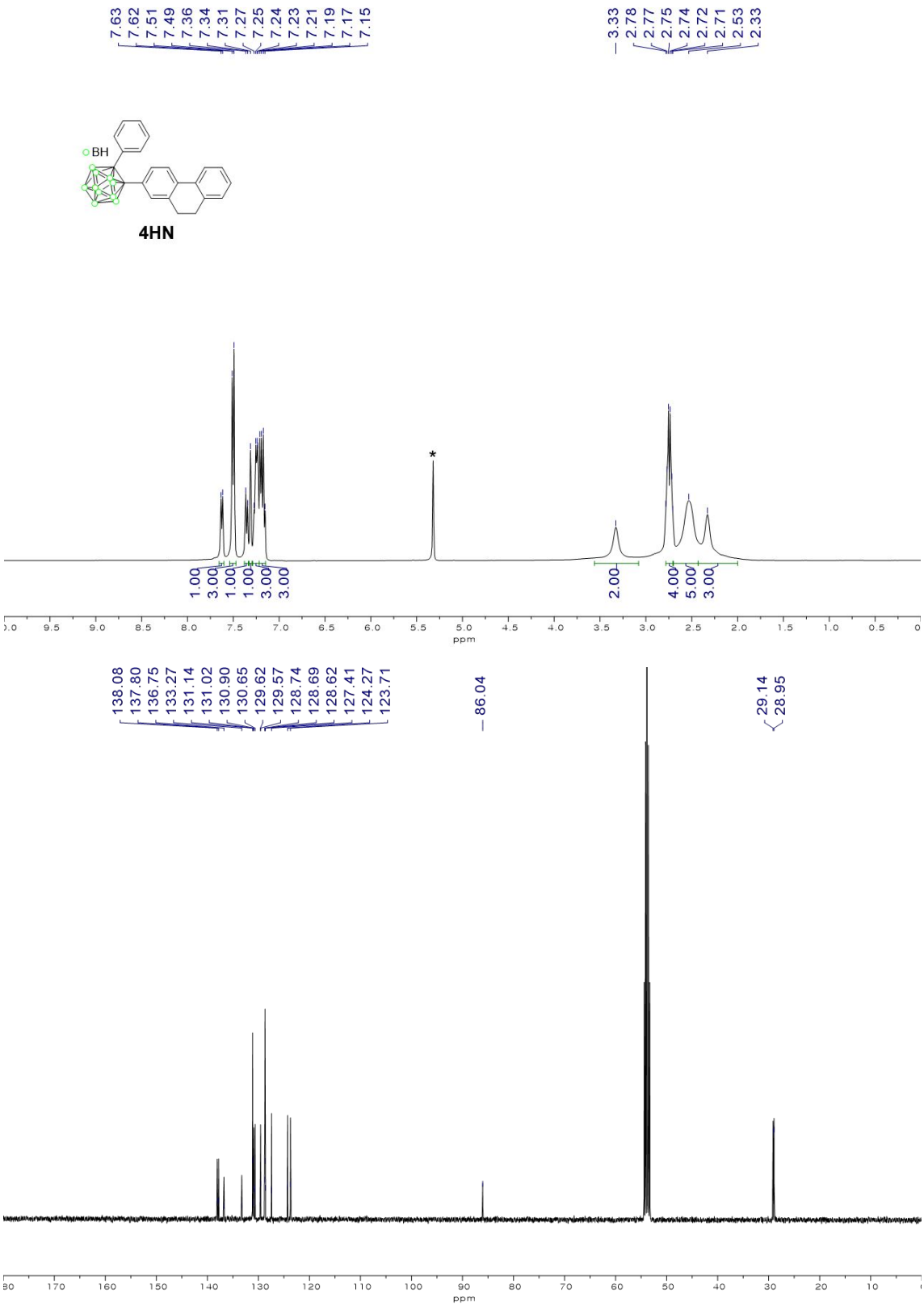


Figure S21. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **4HN** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

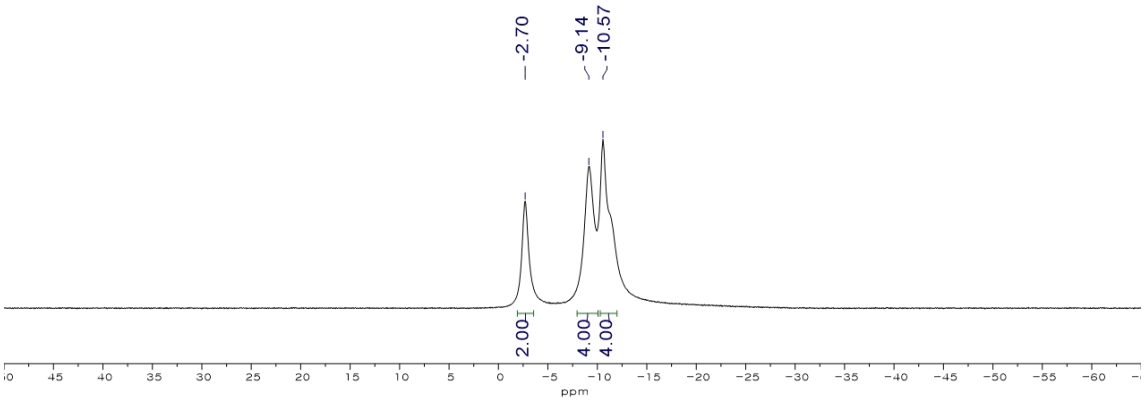


Figure S22. $^{11}B\{^{1}H\}$ NMR spectra of **4HN** in CD_2Cl_2.

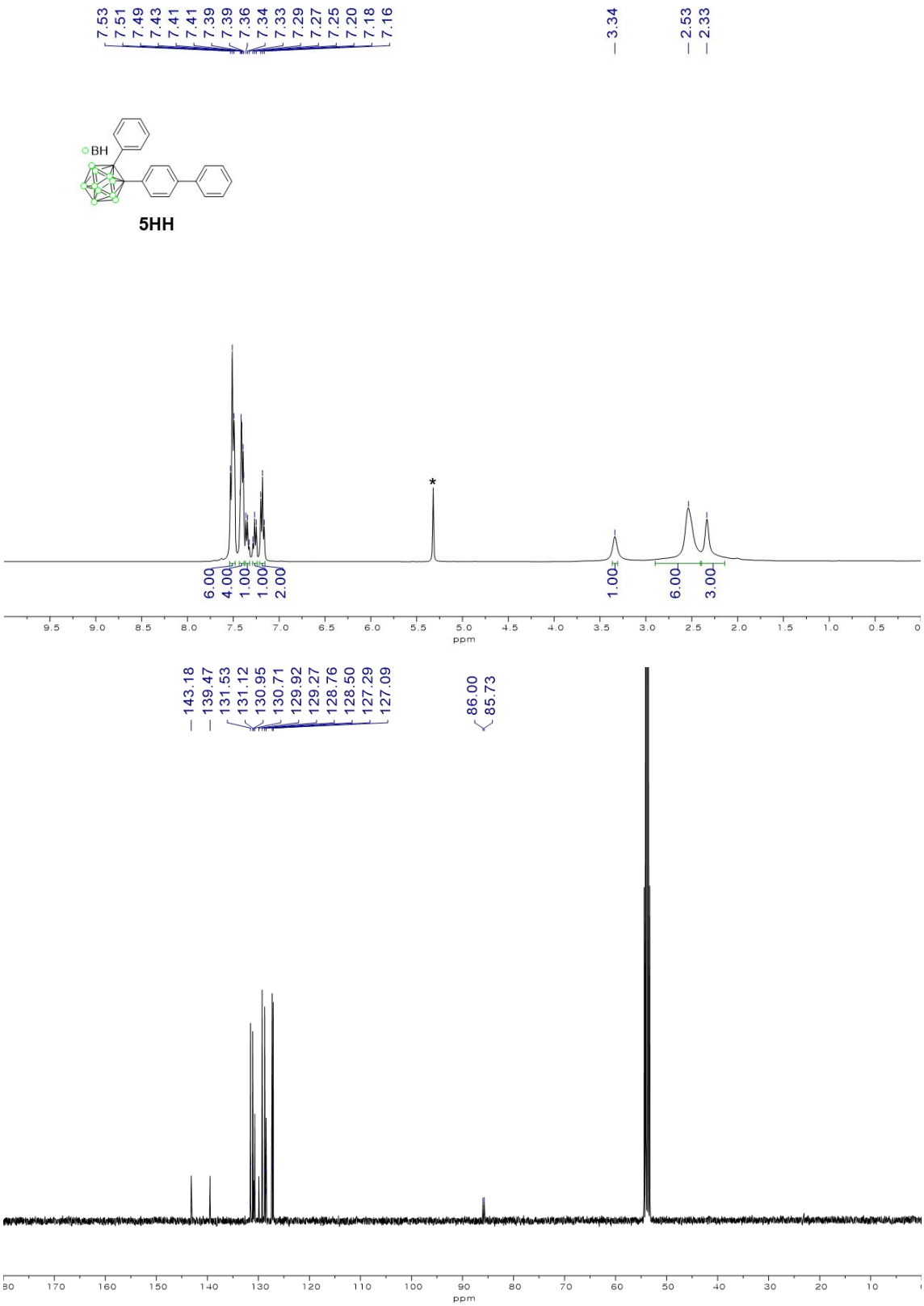


Figure S23. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **5HH** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

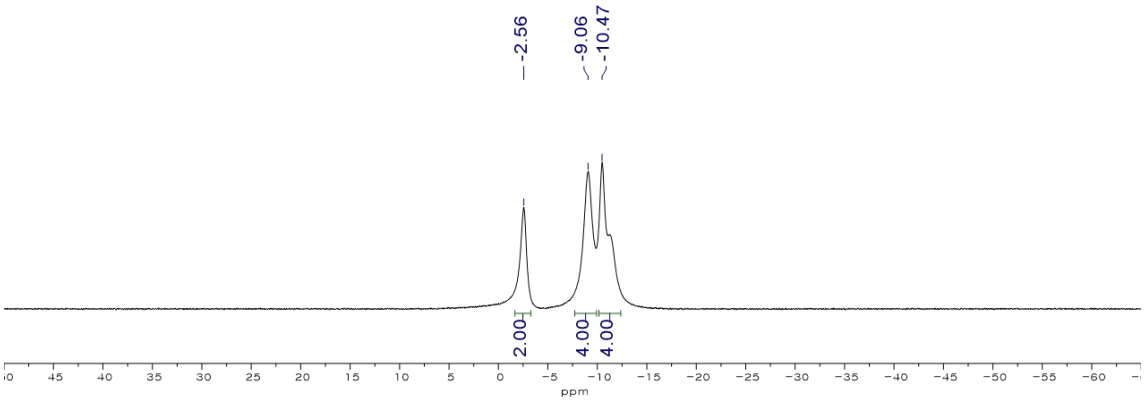


Figure S24. $^{11}B\{^{1}H\}$ NMR spectra of **5HH** in CD_2Cl_2.

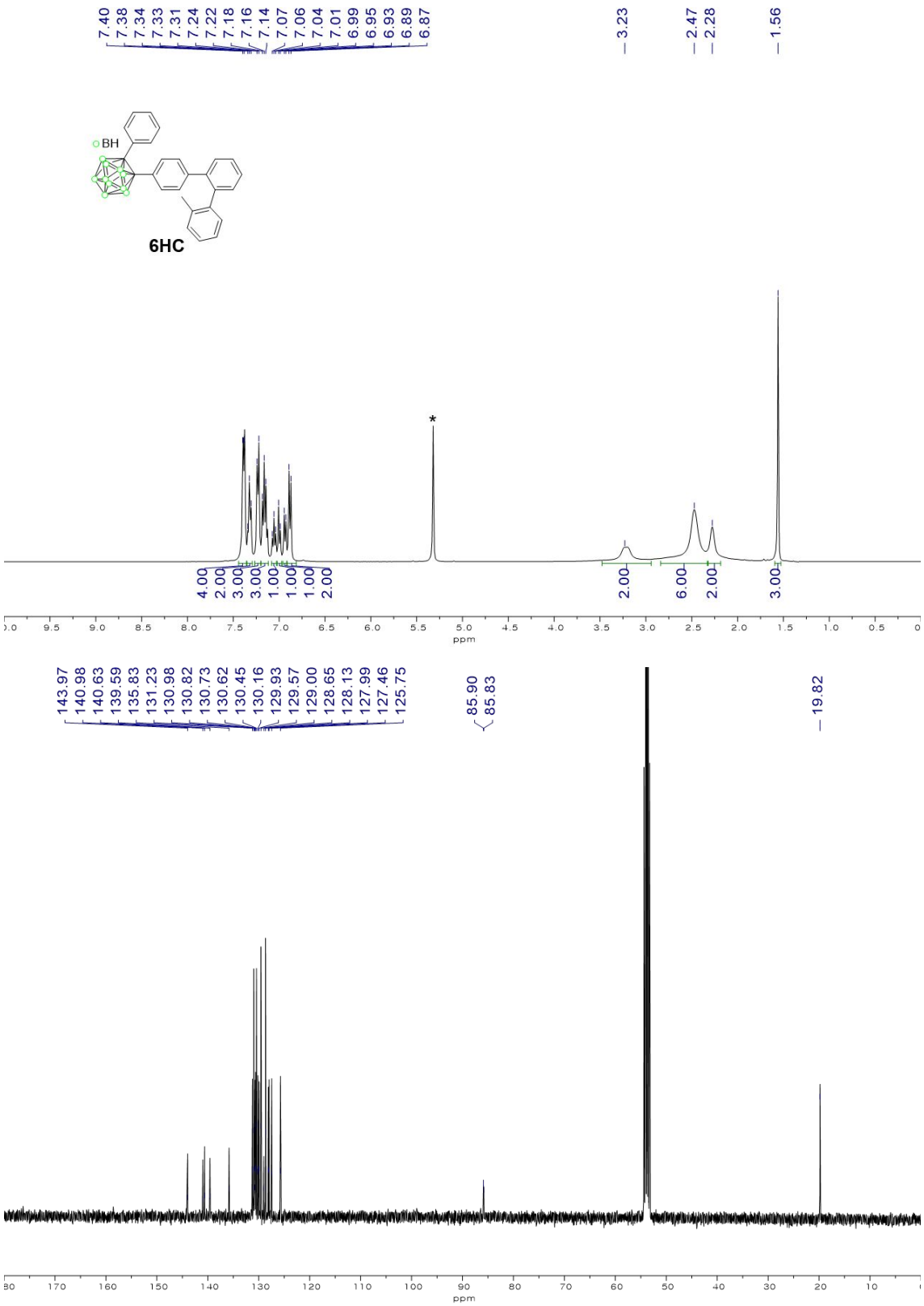


Figure S25. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **6HC** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

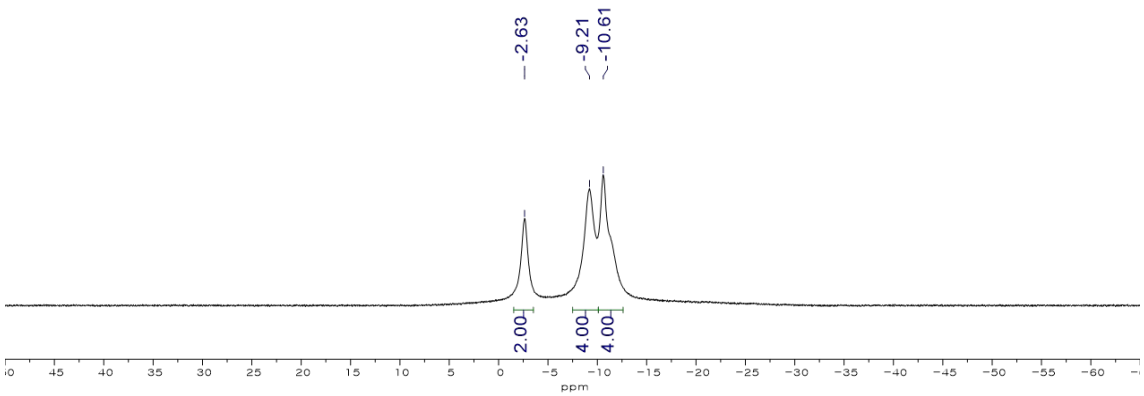


Figure S26. $^{11}B\{^{1}H\}$ NMR spectra of **6HC** in CD_2Cl_2.

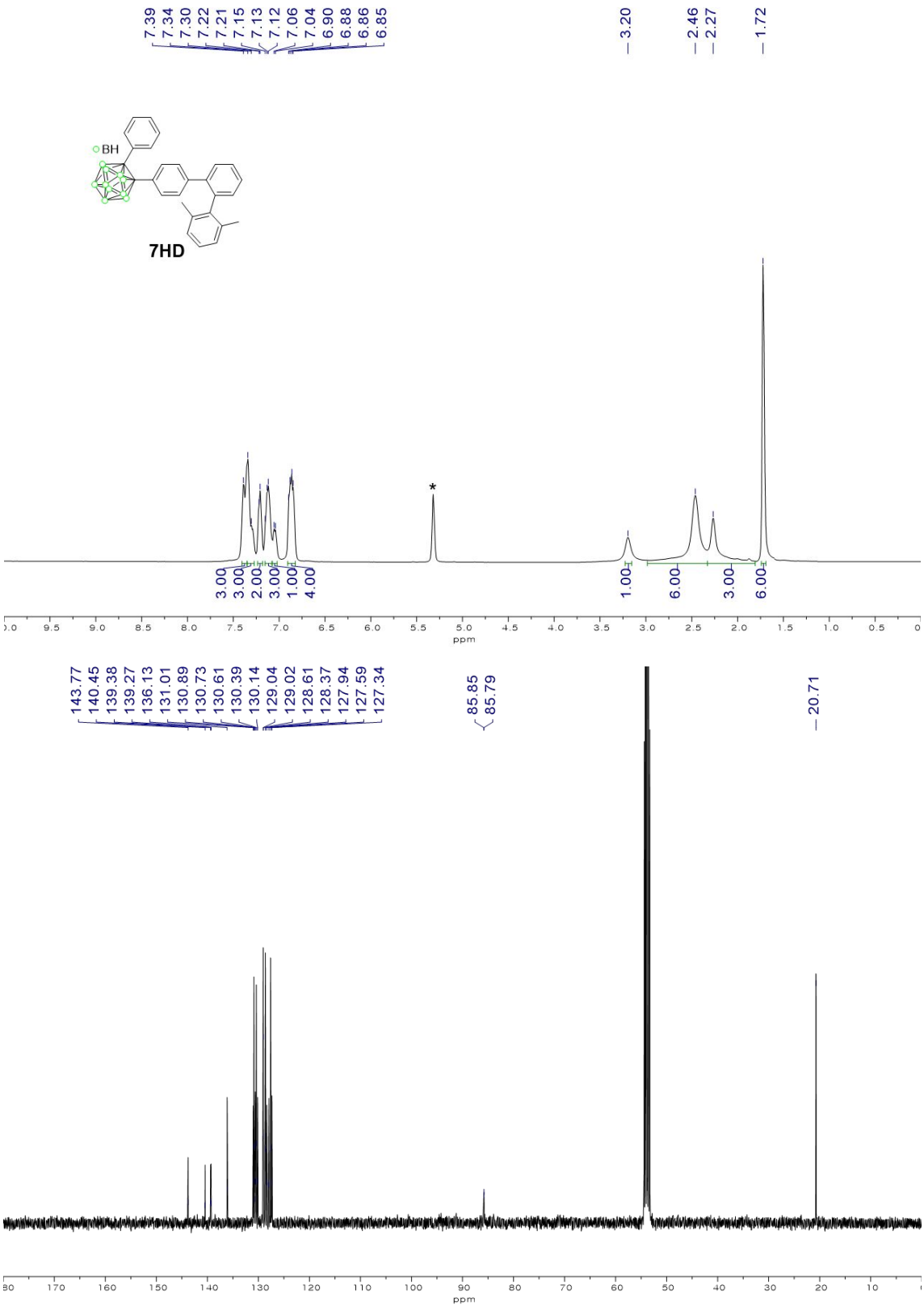


Figure S27. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **7HD** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

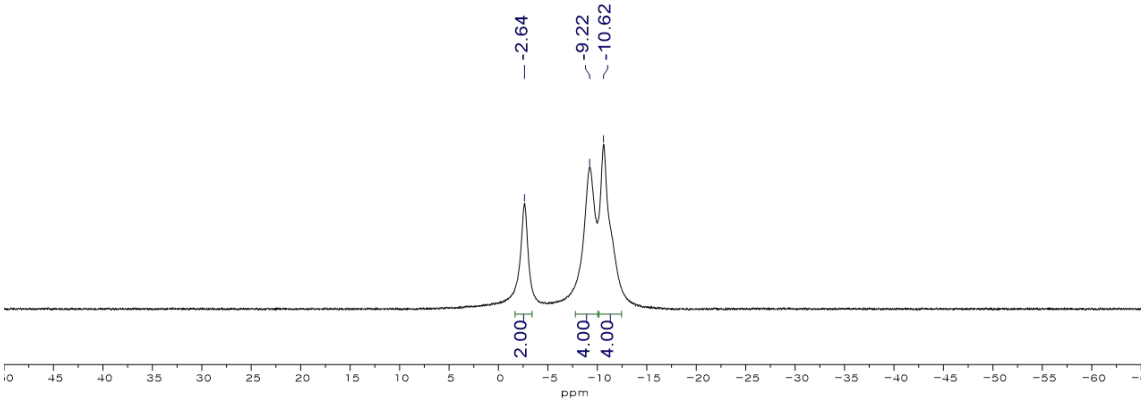


Figure S28. $^{11}B\{^{1}H\}$ NMR spectra of **7HD** in CD_2Cl_2.

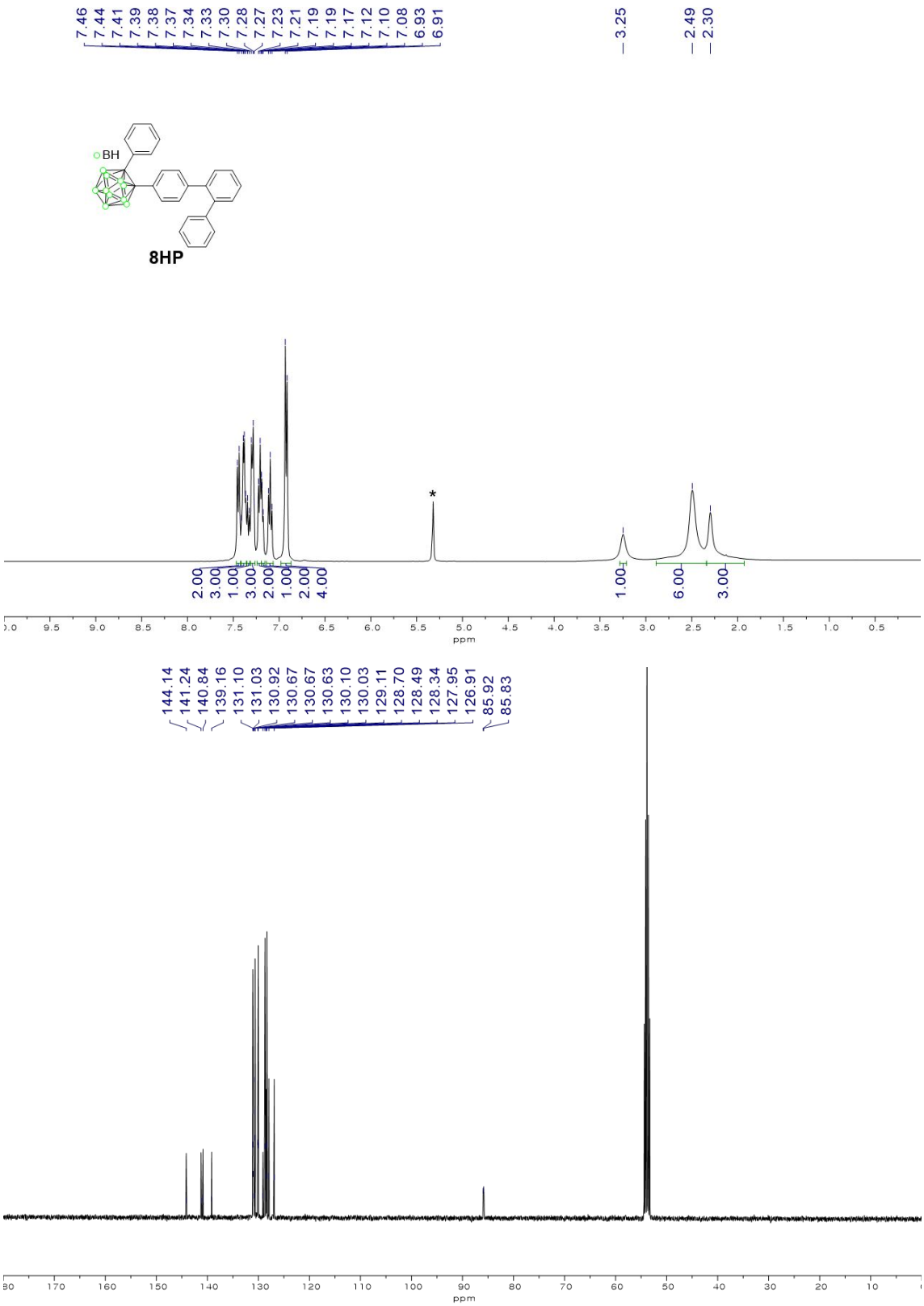


Figure S29. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **8HP** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

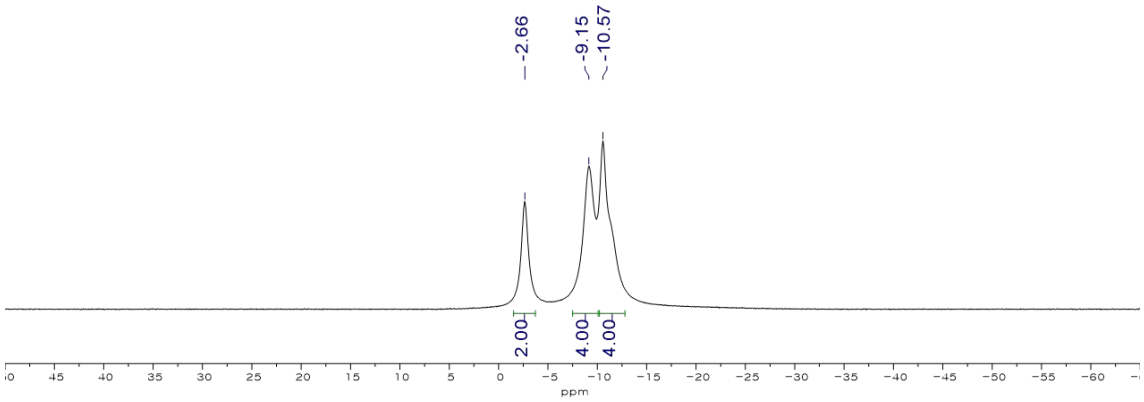


Figure S30. $^{11}B\{^{1}H\}$ NMR spectra of **8HP** in CD_2Cl_2.

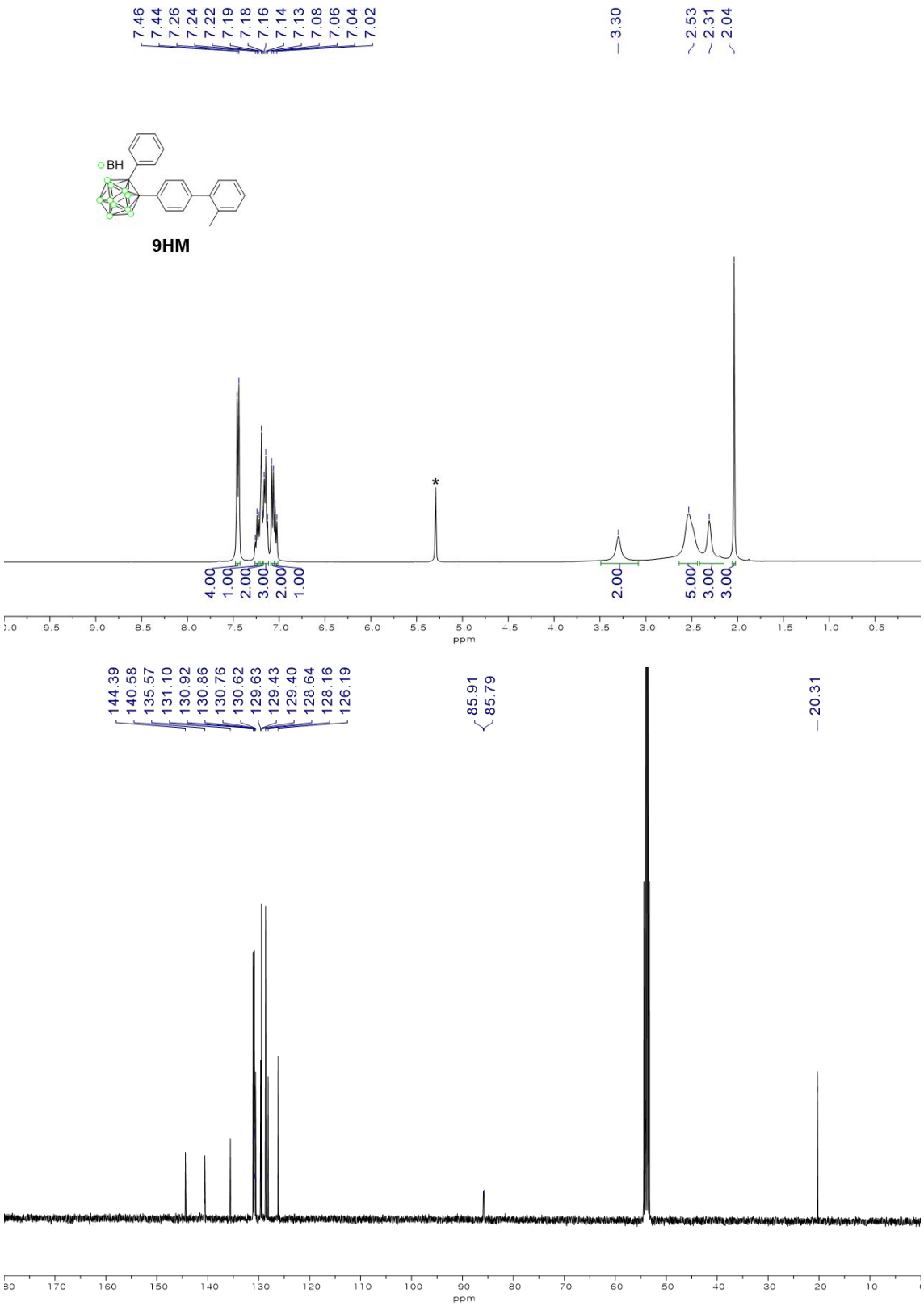


Figure S31. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **9HM** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

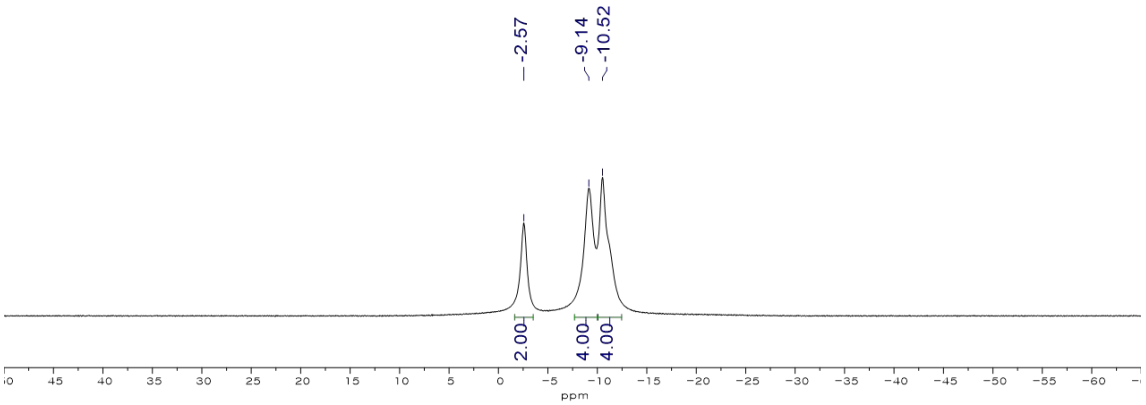


Figure S32. $^{11}B\{^{1}H\}$ NMR spectra of **9HM** in CD_2Cl_2.

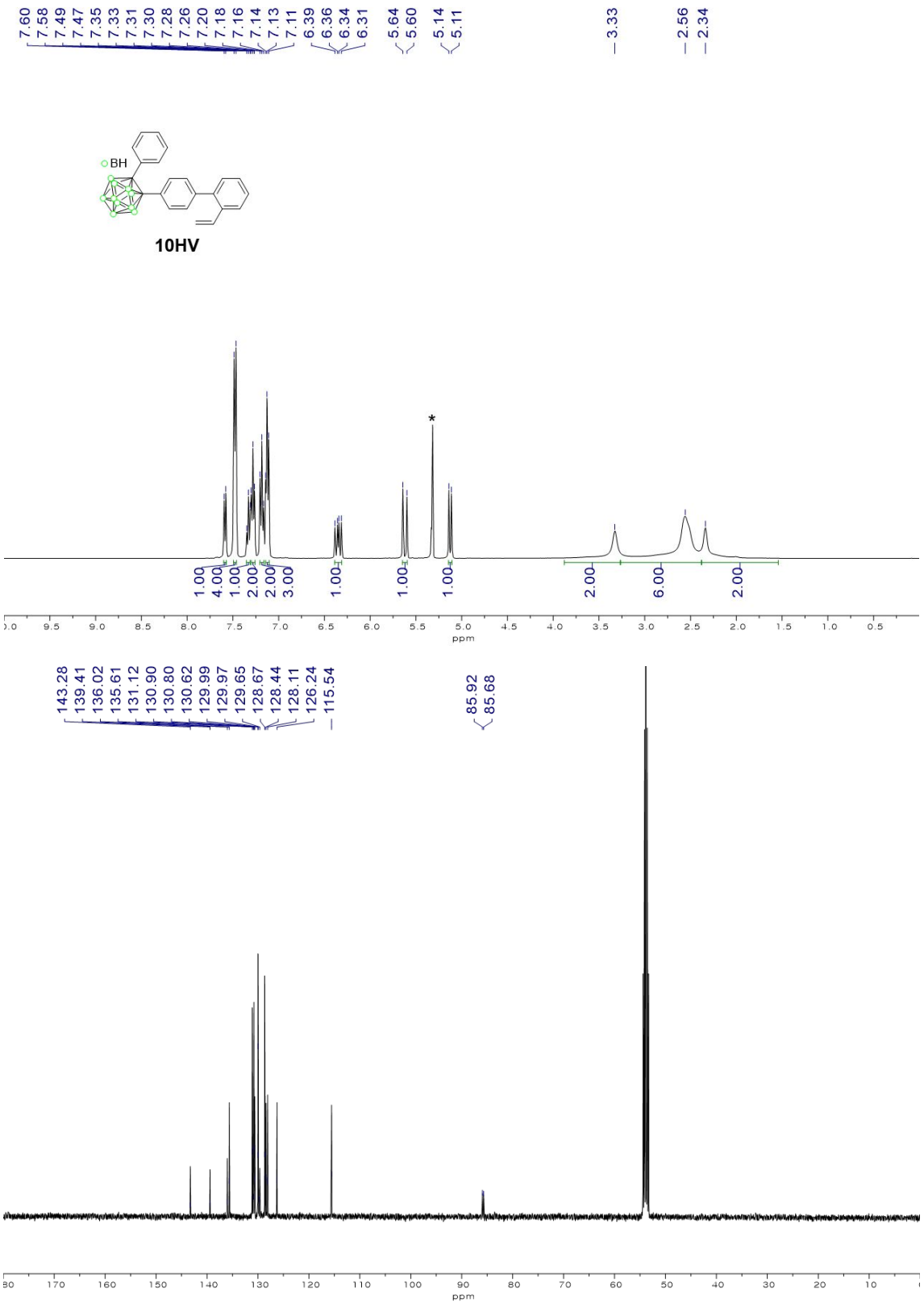


Figure S33. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **10HV** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

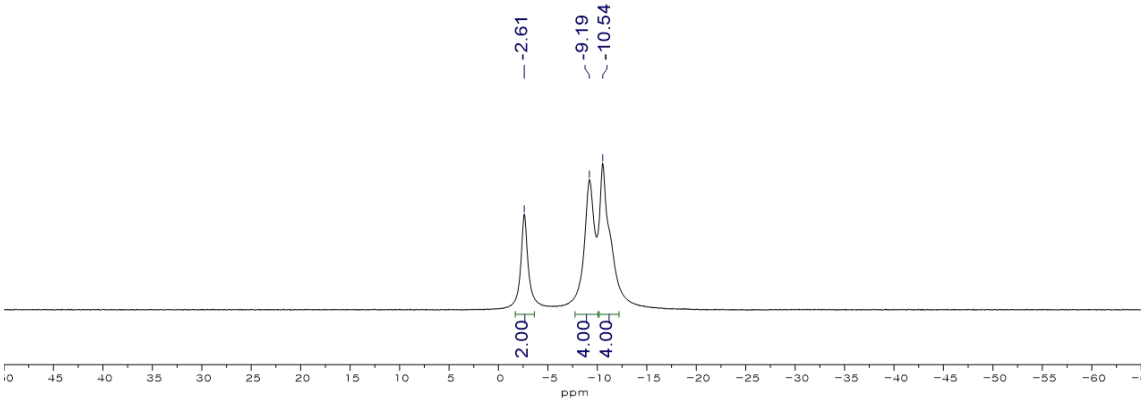


Figure S34. $^{11}B\{^{1}H\}$ NMR spectra of **10HV** in CD_2Cl_2.

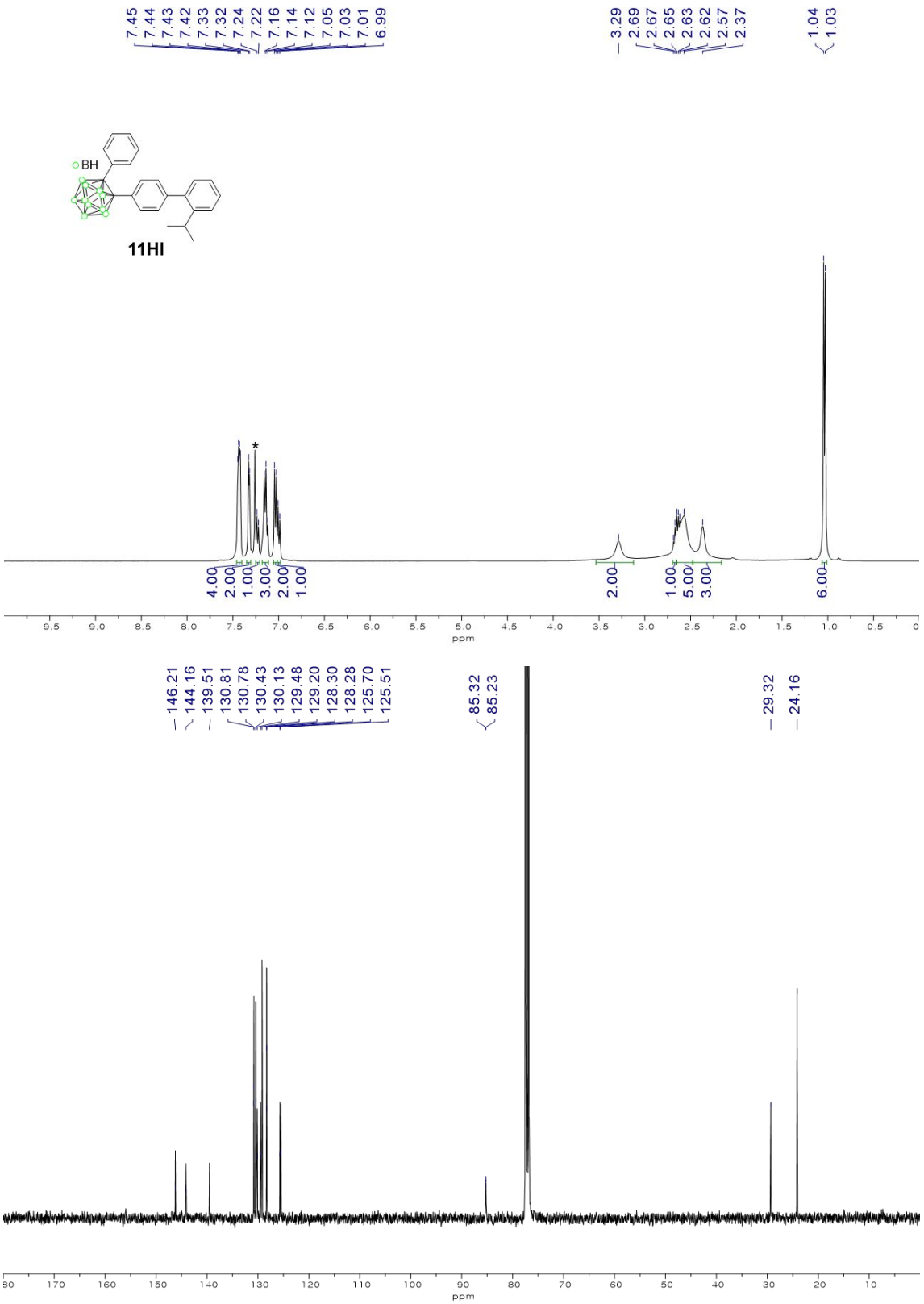


Figure S35. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **11HI** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

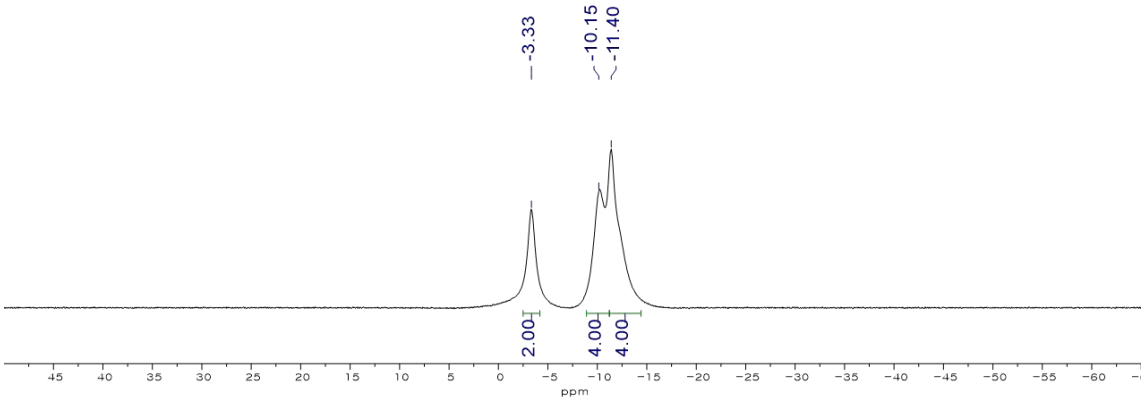


Figure S36. $^{11}B\{^{1}H\}$ NMR spectra of **11HI** in $CDCl_3$.

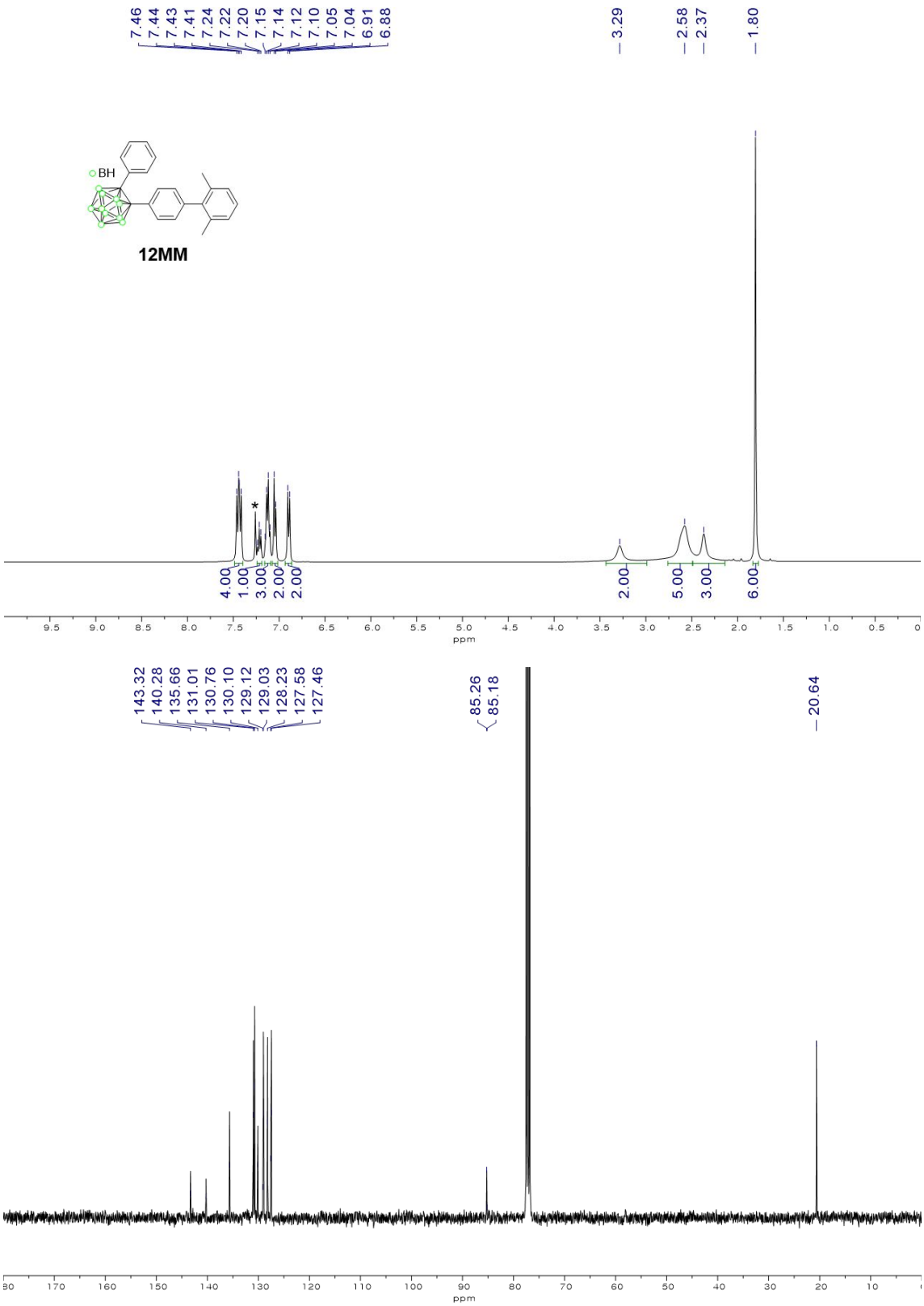


Figure S37. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **12MM** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

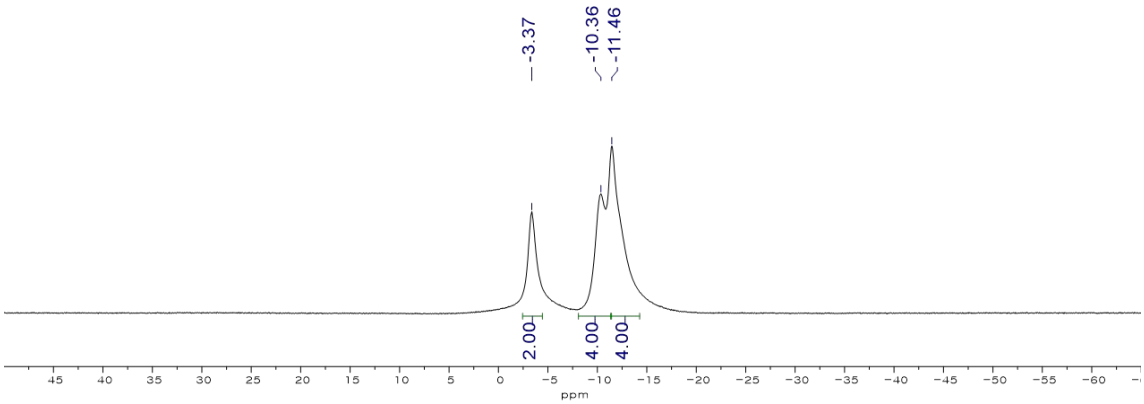


Figure S38. $^{11}B\{^{1}H\}$ NMR spectra of **12MM** in $CDCl_3$.

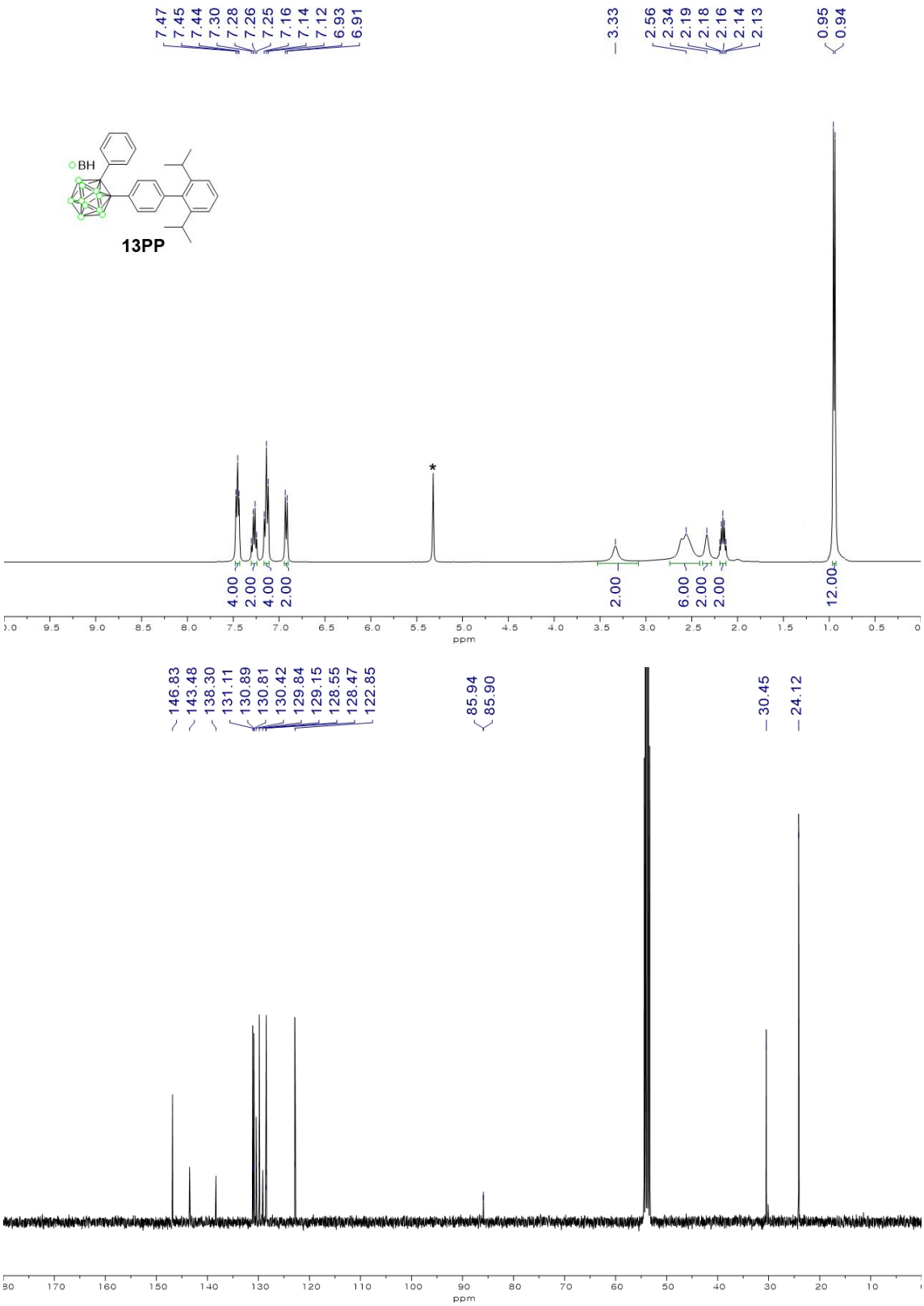


Figure S39. $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **13PP** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

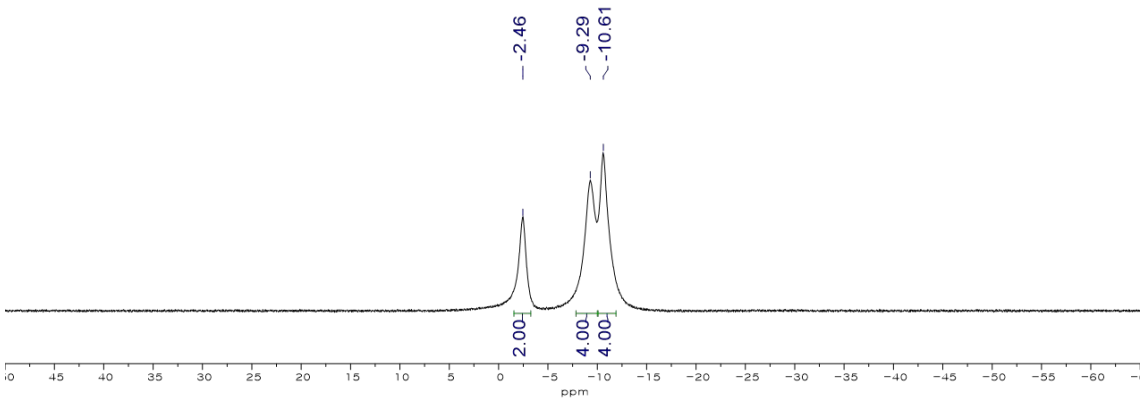


Figure S40. $^{11}B\{^{1}H\}$ NMR spectra of **13PP** in CD_2Cl_2.

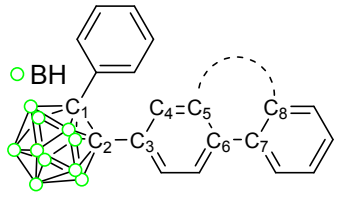
Table S1. Crystallographic data and parameters for the biphenyl-based *o*-carborane compounds

Compound	**1HF**	**2HT**	**3HB**	**4HN**	**5HH**	**6HC**	**7HD**
Formula	$C_{21}H_{24}B_{10}$	$C_{26}H_{26}B_{10}$	$C_{22}H_{24}B_{10}$	$C_{22}H_{26}B_{10}$	$C_{20}H_{24}B_{10}$	$C_{27}H_{30}B_{10}$	$C_{28}H_{32}B_{10}$
Fomula weight	384.50	446.57	396.51	398.53	372.49	462.61	476.63
Crystal system	Triclinic	Triclinic	Trigonal	Trigonal	Triclinic	Triclinic	Triclinic
Space group	P_{-1}	P_{-1}	P_{-3}	P_{-3}	P_{-1}	P_{-1}	P_{-1}
a (Å)	16.697(3)	7.2470(4)	21.7420(5)	21.6636(7)	9.6210(19)	10.842(2)	10.946(2)
b (Å)	19.892(4)	9.7449(5)	21.7420(5)	21.6636(7)	9.974(2)	10.929(2)	11.085(2)
c (Å)	22.032(4)	17.4623(9)	8.3457(3)	8.4570(3)	12.654(3)	12.469(2)	12.538(3)
α (°)	68.42(3)	74.8317(16)	90	90	73.12(3)	98.67(3)	98.03(3)
β (°)	77.35(3)	89.9817(18)	90	90	70.40(3)	107.98(3)	107.22(3)
γ (°)	75.86(3)	80.1985(16)	120	120	81.54(3)	101.39(3)	102.46(3)
V (Å^3)	6531(3)	1171.60(11)	3416.6(2)	3437.2(2)	1093.0(5)	1341.7(5)	1384.7(6)
Z	12	2	6	6	2	2	2
ρ_{calc}(g cm^{-3})	1.173	1.266	1.156	1.155	1.132	1.145	1.143
μ (mm^{-1})	0.059	0.065	0.059	0.059	0.057	0.059	0.059
F(000)	2400	464	1236	1248	388	484	500
T (K)	293(2)	153(2)	173(2)	173(2)	293(2)	293(2)	293(2)
Scan mode	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*
hkl range	–21 → +21, –25 → +25, –25 → +28	–9 → +9, –12 → +12, –22 → +22	–28 → +25, –28 → +28, –10 → +10	–26 → +28, –24 → +28, –11 → +11	–12 → +12, –12 → +12, –16 → +16	–14 → +12, –14 → +14, –15 → +16	–12 → +14, –14 → +14, –16 → +16
Measd reflns	106043	58119	28679	30032	10903	13453	14018
Unique reflns [R_{int}]	29851 [0.0990]	5377 [0.0424]	5185 [0.0485]	5664 [0.0294]	5001 [0.0453]	6108 [0.0810]	6304 [0.0320]
Reflns used for refinement	29851	5377	5185	5664	5001	6108	6304
Refined parameters	1675	355	290	308	271	335	345
R_1[a] (I>2σ(I))	0.0625	0.0484	0.0500	0.0523	0.0599	0.0913	0.0539
wR_2[b] all data	0.1724	0.1360	0.1316	0.1387	0.1469	0.2624	0.1379
GOF on F^2	1.003	1.005	1.025	1.036	1.007	1.032	1.008
ρ_{fin} (max/min) (e Å^{-3})	0.283, –0.248	0.334, –0.222	0.253, –0.222	0.329, –0.229	0.222, –0.179	1.065, –0.300	0.258, –0.234

Compound	**8HP**	**9HM**	**10HV**	**11HI**	**12MM**	**13PP**
Formula	$C_{26}H_{28}B_{10}$	$C_{21}H_{26}B_{10}$	$C_{22}H_{26}B_{10}$	$C_{23}H_{30}B_{10}$	$C_{22}H_{28}B_{10}$	$C_{26}H_{36}B_{10}$
Fomula weight	448.58	386.52	398.53	414.57	400.54	456.65
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	P_{-1}	P_{-1}	$P2_1/n$	$P2_1/n$	$C2/c$
a (Å)	13.1111(7)	9.5380(19)	10.377(2)	12.262(2)	10.303(2)	22.0889(10)
b (Å)	14.3249(8)	9.795(2)	10.518(2)	15.467(3)	16.550(3)	12.0182(6)
c (Å)	13.4063(7)	13.244(3)	12.609(3)	13.498(3)	14.173(3)	24.8327(12)
α (°)	90	103.96(3)	71.67(3)	90	90	90
β (°)	98.9825(17)	103.33(3)	83.43(3)	103.38(3)	102.50(3)	104.5587(16)
γ (°)	90	101.09(3)	61.21(3)	90	90	90
V (Å^3)	2487.0(2)	1127.4(5)	1143.7(5)	2490.5(9)	2359.4(9)	6380.6(5)
Z	4	2	2	4	4	8
ρ_{calc}(g cm^{-3})	1.198	1.139	1.157	1.106	1.128	0.951
μ (mm^{-1})	0.062	0.057	0.059	0.056	0.057	0.049
F(000)	936	404	416	872	840	1936
T (K)	153(2)	293(2)	293(2)	293(2)	293(2)	173(2)
Scan mode	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*	*Ψ and ω scan*
hkl range	–12 → +12, –12 → +12, –16 → +16	–12 → +11, –12 → +12, –17 → +17	–13 → +13, –13 → +13, –16 → +16	–15 → +15, –20 → +20, –16 → +17	–13 → +13, –20 → +21, –18 → +18	–27 → +28, –15 → +15, –32 → +31
Measd reflns	47558	11349	11512	24689	23284	64222
Unique reflns [R_{int}]	5477 [0.0524]	5153 [0.0357]	5217 [0.0305]	5707 [0.0331]	5376 [0.1084]	7271 [0.0679]
Reflns used for refinement	5477	5153	5217	5707	5376	7271
Refined parameters	355	281	289	300	291	331
R_1[a] (I>2σ(I))	0.0458	0.0546	0.0541	0.0589	0.0793	0.0654
wR_2[b] all data	0.1183	0.2035	0.1526	0.1833	0.2031	0.2217
GOF on F^2	1.004	1.005	1.006	1.005	1.006	1.002
ρ_{fin} (max/min) (e Å^{-3})	0.316, –0.236	0.220, –0.349	0.283, –0.197	0.332, –0.215	0.158, –0.152	0.367, –0.277

[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 the biphenyl-based *o*-carborane compounds



	lengths		angles			
	C1–C2	C2–C3	C1–C2–C3	C2–C3–C4	C5–C6–C7	C6–C7–C8
1HF	1.732(7)	1.497(7)	119.0(4)	120.2(5)	120.6(5)	118.4(5)
2HT	1.7280(17)	1.5078(16)	118.57(10)	119.96(11)	118.37(11)	121.93(11)
3HB	1.7210(17)	1.5018(18)	120.87(10)	119.57(12)	117.49(12)	121.69(13)
4HN	1.7218(15)	1.5056(15)	120.13(9)	119.36(10)	117.99(11)	121.73(12)
5HH	1.723(2)	1.504(2)	117.57(12)	119.85(13)	117.07(14)	121.69(14)
6HC	1.720(4)	1.508(3)	118.75(19)	121.9(2)	117.5(2)	121.2(2)
7HD	1.726(2)	1.506(2)	118.51(13)	121.89(14)	117.62(15)	121.41(15)
8HP	1.7207(18)	1.5029(18)	118.51(10)	120.82(12)	118.29(12)	120.77(13)
9HM	1.721(2)	1.5078(18)	117.61(11)	119.23(12)	117.11(14)	121.49(14)
10HV	1.7282(18)	1.5064(17)	116.59(10)	121.38(11)	117.30(13)	121.43(12)
11HI	1.7200(17)	1.5057(16)	118.14(10)	120.14(11)	117.59(13)	121.60(13)
12MM	1.722(3)	1.503(3)	117.00(18)	121.8(2)	116.7(2)	121.9(3)
13PP	1.714(2)	1.5029(19)	116.83(11)	122.08(13)	117.50(13)	121.54(14)

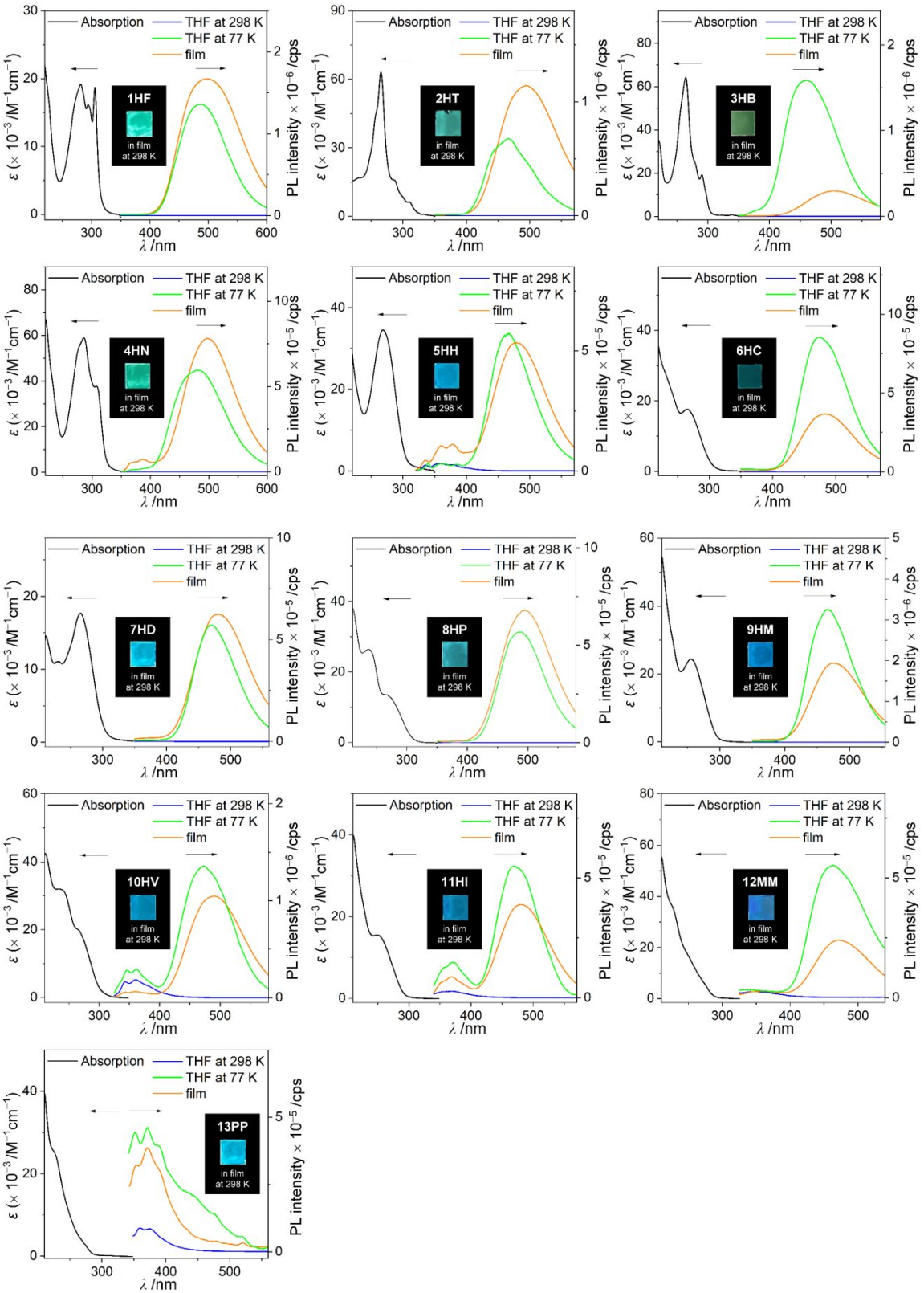


Figure S41. Ultraviolet-visible (UV-vis) absorption (left side) and photoluminescence (PL) spectra (right side) of biphenyl-based *o*-carboranyl compounds (**1HF–13PP**). Black line: absorption spectra in THF (3.0×10^{-5} M); blue line: PL spectra in THF (3.0×10^{-5} M) at 298 K; green line: PL spectra in THF (3.0×10^{-5} M) at 77 K; orange line: PL spectra in film (5 wt% doped with PMMA) at 298 K. Inset figures show the emission color in each state when irradiated by a hand-held UV lamp (λ_{ex} = 265 nm).

Table S3. The photophysical data for biphenyl-based *o*-carboranyl compounds.

	$\lambda_{em,max}$			Φ_{em}[c]	
	at 298 K[a]	at 77 K[a]	film[b]	at 298 K[a]	film[b]
1HF	-[d]	487	498	-[d]	0.292
2HT	-[d]	467	494	-[d]	0.356
3HB	-[d]	459	506	-[d]	0.140
4HN	-[d]	482	387 (sh), 497	-[d]	0.283
5HH	357	358, 467	358, 379, 478	0.02 (LE)	0.197
6HC	-[d]	474	483	-[d]	0.208
7HD	-[d]	471	481	-[d]	0.182
8HP	-[d]	487	495	-[d]	0.197
9HM	-[d]	466	475	-[d]	0.192
10HV	343, 361	346, 361, 473	361 (sh), 489	0.07 (LE)	0.068
11HI	368 (tr)	370 (sh), 468	368 (sh), 480	<0.01 (LE)	0.025
12MM	351 (tr)	463	470	-[d]	0.017
13PP	360, 375	352, 372, 475 (sh)	354, 372	<0.01 (LE)	<0.01 (LE)

[a]$c = 3.0 \times 10^{-5}$ M in THF. [b]Measured in the film state (5 wt% doped in PMMA). [c]Absolute PL quantum yield. [d]Not observed due to weak emission. tr = trace, sh = shoulder peak.

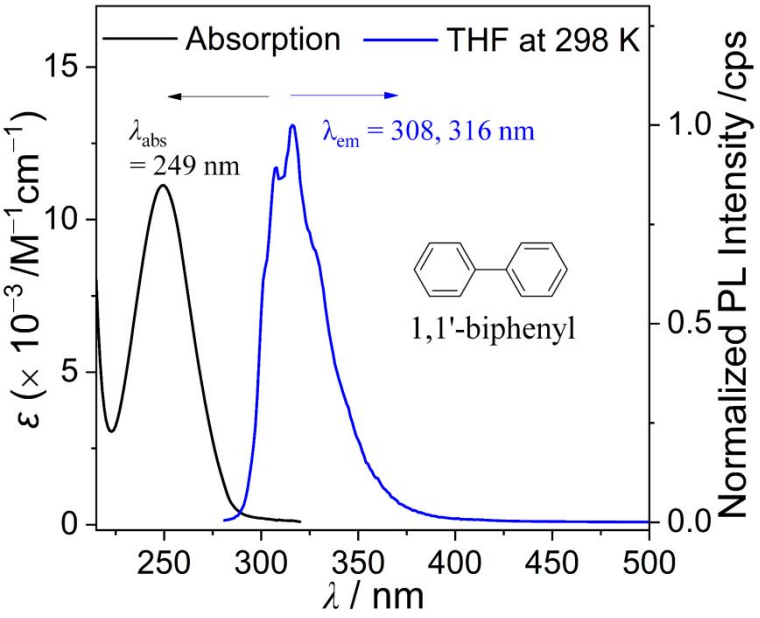


Figure S42. UV-vis absorption and PL spectra for 1,1'-biphenyl (λ_{ex} = 269 nm) in THF (3.0×10^{-5} M) at 298 K.

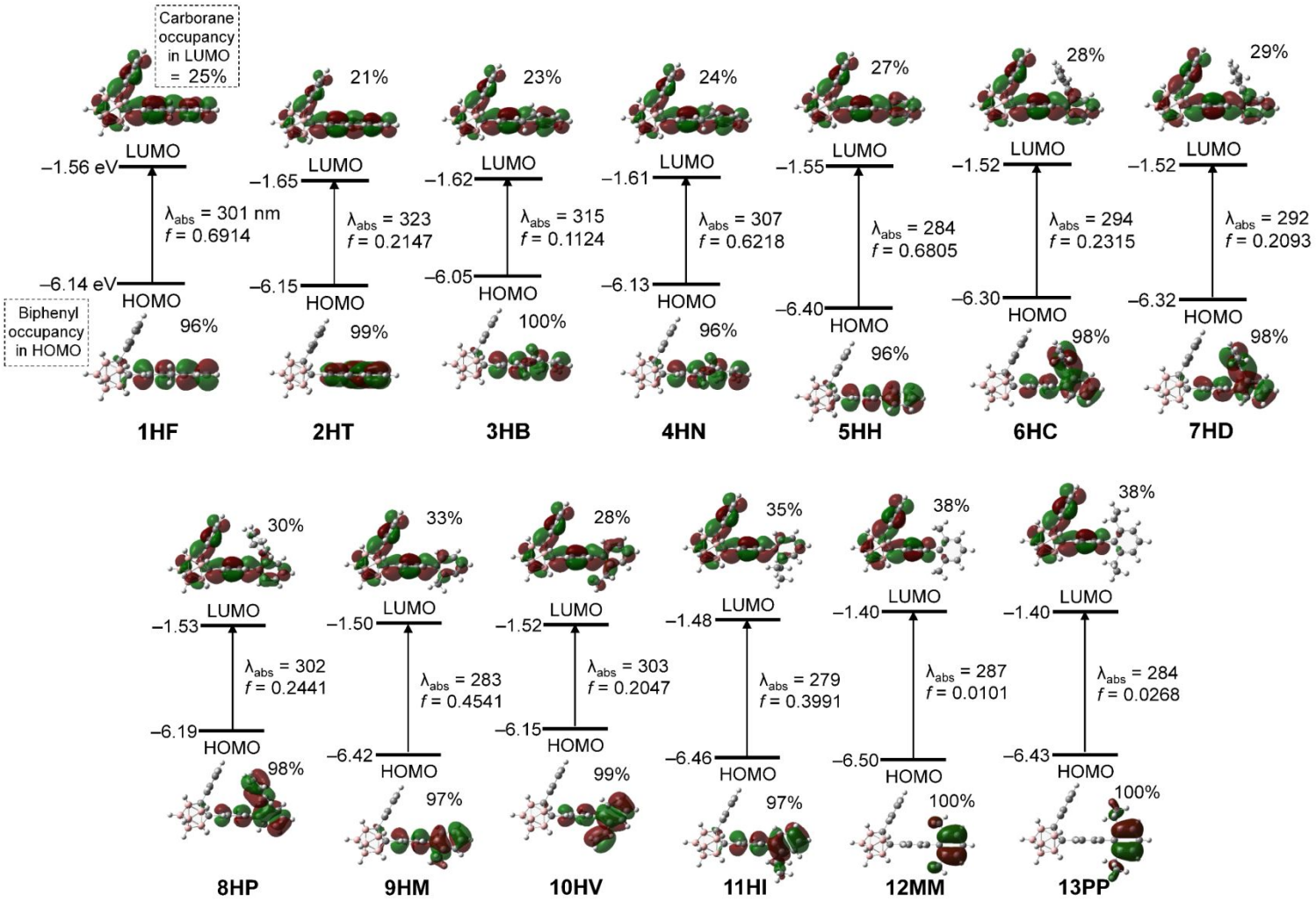


Figure S43. Frontier molecular orbitals of biphenyl-based *o*-carboranyl compounds **1HF–13PP** at ground state (S_0) with their relative energies from density functional theory calculations (Isovalue = 0.04 a.u.) and molecular orbital distributions on the *o*-carborane moieties of the lowest unoccupied molecular orbital (LUMO) levels (%) and on the biphenyl group of the highest occupied molecular orbital (HOMO) level. The transition energy (in nm) was calculated using the TD-B3LYP method with 6-31G(d,p) basis sets.

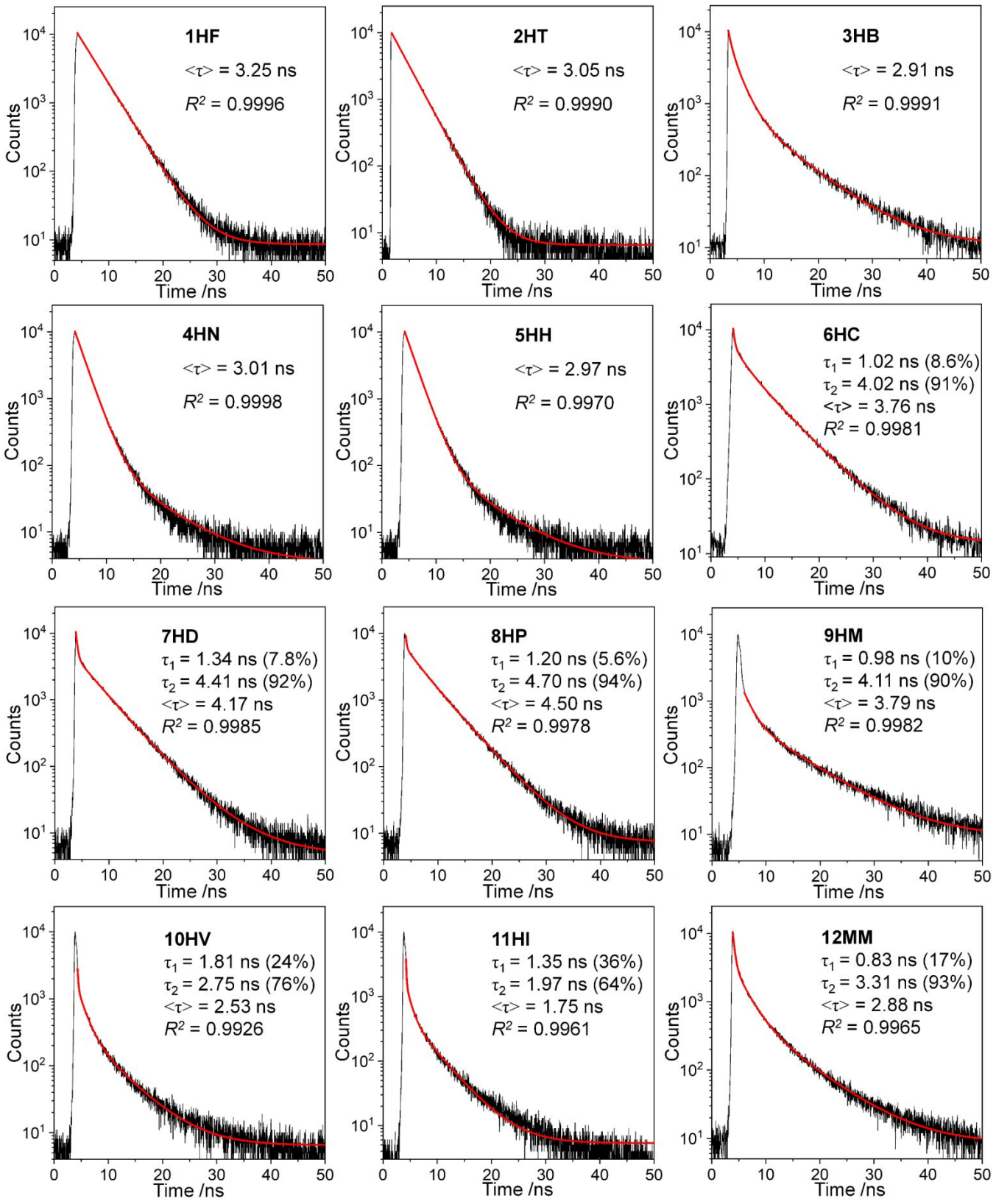


Figure S44. Emission decay curves of biphenyl-based *o*-carboranyl compounds **1HF–12MM** in the crystalline state detected at each intramolecular charge transfer (ICT)-based emission maxima at 298 K. Each red line is its exponential fitting curve for the decay curves.

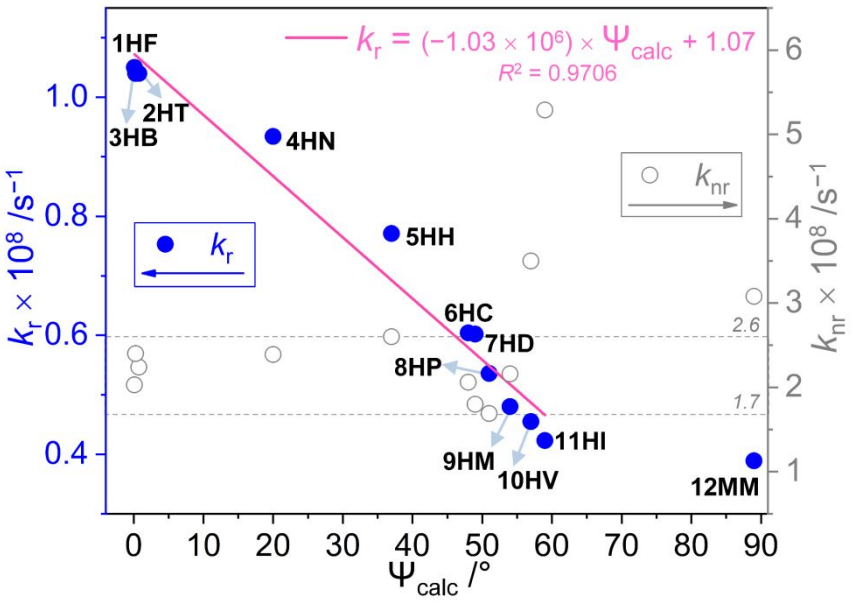
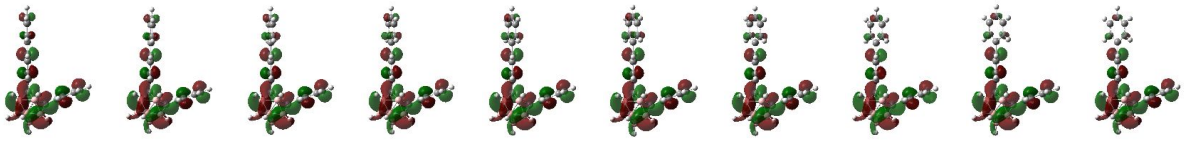
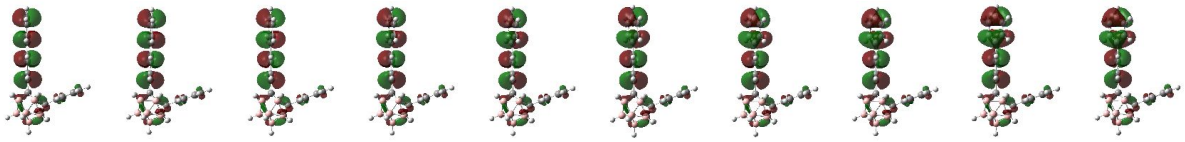
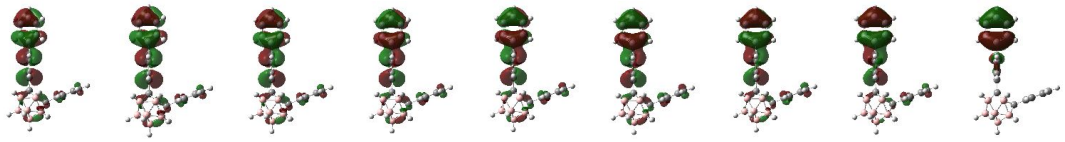


Figure S45. Radiative (k_r, filled blue circle, left) and nonradiative decay constants (k_{nr}, hollow gray circle, right) for biphenyl-based *o*-carboranyl compounds (**1HF–12MM**) in the crystalline state as a function of the calculated dihedral angles (Ψ_{calc}) from each optimized structure in the ground (S_0) state. The pink line is its linear fitting for the k_r values versus Ψ_{calc}.

Table S4. Computed emission wavelengths (λ_{calc}), oscillator strengths (f_{calc}), and molecular orbitals of HOMO and LUMO for **5HH** as a function of the dihedral angle (Ψ) between biphenyl rings in each first excited (S_1) state.

Ψ (°)	0	5	10	15	20	25	30	35	40	45
λ_{calc} /nm	536.95	536.49	535.17	532.86	529.82	526.02	521.48	516.30	510.63	504.35
f_{calc}	0.5439	0.5426	0.5388	0.5324	0.5233	0.5120	0.4983	0.4824	0.4645	0.4445
LUMO										
HOMO										
Ψ (°)	50	55	60	65	70	75	80	85	90	
λ_{calc} (nm)	497.59	490.35	482.55	474.29	465.73	456.77	447.42	437.80	430.11	
f_{calc}	0.4226	0.3989	0.3737	0.3473	0.3199	0.2921	0.2645	0.2390	0.2181	
LUMO										
HOMO										

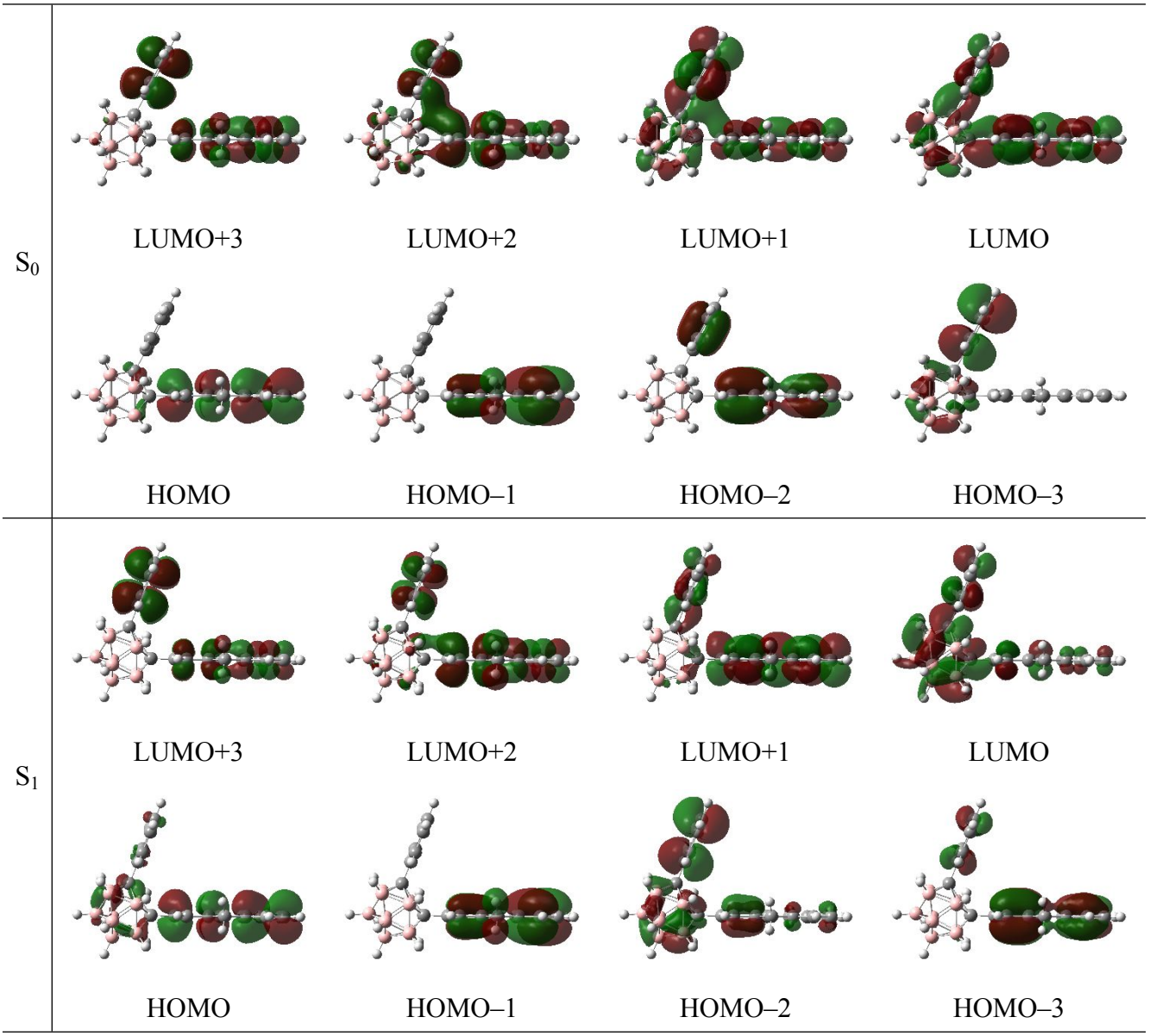


Figure S46. The selected frontier orbitals of **1HF** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S5. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **1HF** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} /nm	f_{calc}	Major contribution
		S_0	
1	300.99	0.6914	HOMO → LUMO (97.60%)
2	271.02	0.0327	HOMO−2 → LUMO (23.91%)
			HOMO−1 → LUMO (8.36%)
			HOMO → LUMO+1 (19.32%)
			HOMO → LUMO+2 (36.86%)
3	268.26	0.0424	HOMO−1 → LUMO (65.44%)
			HOMO → LUMO+1 (18.88%)
			HOMO → LUMO+5 (7.46%)
4	264.61	0.1649	HOMO−1 → LUMO (8.55%)
			HOMO → LUMO+1 (58.97%)
			HOMO → LUMO+2 (18.48%)
5	248.98	0.0084	HOMO−5 → LUMO (52.90%)
			HOMO−2 → LUMO+1 (25.58%)
		S_1	
1	503.44	0.6023	HOMO → LUMO (99.53%)
2	407.72	0.0081	HOMO−3 → LUMO (16.34%)
			HOMO−1 → LUMO (79.96%)
3	380.43	0.3599	HOMO−2 → LUMO (90.19%)
4	379.40	0.0070	HOMO−3 → LUMO (96.71%)
5	376.65	0.1325	HOMO−4 → LUMO (80.26%)

Table S6. Molecular orbital distributions (in %) and energies (in eV) of **1HF** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.38	60.7	2.40	10.2	26.7
LUMO+2	−0.72	27.9	7.44	47.1	17.6
LUMO+1	−1.02	57.0	18.0	12.9	12.1
LUMO	−1.56	10.3	25.4	41.0	23.3
HOMO	−6.14	0.16	4.29	43.8	51.8
HOMO−1	−6.80	0.56	0.20	18.9	80.3
HOMO−2	−7.08	18.5	0.85	59.5	21.1
HOMO−3	−7.16	85.9	13.5	0.27	0.32
			S_1		
LUMO+3	−0.47	75.4	3.00	9.30	12.2
LUMO+2	−0.61	18.7	5.68	45.9	29.7
LUMO+1	−1.20	8.85	5.16	42.4	43.6
LUMO	−3.37	14.9	72.0	9.84	3.29
HOMO	−5.96	1.75	7.71	43.9	46.6
HOMO−1	−6.89	0.02	0.48	29.1	70.4
HOMO−2	−7.14	72.4	21.0	3.44	3.13
HOMO−3	−7.17	2.02	2.04	62.4	33.6

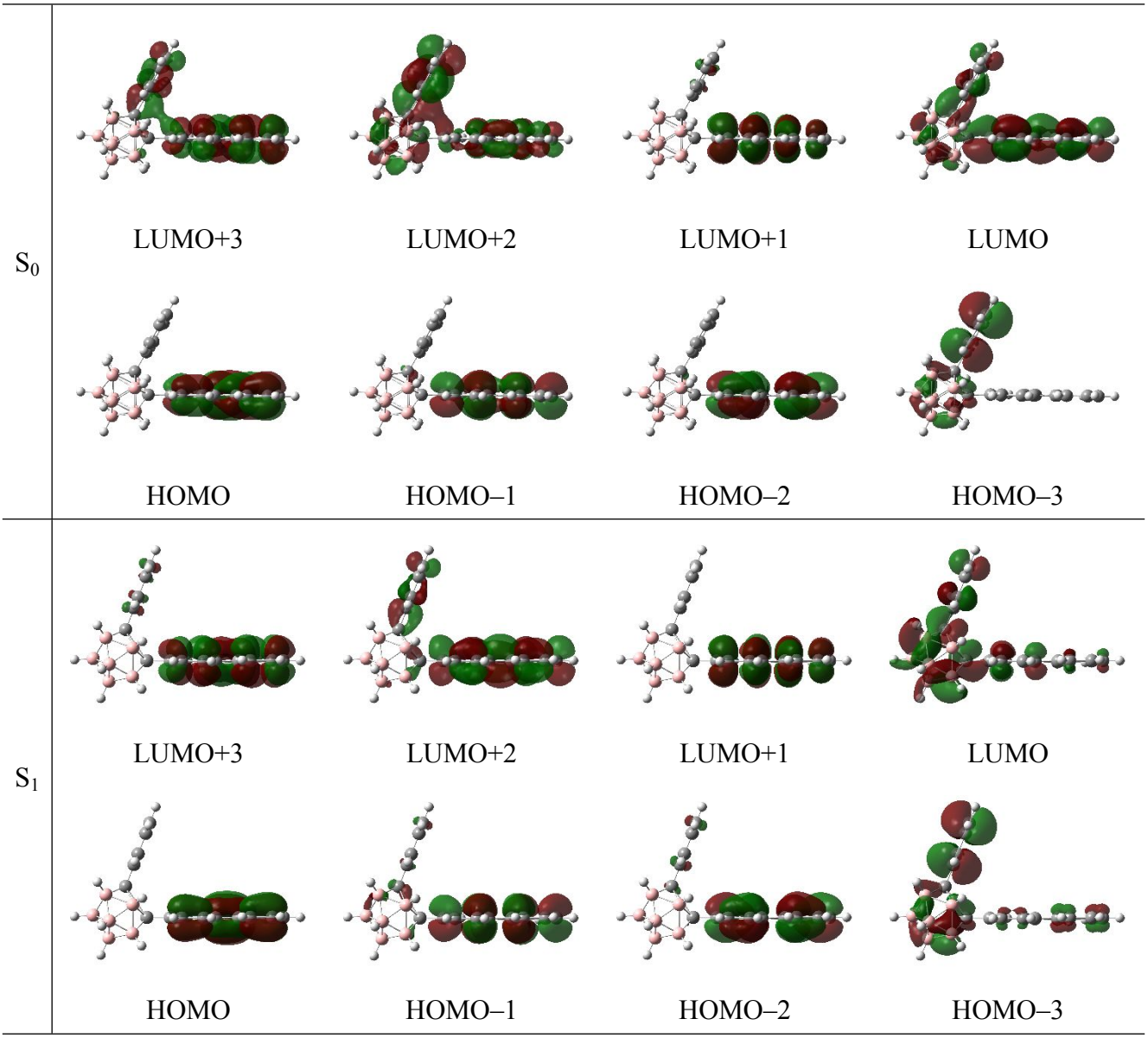


Figure S47. The selected frontier orbitals of **2HT** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S7. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **2HT** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	322.78	0.2147	HOMO−1 → LUMO (7.12%)
			HOMO−1 → LUMO+1 (19.44%)
			HOMO → LUMO (65.18%)
2	311.81	0.1706	HOMO−1 → LUMO (68.80%)
			HOMO → LUMO (12.33%)
			HOMO → LUMO+1 (16.82%)
3	288.79	0.1135	HOMO−1 → LUMO (12.01%)
			HOMO → LUMO+1 (32.13%)
			HOMO → LUMO+2 (10.01%)
			HOMO → LUMO+3 (12.57%)
4	287.40	0.0439	HOMO−2 → LUMO (32.41%)
			HOMO−1 → LUMO+1 (26.57%)
			HOMO−1 → LUMO+3 (12.57%)
5	277.84	0.4812	HOMO−2 → LUMO (24.13%)
			HOMO−1 → LUMO+1 (13.63%)
			HOMO−1 → LUMO+3 (11.03%)
			HOMO → LUMO+1 (15.96%)
			HOMO → LUMO+2 (18.21%)
		S_1	
1	512.28	0.4652	HOMO → LUMO (98.44%)
2	483.35	0.1368	HOMO−1 → LUMO (98.94%)
3	456.30	0.1514	HOMO−2 → LUMO (98.01%)
4	398.35	0.0054	HOMO−3 → LUMO (98.07%)
5	393.43	0.4442	HOMO−4 → LUMO (98.45%)

Table S8. Molecular orbital distributions (in %) and energies (in eV) of **2HT** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−1.00	28.2	9.08	14.4	48.2
LUMO+2	−1.08	33.0	13.2	7.26	46.5
LUMO+1	−1.29	2.11	2.22	41.6	54.0
LUMO	−1.65	6.83	21.4	42.0	29.7
HOMO	−6.15	0.12	0.64	18.0	81.2
HOMO−1	−6.19	0.09	2.35	38.0	59.5
HOMO−2	−6.69	0.63	1.62	33.1	64.6
HOMO−3	−7.17	86.2	13.1	0.24	0.34
			S_1		
LUMO+3	−1.01	2.44	1.74	27.0	68.8
LUMO+2	−1.20	6.81	4.05	34.0	55.1
LUMO+1	−1.43	0.10	1.24	35.5	63.1
LUMO	−3.51	13.1	74.6	9.77	2.57
HOMO	−5.99	0.00	0.26	25.6	74.1
HOMO−1	−6.23	1.40	4.63	31.0	63.0
HOMO−2	−6.69	1.90	2.85	33.9	61.3
HOMO−3	−7.17	74.6	20.0	1.30	4.11

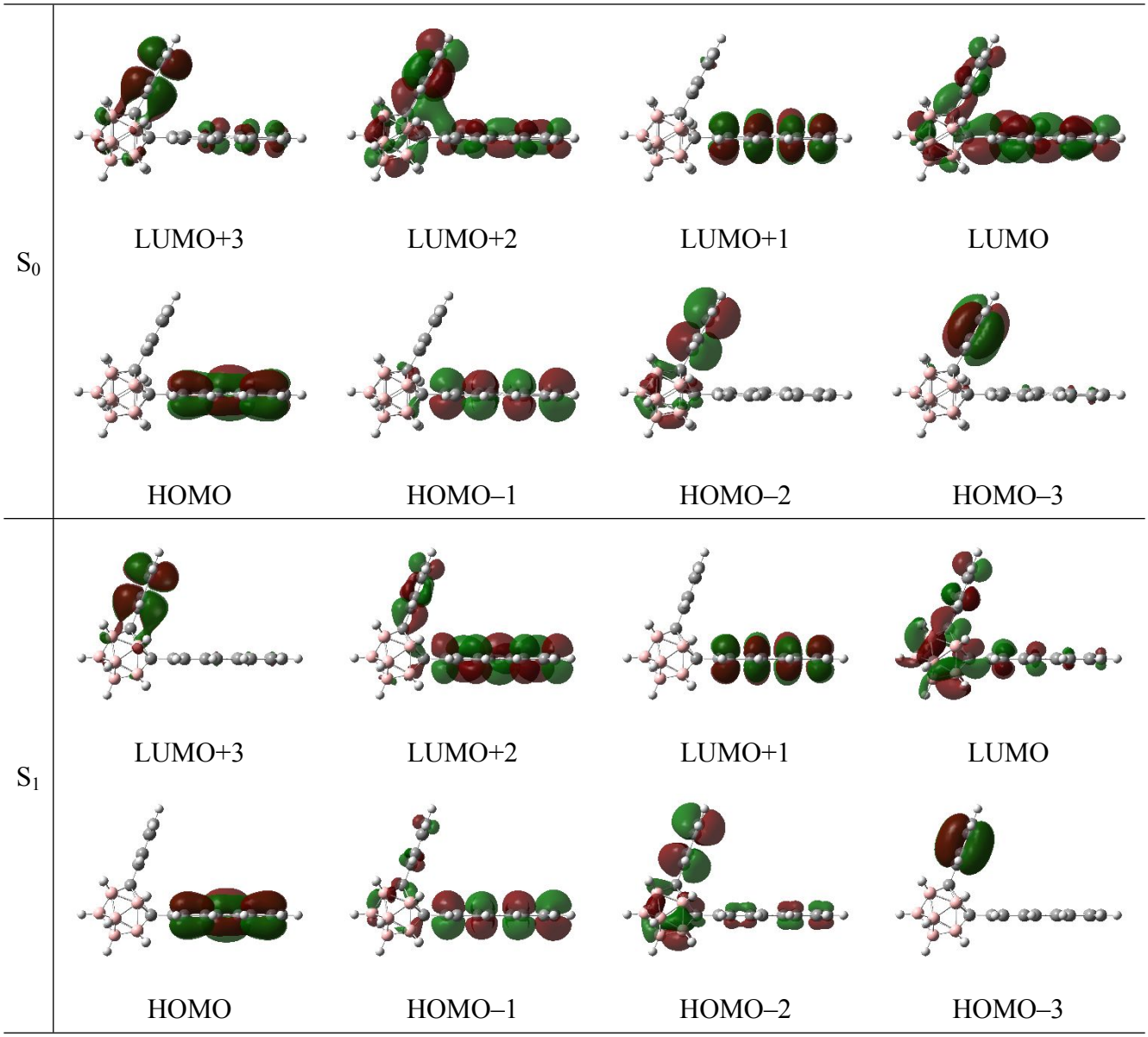


Figure S48. The selected frontier orbitals of **3HB** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S9. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **3HB** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	315.41	0.1124	HOMO−1 → LUMO+1 (17.29%)
			HOMO → LUMO (79.66%)
2	300.26	0.0005	HOMO−1 → LUMO (44.01%)
			HOMO → LUMO+1 (53.32%)
3	280.78	0.0420	HOMO−1 → LUMO+1 (22.22%)
			HOMO → LUMO (10.73%)
			HOMO → LUMO+2 (55.93%)
4	276.63	1.1067	HOMO−1 → LUMO (48.89%)
			HOMO → LUMO+1 (32.60%)
5	263.74	0.1057	HOMO−1 → LUMO+1 (50.22%)
			HOMO → LUMO+2 (34.80%)
		S_1	
1	518.77	0.5041	HOMO → LUMO (99.33%)
2	408.23	0.1423	HOMO−1 → LUMO (98.74%)
3	398.13	0.0056	HOMO−2 → LUMO (97.73%)
4	393.09	0.4359	HOMO−3 → LUMO (98.27%)
5	375.01	0.0048	HOMO−5 → LUMO (11.11%)
			HOMO−4 → LUMO (86.31%)

Table S10. Molecular orbital distributions (in %) and energies (in eV) of **3HB** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.51	82.1	6.83	2.42	8.66
LUMO+2	−1.04	59.7	19.9	9.79	10.7
LUMO+1	−1.35	1.09	2.07	36.2	60.7
LUMO	−1.62	8.60	22.6	42.4	26.3
HOMO	−6.05	0.14	0.27	30.7	68.8
HOMO−1	−6.40	0.15	4.38	43.2	52.3
HOMO−2	−7.17	86.1	13.1	0.39	0.46
HOMO−3	−7.19	95.1	1.32	1.47	2.13
			S_1		
LUMO+3	−0.52	93.1	5.69	0.34	0.90
LUMO+2	−1.12	9.50	4.75	42.4	43.4
LUMO+1	−1.52	0.09	1.19	35.5	63.2
LUMO	−3.51	13.3	75.0	9.27	2.45
HOMO	−5.86	0.00	0.32	32.0	67.7
HOMO−1	−6.48	3.17	7.43	42.4	47.0
HOMO−2	−7.17	73.9	20.0	1.62	4.48
HOMO−3	−7.25	97.0	3.02	0.02	0.00

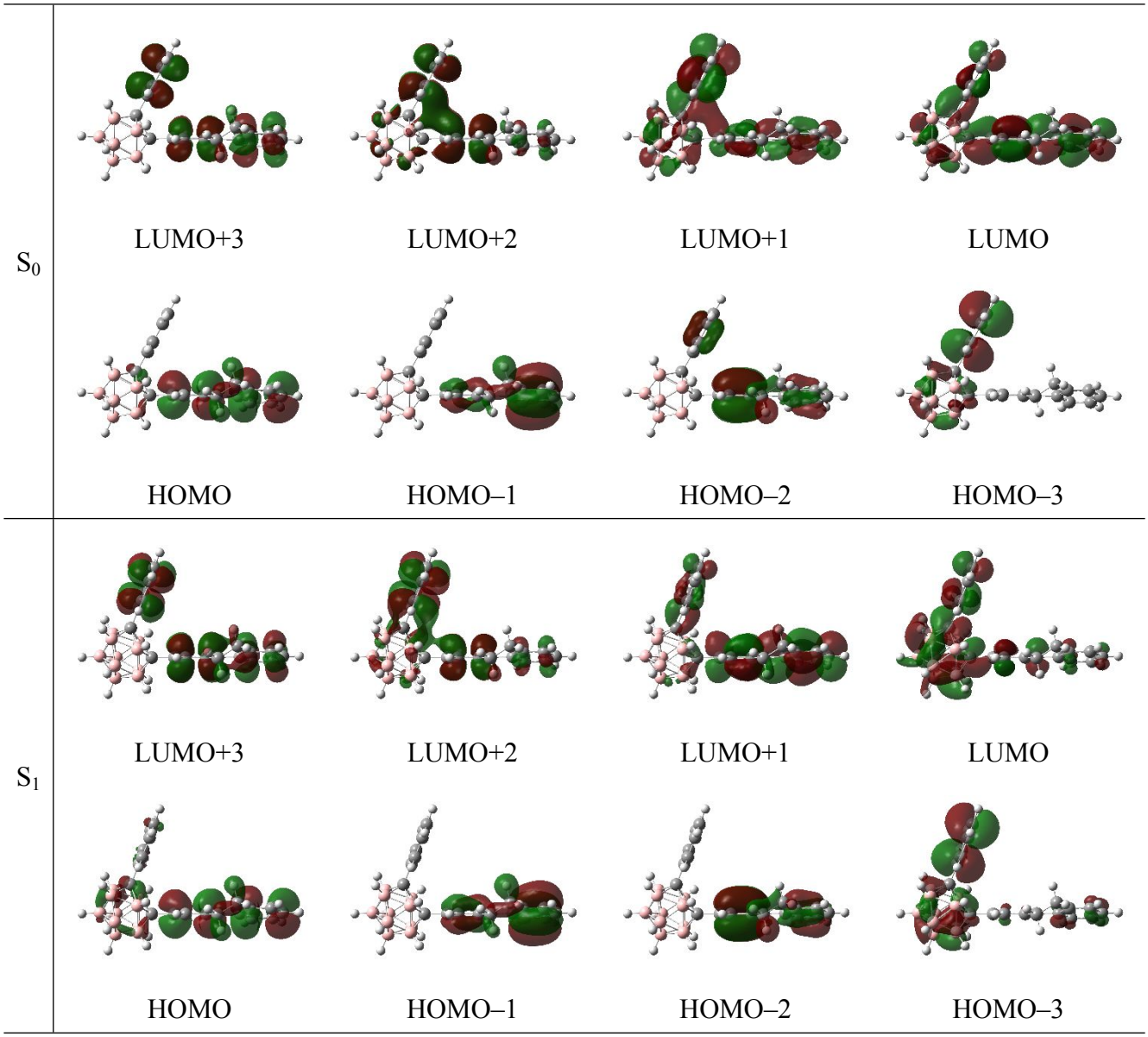


Figure S49. The selected frontier orbitals of **4HN** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S11. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **4HN** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	307.23	0.6218	HOMO → LUMO (97.65%)
2	275.95	0.0097	HOMO−2 → LUMO (9.91%)
			HOMO−1 → LUMO (48.83%)
			HOMO → LUMO+1 (14.02%)
			HOMO → LUMO+2 (14.58%)
3	268.37	0.1269	HOMO−2 → LUMO (14.96%)
			HOMO → LUMO+1 (71.18%)
			HOMO → LUMO+2 (9.28%)
4	267.26	0.0589	HOMO−2 → LUMO (35.28%)
			HOMO−1 → LUMO (30.87%)
			HOMO → LUMO+1 (13.15%)
5	250.51	0.0199	HOMO−4 → LUMO (62.32%)
			HOMO−2 → LUMO (11.26%)
			HOMO → LUMO+2 (8.55%)
		S_1	
1	503.25	0.5003	HOMO → LUMO (99.44%)
2	415.17	0.0378	HOMO−2 → LUMO (40.36%)
			HOMO−1 → LUMO (58.78%)
3	395.68	0.0188	HOMO−2 → LUMO (58.70%)
			HOMO−1 → LUMO (39.88%)
4	381.37	0.0480	HOMO−4 → LUMO (10.01%)
			HOMO−3 → LUMO (87.18%)
5	380.59	0.4209	HOMO−4 → LUMO (87.64%)
			HOMO−3 → LUMO (10.05%)

Table S12. Molecular orbital distributions (in %) and energies (in eV) of **4HN** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.33	44.3	1.08	26.2	28.4
LUMO+2	−0.68	44.2	8.65	40.8	6.27
LUMO+1	−1.04	58.3	18.9	11.2	11.6
LUMO	−1.61	9.09	24.3	43.1	23.5
HOMO	−6.13	0.15	3.80	43.5	52.6
HOMO−1	−6.77	0.26	0.35	10.4	89.0
HOMO−2	−6.99	6.76	0.87	81.8	10.6
HOMO−3	−7.16	85.8	13.6	0.22	0.33
			S_1		
LUMO+3	−0.43	26.8	1.34	44.9	27.0
LUMO+2	−0.56	67.2	7.64	19.3	5.83
LUMO+1	−1.29	7.80	5.46	43.1	43.6
LUMO	−3.39	14.7	72.1	10.1	3.13
HOMO	−5.93	1.50	6.87	44.1	47.6
HOMO−1	−6.85	1.19	1.06	21.6	76.1
HOMO−2	−7.05	0.02	1.18	76.6	22.2
HOMO−3	−7.15	73.3	21.1	1.16	4.52

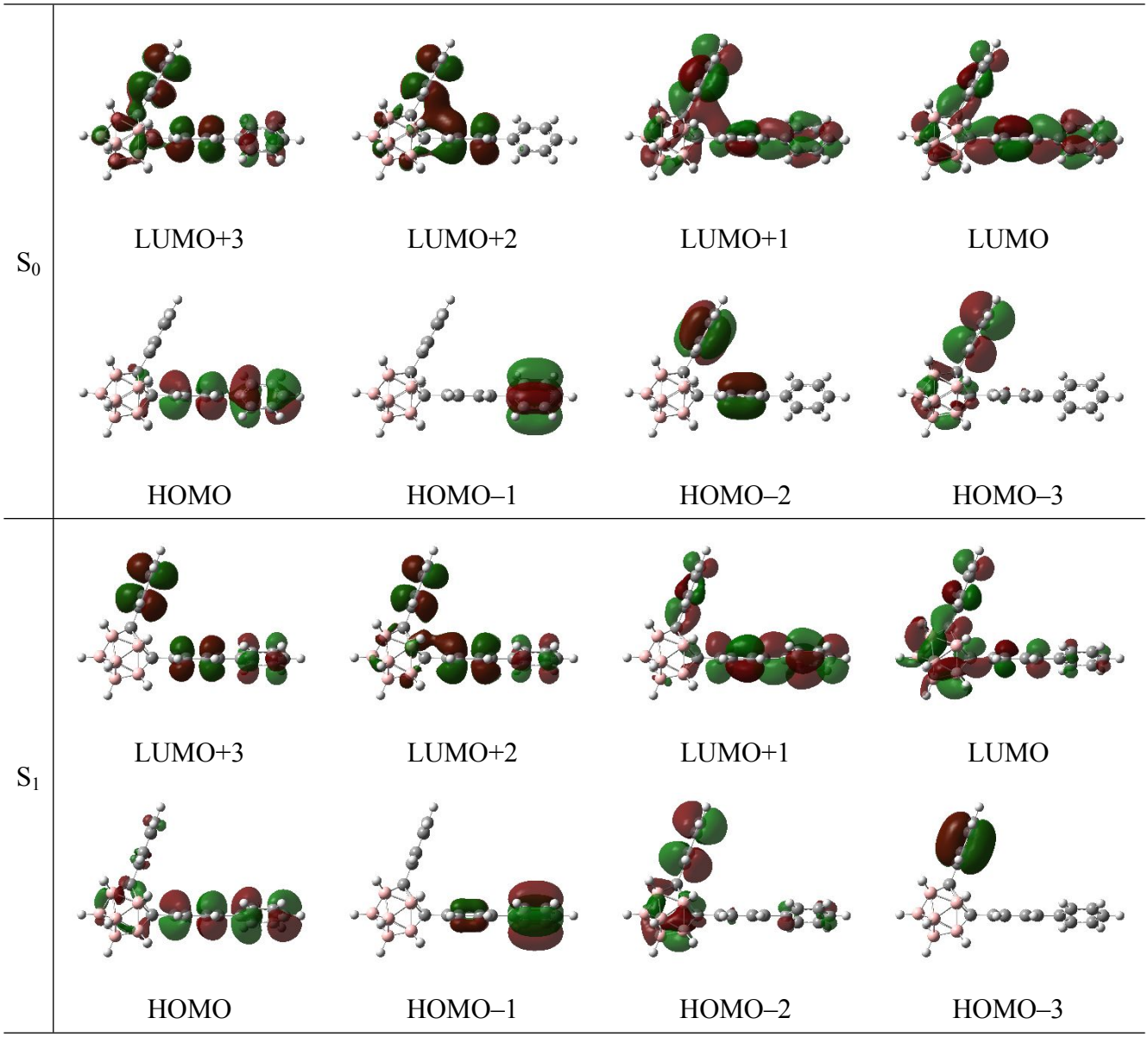


Figure S50. The selected frontier orbitals of **5HH** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S13. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **5HH** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	284.29	0.6805	HOMO → LUMO (98.21%)
2	259.43	0.0015	HOMO−4 → LUMO (16.45%)
			HOMO−2 → LUMO (22.99%)
			HOMO−1 → LUMO (17.62%)
			HOMO → LUMO+2 (28.06%)
			HOMO → LUMO+3 (7.33%)
3	257.22	0.0007	HOMO−2 → LUMO (9.04%)
			HOMO−1 → LUMO (60.33%)
			HOMO → LUMO+5 (12.72%)
4	252.49	0.1835	HOMO → LUMO+1 (95.30%)
5	248.13	0.0070	HOMO−4 → LUMO (34.84%)
			HOMO−3 → LUMO+2 (6.20%)
			HOMO−2 → LUMO (43.00%)
		S_1	
1	528.60	0.5244	HOMO → LUMO (99.33%)
2	385.33	0.0007	HOMO−4 → LUMO (43.86%)
			HOMO−1 → LUMO (53.93%)
3	383.40	0.0104	HOMO−2 → LUMO (95.62%)
4	382.89	0.2365	HOMO−3 → LUMO (97.77%)
5	370.61	0.0055	HOMO−4 → LUMO (53.84%)
			HOMO−1 → LUMO (43.50%)

Table S14. Molecular orbital distributions (in %) and energies (in eV) of **5HH** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.32	46.4	1.31	33.6	18.7
LUMO+2	−0.71	41.3	9.11	48.0	1.60
LUMO+1	−1.01	57.0	17.2	13.7	12.1
LUMO	−1.55	11.4	26.8	43.0	18.8
HOMO	−6.40	0.18	4.24	41.9	53.7
HOMO−1	−6.99	0.03	0.02	0.52	99.4
HOMO−2	−7.15	78.5	10.8	10.3	0.39
HOMO−3	−7.17	61.5	3.47	34.6	0.35
			S_1		
LUMO+3	−0.46	49.4	1.50	29.3	19.8
LUMO+2	−0.60	44.1	7.92	36.1	11.9
LUMO+1	−1.32	7.95	5.57	43.0	43.5
LUMO	−3.54	14.5	71.8	10.6	3.04
HOMO	−5.89	2.03	7.66	43.7	46.6
HOMO−1	−7.10	73.6	21.1	1.12	4.27
HOMO−2	−7.16	0.41	0.44	14.7	84.5
HOMO−3	−7.27	0.02	2.35	82.6	15.0

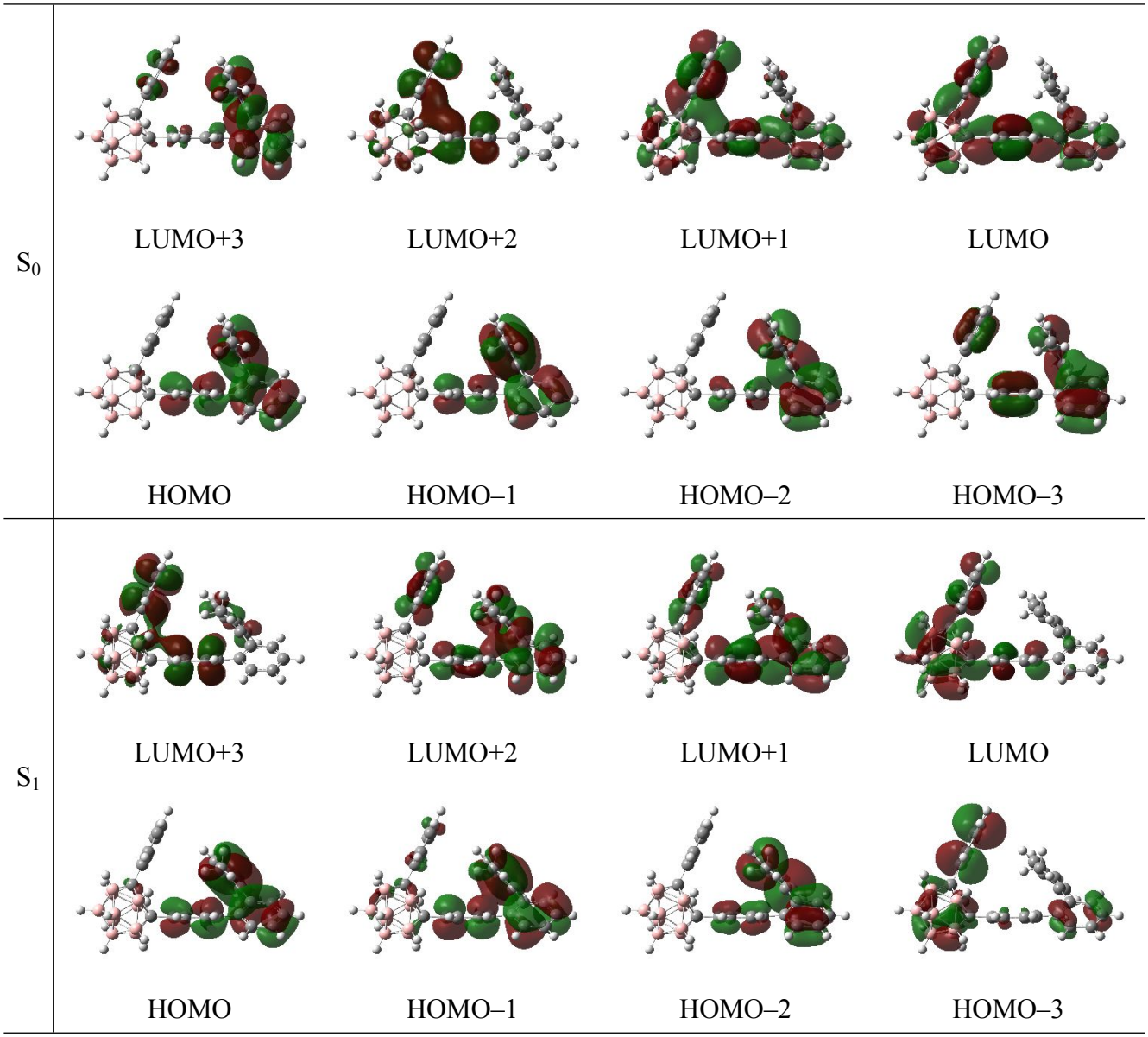


Figure S51. The selected frontier orbitals of **6HC** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S15. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **6HC** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	293.71	0.2315	HOMO → LUMO (96.21%)
2	274.54	0.1541	HOMO−1 → LUMO (96.86%)
3	265.21	0.0554	HOMO−2 → LUMO (87.34%)
4	259.15	0.0627	HOMO−3 → LUMO (8.42%)
			HOMO → LUMO+1 (71.48%)
5	257.94	0.0324	HOMO−6 → LUMO (9.24%)
			HOMO−3 → LUMO (30.38%)
			HOMO → LUMO+1 (19.52%)
			HOMO → LUMO+2 (18.71%)
		S_1	
1	502.25	0.3158	HOMO → LUMO (99.56%)
2	423.54	0.1778	HOMO−1 → LUMO (97.94%)
3	400.15	0.1022	HOMO−2 → LUMO (98.38%)
4	385.64	0.0287	HOMO−4 → LUMO (20.70%)
			HOMO−3 → LUMO (70.40%)
5	384.86	0.0102	HOMO−5 → LUMO (21.55%)
			HOMO−4 → LUMO (69.29%)

Table S16. Molecular orbital distributions (in %) and energies (in eV) of **6HC** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.47	5.65	1.14	2.93	90.3
LUMO+2	−0.69	46.0	9.10	41.5	3.36
LUMO+1	−1.01	54.1	15.5	14.1	16.3
LUMO	−1.52	13.7	28.0	40.3	18.0
HOMO	−6.30	0.07	2.03	23.0	74.9
HOMO−1	−6.57	0.05	1.46	15.5	83.0
HOMO−2	−6.75	0.67	0.97	7.47	90.9
HOMO−3	−7.06	8.09	0.50	31.3	60.1
			S_1		
LUMO+3	−0.60	73.2	7.43	16.9	2.48
LUMO+2	−0.68	12.8	1.99	11.3	73.8
LUMO+1	−1.24	7.41	4.22	30.6	57.8
LUMO	−3.42	13.5	72.8	11.4	2.32
HOMO	−5.89	0.59	2.84	18.2	78.4
HOMO−1	−6.57	2.30	5.04	28.2	64.5
HOMO−2	−6.68	0.71	0.85	8.04	90.4
HOMO−3	−7.16	70.9	20.0	1.23	7.97

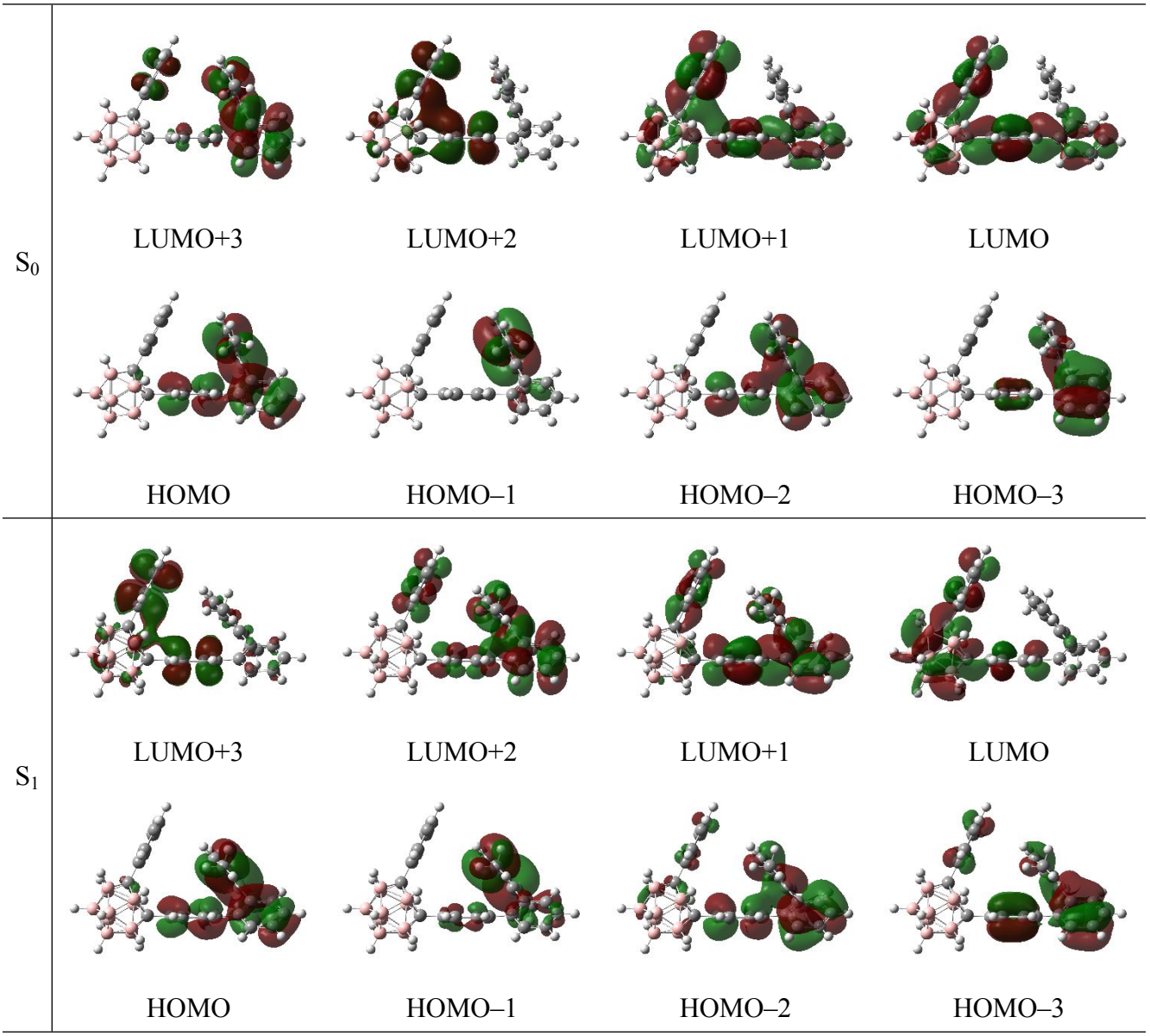


Figure S52. The selected frontier orbitals of **7HD** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S17. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **7HD** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	292.30	0.2093	HOMO → LUMO (96.04%)
2	281.16	0.0076	HOMO−1 → LUMO (97.46%)
3	273.74	0.3021	HOMO−2 → LUMO (92.48%)
4	259.65	0.0044	HOMO−6 → LUMO (6.42%)
			HOMO−3 → LUMO (53.09%)
			HOMO → LUMO+2 (12.72%)
5	257.45	0.0871	HOMO → LUMO+1 (91.32%)
		S_1	
1	511.34	0.3021	HOMO → LUMO (99.56%)
2	423.47	0.0547	HOMO−1 → LUMO (98.39%)
3	411.01	0.2824	HOMO−2 → LUMO (97.41%)
4	393.04	0.0172	HOMO−6 → LUMO (22.69%)
			HOMO−3 → LUMO (74.29%)
5	386.14	0.0283	HOMO−4 → LUMO (91.21%)

Table S18. Molecular orbital distributions (in %) and energies (in eV) of **7HD** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.42	8.68	0.69	2.37	88.3
LUMO+2	−0.69	44.3	9.07	43.1	3.53
LUMO+1	−1.00	53.0	15.4	15.9	15.7
LUMO	−1.52	14.3	29.3	40.1	16.3
HOMO	−6.32	0.07	1.97	22.4	75.6
HOMO−1	−6.46	0.14	0.05	0.77	99.0
HOMO−2	−6.60	0.38	2.47	22.9	74.3
HOMO−3	−6.95	0.85	0.10	8.11	90.9
			S_1		
LUMO+3	−0.57	77.0	7.31	13.3	2.46
LUMO+2	−0.64	9.84	1.46	8.23	80.5
LUMO+1	−1.19	8.83	4.55	34.0	52.6
LUMO	−3.42	13.5	72.9	11.4	2.25
HOMO	−5.90	0.56	2.80	18.6	78.0
HOMO−1	−6.46	0.29	0.49	4.83	94.4
HOMO−2	−6.57	2.80	5.37	27.6	64.3
HOMO−3	−7.11	9.35	3.59	47.0	40.1

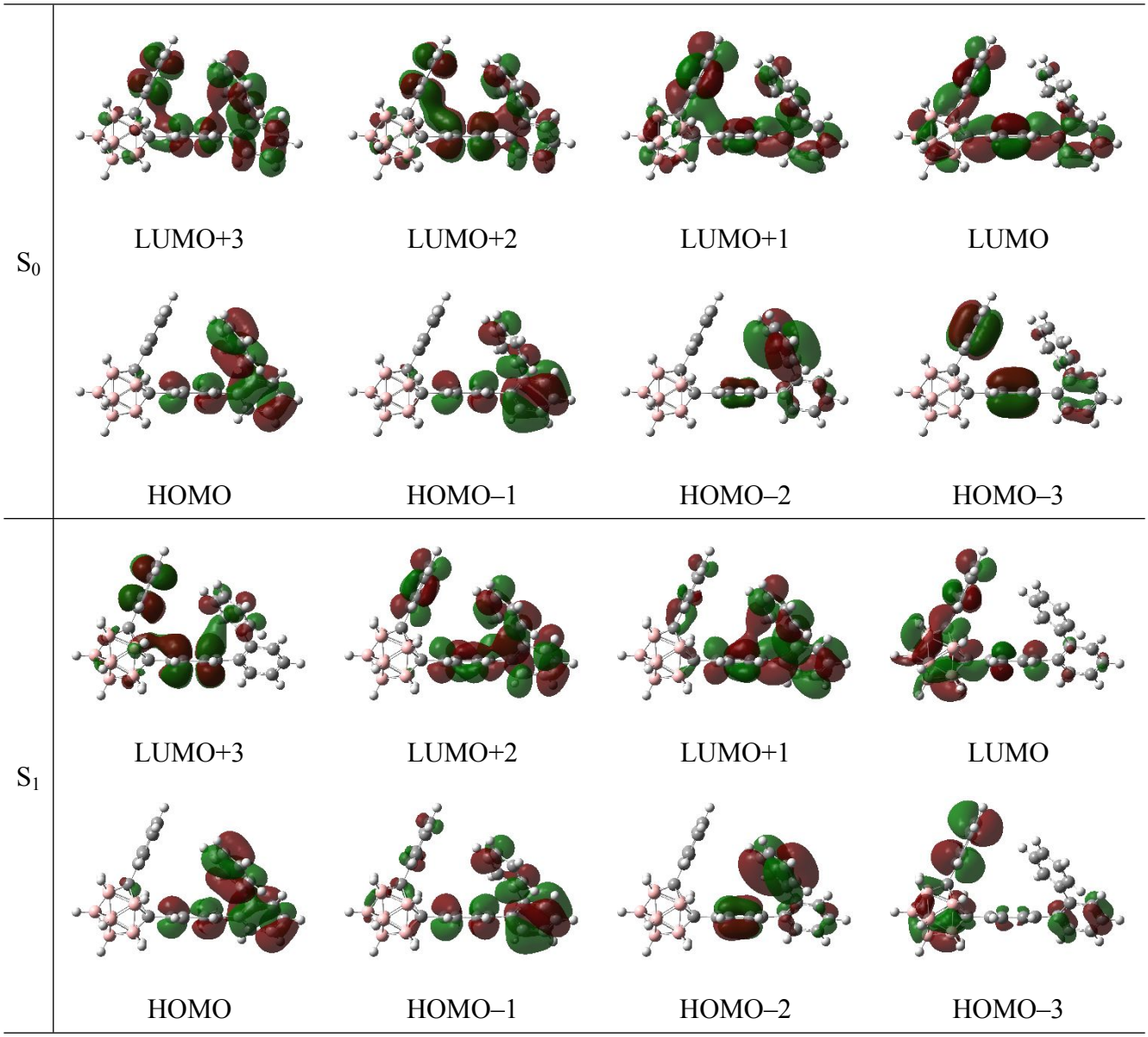


Figure S53. The selected frontier orbitals of **8HP** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S19. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **8HP** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	301.60	0.2441	HOMO → LUMO (97.19%)
2	271.44	0.1757	HOMO−1 → LUMO (79.88%)
			HOMO → LUMO+3 (5.79%)
3	266.44	0.0859	HOMO → LUMO+1 (91.04%)
4	262.19	0.0216	HOMO−3 → LUMO (15.38%)
			HOMO−2 → LUMO (31.44%)
			HOMO → LUMO+2 (23.13%)
5	257.01	0.0209	HOMO−3 → LUMO (13.34%)
			HOMO−2 → LUMO (53.17%)
			HOMO → LUMO+2 (17.90%)
		S_1	
1	513.55	0.3047	HOMO → LUMO (99.53%)
2	429.62	0.1632	HOMO−1 → LUMO (98.13%)
3	400.17	0.0143	HOMO−2 → LUMO (93.15%)
4	385.53	0.0069	HOMO−3 → LUMO (96.26%)
5	383.60	0.4139	HOMO−4 → LUMO (96.47%)

Table S20. Molecular orbital distributions (in %) and energies (in eV) of **8HP** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.63	28.6	5.09	12.7	53.7
LUMO+2	−0.73	31.5	7.02	33.8	27.7
LUMO+1	−1.03	47.6	13.5	12.9	26.0
LUMO	−1.53	16.2	30.0	36.9	17.2
HOMO	−6.19	0.07	1.76	20.5	77.7
HOMO−1	−6.67	0.30	2.55	21.6	75.5
HOMO−2	−6.88	0.24	0.11	6.15	93.5
HOMO−3	−7.13	23.5	1.27	64.2	11.0
			S_1		
LUMO+3	−0.61	54.6	7.77	31.1	6.56
LUMO+2	−0.74	14.5	2.67	20.9	62.0
LUMO+1	−1.35	4.58	3.29	22.3	70.0
LUMO	−3.41	13.5	72.7	11.4	2.37
HOMO	−5.88	0.62	3.09	19.0	77.3
HOMO−1	−6.62	3.08	5.40	26.8	64.8
HOMO−2	−6.91	0.67	0.78	22.6	76.0
HOMO−3	−7.16	69.9	19.7	1.71	8.69

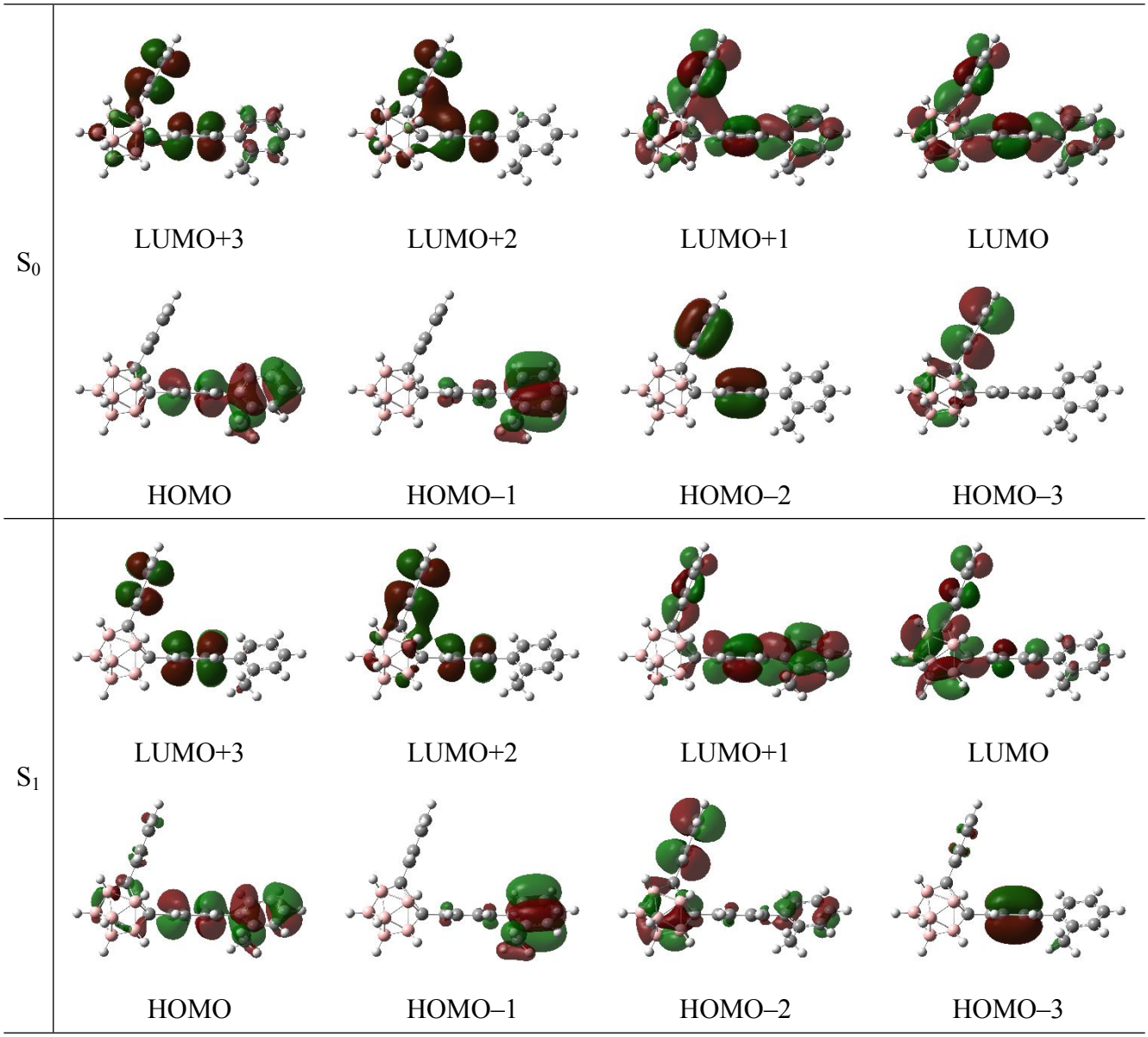


Figure S54. The selected frontier orbitals of **9HM** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S21. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **9HM** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	282.50	0.4541	HOMO → LUMO (97.69%)
2	265.17	0.0358	HOMO−1 → LUMO (85.98%)
3	255.74	0.0026	HOMO−4 → LUMO (15.10%)
			HOMO−2 → LUMO (40.39%)
			HOMO → LUMO+2 (28.63%)
4	249.62	0.1385	HOMO → LUMO+1 (93.27%)
5	247.29	0.0072	HOMO−4 → LUMO (41.10%)
			HOMO−3 → LUMO+2 (8.02%)
			HOMO−2 → LUMO (34.07%)
		S_1	
1	508.88	0.3486	HOMO → LUMO (99.26%)
2	409.26	0.0171	HOMO−1 → LUMO (98.84%)
3	386.66	0.0111	HOMO−4 → LUMO (7.19%)
			HOMO−2 → LUMO (88.79%)
4	384.50	0.2041	HOMO−4 → LUMO (42.39%)
			HOMO−3 → LUMO (54.22%)
5	384.33	0.2620	HOMO−4 → LUMO (53.14%)
			HOMO−3 → LUMO (9.00%)
			HOMO−2 → LUMO (36.00%)

Table S22. Molecular orbital distributions (in %) and energies (in eV) of **9HM** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	-0.31	49.5	1.28	41.3	7.91
LUMO+2	-0.70	43.4	9.17	45.8	1.66
LUMO+1	-0.96	51.2	13.7	22.2	12.9
LUMO	-1.50	18.3	32.7	38.2	10.8
HOMO	-6.42	0.14	3.25	32.3	64.3
HOMO−1	-6.73	0.03	0.43	3.81	95.7
HOMO−2	-7.14	82.0	12.7	4.42	0.84
HOMO−3	-7.17	49.0	1.79	48.8	0.43
			S_1		
LUMO+3	-0.40	19.6	2.78	74.9	2.81
LUMO+2	-0.56	75.4	8.36	15.8	0.40
LUMO+1	-1.18	9.86	5.16	43.8	41.2
LUMO	-3.42	14.5	72.6	10.5	2.43
HOMO	-6.12	1.79	6.79	39.1	52.4
HOMO−1	-6.83	0.80	0.65	2.56	96.0
HOMO−2	-7.14	71.0	20.2	1.82	7.02
HOMO−3	-7.25	0.09	2.36	96.9	0.67

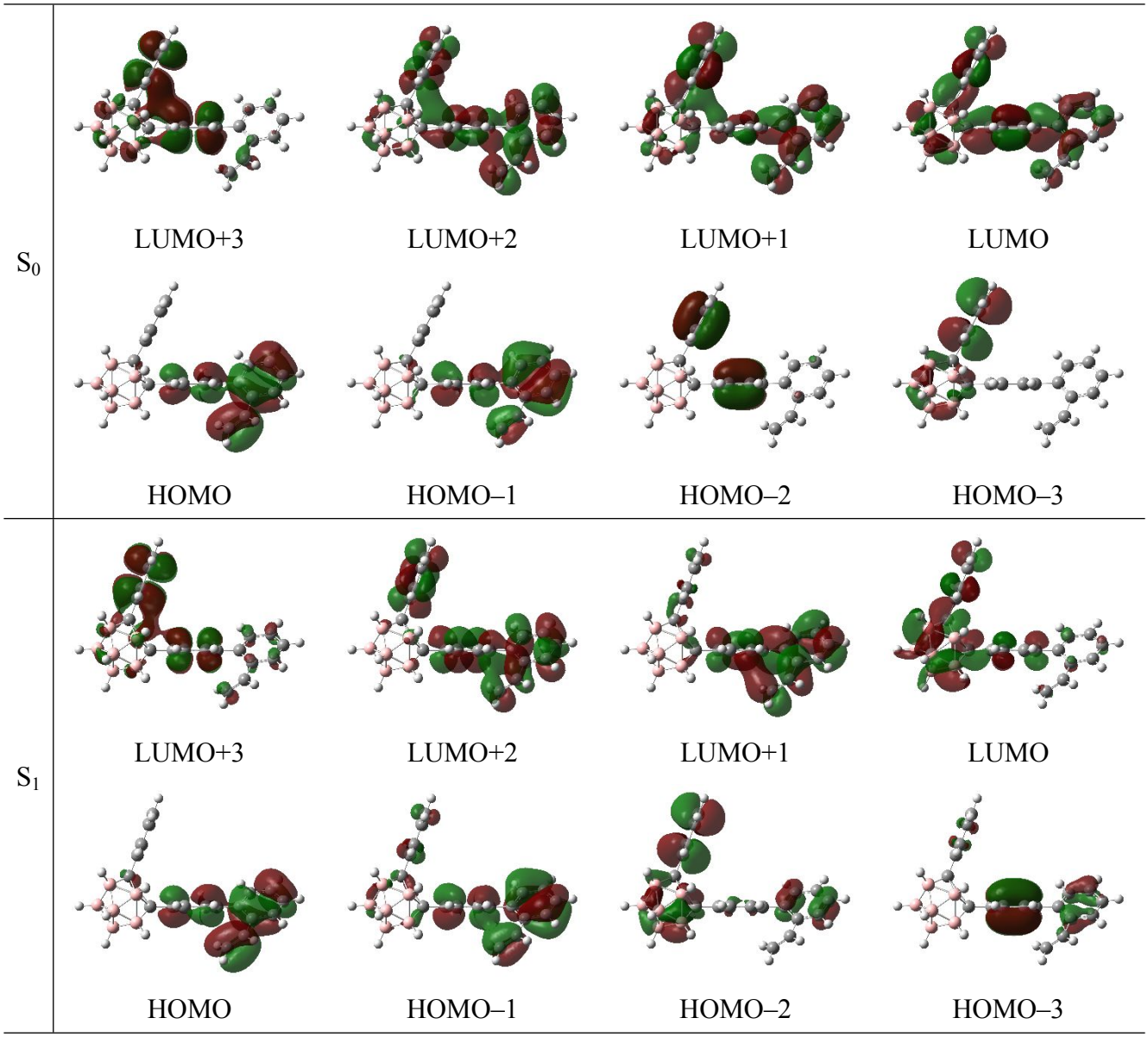


Figure S55. The selected frontier orbitals of **10HV** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S23. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **10HV** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	303.25	0.2047	HOMO → LUMO (96.42%)
2	271.48	0.1528	HOMO−1 → LUMO (67.52%)
			HOMO−1 → LUMO+1 (7.80%)
			HOMO → LUMO+2 (13.51%)
3	267.30	0.0316	HOMO → LUMO+1 (89.11%)
4	260.42	0.0014	HOMO−4 → LUMO (10.15%)
			HOMO−2 → LUMO (23.18%)
			HOMO → LUMO+3 (43.74%)
			HOMO → LUMO+4 (7.09%)
5	251.92	0.1369	HOMO−1 → LUMO (26.68%)
			HOMO−1 → LUMO+1 (24.67%)
			HOMO → LUMO+2 (23.98%)
		S_1	
1	522.50	0.3546	HOMO → LUMO (99.55%)
2	402.13	0.1398	HOMO−1 → LUMO (97.55%)
3	389.30	0.0086	HOMO−3 → LUMO (7.51%)
			HOMO−2 → LUMO (88.82%)
4	387.85	0.0085	HOMO−4 → LUMO (7.71%)
			HOMO−3 → LUMO (90.40%)
5	384.97	0.2358	HOMO−4 → LUMO (96.17%)

Table S24. Molecular orbital distributions (in %) and energies (in eV) of **10HV** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.69	45.2	9.27	39.8	5.67
LUMO+2	−0.72	18.2	6.74	23.0	52.1
LUMO+1	−1.06	39.6	13.9	6.08	40.5
LUMO	−1.52	14.7	28.3	36.7	20.2
HOMO	−6.15	0.06	1.41	17.3	81.2
HOMO−1	−6.72	0.23	2.88	23.7	73.2
HOMO−2	−7.14	37.5	1.35	59.0	2.14
HOMO−3	−7.17	83.9	13.2	1.83	1.15
			S_1		
LUMO+3	−0.55	73.7	7.98	15.8	2.54
LUMO+2	−0.69	18.5	3.50	26.4	51.6
LUMO+1	−1.48	2.84	3.15	21.1	72.9
LUMO	−3.42	13.4	73.0	11.2	2.38
HOMO	−5.83	0.69	3.20	21.5	74.6
HOMO−1	−6.68	4.56	5.87	27.8	61.7
HOMO−2	−7.14	70.4	19.3	1.08	9.27
HOMO−3	−7.22	0.17	2.04	90.9	6.86

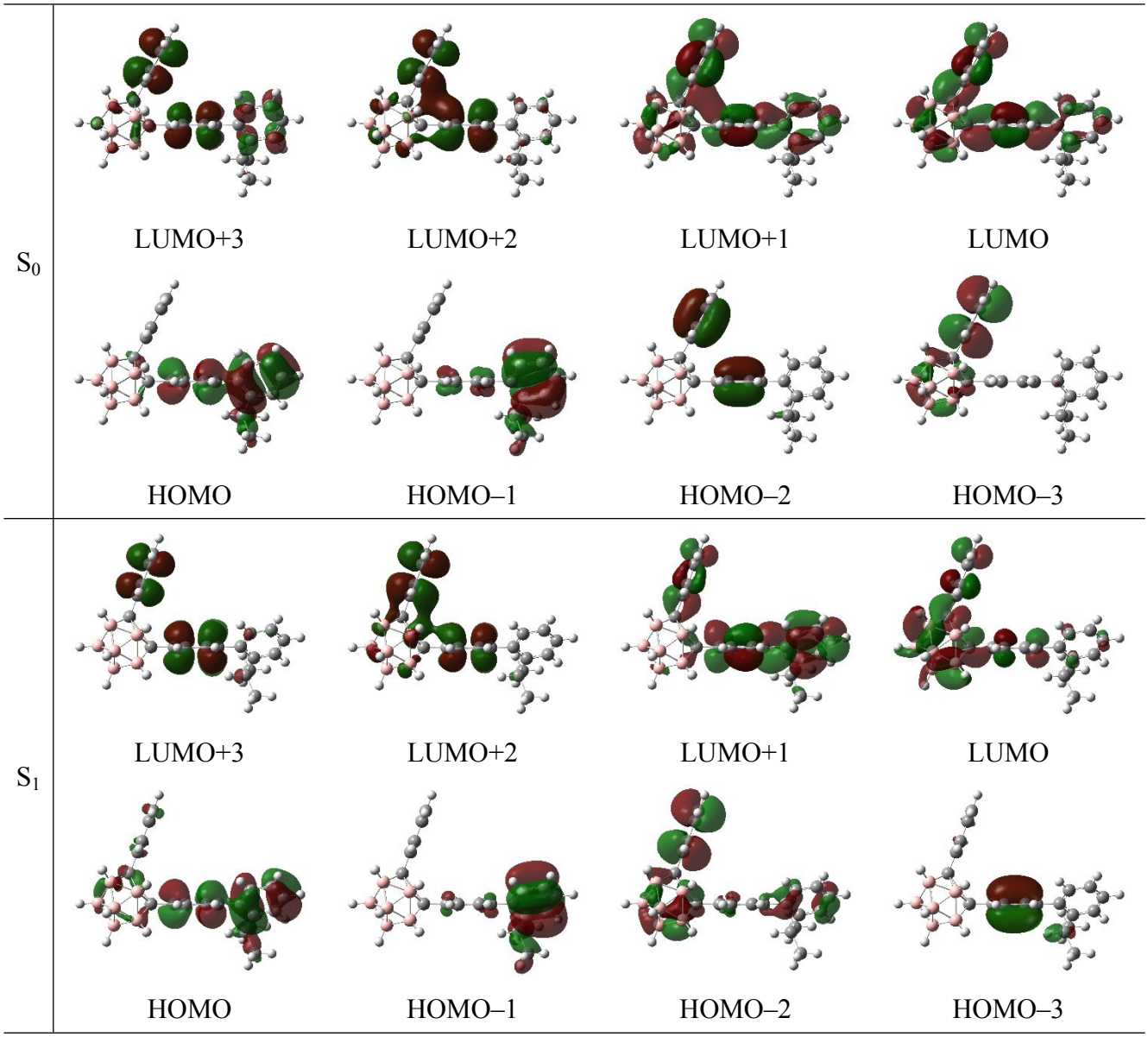


Figure S56. The selected frontier orbitals of **11HI** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S25. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **11HI** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	279.04	0.3991	HOMO → LUMO (97.22%)
2	264.11	0.0313	HOMO−1 → LUMO (86.04%)
3	254.20	0.0039	HOMO−4 → LUMO (13.13%)
			HOMO−2 → LUMO (41.99%)
			HOMO → LUMO+2 (27.20%)
4	247.22	0.1083	HOMO → LUMO+1 (90.67%)
5	246.74	0.0078	HOMO−4 → LUMO (41.82%)
			HOMO−3 → LUMO+2 (8.02%)
			HOMO−2 → LUMO (31.60%)
		S_1	
1	498.13	0.2446	HOMO → LUMO (99.24%)
2	413.17	0.0156	HOMO−1 → LUMO (98.99%)
3	387.51	0.0037	HOMO−2 → LUMO (94.70%)
4	384.87	0.4566	HOMO−3 → LUMO (96.44%)
5	384.51	0.0142	HOMO−4 → LUMO (92.43%)

Table S26. Molecular orbital distributions (in %) and energies (in eV) of **11HI** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.33	50.7	1.29	34.5	13.5
LUMO+2	−0.72	40.7	8.96	47.4	3.00
LUMO+1	−0.93	48.5	12.8	26.9	11.8
LUMO	−1.48	21.7	34.8	35.8	7.65
HOMO	−6.46	0.14	3.10	30.9	65.9
HOMO−1	−6.71	0.04	0.48	4.52	95.0
HOMO−2	−7.14	84.1	13.6	0.88	1.44
HOMO−3	−7.17	43.6	0.92	54.5	1.00
			S_1		
LUMO+3	−0.41	22.1	2.49	71.5	3.86
LUMO+2	−0.57	72.7	8.47	18.2	0.64
LUMO+1	−1.14	10.7	5.02	44.3	40.1
LUMO	−3.40	14.5	72.8	10.5	2.22
HOMO	−6.12	1.76	6.67	38.6	53.0
HOMO−1	−6.80	0.68	0.66	2.72	95.9
HOMO−2	−7.14	70.1	19.9	2.23	7.76
HOMO−3	−7.24	0.12	2.25	95.6	2.07

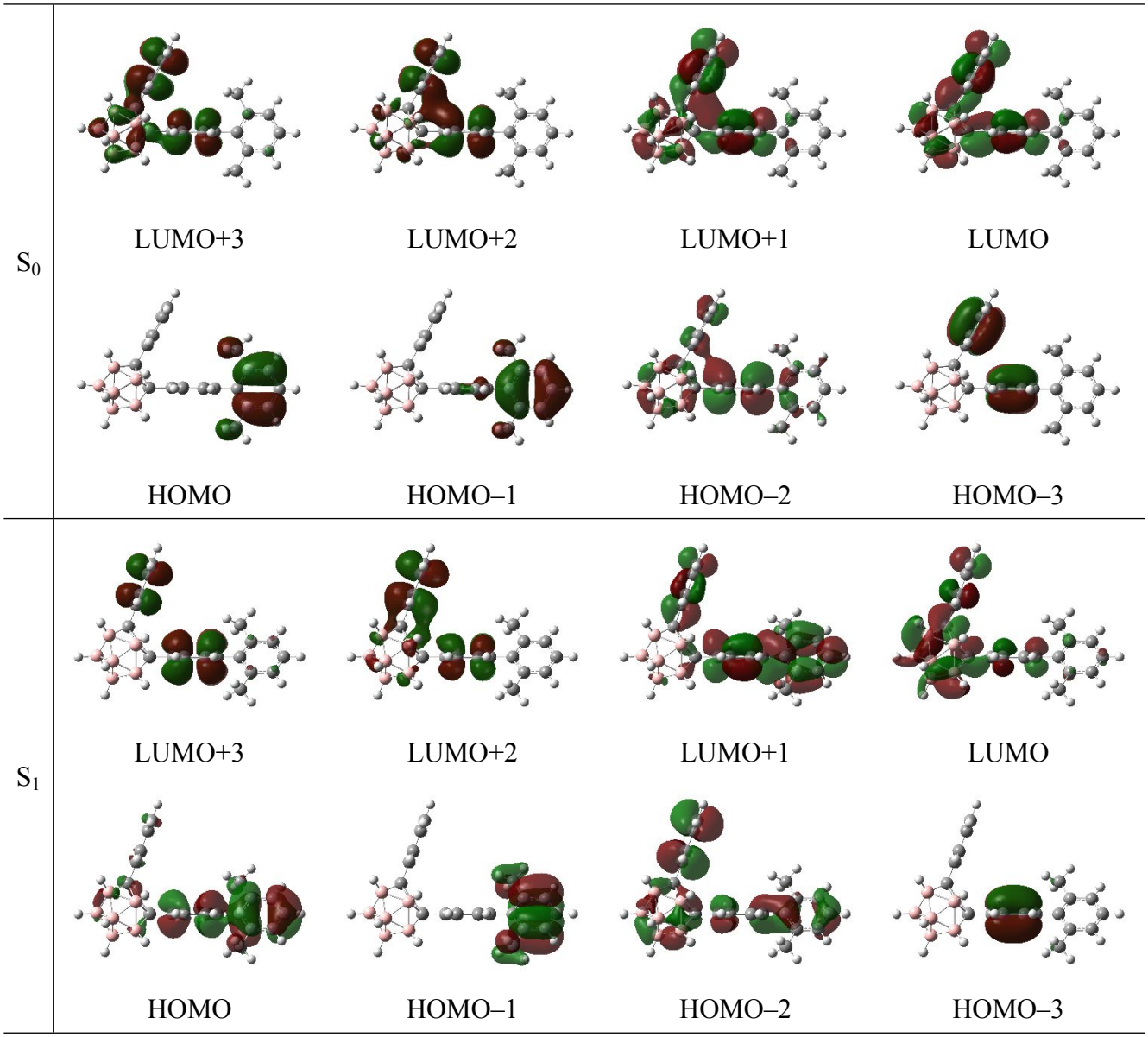


Figure S57. The selected frontier orbitals of **12MM** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S27. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **12MM** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	287.21	0.0101	HOMO → LUMO (93.48%)
2	268.23	0.0003	HOMO−1 → LUMO (88.92%)
			HOMO−1 → LUMO+1 (8.24%)
3	247.94	0.0308	HOMO−3 → LUMO (66.15%)
			HOMO−2 → LUMO (9.64%)
			HOMO−2 → LUMO+2 (12.26%)
4	245.67	0.2758	HOMO−2 → LUMO (84.51%)
5	243.50	0.0010	HOMO−5 → LUMO (66.54%)
			HOMO−4 → LUMO+2 (10.97%)
		S_1	
1	500.98	0.1012	HOMO → LUMO (99.24%)
2	418.65	0.0018	HOMO−1 → LUMO (99.80%)
3	392.64	0.2513	HOMO−2 → LUMO (98.48%)
4	390.29	0.0040	HOMO−3 → LUMO (96.02%)
5	386.24	0.0073	HOMO−4 → LUMO (95.16%)

Table S28. Molecular orbital distributions (in %) and energies (in eV) of **12MM** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.32	53.2	1.44	43.2	2.11
LUMO+2	−0.72	41.1	9.06	48.6	1.27
LUMO+1	−0.84	42.6	13.9	42.0	1.58
LUMO	−1.40	31.2	38.2	29.4	1.15
HOMO	−6.50	0.00	0.00	0.16	99.8
HOMO−1	−6.60	0.00	0.05	3.92	96.0
HOMO−2	−7.05	4.74	12.1	77.9	5.21
HOMO−3	−7.15	47.8	2.02	49.7	0.40
			S_1		
LUMO+3	−0.39	18.5	2.71	75.1	3.77
LUMO+2	−0.56	76.3	8.14	15.1	0.49
LUMO+1	−1.06	12.7	4.97	45.2	37.2
LUMO	−3.43	14.2	73.3	10.7	1.82
HOMO	−6.14	1.49	5.53	32.3	60.7
HOMO−1	−6.61	0.00	0.00	0.04	99.9
HOMO−2	−7.10	56.9	17.5	11.5	14.0
HOMO−3	−7.23	0.04	2.31	96.8	8.52

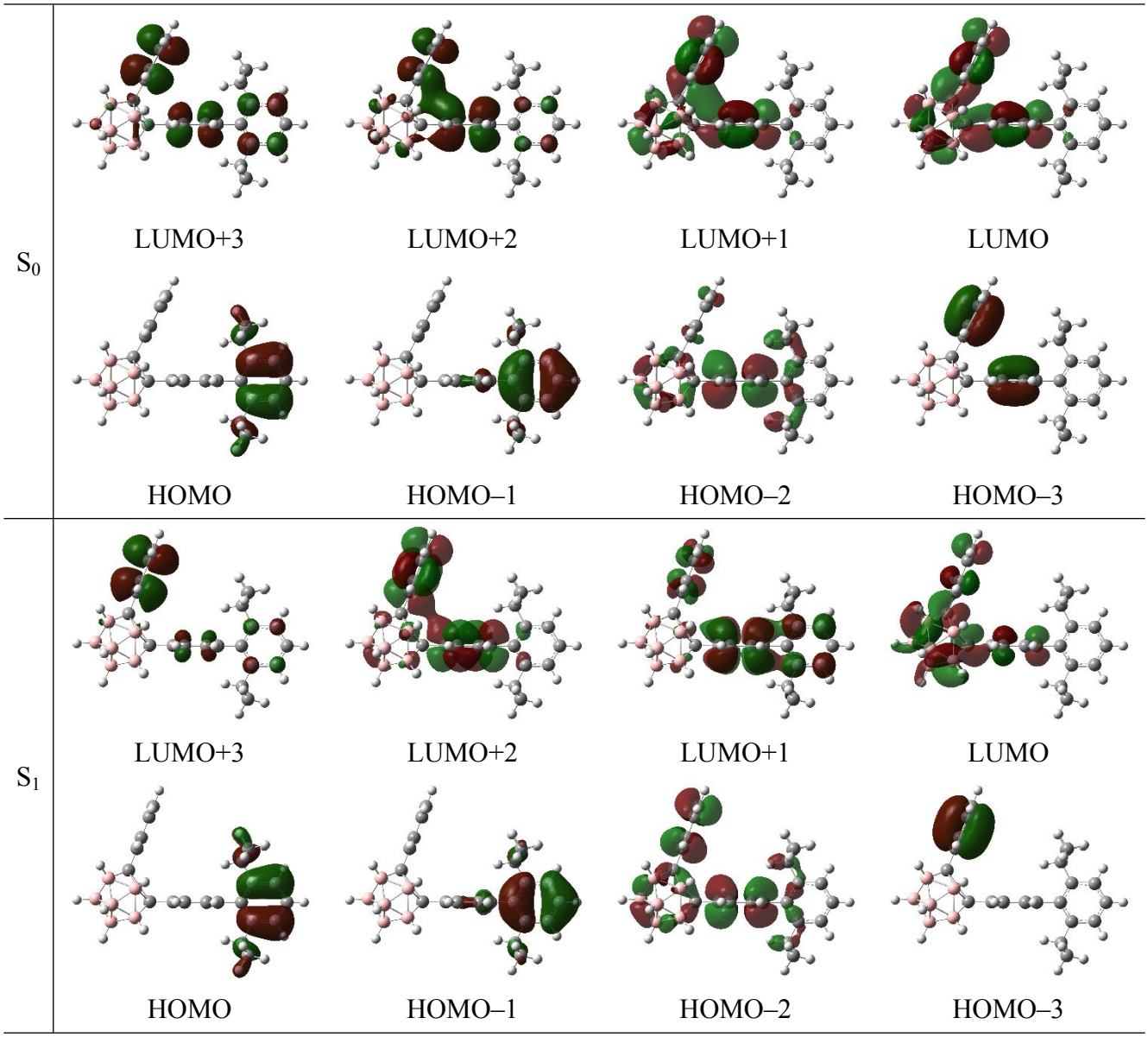


Figure S58. The selected frontier orbitals of **13PP** from B3LYP calculations (Isovalue = 0.04 a.u.) at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF.

Table S29. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **13PP** from TD-B3LYP calculations using the B3LYP geometries at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

state	λ_{calc} (nm)	f_{calc}	Major contribution
		S_0	
1	284.21	0.0268	HOMO → LUMO (95.39%)
2	265.99	0.0000	HOMO−1 → LUMO (90.74%)
			HOMO−1 → LUMO+1 (8.19%)
3	248.13	0.0087	HOMO−3 → LUMO (67.89%)
			HOMO−2 → LUMO+2 (17.11%)
4	247.91	0.3050	HOMO−2 → LUMO (94.28%)
5	243.83	0.0014	HOMO−5 → LUMO (59.44%)
			HOMO−4 → LUMO+2 (9.10%)
			HOMO−3 → LUMO (8.88%)
		S_1	
1	521.05	0.0297	HOMO → LUMO (99.88%)
2	435.37	0.0043	HOMO−2 → LUMO (13.63%)
			HOMO−1 → LUMO (85.95%)
3	412.13	0.0985	HOMO−2 → LUMO (85.67%)
			HOMO−1 → LUMO (13.68%)
4	399.86	0.0045	HOMO−3 → LUMO (96.39%)
5	394.25	0.0055	HOMO−4 → LUMO (95.65%)

Table S30. Molecular orbital distributions (in %) and energies (in eV) of **13PP** at their ground state (S_0) and the first excited state (S_1) fully optimized geometries in THF

	E (eV)	car-phenyl	carborane	bridged phenyl	terminal phenyl
			S_0		
LUMO+3	−0.27	6.3	1.68	26.4	11.6
LUMO+2	−0.37	32.1	8.21	53.2	6.43
LUMO+1	−0.76	42.7	13.7	42.1	1.49
LUMO	−1.40	31.1	38.3	29.5	1.14
HOMO	−6.43	0.00	0.00	0.34	99.6
HOMO−1	−6.63	0.00	0.05	3.88	96.1
HOMO−2	−7.00	2.67	11.2	78.3	7.88
HOMO−3	−7.15	49.3	0.92	49.1	0.30
			S_1		
LUMO+3	−0.48	85.8	3.55	6.03	4.67
LUMO+2	−0.70	44.6	7.29	46.2	1.87
LUMO+1	−0.70	8.44	5.44	68.0	18.1
LUMO	−3.50	12.4	75.3	11.8	0.54
HOMO	−6.12	0.00	0.00	0.20	99.8
HOMO−1	−6.78	0.05	0.11	4.08	95.8
HOMO−2	−6.90	24.3	15.4	55.4	4.95
HOMO−3	−7.23	55.9	21.2	20.6	2.22

Table S31. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **1HF** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.589259	-1.057288	0.119742
C	2.667941	0.333029	-0.055707
B	2.638910	-0.583075	1.403211
H	2.174195	-0.100896	2.370658
B	2.405058	-2.290559	0.972918
H	1.747169	-2.961912	1.690559
B	2.210550	-2.361968	-0.789255
H	1.417815	-3.082563	-1.290465
B	2.330071	-0.696717	-1.395148
H	1.661053	-0.287006	-2.272329
B	3.713314	-1.785359	-1.538263
H	4.049878	-2.179987	-2.604249
B	3.775370	-2.774293	-0.051911
H	4.160625	-3.895536	-0.048854
B	4.029658	-1.668928	1.328219
H	4.593537	-1.980123	2.323413
B	4.163398	-0.018662	0.686905
H	4.722175	0.885040	1.206422
B	3.969133	-0.090656	-1.075129
H	4.394274	0.763092	-1.774530
B	4.857280	-1.376547	-0.227955
H	6.031786	-1.478097	-0.353650
C	0.107812	-0.836992	0.273498
C	-0.467418	-0.718293	1.551275
H	0.164350	-0.766238	2.429083
C	-1.840969	-0.556058	1.717267
H	-2.255658	-0.469419	2.717117
C	-2.663327	-0.515278	0.590721
C	-2.098728	-0.649260	-0.693850
C	-0.731306	-0.811415	-0.855740
H	-0.312254	-0.929676	-1.847901
C	-5.114415	-0.194683	1.415522
C	-6.439095	-0.071043	0.994789
C	-6.761873	-0.112923	-0.366444
C	-5.763399	-0.279519	-1.331949
C	-4.441545	-0.403232	-0.919230
C	-4.115945	-0.360913	0.452855
H	-4.869138	-0.161789	2.473265
H	-7.227664	0.058645	1.730077
H	-7.798235	-0.015453	-0.675970
H	-6.022513	-0.311600	-2.386889
C	1.246960	3.660384	-1.257331
C	1.098747	4.359089	-0.059470
C	1.459199	3.746808	1.140497
C	1.953795	2.443911	1.144976
C	2.092066	1.725842	-0.052350
C	1.740859	2.357340	-1.255182
H	0.982680	4.129444	-2.200171
H	0.713669	5.374313	-0.061944
H	1.360864	4.283363	2.079201
H	2.243679	1.990759	2.084552
H	1.864599	1.835953	-2.196106
C	-3.186385	-0.591435	-1.747034
H	-3.223297	-1.509980	-2.347470
H	-3.030707	0.235052	-2.452904

Table S32. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **1HF** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.243839	-1.328480	0.060106
C	2.983157	0.307079	-0.049315
B	2.367367	-0.787062	1.206998
H	1.957777	-0.286445	2.201834
B	1.962062	-2.567802	0.857184
H	1.286116	-3.211042	1.592860
B	1.799973	-2.513892	-0.926065
H	0.999597	-3.112816	-1.568347
B	2.153491	-0.711649	-1.234272
H	1.585293	-0.155629	-2.114660
B	3.367207	-2.040921	-1.590505
H	3.665461	-2.414996	-2.680144
B	3.280435	-3.152435	-0.178102
H	3.533868	-4.314149	-0.235805
B	3.621989	-2.128551	1.261327
H	4.107884	-2.563381	2.256730
B	4.130584	-0.518715	0.739561
H	4.886308	0.114824	1.401818
B	3.972698	-0.467093	-1.073017
H	4.604524	0.209153	-1.817811
B	4.559472	-1.949116	-0.253708
H	5.702632	-2.263944	-0.363905
C	-0.215392	-1.035906	0.210741
C	-0.818999	-1.066504	1.501150
H	-0.202780	-1.308371	2.358368
C	-2.158106	-0.782507	1.681826
H	-2.593052	-0.797800	2.675587
C	-2.945168	-0.475598	0.550912
C	-2.355539	-0.465525	-0.750006
C	-1.012523	-0.745550	-0.917098
H	-0.564895	-0.736707	-1.903690
C	-5.342459	-0.040996	1.420988
C	-6.625540	0.284990	1.020123
C	-6.919748	0.498667	-0.345357
C	-5.929789	0.388681	-1.335718
C	-4.642698	0.064910	-0.951261
C	-4.337365	-0.153688	0.432089
H	-5.110747	-0.206499	2.467481
H	-7.417969	0.379370	1.754523
H	-7.934397	0.753856	-0.633236
H	-6.179431	0.557033	-2.378090
C	2.306211	3.878224	-1.091518
C	2.307459	4.538316	0.141822
C	2.528808	3.805078	1.312320
C	2.740862	2.431484	1.253981
C	2.741388	1.748623	0.016699
C	2.516809	2.504687	-1.155977
H	2.141365	4.438291	-2.007476
H	2.140333	5.610000	0.189914
H	2.537402	4.307757	2.275137
H	2.914911	1.874551	2.168111
H	2.516968	2.004878	-2.118448
C	-3.397955	-0.117887	-1.788479
H	-3.518336	-0.913134	-2.534037
H	-3.138744	0.792787	-2.341886

Table S33. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **2HT** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-2.163018	0.538547	-0.909760
C	-3.258598	-0.194750	0.260313
B	-2.755902	1.444028	0.433153
H	-2.011843	1.725490	1.300448
B	-2.643004	2.152164	-1.191972
H	-1.780385	2.933443	-1.401660
B	-3.016403	0.863365	-2.353101
H	-2.409994	0.752969	-3.362495
B	-3.349490	-0.605418	-1.412453
H	-2.999906	-1.676736	-1.751222
B	-4.688589	0.335167	-2.075759
H	-5.340849	-0.105710	-2.961917
B	-4.258798	2.062610	-1.926701
H	-4.604760	2.875524	-2.717215
B	-4.080330	2.432473	-0.187821
H	-4.293397	3.500042	0.281331
B	-4.436878	0.951329	0.724393
H	-4.815595	0.897066	1.843458
B	-4.809625	-0.337596	-0.436849
H	-5.449549	-1.280232	-0.119930
B	-5.363079	1.322428	-0.748046
H	-6.515012	1.594189	-0.679808
C	-0.712301	0.135357	-0.923737
C	-0.264867	-0.951925	-1.697554
H	-0.964623	-1.530767	-2.286362
C	1.075569	-1.280586	-1.724946
H	1.373980	-2.121873	-2.337453
C	2.044916	-0.557113	-0.997693
C	1.608367	0.555994	-0.232521
C	0.234186	0.870699	-0.219703
H	-0.104737	1.724260	0.347465
C	3.925722	-2.034046	-1.762700
C	5.263523	-2.382492	-1.794216
C	6.193966	-1.618841	-1.077605
C	5.766162	-0.526304	-0.345137
C	4.406016	-0.147589	-0.295482
C	3.463294	-0.921303	-1.025110
H	5.586451	-3.243618	-2.371170
H	7.247568	-1.880767	-1.093216
H	6.506603	0.044356	0.201178
C	-1.834414	-3.175302	3.045961
C	-1.728629	-1.819770	3.355485
C	-2.176540	-0.854974	2.454901
C	-2.733672	-1.229168	1.223080
C	-2.848481	-2.596421	0.928335
C	-2.401336	-3.559195	1.830876
H	-1.485049	-3.925934	3.748400
H	-1.299515	-1.507029	4.302416
H	-2.100188	0.191861	2.719904
H	-3.299746	-2.912661	-0.003918
H	-2.501219	-4.611276	1.582113
C	3.958220	1.010887	0.485787
C	4.869614	1.804884	1.217222
C	2.580107	1.356742	0.521084
C	4.456223	2.896643	1.958703
H	5.925425	1.565017	1.205622
C	2.184371	2.476007	1.286816
C	3.097840	3.236060	1.994369
H	5.184393	3.485363	2.508273
H	1.140987	2.762701	1.330849
H	2.759269	4.091076	2.571435
H	3.224725	-2.641737	-2.321360

Table S34. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **2HT** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.868025	1.145288	-0.736191
C	-3.598371	-0.261147	0.140060
B	-2.671911	1.070481	0.773529
H	-2.013652	0.867568	1.741930
B	-2.346126	2.619197	-0.214453
H	-1.491970	3.395025	0.074643
B	-2.678449	2.006148	-1.864637
H	-2.082792	2.311551	-2.847869
B	-3.121767	0.237707	-1.461506
H	-2.815325	-0.613518	-2.231589
B	-4.368933	1.506546	-1.919700
H	-4.943230	1.559235	-2.961960
B	-3.889915	2.983635	-1.011487
H	-4.133611	4.091930	-1.375126
B	-3.836454	2.488928	0.717710
H	-4.020113	3.261428	1.605792
B	-4.511392	0.865417	0.881855
H	-5.071807	0.535634	1.876930
B	-4.844729	0.247194	-0.777246
H	-5.664109	-0.562855	-1.069234
B	-5.161813	1.952098	-0.370336
H	-6.283487	2.346700	-0.290634
C	-0.445507	0.746606	-0.877573
C	0.036906	0.151268	-2.057231
H	-0.639784	-0.018009	-2.886806
C	1.374113	-0.230344	-2.191465
H	1.671815	-0.680470	-3.129770
C	2.304498	-0.041889	-1.165892
C	1.844805	0.574798	0.035228
C	0.476387	0.952522	0.142419
H	0.121493	1.422640	1.047548
C	4.185925	-1.086269	-2.451410
C	5.522668	-1.473503	-2.576117
C	6.425762	-1.235805	-1.536407
C	5.979333	-0.614508	-0.383858
C	4.624319	-0.208737	-0.230926
C	3.708534	-0.452206	-1.298356
H	5.851933	-1.962177	-3.486935
H	7.463605	-1.535462	-1.626795
H	6.690001	-0.443650	0.413037
C	-3.016042	-4.291693	1.525225
C	-2.893541	-3.215703	2.408726
C	-3.077196	-1.909721	1.960557
C	-3.392432	-1.640868	0.612770
C	-3.514420	-2.737755	-0.264778
C	-3.330070	-4.042623	0.186326
H	-2.871682	-5.309269	1.875478
H	-2.655634	-3.394319	3.453639
H	-2.983443	-1.084522	2.658324
H	-3.761538	-2.559641	-1.305807
H	-3.434061	-4.869306	-0.510876
C	4.167149	0.432490	0.978901
C	5.046776	0.704232	2.057877
C	2.765670	0.815082	1.116806
C	4.602833	1.302900	3.211986
H	6.092628	0.441877	1.985490
C	2.350897	1.427368	2.331821
C	3.236046	1.666309	3.351922
H	5.297069	1.499309	4.021484
H	1.318937	1.716092	2.467928
H	2.894918	2.135383	4.267957
H	3.519176	-1.294486	-3.277941

Table S35. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **3HB** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.749520	-1.060653	-0.048463
C	2.811220	0.343981	-0.039219
B	2.582634	-0.600883	1.386703
H	1.971534	-0.139554	2.280337
B	2.446637	-2.302118	0.896983
H	1.697749	-2.995601	1.494217
B	2.519609	-2.339618	-0.875501
H	1.824207	-3.063095	-1.501283
B	2.700181	-0.662578	-1.432515
H	2.155097	-0.252545	-2.391418
B	4.107423	-1.727261	-1.382865
H	4.605907	-2.097822	-2.392455
B	3.963040	-2.743957	0.079450
H	4.363504	-3.859042	0.119588
B	3.988703	-1.662489	1.500668
H	4.404319	-1.982696	2.563610
B	4.185467	0.001536	0.913046
H	4.645668	0.902908	1.524800
B	4.260120	-0.037238	-0.859522
H	4.768219	0.838405	-1.470864
B	5.033915	-1.326284	0.090732
H	6.215526	-1.407076	0.142454
C	0.258957	-0.863228	-0.130580
C	-0.406437	-0.940713	-1.376679
H	0.160867	-1.127114	-2.279867
C	-1.776589	-0.799399	-1.461527
H	-2.237850	-0.871639	-2.439640
C	-2.574772	-0.574055	-0.317428
C	-1.911061	-0.511897	0.941959
C	-0.508671	-0.660816	1.006686
H	-0.039598	-0.622337	1.982467
C	-4.758234	-0.456153	-1.575059
C	-6.132287	-0.301739	-1.583622
C	-6.833092	-0.097653	-0.380449
C	-6.141142	-0.051198	0.813364
C	-4.736146	-0.206236	0.848103
C	-4.020782	-0.414738	-0.368906
H	-6.672175	-0.338461	-2.525021
H	-7.912123	0.022563	-0.392952
H	-6.670552	0.106033	1.749346
C	1.179457	4.343558	-0.155912
C	1.475631	3.738254	1.065130
C	1.989822	2.443700	1.101739
C	2.214206	1.727571	-0.084030
C	1.927480	2.352068	-1.306979
C	1.412218	3.646562	-1.341051
H	0.778066	5.352042	-0.183813
H	1.310892	4.273714	1.995113
H	2.228815	1.995042	2.057962
H	2.115891	1.832709	-2.237965
H	1.197236	4.109961	-2.299046
C	-4.023810	-0.156066	2.093300
C	-2.673217	-0.301451	2.140051
H	-4.245934	-0.610747	-2.517944
H	-2.144816	-0.261552	3.088479
H	-4.592714	0.002159	3.005443

Table S36. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **3HB** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.399638	-1.346774	-0.095202
C	3.147310	0.292088	-0.004891
B	2.382882	-0.748317	1.168323
H	1.844566	-0.227867	2.090882
B	2.019982	-2.547295	0.825724
H	1.253438	-3.179788	1.479367
B	2.100882	-2.540717	-0.963464
H	1.400224	-3.171585	-1.688787
B	2.492469	-0.736289	-1.254791
H	2.039955	-0.206375	-2.217348
B	3.738765	-2.075928	-1.424205
H	4.176056	-2.480888	-2.455510
B	3.465539	-3.152207	-0.008371
H	3.723122	-4.315546	-0.002535
B	3.608448	-2.090081	1.437291
H	3.949247	-2.505497	2.500374
B	4.206101	-0.504170	0.940932
H	4.871522	0.152111	1.675309
B	4.287343	-0.495225	-0.860153
H	5.015805	0.168482	-1.524707
B	4.749296	-1.952080	0.056259
H	5.892451	-2.284764	0.106917
C	-0.051605	-1.035306	-0.161235
C	-0.716227	-0.911320	-1.401203
H	-0.151819	-1.050573	-2.316050
C	-2.080952	-0.614046	-1.501019
H	-2.510395	-0.535502	-2.492527
C	-2.867166	-0.424745	-0.363450
C	-2.213652	-0.555909	0.904951
C	-0.823330	-0.860500	0.977827
H	-0.372372	-0.953297	1.959556
C	-5.016476	0.040700	-1.593209
C	-6.384100	0.344178	-1.576751
C	-7.081102	0.510117	-0.370108
C	-6.398403	0.369861	0.821631
C	-5.006883	0.060812	0.830740
C	-4.295946	-0.108278	-0.405380
H	-6.908754	0.451990	-2.520104
H	-8.139079	0.744929	-0.377240
H	-6.908399	0.492537	1.771605
C	2.524201	4.547362	-0.007317
C	2.582749	3.841953	1.197897
C	2.779753	2.463168	1.200095
C	2.927602	1.747833	-0.006227
C	2.868316	2.474927	-1.212992
C	2.671010	3.853744	-1.211778
H	2.369617	5.622098	-0.007727
H	2.476489	4.368718	2.142112
H	2.827509	1.929096	2.143039
H	2.984787	1.949993	-2.155021
H	2.633672	4.389616	-2.156095
C	-4.321674	-0.080492	2.052380
C	-2.955601	-0.381806	2.088451
H	-4.528325	-0.076069	-2.552960
H	-2.458360	-0.482803	3.047303
H	-4.864266	0.047134	2.983154

Table S37. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **4HN** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.776312	-1.069040	-0.048481
C	-2.844773	0.343719	-0.036462
B	-2.756155	-0.687268	-1.415391
H	-2.240963	-0.289919	-2.394518
B	-2.566635	-2.357320	-0.839422
H	-1.887945	-3.093113	-1.469151
B	-2.457171	-2.289491	0.929783
H	-1.702417	-2.977995	1.525587
B	-2.582311	-0.579520	1.395410
H	-1.953062	-0.110997	2.270985
B	-3.985655	-1.640706	1.556098
H	-4.380414	-1.947675	2.631955
B	-3.989944	-2.744192	0.152585
H	-4.391852	-3.858996	0.220236
B	-4.163593	-1.750838	-1.320899
H	-4.686225	-2.137261	-2.313392
B	-4.306133	-0.053884	-0.820174
H	-4.832497	0.807350	-1.436527
B	-4.196933	0.013637	0.948924
H	-4.647639	0.921746	1.557938
B	-5.059982	-1.327535	0.164396
H	-6.241597	-1.410003	0.240756
C	-0.288014	-0.875449	-0.149939
C	0.353946	-0.856114	-1.396717
H	-0.218612	-0.951752	-2.310648
C	1.734495	-0.714207	-1.478880
H	2.192453	-0.676176	-2.461292
C	2.529480	-0.599478	-0.328161
C	1.887862	-0.617429	0.930621
C	0.503224	-0.758532	1.002555
H	0.039952	-0.784682	1.981942
C	-1.410097	3.734558	0.952833
C	-1.220807	4.338420	-0.290665
C	-1.556938	3.641232	-1.451555
C	-2.069222	2.347253	-1.371631
C	-2.249975	1.725205	-0.126324
C	-1.922013	2.440649	1.035990
H	-1.163268	4.269954	1.864216
H	-0.821669	5.345962	-0.354162
H	-1.424935	4.103252	-2.424831
H	-2.336838	1.828541	-2.283650
H	-2.074403	1.995210	2.011087
C	6.076534	0.226064	0.672853
C	4.689378	0.070138	0.728075
C	4.004064	-0.459856	-0.389423
C	4.743472	-0.839476	-1.522223
C	6.126698	-0.679422	-1.563533
C	6.797607	-0.139626	-0.464524
H	6.596956	0.635285	1.535003
H	4.238475	-1.284790	-2.373217
H	6.679052	-0.983966	-2.447352
H	7.876182	-0.015562	-0.487574
C	3.897110	0.469108	1.953601
H	3.499909	1.485977	1.819997
H	4.549000	0.499042	2.831974
C	2.729548	-0.498505	2.181590
H	2.113388	-0.171192	3.024400
H	3.129931	-1.487929	2.446095

Table S38. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **4HN** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.453083	-1.353040	0.049614
C	-3.157415	0.316865	-0.055281
B	-2.499388	-0.871609	-1.195682
H	-2.019544	-0.451286	-2.196495
B	-2.156052	-2.629619	-0.700315
H	-1.456419	-3.338359	-1.348524
B	-2.091681	-2.455065	1.080808
H	-1.343937	-3.024330	1.807815
B	-2.424033	-0.628115	1.242479
H	-1.898477	-0.023578	2.117243
B	-3.683599	-1.906418	1.618832
H	-4.050694	-2.197811	2.712813
B	-3.543083	-3.115375	0.294210
H	-3.824954	-4.265571	0.416823
B	-3.779274	-2.190073	-1.229694
H	-4.216961	-2.684971	-2.219537
B	-4.280579	-0.537670	-0.849663
H	-4.982729	0.063016	-1.596251
B	-4.225230	-0.363392	0.959106
H	-4.882614	0.376623	1.616052
B	-4.797263	-1.886614	0.211540
H	-5.951401	-2.173059	0.276466
C	0.013282	-1.088467	-0.048434
C	0.704810	-1.307304	-1.270612
H	0.155737	-1.662940	-2.133927
C	2.052672	-1.047206	-1.381185
H	2.532182	-1.185786	-2.342544
C	2.802892	-0.566737	-0.276092
C	2.113011	-0.358548	0.964289
C	0.749066	-0.620992	1.049981
H	0.244908	-0.455518	1.994841
C	-2.460464	3.941408	0.771225
C	-2.379153	4.512295	-0.503105
C	-2.551686	3.701826	-1.629884
C	-2.797242	2.339790	-1.487523
C	-2.880831	1.746664	-0.207944
C	-2.704452	2.579699	0.919446
H	-2.334304	4.561920	1.653793
H	-2.186226	5.574704	-0.616474
H	-2.496012	4.134690	-2.624549
H	-2.932755	1.722568	-2.368906
H	-2.769112	2.149665	1.912958
C	6.220801	0.752186	0.578865
C	4.856452	0.493903	0.662062
C	4.222617	-0.292645	-0.363423
C	5.019752	-0.784187	-1.434461
C	6.371075	-0.513859	-1.493253
C	6.979187	0.261443	-0.484916
H	6.696696	1.347118	1.351941
H	4.570330	-1.404593	-2.199741
H	6.969041	-0.904930	-2.309076
H	8.042270	0.472874	-0.533812
C	4.020908	1.055187	1.776875
H	3.580026	2.005182	1.440428
H	4.649297	1.289253	2.639969
C	2.886237	0.099406	2.168979
H	2.216620	0.569667	2.893246
H	3.319335	-0.780931	2.666017

Table S39. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **5HH** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.544059	-1.067191	-0.074058
C	-2.608142	0.333237	0.035792
B	-2.448169	-0.539507	-1.442966
H	-1.879607	-0.034498	-2.341013
B	-2.285066	-2.262110	-1.043659
H	-1.566021	-2.922796	-1.710881
B	-2.271317	-2.388278	0.726293
H	-1.543663	-3.137741	1.280732
B	-2.426074	-0.740701	1.371341
H	-1.838841	-0.373700	2.322743
B	-3.833038	-1.806864	1.338935
H	-4.281439	-2.227248	2.352509
B	-3.759071	-2.750386	-0.176557
H	-4.159349	-3.863692	-0.252634
B	-3.855984	-1.600490	-1.540255
H	-4.322134	-1.871144	-2.595990
B	-4.027144	0.032122	-0.863535
H	-4.517563	0.960848	-1.407177
B	-4.013387	-0.094118	0.906470
H	-4.492478	0.748009	1.584692
B	-4.831400	-1.338035	-0.066397
H	-6.014007	-1.421060	-0.063446
C	-0.051754	-0.869359	-0.065049
C	0.675574	-0.941515	1.132354
H	0.160777	-1.113059	2.069554
C	2.058856	-0.798469	1.139434
H	2.587622	-0.832721	2.086657
C	2.776512	-0.583578	-0.047909
C	2.045776	-0.528897	-1.245454
H	2.570081	-0.403554	-2.187474
C	0.662159	-0.670477	-1.255910
H	0.139473	-0.646066	-2.203917
C	4.886688	0.477709	-0.905055
C	6.272511	0.624668	-0.896028
C	7.053789	-0.131866	-0.021069
C	6.437404	-1.036562	0.844909
C	5.051566	-1.183125	0.836601
C	4.252326	-0.428418	-0.038593
H	6.741914	1.337216	-1.568010
H	8.133623	-0.017707	-0.014389
H	7.037184	-1.636568	1.523016
C	-0.983413	4.329663	0.283633
C	-1.304759	3.775539	-0.955223
C	-1.816493	2.481927	-1.035636
C	-2.012714	1.715378	0.123236
C	-1.701125	2.288754	1.365106
C	-1.188610	3.582416	1.443026
H	-0.584490	5.337625	0.345561
H	-1.162416	4.350646	-1.865035
H	-2.075516	2.073770	-2.004598
H	-1.868933	1.730030	2.277112
H	-0.954432	4.005756	2.414950
H	4.286063	1.090014	-1.570951
H	4.584855	-1.909522	1.495014

Table S40. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **5HH** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.175431	-1.329008	0.033661
C	-2.926563	0.296121	-0.013301
B	-2.204218	-0.789245	-1.207440
H	-1.716839	-0.286996	-2.165403
B	-1.815605	-2.569146	-0.826033
H	-1.073849	-3.206483	-1.501096
B	-1.812294	-2.516903	0.967025
H	-1.067584	-3.115537	1.673379
B	-2.196089	-0.717374	1.243909
H	-1.702173	-0.157736	2.166341
B	-3.431304	-2.053400	1.493091
H	-3.821699	-2.429274	2.552535
B	-3.215937	-3.162137	0.092130
H	-3.466055	-4.325467	0.127283
B	-3.438368	-2.137917	-1.371021
H	-3.833038	-2.577695	-2.403971
B	-4.003508	-0.535621	-0.894370
H	-4.704815	0.095451	-1.616175
B	-3.996593	-0.480139	0.924027
H	-4.693411	0.193033	1.611282
B	-4.504536	-1.966427	0.060575
H	-5.650674	-2.289165	0.073777
C	0.283392	-1.030739	0.025058
C	1.006077	-0.893095	1.234468
H	0.490785	-1.023137	2.178367
C	2.352501	-0.590080	1.232284
H	2.868303	-0.508181	2.181446
C	3.074969	-0.439882	0.014254
C	2.347156	-0.611836	-1.197890
H	2.844706	-0.480864	-2.151219
C	0.996125	-0.894169	-1.189874
H	0.468462	-1.001228	-2.129660
C	5.304601	-0.409595	-1.132524
C	6.656392	-0.123427	-1.129724
C	7.252378	0.458815	0.001891
C	6.476243	0.746018	1.137205
C	5.126025	0.451827	1.147390
C	4.493501	-0.134092	0.009446
H	7.260064	-0.354519	-2.000431
H	8.312907	0.687188	-0.001491
H	6.936199	1.206181	2.004777
C	-2.271741	4.533651	-0.137997
C	-2.376600	3.800394	-1.324689
C	-2.581076	2.424938	-1.287362
C	-2.691860	1.740456	-0.056074
C	-2.584713	2.496556	1.132937
C	-2.379971	3.871814	1.089604
H	-2.109912	5.606762	-0.169520
H	-2.299714	4.304565	-2.283676
H	-2.664137	1.867871	-2.214130
H	-2.670614	1.995081	2.090681
H	-2.305631	4.431757	2.017344
H	4.866504	-0.884709	-2.001319
H	4.536052	0.706660	2.018823

Table S41. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **6HC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.529129	-1.126502	0.311332
C	3.338412	0.381775	-0.102532
B	3.150687	-0.092848	1.543615
H	2.395811	0.497652	2.225890
B	3.339309	-1.856799	1.624607
H	2.669244	-2.453918	2.394698
B	3.568465	-2.436117	-0.037104
H	3.056158	-3.433268	-0.413887
B	3.513780	-1.014139	-1.099232
H	2.994514	-1.024461	-2.155250
B	5.069340	-1.730152	-0.670554
H	5.707383	-2.297627	-1.492793
B	4.972228	-2.245967	1.037271
H	5.547130	-3.197877	1.448220
B	4.697679	-0.788286	2.032860
H	5.068023	-0.679326	3.153611
B	4.665536	0.615693	0.946082
H	4.913851	1.732726	1.244945
B	4.893738	0.036203	-0.715395
H	5.301479	0.753298	-1.562877
B	5.788438	-0.724061	0.619387
H	6.958652	-0.566052	0.724923
C	1.037125	-1.236719	0.143125
C	0.164204	-0.909760	1.191376
H	0.559810	-0.565983	2.138908
C	-1.213376	-1.037530	1.045962
H	-1.857138	-0.782073	1.879296
C	-1.777221	-1.504921	-0.151198
C	-0.897866	-1.855511	-1.188925
H	-1.300832	-2.221632	-2.128216
C	0.480228	-1.725202	-1.047332
H	1.122674	-2.011826	-1.870580
C	-4.198388	-0.704205	0.046127
C	-5.562292	-0.994506	-0.116340
C	-5.997555	-2.211487	-0.636782
C	-5.060004	-3.173886	-1.007515
C	-3.703087	-2.907915	-0.846243
C	-3.246165	-1.687551	-0.318804
H	-6.287681	-0.234768	0.159447
H	-7.060126	-2.403359	-0.752600
H	-5.380507	-4.130395	-1.409406
C	1.657776	2.828400	-2.494689
C	1.092516	3.750401	-1.613748
C	1.254503	3.574474	-0.239809
C	1.968195	2.482344	0.250594
C	2.528524	1.541015	-0.625549
C	2.370841	1.735294	-2.006410
H	1.550584	2.959759	-3.567080
H	0.539859	4.603747	-1.995339
H	0.829742	4.289843	0.457556
H	2.096505	2.371258	1.319774
H	2.816629	1.038502	-2.705192
H	-2.973958	-3.670543	-1.102916
C	-3.836775	0.640433	0.599672
C	-3.211515	1.636762	-0.182934
C	-4.197521	0.933399	1.924492
C	-2.945370	2.878875	0.408120
C	-3.922417	2.174777	2.495234
C	-3.286212	3.152241	1.731866
H	-2.467198	3.649043	-0.191794
H	-4.205285	2.374984	3.524448
H	-3.066955	4.126613	2.159018
C	-2.846912	1.407193	-1.630872
H	-3.632747	0.862549	-2.162430
H	-2.684396	2.359274	-2.143294
H	-1.926625	0.820514	-1.726316
H	-4.693258	0.165579	2.512238

Table S42. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **6HC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.193227	-1.545306	0.359310
C	3.466222	0.405054	-0.142862
B	2.939230	-0.355329	1.339724
H	2.253775	0.287047	2.064893
B	3.044635	-2.193841	1.595999
H	2.432322	-2.758864	2.443965
B	3.213546	-2.733880	-0.105699
H	2.730813	-3.716489	-0.569728
B	3.168724	-1.095754	-0.980881
H	2.646479	-1.036139	-2.045277
B	4.712727	-2.053231	-0.741814
H	5.287815	-2.645211	-1.600467
B	4.637667	-2.650301	0.952220
H	5.172967	-3.647956	1.323232
B	4.443257	-1.183826	1.973649
H	4.824261	-1.136957	3.101111
B	4.644136	0.256372	0.972349
H	5.082903	1.261777	1.430047
B	4.814177	-0.289606	-0.738294
H	5.383350	0.292605	-1.604271
B	5.579770	-1.210692	0.583500
H	6.765548	-1.207613	0.700856
C	0.719502	-1.608256	0.210996
C	-0.139576	-1.131754	1.212554
H	0.274732	-0.759260	2.141851
C	-1.519906	-1.119985	1.032201
H	-2.152915	-0.780372	1.844140
C	-2.104244	-1.588289	-0.165672
C	-1.246489	-2.138044	-1.140045
H	-1.660342	-2.511493	-2.071433
C	0.127240	-2.139143	-0.960503
H	0.764712	-2.531455	-1.744584
C	-4.325678	-0.367747	0.023309
C	-5.736573	-0.423062	-0.059944
C	-6.374702	-1.506802	-0.636245
C	-5.615599	-2.593617	-1.107962
C	-4.232569	-2.590703	-0.982262
C	-3.555357	-1.508353	-0.396801
H	-6.316210	0.433227	0.267054
H	-7.454535	-1.511644	-0.736789
H	-6.114514	-3.451964	-1.545681
C	2.088140	3.122463	-2.398726
C	1.723284	4.105164	-1.473280
C	1.934941	3.871252	-0.110693
C	2.495227	2.671512	0.321309
C	2.867675	1.668701	-0.599128
C	2.650904	1.922851	-1.970398
H	1.937298	3.293132	-3.460944
H	1.288728	5.041862	-1.809121
H	1.668257	4.630410	0.619405
H	2.656784	2.505382	1.380794
H	2.933815	1.172221	-2.700225
H	-3.664299	-3.461558	-1.289545
C	-3.715445	0.861027	0.541275
C	-2.644178	1.564623	-0.125928
C	-4.237901	1.395150	1.750066
C	-2.080096	2.674291	0.514516
C	-3.660781	2.493445	2.351086
C	-2.562370	3.132919	1.733184
H	-1.265755	3.199990	0.026239
H	-4.035144	2.855356	3.302106
H	-2.110948	4.000516	2.202301
C	-2.193084	1.251772	-1.526849
H	-2.778745	0.466508	-2.000710
H	-2.279740	2.155246	-2.140007
H	-1.137776	0.961042	-1.537686
H	-5.053854	0.876126	2.239658

Table S43. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **7HD** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.666392	-1.134142	0.292930
C	3.502496	0.380958	-0.063694
B	3.244132	-0.121311	1.564564
H	2.467793	0.459342	2.229262
B	3.420480	-1.888378	1.623866
H	2.721752	-2.495799	2.359641
B	3.711942	-2.442644	-0.036095
H	3.213186	-3.432346	-0.448962
B	3.705882	-1.002008	-1.075349
H	3.234032	-0.991725	-2.152278
B	5.239891	-1.735331	-0.596754
H	5.909724	-2.293819	-1.401016
B	5.072287	-2.278160	1.096110
H	5.626979	-3.240425	1.514650
B	4.766901	-0.835760	2.103444
H	5.095305	-0.749764	3.240156
B	4.787095	0.585930	1.041066
H	5.034530	1.694478	1.370678
B	5.077027	0.032083	-0.618794
H	5.528722	0.757080	-1.436532
B	5.912896	-0.756082	0.736679
H	7.080491	-0.609377	0.891632
C	1.181173	-1.231145	0.069845
C	0.278121	-0.956440	1.108200
H	0.642943	-0.660755	2.084042
C	-1.094551	-1.076185	0.915169
H	-1.758854	-0.865706	1.744293
C	-1.623116	-1.481207	-0.320495
C	-0.712964	-1.775754	-1.349799
H	-1.085785	-2.092214	-2.318758
C	0.660652	-1.654663	-1.161497
H	1.324132	-1.897259	-1.982042
C	-4.048113	-0.675697	-0.191948
C	-5.400396	-0.930154	-0.471523
C	-5.815896	-2.111491	-1.083193
C	-4.868428	-3.073594	-1.432311
C	-3.521836	-2.837933	-1.168502
C	-3.086050	-1.651612	-0.550403
H	-6.134540	-0.172988	-0.211229
H	-6.869836	-2.276343	-1.285984
H	-5.173610	-4.003163	-1.903134
C	1.970605	2.885560	-2.491839
C	1.337825	3.777607	-1.625208
C	1.405540	3.563049	-0.248311
C	2.093508	2.461952	0.259710
C	2.721216	1.551116	-0.603766
C	2.657443	1.782853	-1.987056
H	1.934952	3.046379	-3.564701
H	0.803317	4.636424	-2.019294
H	0.925682	4.253894	0.437543
H	2.145237	2.322128	1.331938
H	3.152800	1.109193	-2.675248
H	-2.786611	-3.594491	-1.425427
C	-3.697932	0.642243	0.437966
C	-3.151208	1.679863	-0.349603
C	-3.974199	0.859201	1.807304
C	-2.868353	2.912575	0.252114
C	-3.673311	2.104118	2.373410
C	-3.121804	3.126613	1.604692
H	-2.448032	3.711096	-0.353411
H	-3.875986	2.268320	3.428434
H	-2.895613	4.087966	2.057160
C	-4.582254	-0.223024	2.673448
H	-4.553658	0.064724	3.727515
H	-5.628258	-0.413686	2.409153
H	-4.057106	-1.177965	2.566900
C	-2.877458	1.491994	-1.824524
H	-3.740142	1.062550	-2.343535
H	-2.635858	2.447549	-2.297018
H	-2.032943	0.815031	-1.994812

Table S44. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **7HD** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-2.346343	-1.543325	-0.374684
C	-3.618730	0.413913	0.107073
B	-3.053430	-0.337259	-1.365059
H	-2.341140	0.305783	-2.063415
B	-3.166234	-2.172643	-1.642117
H	-2.533827	-2.735340	-2.476846
B	-3.390096	-2.726873	0.048656
H	-2.929511	-3.717783	0.517629
B	-3.357797	-1.096290	0.939372
H	-2.867497	-1.050377	2.019585
B	-4.901735	-2.039307	0.646353
H	-5.506906	-2.634282	1.482036
B	-4.781242	-2.621637	-1.050370
H	-5.313220	-3.611512	-1.446305
B	-4.544663	-1.147584	-2.051857
H	-4.891364	-1.087722	-3.189785
B	-4.764474	0.284884	-1.043735
H	-5.181892	1.297854	-1.504781
B	-4.989387	-0.275044	0.655764
H	-5.579567	0.304059	1.509725
B	-5.722529	-1.177895	-0.696428
H	-6.904295	-1.164305	-0.848798
C	-0.878378	-1.620753	-0.184245
C	0.013344	-1.150460	-1.159009
H	-0.370146	-0.771068	-2.098741
C	1.388501	-1.155423	-0.939772
H	2.046623	-0.825447	-1.735149
C	1.935255	-1.631425	0.272549
C	1.043619	-2.172324	1.221323
H	1.426640	-2.551321	2.163645
C	-0.324474	-2.159554	1.002413
H	-0.987829	-2.546480	1.767540
C	4.158699	-0.410983	0.182599
C	5.554242	-0.432177	0.389734
C	6.167609	-1.507754	1.011129
C	5.400121	-2.617904	1.402920
C	4.030567	-2.638033	1.173891
C	3.378771	-1.558040	0.554939
H	6.140619	0.439403	0.122563
H	7.234485	-1.485763	1.205458
H	5.881176	-3.471123	1.869842
C	-2.294413	3.102956	2.428406
C	-1.897035	4.092257	1.523441
C	-2.068296	3.871570	0.153076
C	-2.621174	2.678701	-0.306564
C	-3.026664	1.669834	0.592916
C	-2.850184	1.910349	1.972244
H	-2.175124	3.263329	3.496242
H	-1.468820	5.023886	1.880907
H	-1.775391	4.635594	-0.561736
H	-2.751289	2.522877	-1.371952
H	-3.158756	1.154612	2.686234
H	3.453853	-3.517154	1.439534
C	3.540123	0.806436	-0.371556
C	2.517540	1.513565	0.373167
C	3.968557	1.309091	-1.644583
C	1.904403	2.627136	-0.205252
C	3.320259	2.417989	-2.165590
C	2.293560	3.077585	-1.457511
H	1.131972	3.151921	0.346940
H	3.589809	2.772548	-3.154981
H	1.815811	3.946774	-1.896757
C	5.021785	0.618818	-2.481071
H	4.938893	0.936501	-3.522397
H	6.033614	0.867285	-2.144876
H	4.927571	-0.469044	-2.445277
C	2.167369	1.185118	1.799430
H	2.393630	2.052298	2.430462
H	1.093741	0.995674	1.894481
H	2.714270	0.333561	2.197580

Table S45. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **8HP** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.400818	-1.125072	-0.306260
C	3.256479	0.366113	0.105993
B	3.411951	-1.043139	1.087435
H	2.918303	-1.055163	2.154267
B	3.415754	-2.458899	0.014407
H	2.890857	-3.448739	0.393032
B	3.171914	-1.861403	-1.638097
H	2.479256	-2.438741	-2.403216
B	3.024369	-0.093341	-1.539535
H	2.271782	0.519664	-2.203025
B	4.546464	-0.822126	-2.062012
H	4.902425	-0.714786	-3.188572
B	4.804158	-2.293197	-1.083015
H	5.350963	-3.255501	-1.511681
B	4.943238	-1.793409	0.625613
H	5.584073	-2.383446	1.430963
B	4.811762	-0.024447	0.687510
H	5.255693	0.673288	1.532895
B	4.568281	0.572649	-0.965037
H	4.843922	1.683487	-1.262767
B	5.663276	-0.795697	-0.668688
H	6.836345	-0.666323	-0.795026
C	0.909614	-1.203205	-0.119001
C	0.355081	-1.646971	1.090030
H	0.996357	-1.916249	1.919912
C	-1.024349	-1.757054	1.243276
H	-1.425433	-2.092991	2.194329
C	-1.902432	-1.428757	0.199043
C	-1.341907	-1.002275	-1.015432
C	0.035435	-0.894085	-1.173420
H	0.427957	-0.580753	-2.132858
C	1.315499	3.642640	0.283140
C	1.133509	3.793270	1.658504
C	1.635874	2.824578	2.528327
C	2.308730	1.711096	2.028019
C	2.486052	1.543732	0.645471
C	1.987075	2.529374	-0.220170
H	0.940391	4.394290	-0.404139
H	0.613365	4.662290	2.049531
H	1.510756	2.934581	3.600876
H	2.704855	0.979243	2.720757
H	2.129906	2.438765	-1.289631
C	-4.545384	1.308153	-1.589440
C	-4.243404	2.606137	-2.003687
C	-3.342530	3.383582	-1.273894
C	-2.746842	2.853153	-0.126918
C	-3.046870	1.555427	0.285129
C	-3.949204	0.760326	-0.441254
H	-5.239206	0.705226	-2.168073
H	-4.710074	3.007259	-2.898682
H	-3.107068	4.393851	-1.595243
H	-2.046396	3.449615	0.450083
H	-2.585593	1.156692	1.182854
H	-1.990070	-0.763509	-1.851438
C	-5.688718	-0.911846	0.146938
C	-4.322397	-0.610037	0.016514
C	-3.373533	-1.603947	0.365531
C	-3.833080	-2.839131	0.854000
C	-5.192049	-3.115393	0.983992
C	-6.126914	-2.146540	0.620547
H	-6.415907	-0.145360	-0.103306
H	-3.104726	-3.604490	1.104452
H	-5.515423	-4.082464	1.356792
H	-7.190454	-2.344309	0.714118

Table S46. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **8HP** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.112200	-1.516214	-0.326635
C	3.446021	0.407717	0.118293
B	3.133609	-1.080726	0.979882
H	2.646522	-0.994301	2.058884
B	3.115062	-2.727356	0.120430
H	2.620021	-3.692418	0.607607
B	2.911617	-2.196509	-1.580623
H	2.260911	-2.752393	-2.405709
B	2.857109	-0.353766	-1.340188
H	2.163213	0.295026	-2.051507
B	4.322993	-1.225656	-2.008717
H	4.672037	-1.199202	-3.147054
B	4.510262	-2.687275	-0.979077
H	5.010188	-3.700769	-1.356268
B	4.647465	-2.077074	0.706518
H	5.233383	-2.673707	1.554468
B	4.790179	-0.316608	0.682590
H	5.398148	0.257835	1.527010
B	4.586140	0.218985	-1.029034
H	5.035275	1.209198	-1.509088
B	5.496709	-1.267978	-0.651149
H	6.678535	-1.294111	-0.800569
C	0.639233	-1.549866	-0.152566
C	0.056841	-1.988037	1.058893
H	0.698856	-2.322816	1.865441
C	-1.316941	-1.976833	1.244687
H	-1.727875	-2.287203	2.200194
C	-2.180081	-1.504892	0.233978
C	-1.602803	-1.110486	-0.994787
C	-0.225987	-1.140577	-1.181473
H	0.185192	-0.835395	-2.136460
C	1.954263	3.891559	0.118467
C	1.833571	4.151484	1.487274
C	2.248595	3.181605	2.405314
C	2.769533	1.968518	1.963627
C	2.893714	1.687739	0.586070
C	2.474367	2.678631	-0.326852
H	1.647397	4.640229	-0.606594
H	1.429683	5.098130	1.833335
H	2.168195	3.372739	3.471691
H	3.090026	1.226983	2.687247
H	2.565386	2.492253	-1.391319
C	-4.494391	1.668554	-1.484426
C	-3.967707	2.878484	-1.895157
C	-2.822693	3.403988	-1.265096
C	-2.205785	2.701744	-0.224463
C	-2.710358	1.474646	0.176276
C	-3.867353	0.919616	-0.451290
H	-5.360973	1.259065	-1.990417
H	-4.432892	3.422965	-2.709470
H	-2.423812	4.360454	-1.585714
H	-1.334041	3.114640	0.270823
H	-2.253779	0.951356	1.005812
H	-2.242653	-0.810851	-1.817632
C	-5.852942	-0.457611	0.060196
C	-4.441947	-0.346586	-0.007049
C	-3.634479	-1.455544	0.446785
C	-4.279213	-2.548815	1.046887
C	-5.662900	-2.605796	1.144615
C	-6.456611	-1.557932	0.636621
H	-6.463857	0.372458	-0.274780
H	-3.682653	-3.389835	1.381774
H	-6.136138	-3.475086	1.588878
H	-7.536910	-1.605994	0.717114

Table S47. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **9HM** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.686300	-1.047365	-0.132472
C	-2.803479	0.311167	0.040314
B	-2.619369	-0.495053	-1.473033
H	-2.077497	0.062134	-2.355120
B	-2.391039	-2.226032	-1.144924
H	-1.657597	-2.835651	-1.844209
B	-2.359601	-2.424274	0.617462
H	-1.604373	-3.171152	1.137444
B	-2.568918	-0.810148	1.329423
H	-1.993709	-0.461218	2.293513
B	-3.936773	-1.925761	1.260884
H	-4.364894	-2.404706	2.258231
B	-3.839442	-2.803105	-0.291257
H	-4.201297	-3.927133	-0.411084
B	-3.988152	-1.603474	-1.605467
H	-4.453388	-1.850621	-2.668405
B	-4.215092	-0.007408	-0.862768
H	-4.746985	0.921051	-1.366367
B	-4.183371	-0.205513	0.899882
H	-4.693223	0.585903	1.615606
B	-4.961643	-1.438065	-0.117566
H	-6.141464	-1.567312	-0.110903
C	-0.202583	-0.793684	-0.130631
C	0.535153	-0.839437	1.062032
H	0.037171	-1.027516	2.005064
C	1.913667	-0.648177	1.057505
H	2.449007	-0.668332	2.000584
C	2.612093	-0.407619	-0.135921
C	1.869771	-0.371062	-1.327234
H	2.381772	-0.206113	-2.270011
C	0.491515	-0.564249	-1.328066
H	-0.038208	-0.549431	-2.272449
C	4.545607	0.997056	-0.810176
C	5.902682	1.305031	-0.868690
C	6.825675	0.444413	-0.274742
C	6.377919	-0.712281	0.361830
C	5.016325	-1.038060	0.438206
C	4.081451	-0.157874	-0.156514
H	6.233726	2.208392	-1.372038
H	7.888221	0.665866	-0.312829
H	7.101502	-1.391445	0.805473
C	4.612577	-2.326808	1.121238
H	5.442633	-3.038386	1.110496
H	4.341124	-2.165777	2.171183
H	3.753538	-2.796930	0.635975
C	-1.320932	4.346270	0.464997
C	-1.586309	3.824589	-0.801568
C	-2.052883	2.518420	-0.940814
C	-2.257984	1.708253	0.187014
C	-2.002255	2.247675	1.457440
C	-1.535533	3.554164	1.593364
H	-0.957167	5.363449	0.572140
H	-1.434633	4.433789	-1.687017
H	-2.266274	2.137269	-1.931592
H	-2.175899	1.654461	2.346452
H	-1.343907	3.951385	2.585142
H	3.821753	1.669646	-1.261136

Table S48. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **9HM** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.338805	-1.305766	-0.155343
C	-3.129175	0.263689	0.046608
B	-2.407619	-0.635485	-1.293623
H	-1.952242	0.000041	-2.186391
B	-1.971298	-2.439654	-1.155608
H	-1.230388	-2.968392	-1.919571
B	-1.929834	-2.617770	0.628474
H	-1.157029	-3.282439	1.239649
B	-2.352499	-0.879872	1.143363
H	-1.853974	-0.433765	2.123441
B	-3.548310	-2.269967	1.239716
H	-3.905690	-2.792116	2.247839
B	-3.336793	-3.182114	-0.297076
H	-3.558270	-4.346618	-0.408931
B	-3.613856	-1.983387	-1.610399
H	-4.019723	-2.294945	-2.685006
B	-4.206542	-0.471889	-0.917319
H	-4.937015	0.230369	-1.537508
B	-4.166930	-0.654266	0.889749
H	-4.866122	-0.093562	1.669602
B	-4.654189	-2.027079	-0.150892
H	-5.791374	-2.380700	-0.160722
C	0.111729	-0.970308	-0.157097
C	0.853671	-0.926789	1.045884
H	0.352286	-1.122150	1.986041
C	2.201514	-0.620654	1.047174
H	2.719011	-0.550859	1.994845
C	2.890358	-0.321289	-0.159297
C	2.134340	-0.356515	-1.365120
H	2.627784	-0.166320	-2.311617
C	0.795762	-0.697781	-1.363951
H	0.258971	-0.750821	-2.303472
C	4.702473	1.041690	-1.137437
C	6.000498	1.498297	-1.194168
C	6.965043	0.948272	-0.327366
C	6.607543	-0.056030	0.575077
C	5.301792	-0.532459	0.670385
C	4.297992	0.048630	-0.194250
H	6.276476	2.279980	-1.892923
H	7.993053	1.292255	-0.370965
H	7.372209	-0.496916	1.206352
C	5.025147	-1.674675	1.612585
H	5.942493	-2.240489	1.790180
H	4.682229	-1.313115	2.589915
H	4.265526	-2.357310	1.228271
C	-2.582780	4.500420	0.455957
C	-2.702173	3.923065	-0.812395
C	-2.872407	2.548867	-0.948023
C	-2.932438	1.708801	0.186257
C	-2.811418	2.308505	1.459639
C	-2.641515	3.683262	1.589675
H	-2.448005	5.572753	0.559587
H	-2.663770	4.548068	-1.699948
H	-2.967504	2.113575	-1.936773
H	-2.858646	1.686037	2.346470
H	-2.555602	4.120881	2.580106
H	3.951742	1.486576	-1.779181

Table S49. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **10HV** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.769483	-1.018770	0.137138
C	2.918138	0.311701	-0.051649
B	2.730048	-0.484441	1.466112
H	2.209896	0.088414	2.351309
B	2.456203	-2.210532	1.146451
H	1.715977	-2.800240	1.855547
B	2.401309	-2.414183	-0.614723
H	1.622684	-3.143976	-1.124407
B	2.642637	-0.808015	-1.334196
H	2.067959	-0.447741	-2.294340
B	3.983539	-1.956404	-1.275708
H	4.389721	-2.448787	-2.275695
B	3.881075	-2.825770	0.280372
H	4.216604	-3.957884	0.400783
B	4.072608	-1.625650	1.588713
H	4.542426	-1.880787	2.647758
B	4.330925	-0.038121	0.838101
H	4.890388	0.878901	1.332744
B	4.275850	-0.241489	-0.923313
H	4.797450	0.534596	-1.647306
B	5.034392	-1.489229	0.090277
H	6.210582	-1.647311	0.071717
C	0.292674	-0.728203	0.153589
C	-0.458235	-0.728629	-1.033523
H	0.025658	-0.909908	-1.985122
C	-1.829731	-0.502205	-1.010763
H	-2.383397	-0.503047	-1.943541
C	-2.507018	-0.269762	0.196532
C	-1.755870	-0.275767	1.380470
H	-2.253699	-0.111246	2.330980
C	-0.382035	-0.506638	1.362346
H	0.157872	-0.523601	2.300939
C	-4.335786	1.284968	0.784187
C	-5.658403	1.724802	0.782433
C	-6.642827	0.931124	0.194508
C	-6.292096	-0.296986	-0.359209
C	-4.969064	-0.776849	-0.339280
C	-3.963442	0.054055	0.220250
H	-5.910983	2.685930	1.219633
H	-7.676280	1.263105	0.168357
H	-7.062698	-0.922932	-0.801238
C	-4.760035	-2.140500	-0.873010
H	-5.487251	-2.434349	-1.629608
C	1.529171	4.379476	-0.480963
C	1.786435	3.854839	0.786051
C	2.222879	2.538461	0.927147
C	2.405234	1.720971	-0.199245
C	2.157919	2.263088	-1.470230
C	1.721475	3.579786	-1.608020
H	1.188967	5.404631	-0.589535
H	1.651954	4.469610	1.670432
H	2.430537	2.154885	1.918184
H	2.314592	1.663655	-2.358262
H	1.535926	3.978914	-2.600188
H	-3.560617	1.919085	1.204215
C	-3.864528	-3.054661	-0.481222
H	-3.853916	-4.042452	-0.931469
H	-3.129313	-2.864092	0.292448

Table S50. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **10HV** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.409245	-1.272733	0.182093
C	3.241592	0.232604	-0.062761
B	2.532370	-0.614849	1.293601
H	2.109239	0.041789	2.187503
B	2.036616	-2.402695	1.184872
H	1.296582	-2.903591	1.969135
B	1.959930	-2.603199	-0.594802
H	1.162284	-3.259433	-1.183461
B	2.428768	-0.885542	-1.134618
H	1.932772	-0.438001	-2.115636
B	3.578544	-2.312829	-1.234888
H	3.900722	-2.859695	-2.242553
B	3.365432	-3.198776	0.314610
H	3.550524	-4.369219	0.437566
B	3.699189	-1.996306	1.609376
H	4.107877	-2.311969	2.682392
B	4.331957	-0.515833	0.884944
H	5.092424	0.176821	1.480049
B	4.256638	-0.716403	-0.908714
H	4.958641	-0.178871	-1.702803
B	4.716963	-2.089072	0.134950
H	5.840779	-2.484669	0.131396
C	-0.022285	-0.873714	0.207659
C	-0.768809	-0.767902	-0.976928
H	-0.290666	-0.958636	-1.930400
C	-2.112064	-0.407340	-0.951382
H	-2.646800	-0.293241	-1.887718
C	-2.769319	-0.131424	0.271633
C	-2.015845	-0.219570	1.458568
H	-2.494354	-0.031136	2.414422
C	-0.682112	-0.599864	1.427325
H	-0.135630	-0.692680	2.358731
C	-4.552632	1.381006	1.096645
C	-5.838116	1.907663	1.041725
C	-6.804674	1.358699	0.173582
C	-6.478846	0.263139	-0.599541
C	-5.198997	-0.341306	-0.509897
C	-4.178147	0.287749	0.302319
H	-6.087699	2.774175	1.644826
H	-7.798366	1.789323	0.124286
H	-7.223362	-0.190153	-1.245456
C	-5.044132	-1.610994	-1.176025
H	-5.772424	-1.811819	-1.958738
C	2.838223	4.487580	-0.515346
C	2.960654	3.920562	0.756644
C	3.085126	2.541881	0.905495
C	3.094082	1.687478	-0.217339
C	2.970937	2.276040	-1.493700
C	2.846959	3.655272	-1.638493
H	2.739793	5.562835	-0.629770
H	2.960852	4.556085	1.637695
H	3.183182	2.115447	1.897884
H	2.979463	1.642261	-2.373761
H	2.757967	4.083026	-2.633103
H	-3.802302	1.864039	1.711912
C	-4.175727	-2.615830	-0.860429
H	-4.176634	-3.531281	-1.440904
H	-3.507587	-2.567858	-0.011220

Table S51. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **11HI** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.972028	-1.043056	0.206878
C	-3.227718	0.167941	-0.074971
B	-2.823696	-0.986458	-1.290837
H	-2.258592	-0.626022	-2.256688
B	-2.459826	-2.525860	-0.482454
H	-1.607454	-3.208237	-0.936826
B	-2.575442	-2.238558	1.264140
H	-1.803463	-2.722682	2.017960
B	-3.007863	-0.529702	1.486397
H	-2.562633	0.131549	2.350512
B	-4.247407	-1.778493	1.642147
H	-4.718975	-2.020149	2.703560
B	-3.918900	-3.021830	0.403287
H	-4.156204	-4.171799	0.576570
B	-4.059271	-2.245419	-1.198632
H	-4.395739	-2.822315	-2.179116
B	-4.509763	-0.547585	-0.943225
H	-5.079573	0.141232	-1.717428
B	-4.625956	-0.260711	0.803542
H	-5.275902	0.626781	1.237663
B	-5.180360	-1.804828	0.119636
H	-6.337297	-2.067680	0.086053
C	-0.526969	-0.622280	0.235189
C	0.250539	-0.630918	-0.932967
H	-0.190611	-0.913074	-1.880726
C	1.597196	-0.281226	-0.896982
H	2.165468	-0.276772	-1.821528
C	2.223718	0.082247	0.305475
C	1.443252	0.082246	1.471716
H	1.901236	0.345743	2.419930
C	0.095830	-0.266673	1.440773
H	-0.464365	-0.273125	2.367544
C	3.921220	1.795557	0.865070
C	5.217496	2.298047	0.927414
C	6.277271	1.509960	0.476932
C	6.024282	0.231519	-0.014696
C	4.725875	-0.298488	-0.085130
C	3.652510	0.512456	0.353430
H	3.089262	2.409458	1.197877
H	5.396569	3.295556	1.317252
H	7.295851	1.885281	0.512955
H	6.860484	-0.378105	-0.345306
C	-2.439439	3.836936	0.597967
H	-2.195831	4.317495	-0.689070
C	-2.285201	3.447252	-1.776006
H	-2.605704	2.105110	-1.578178
H	-2.838005	1.608278	-0.286056
H	-2.760098	2.495328	0.799057
C	-2.384447	4.505591	1.451218
H	-1.945895	5.362427	-0.844353
H	-2.109277	3.810528	-2.783581
H	-2.684243	1.449556	-2.436387
C	-2.959403	2.145615	1.804230
C	4.539140	-1.732766	-0.576801
C	5.281321	-2.738915	0.324923
C	5.081330	-3.763823	-0.005459
C	4.958858	-2.648986	1.366944
C	6.365304	-2.585941	0.294746
H	4.963001	-1.897175	-2.048741
H	4.775872	-2.921469	-2.388294
H	6.030663	-1.692334	-2.182877
H	4.410274	-1.216329	-2.704168
H	3.475376	-1.976507	-0.513649

Table S52. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **11HI** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-1.672778	-1.268291	0.292333
C	-3.566480	0.131565	-0.115719
B	-2.640353	-1.014464	-1.084781
H	-2.122982	-0.595669	-2.067156
B	-2.112493	-2.673718	-0.426077
H	-1.255857	-3.312246	-0.946643
B	-2.272239	-2.380836	1.335843
H	-1.538169	-2.794988	2.173625
B	-2.855657	-0.613239	1.321395
H	-2.503955	0.116118	2.189089
B	-3.968917	-2.031772	1.669767
H	-4.410993	-2.302966	2.741083
B	-3.522762	-3.288663	0.461654
H	-3.658577	-4.457343	0.644618
B	-3.715344	-2.501769	-1.145283
H	-3.970817	-3.117960	-2.131038
B	-4.478677	-0.923312	-0.944254
H	-5.173396	-0.475365	-1.797612
B	-4.637310	-0.623790	0.840143
H	-5.455856	0.055564	1.369196
B	-4.916093	-2.258373	0.164787
H	-6.020508	-2.703491	0.140216
C	-0.256053	-0.813353	0.347607
C	0.543713	-0.769581	-0.816772
H	0.112384	-1.053622	-1.768938
C	1.861121	-0.352814	-0.765872
H	2.426616	-0.284166	-1.687435
C	2.454474	0.063683	0.457055
C	1.639572	0.033759	1.621470
H	2.063286	0.321070	2.577584
C	0.335532	-0.420619	1.570888
H	-0.247514	-0.468479	2.482762
C	4.049095	1.711237	1.357767
C	5.272463	2.342533	1.386172
C	6.332484	1.830773	0.610585
C	6.150420	0.681802	-0.159763
C	4.929146	0.009284	-0.207347
C	3.818898	0.570479	0.531272
H	3.217499	2.128075	1.913372
H	5.415598	3.234676	1.985457
H	7.301737	2.317954	0.629833
H	6.996786	0.283305	-0.708269
C	-3.483508	3.863494	0.499259
H	-3.334815	4.361992	-0.799075
C	-3.260363	3.468209	-1.872418
H	-3.327767	2.095959	-1.652968
H	-3.476858	1.575465	-0.348156
H	-3.551708	2.492124	0.724175
C	-3.548106	4.547943	1.340228
H	-3.279958	5.432405	-0.972340
H	-3.150451	3.843711	-2.885724
H	-3.272166	1.413258	-2.493805
C	-3.670743	2.117961	1.735120
C	4.857680	-1.328729	-0.928822
C	5.805457	-2.355688	-0.268326
C	5.686353	-3.328436	-0.754757
C	5.580868	-2.476137	0.795338
C	6.854066	-2.057341	-0.364034
H	5.158247	-1.191564	-2.434882
H	5.051221	-2.165196	-2.922401
H	6.180069	-0.841029	-2.610956
H	4.476531	-0.489125	-2.924299
H	3.848422	-1.729134	-0.818865

Table S53. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **12MM** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.835244	-1.077708	0.000794
C	2.927550	0.301727	-0.009400
B	2.745915	-0.667962	1.405177
H	2.185493	-0.214238	2.335067
B	2.547109	-2.354081	0.885518
H	1.811652	-3.044274	1.503153
B	2.535849	-2.355599	-0.888884
H	1.793898	-3.048657	-1.495380
B	2.728514	-0.671133	-1.417509
H	2.152337	-0.226098	-2.341904
B	4.111855	-1.766937	-1.456897
H	4.554252	-2.125069	-2.496648
B	4.012920	-2.812070	-0.011241
H	4.389030	-3.936331	-0.012674
B	4.130325	-1.762933	1.429839
H	4.587347	-2.116615	2.464781
B	4.337752	-0.090796	0.869047
H	4.845920	0.787277	1.476739
B	4.327267	-0.092806	-0.905342
H	4.825836	0.784728	-1.521804
B	5.115559	-1.418793	-0.020546
H	6.296112	-1.526642	-0.027358
C	0.346527	-0.846853	0.003639
C	-0.376543	-0.816112	-1.197838
H	0.137194	-0.940514	-2.143116
C	-1.758200	-0.641876	-1.195777
H	-2.295090	-0.621475	-2.139675
C	-2.469562	-0.496682	0.003098
C	-1.746226	-0.543949	1.202520
H	-2.273795	-0.446668	2.146877
C	-0.364408	-0.718583	1.205544
H	0.157938	-0.765842	2.152870
C	-4.492124	0.999139	-0.036044
C	-5.882582	1.158724	-0.036615
C	-6.729630	0.054192	0.000348
C	-6.191955	-1.229625	0.038480
C	-4.806693	-1.430023	0.040111
C	-3.955458	-0.305289	0.002492
H	-6.300208	2.161588	-0.066550
H	-7.806876	0.193666	-0.000554
H	-6.851347	-2.092933	0.067572
C	-3.593055	2.214569	-0.076650
H	-4.183726	3.133672	-0.109657
H	-2.939478	2.264896	0.800969
H	-2.936061	2.203671	-0.953051
C	-4.247622	-2.834563	0.082236
H	-5.053076	-3.572667	0.113037
H	-3.626484	-3.050133	-0.793859
H	-3.612492	-2.991718	0.960689
C	1.388594	4.339720	0.022883
C	1.700347	3.694958	1.219650
C	2.184417	2.388283	1.209129
C	2.361781	1.699201	-0.000319
C	2.059840	2.362950	-1.198801
C	1.575221	3.669645	-1.185820
H	1.011929	5.358067	0.031734
H	1.572422	4.209074	2.167314
H	2.436521	1.909007	2.146881
H	2.213715	1.864753	-2.147619
H	1.348935	4.163953	-2.125613

Table S54. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **12MM** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	1.486509	-1.336260	0.166080
C	3.266121	0.243100	-0.057873
B	2.533474	-0.613272	1.297006
H	2.056160	0.046839	2.160348
B	2.117104	-2.425546	1.214583
H	1.369769	-2.938917	1.983036
B	2.108917	-2.664144	-0.562948
H	1.355536	-3.359668	-1.164248
B	2.524400	-0.939590	-1.127128
H	2.039738	-0.532610	-2.131144
B	3.734379	-2.320378	-1.157168
H	4.113727	-2.873493	-2.140737
B	3.504931	-3.182073	0.405545
H	3.735013	-4.340206	0.560624
B	3.746271	-1.937345	1.682217
H	4.134772	-2.209307	2.774145
B	4.339201	-0.445734	0.947376
H	5.051719	0.286173	1.554305
B	4.333944	-0.689074	-0.849454
H	5.041680	-0.145924	-1.634247
B	4.814325	-2.020016	0.243839
H	5.953912	-2.364082	0.286098
C	0.035875	-1.010289	0.131507
C	-0.683470	-1.004972	-1.084235
H	-0.165307	-1.224441	-2.010018
C	-2.036523	-0.718161	-1.114621
H	-2.549515	-0.692464	-2.068773
C	-2.741993	-0.378853	0.068596
C	-2.014054	-0.375812	1.285918
H	-2.528507	-0.168843	2.216921
C	-0.672347	-0.712560	1.316921
H	-0.154171	-0.742492	2.268061
C	-4.649828	1.157388	0.671320
C	-6.004345	1.446382	0.609035
C	-6.902665	0.580869	-0.029589
C	-6.446714	-0.598809	-0.633602
C	-5.101876	-0.934644	-0.627334
C	-4.166606	-0.051624	0.037746
H	-6.372351	2.368679	1.045597
H	-7.959353	0.825416	-0.055877
H	-7.161161	-1.270922	-1.096775
C	-3.726661	2.158822	1.318276
H	-4.215752	3.133450	1.375361
H	-3.470297	1.867611	2.343099
H	-2.789878	2.270875	0.769245
C	-4.681598	-2.248465	-1.235908
H	-5.546214	-2.908564	-1.331080
H	-4.267524	-2.113872	-2.241523
H	-3.921276	-2.754520	-0.637971
C	2.695831	4.461352	-0.620909
C	2.797425	3.928131	0.667923
C	2.975816	2.560427	0.853031
C	3.061831	1.682875	-0.250150
C	2.958624	2.238121	-1.544511
C	2.780483	3.606476	-1.724561
H	2.555006	5.528463	-0.763392
H	2.738931	4.582327	1.533121
H	3.057006	2.159915	1.857637
H	3.025959	1.586278	-2.408674
H	2.708631	4.009211	-2.730837

Table S55. Cartesian coordinates of the ground state (S_0) fully optimized geometry of **13PP** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.360049	-1.140310	-0.000123
C	3.510778	0.191247	0.000004
B	3.278605	-0.771206	1.411148
H	2.729798	-0.298168	2.338306
B	3.010668	-2.446455	0.886965
H	2.242769	-3.105597	1.498995
B	3.010630	-2.446247	-0.887537
H	2.242706	-3.105250	-1.499686
B	3.278542	-0.770875	-1.411351
H	2.729676	-0.297644	-2.338377
B	4.614181	-1.924763	-1.443762
H	5.048150	-2.299500	-2.481210
B	4.461101	-2.966486	-0.000383
H	4.788540	-4.105881	-0.000525
B	4.614246	-1.925099	1.443229
H	5.048267	-2.300071	2.480570
B	4.897320	-0.262495	0.887142
H	5.437915	0.592835	1.499335
B	4.897284	-0.262284	-0.887309
H	5.437842	0.593193	-1.499329
B	5.622719	-1.621884	-0.000255
H	6.797580	-1.780288	-0.000298
C	0.882575	-0.846870	-0.000079
C	0.168977	-0.738003	-1.202546
H	0.682732	-0.845037	-2.149825
C	-1.204404	-0.507381	-1.200042
H	-1.733334	-0.427164	-2.144992
C	-1.918236	-0.382097	-0.000032
C	-1.204358	-0.507345	1.199952
H	-1.733247	-0.427097	2.144922
C	0.169023	-0.737974	1.202410
H	0.682815	-0.844969	2.149674
C	-3.883638	1.198330	-0.000202
C	-5.267984	1.409228	-0.000215
C	-6.158566	0.340578	-0.000043
C	-5.672715	-0.962841	0.000147
C	-4.296793	-1.223663	0.000161
C	-3.398427	-0.130666	-0.000017
H	-5.653638	2.424761	-0.000361
H	-7.229492	0.523245	-0.000055
H	-6.373248	-1.792991	0.000282
C	2.146444	4.291681	0.000648
C	2.367658	3.624105	1.205002
C	2.795713	2.297849	1.205977
C	3.005605	1.611750	0.000218
C	2.795200	2.298070	-1.205324
C	2.367146	3.624327	-1.203922
H	1.814097	5.325398	0.000815
H	2.212651	4.135362	2.150160
H	2.978111	1.800874	2.150517
H	2.977187	1.801269	-2.150034
H	2.211736	4.135758	-2.148919
C	-2.948636	2.407085	-0.000393
H	-1.919193	2.038568	-0.000257
C	-3.816609	-2.674362	0.000365
H	-2.723198	-2.668331	0.000283
C	-3.123210	3.261759	1.269356
H	-2.408230	4.091735	1.274324
H	-4.129466	3.689747	1.332255
H	-2.958624	2.666780	2.173150
C	-3.123068	3.261223	-1.270524
H	-2.958378	2.665863	-2.174048
H	-2.408096	4.091205	-1.275761
H	-4.129322	3.689173	-1.333715
C	-4.264772	-3.422317	1.270481
H	-3.866457	-4.442654	1.275066
H	-5.356068	-3.491584	1.333706
H	-3.911309	-2.916308	2.174350
C	-4.264955	-3.422750	-1.269432
H	-3.866627	-4.443083	-1.273729
H	-3.911632	-2.917044	-2.173526
H	-5.356258	-3.492054	-1.332473

Table S56. Cartesian coordinates of the first-excited state (S_1) fully optimized geometry of **13PP** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.038003	-1.466308	0.007547
C	3.866900	0.081770	-0.002781
B	3.126420	-0.895254	1.217866
H	2.661251	-0.341332	2.160314
B	2.665086	-2.672827	0.913118
H	1.911602	-3.276711	1.607942
B	2.665609	-2.685300	-0.880804
H	1.912519	-3.298794	-1.567593
B	3.127053	-0.912210	-1.210013
H	2.662252	-0.371596	-2.160327
B	4.301798	-2.307182	-1.417914
H	4.668807	-2.747411	-2.463067
B	4.041837	-3.353208	0.021238
H	4.241195	-4.528778	0.029506
B	4.301011	-2.287279	1.445872
H	4.667399	-2.712827	2.497298
B	4.950856	-0.740138	0.900659
H	5.678542	-0.099818	1.589623
B	4.951377	-0.752636	-0.894011
H	5.679542	-0.122031	-1.591373
B	5.385149	-2.217757	0.013726
H	6.511090	-2.609866	0.016788
C	0.613083	-1.079700	0.004536
C	-0.093376	-0.900492	-1.200130
H	0.417863	-1.050736	-2.144365
C	-1.436707	-0.534599	-1.204356
H	-1.952420	-0.403774	-2.151671
C	-2.126511	-0.333611	-0.001070
C	-1.436323	-0.515626	1.205015
H	-1.951806	-0.369956	2.150280
C	-0.093065	-0.881745	1.206337
H	0.418269	-1.017368	2.152729
C	-3.931964	1.431933	0.005246
C	-5.335518	1.802113	0.013492
C	-6.341998	0.851852	0.006198
C	-5.978044	-0.484239	-0.006446
C	-4.587828	-0.901181	-0.008785
C	-3.570476	0.070729	-0.002182
H	-5.590573	2.854499	0.025869
H	-7.384113	1.144544	0.010662
H	-6.744986	-1.248756	-0.013448
C	3.457716	4.369161	-0.032831
C	3.524905	3.673095	1.176964
C	3.653453	2.285669	1.187691
C	3.721044	1.551186	-0.013092
C	3.654507	2.268867	-1.224048
C	3.525965	3.656308	-1.232753
H	3.357376	5.450405	-0.040405
H	3.479066	4.213145	2.118710
H	3.707765	1.759286	2.134563
H	3.709633	1.729359	-2.163455
H	3.480967	4.183188	-2.181967
C	-2.920015	2.545768	0.010091
H	-1.927320	2.096416	-0.023342
C	-4.306273	-2.380043	-0.019361
H	-3.224245	-2.514084	-0.014830
C	-3.021082	3.371699	1.315506
H	-2.241958	4.138636	1.305107
H	-3.986830	3.877366	1.413176
H	-2.870992	2.741423	2.195921
C	-3.074476	3.448064	-1.236934
H	-2.977979	2.870206	-2.159887
H	-2.284115	4.203305	-1.221502
H	-4.034910	3.972551	-1.256725
C	-4.872862	-3.061460	1.248877
H	-4.601427	-4.120380	1.228234
H	-5.964200	-2.998785	1.303992
H	-4.455853	-2.618384	2.157066
C	-4.859286	-3.038248	-1.305831
H	-4.591194	-4.098201	-1.300142
H	-4.430138	-2.580727	-2.201124
H	-5.949691	-2.970825	-1.372649