Electronic Supplementary Information

Effects of molecular geometry on the efficiency of intramolecular charge transfer–based luminescence in *o*-carboranyl-substituted 1*H*-phenanthro[9,10-*d*]imidazoles

Sehee Im,[a] Chan Hee Ryu,[a] Mingi Kim,[a] Dong Kyun You,[a] Sanghee Yi,[a] Wonchul Lee,[a] and Kang Mun Lee*[a]

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

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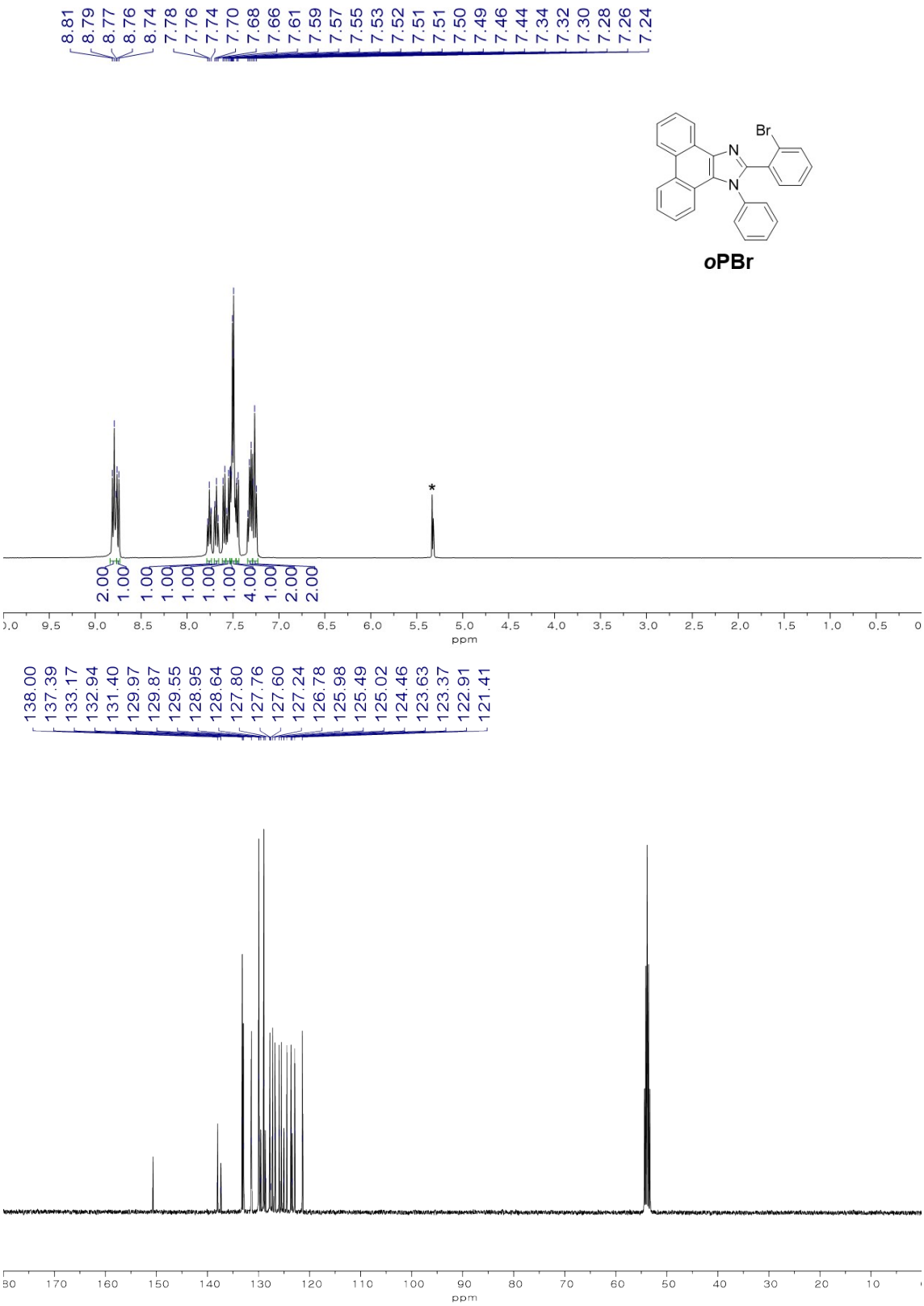

Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***o*PBr** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

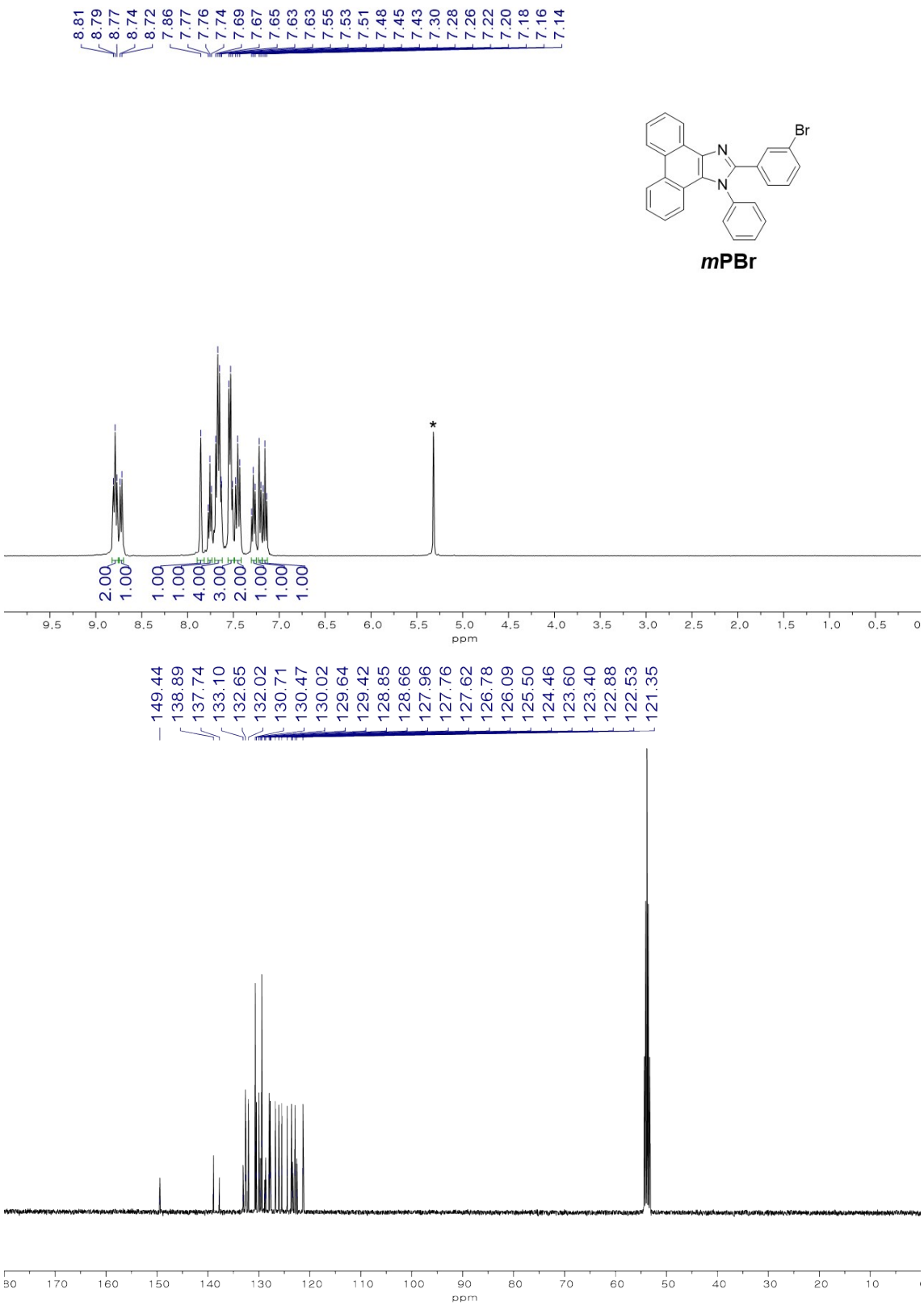

Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***m*PBr** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

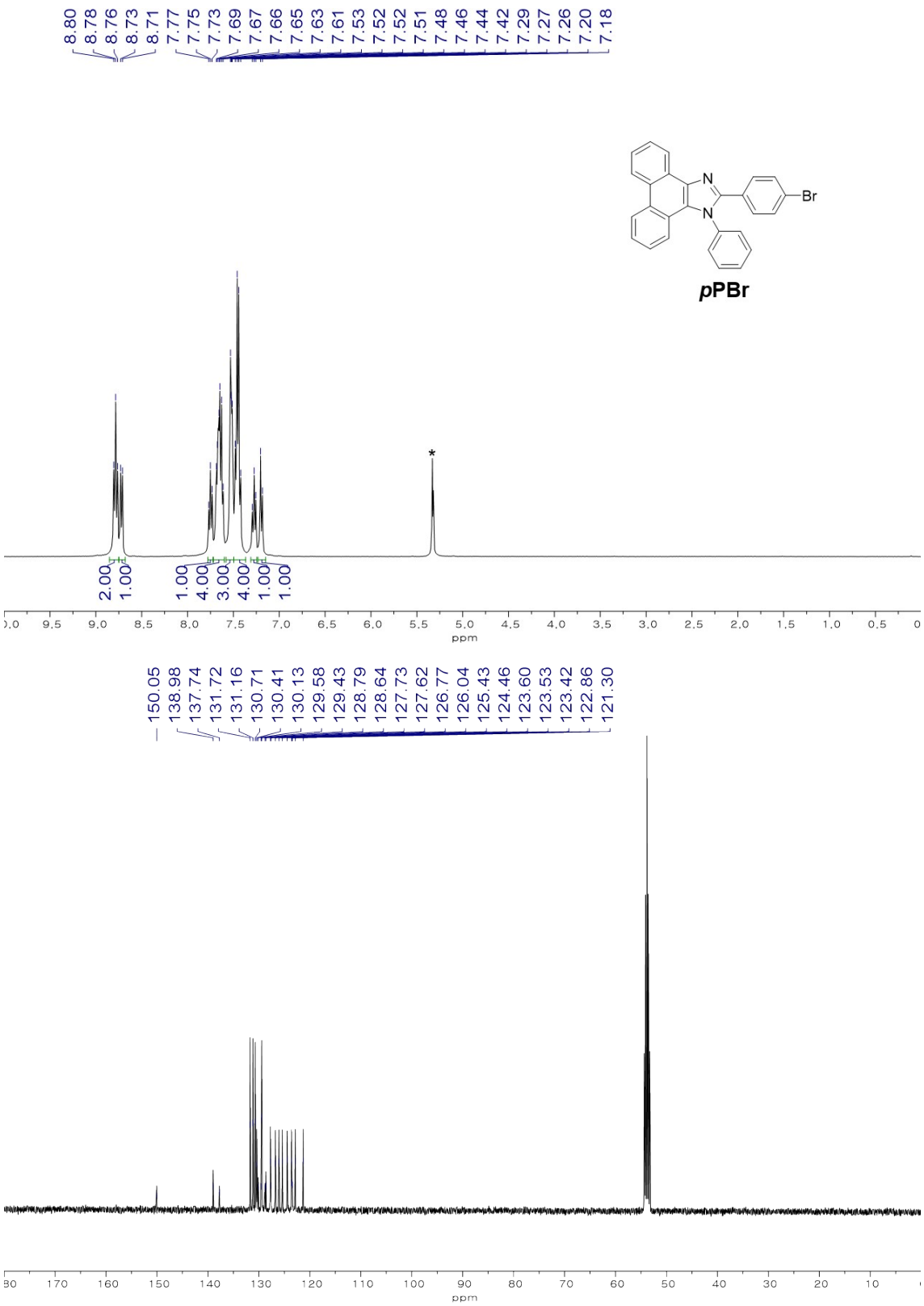

Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***p*PBr** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

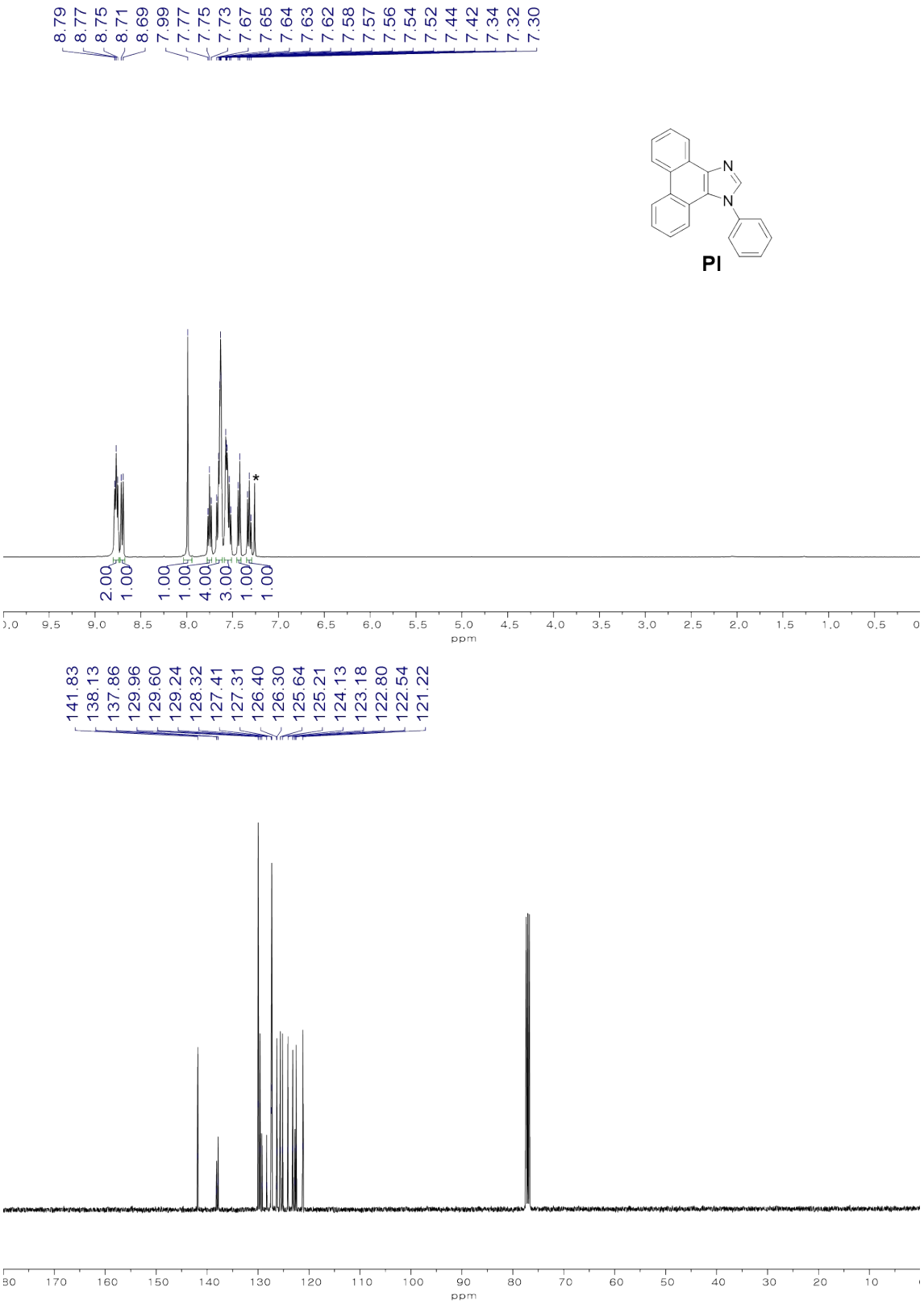

Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **PI** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

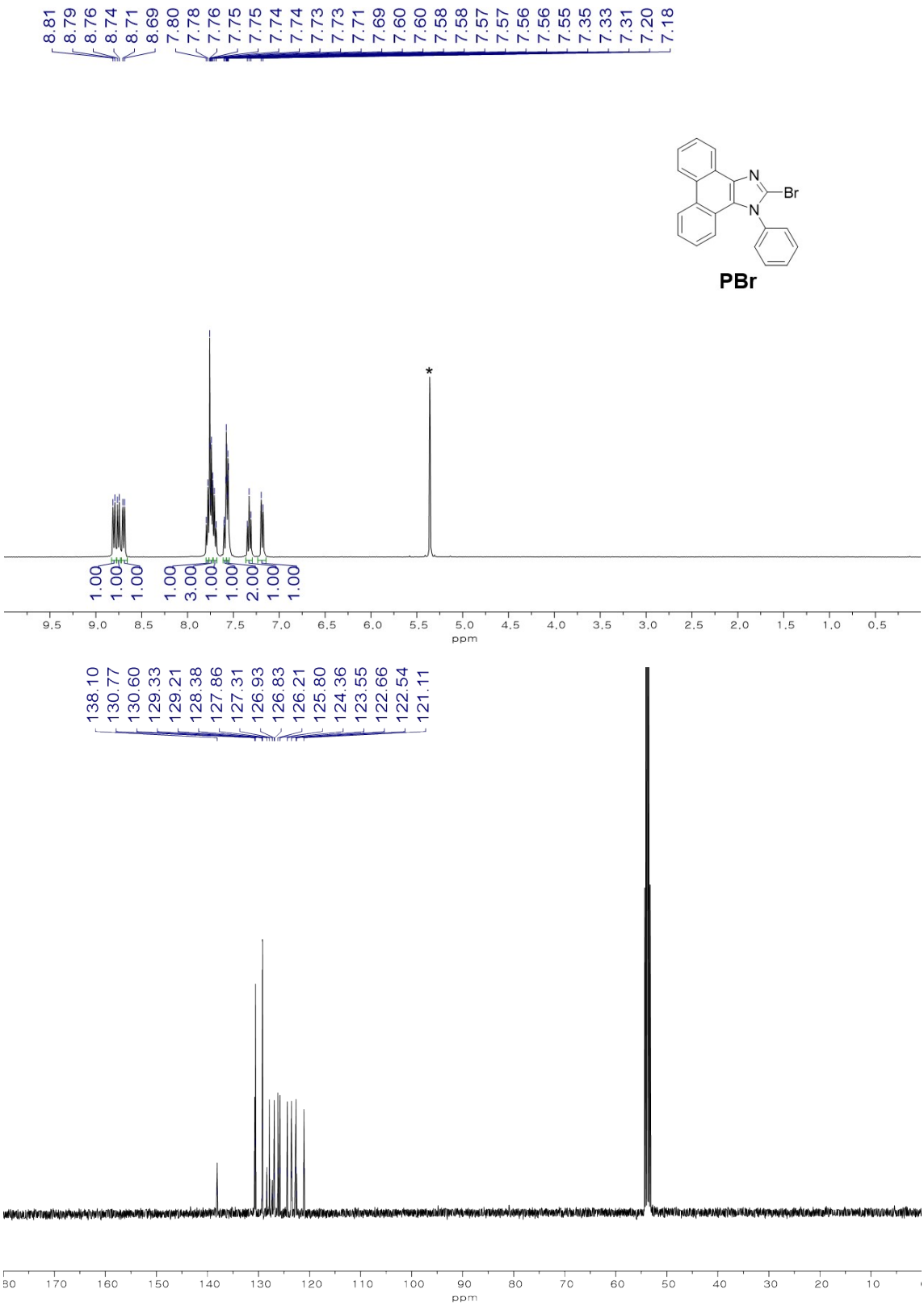

Fig. S5 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **PBr** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

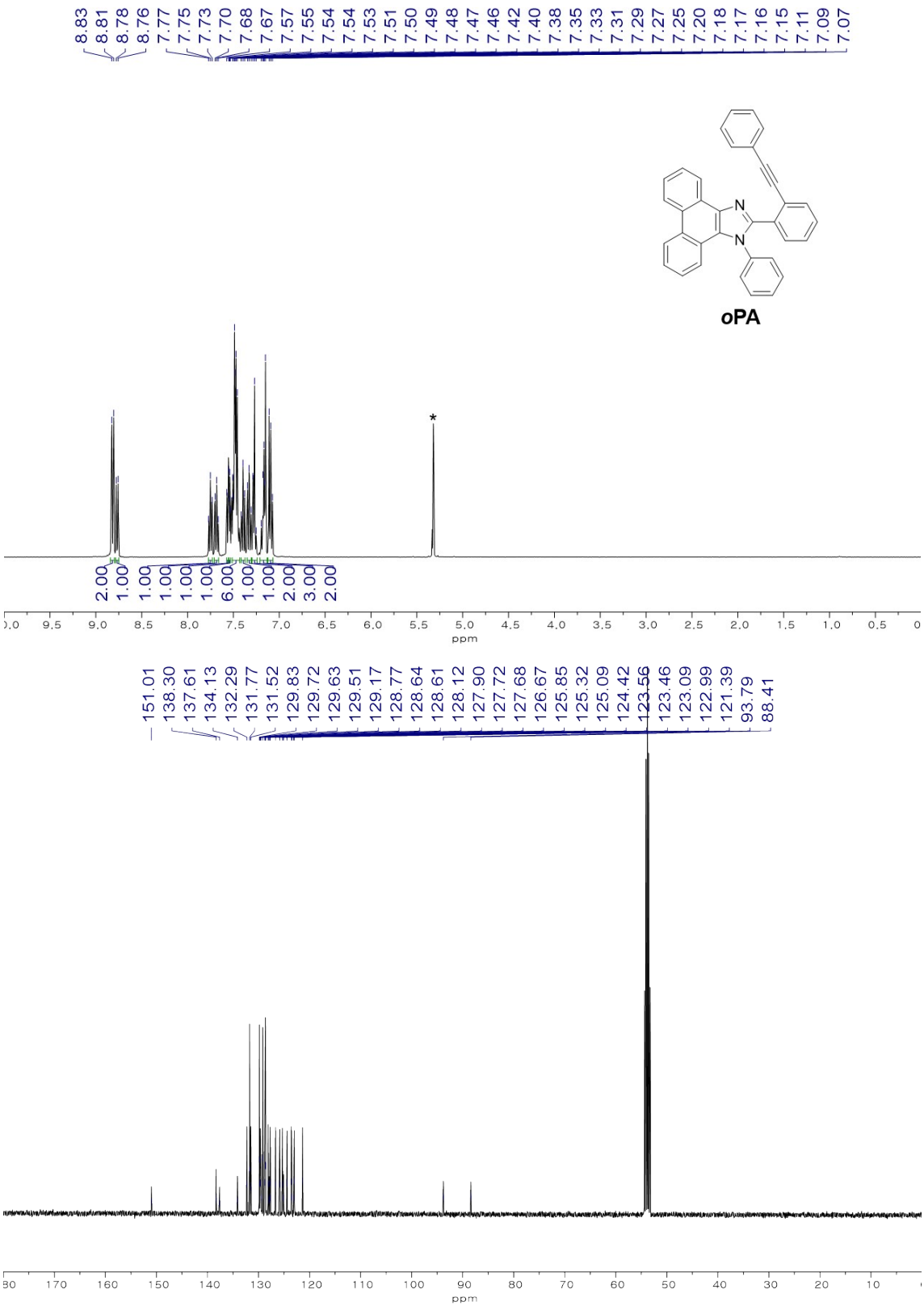

Fig. S6 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***o*PA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

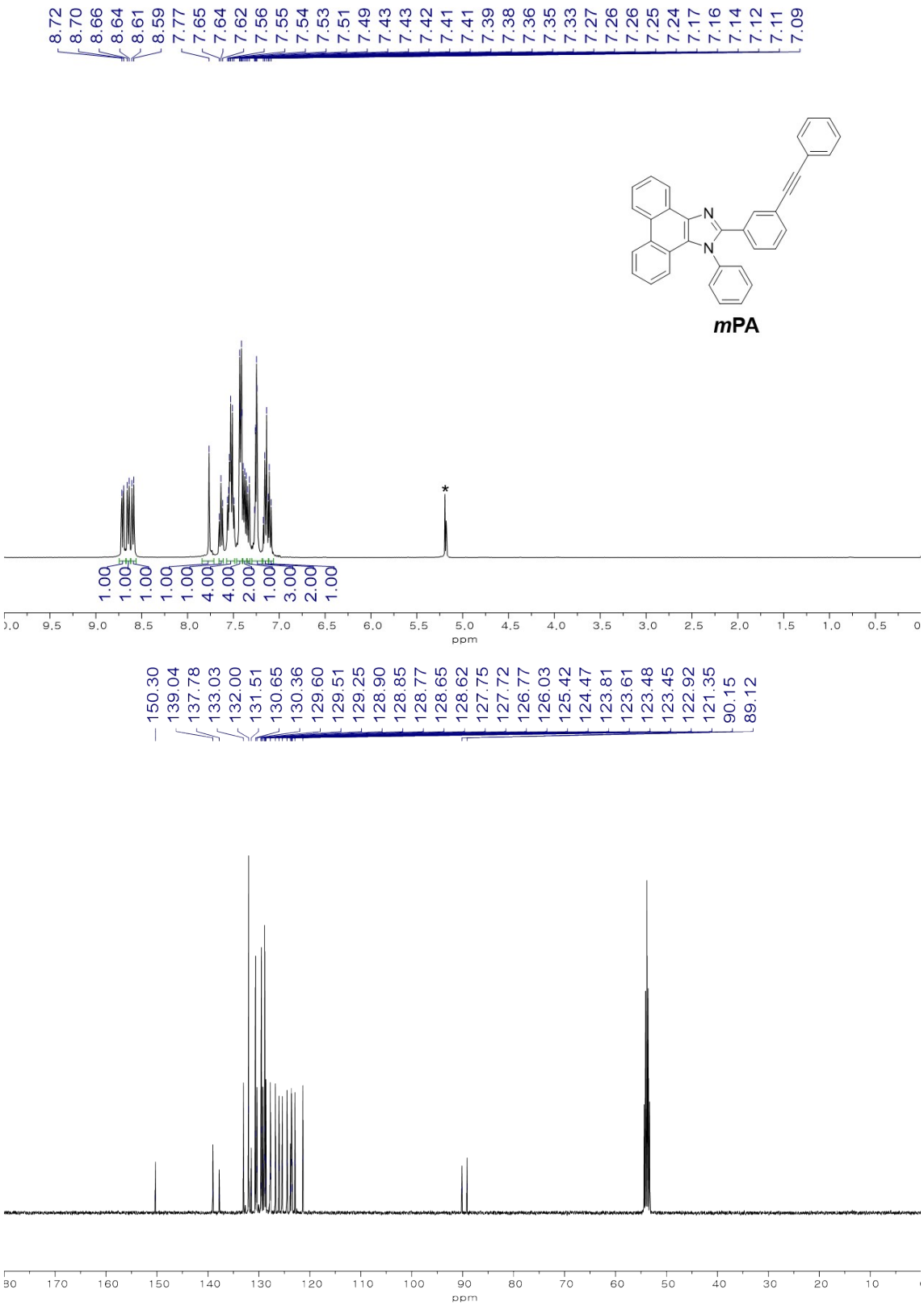

Fig. S7 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***m*PA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

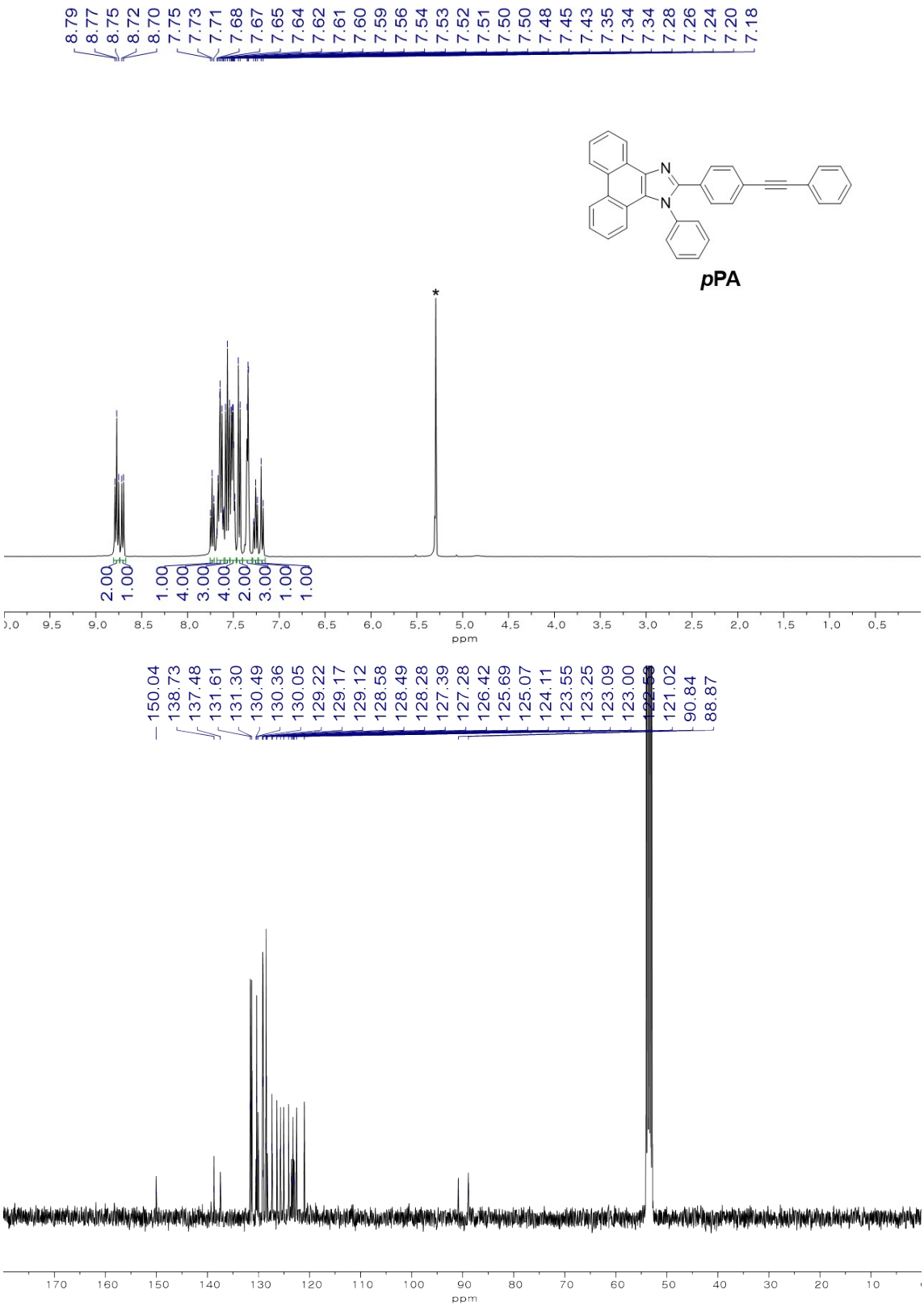

Fig. S8 ^{1}H (top) and ^{13}C (bottom) NMR spectra of ***p*PA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

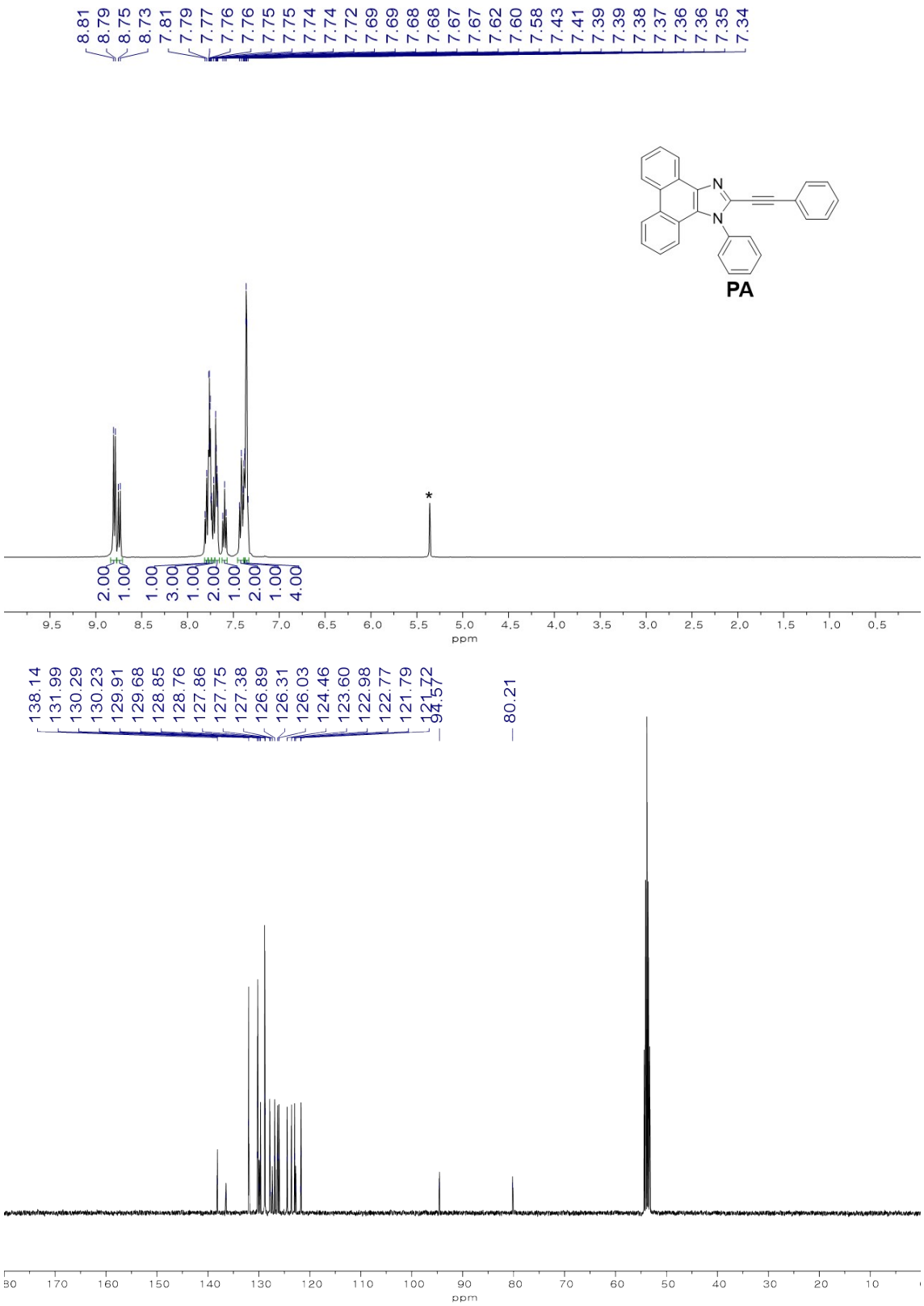

Fig. S9 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **PA** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

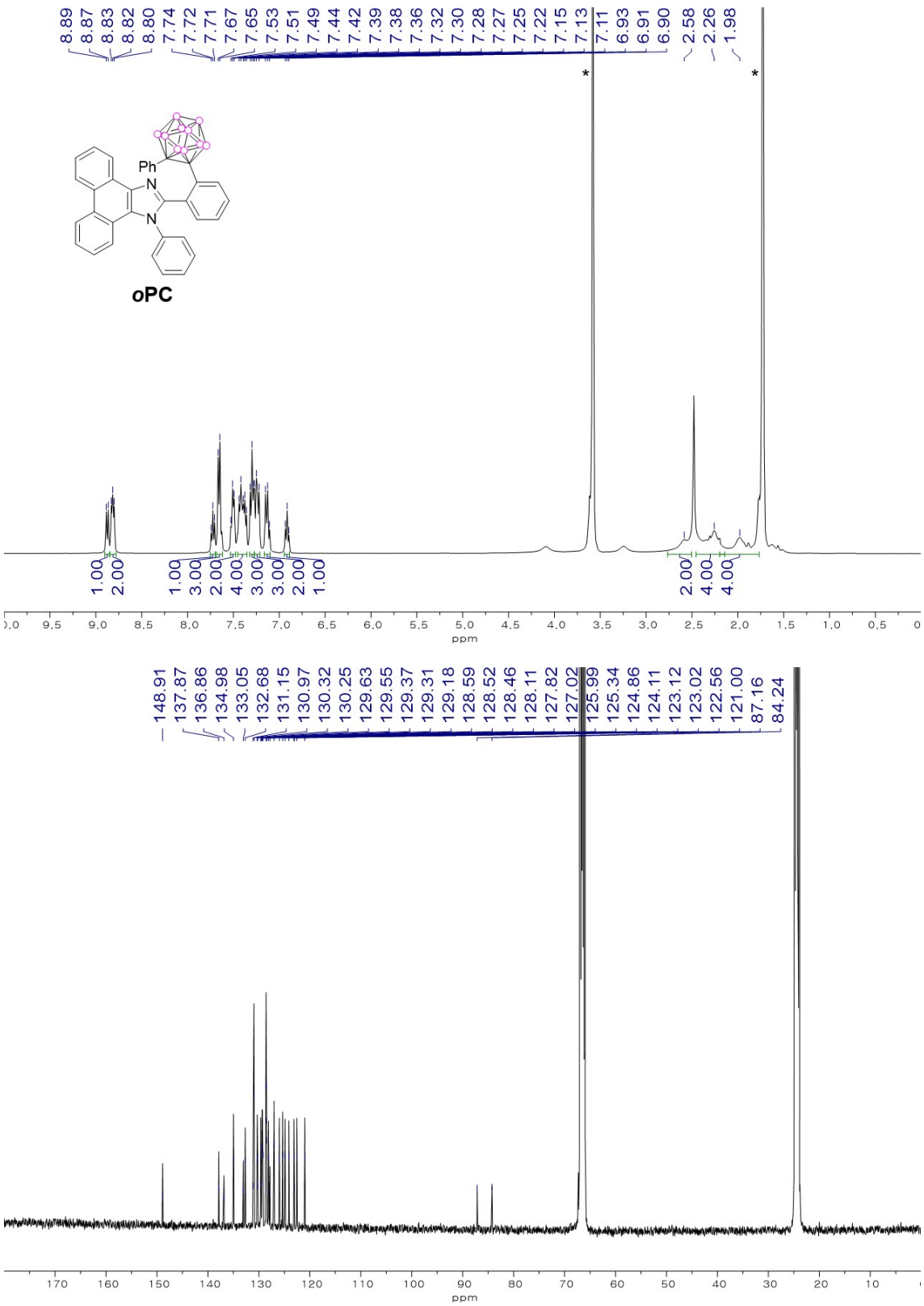

Fig. S10 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of ***o*PC** in THF-d_8 (* from residual THF in THF-d_8).

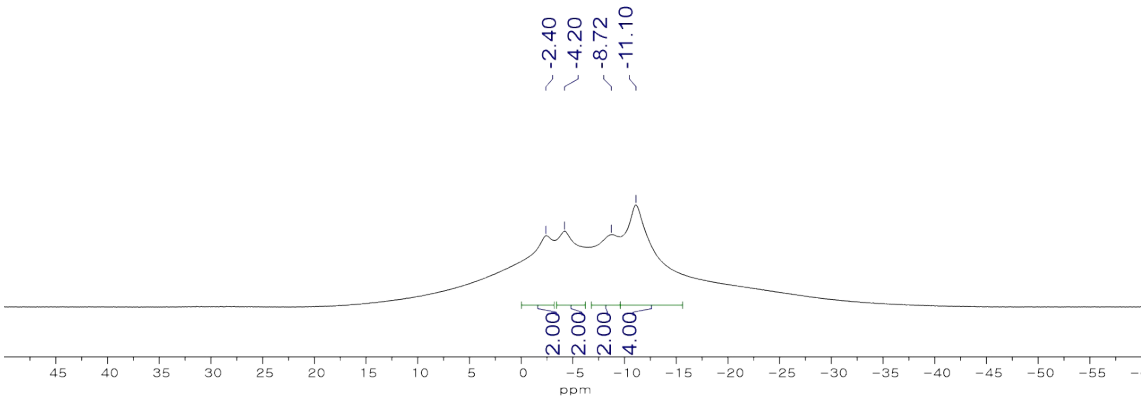

Fig. S11 $^{11}B\{^{1}H\}$ NMR spectra of ***o*PC** in THF-d_8.

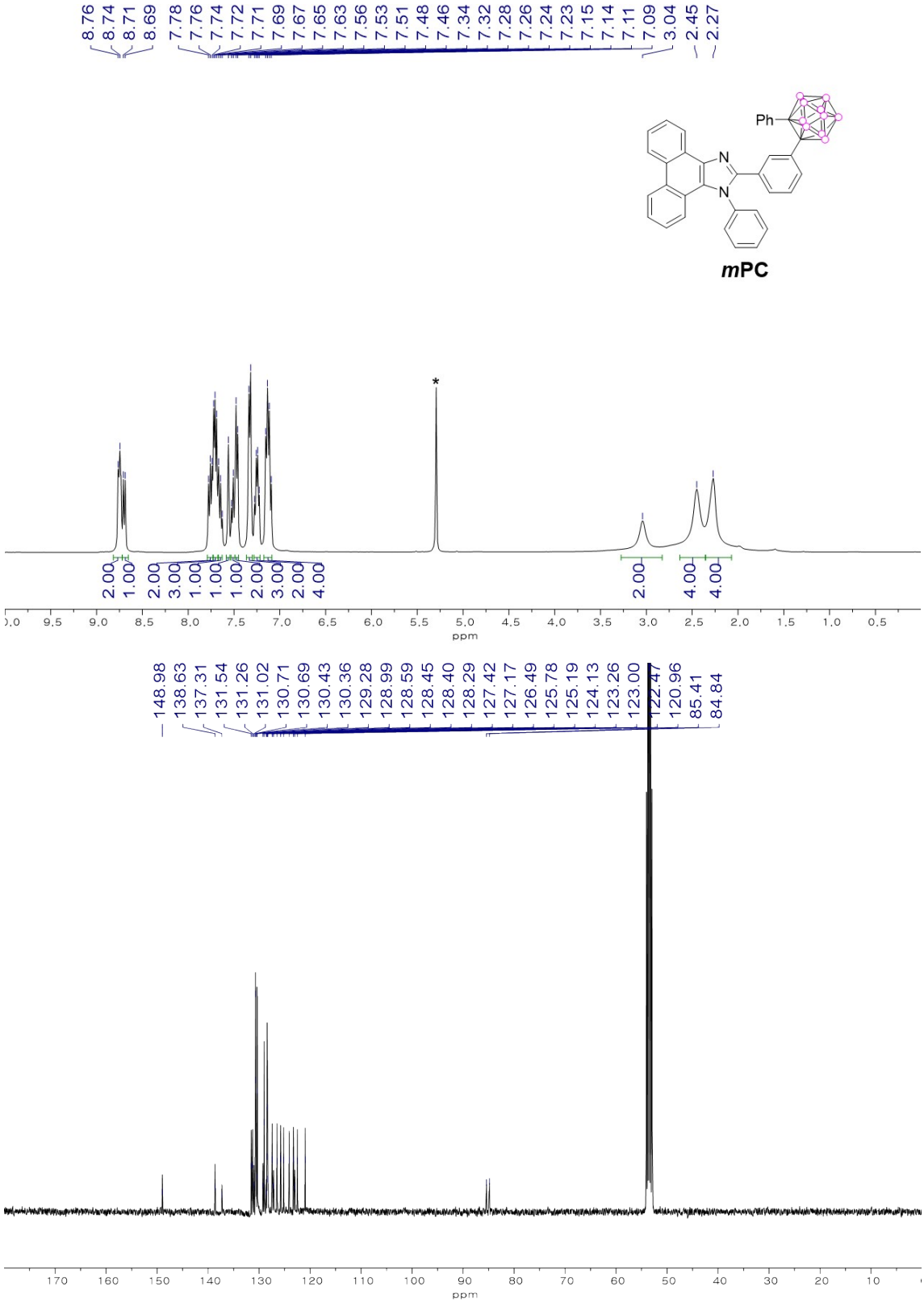

Fig. S12 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of ***m*PC** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

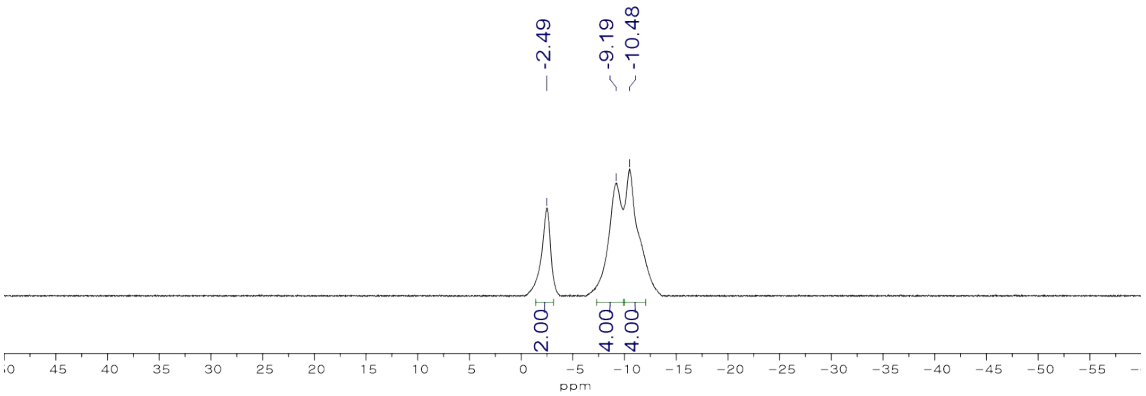

Fig. S13 $^{11}B\{^{1}H\}$ NMR spectra of ***m*PC** in CD_2Cl_2.

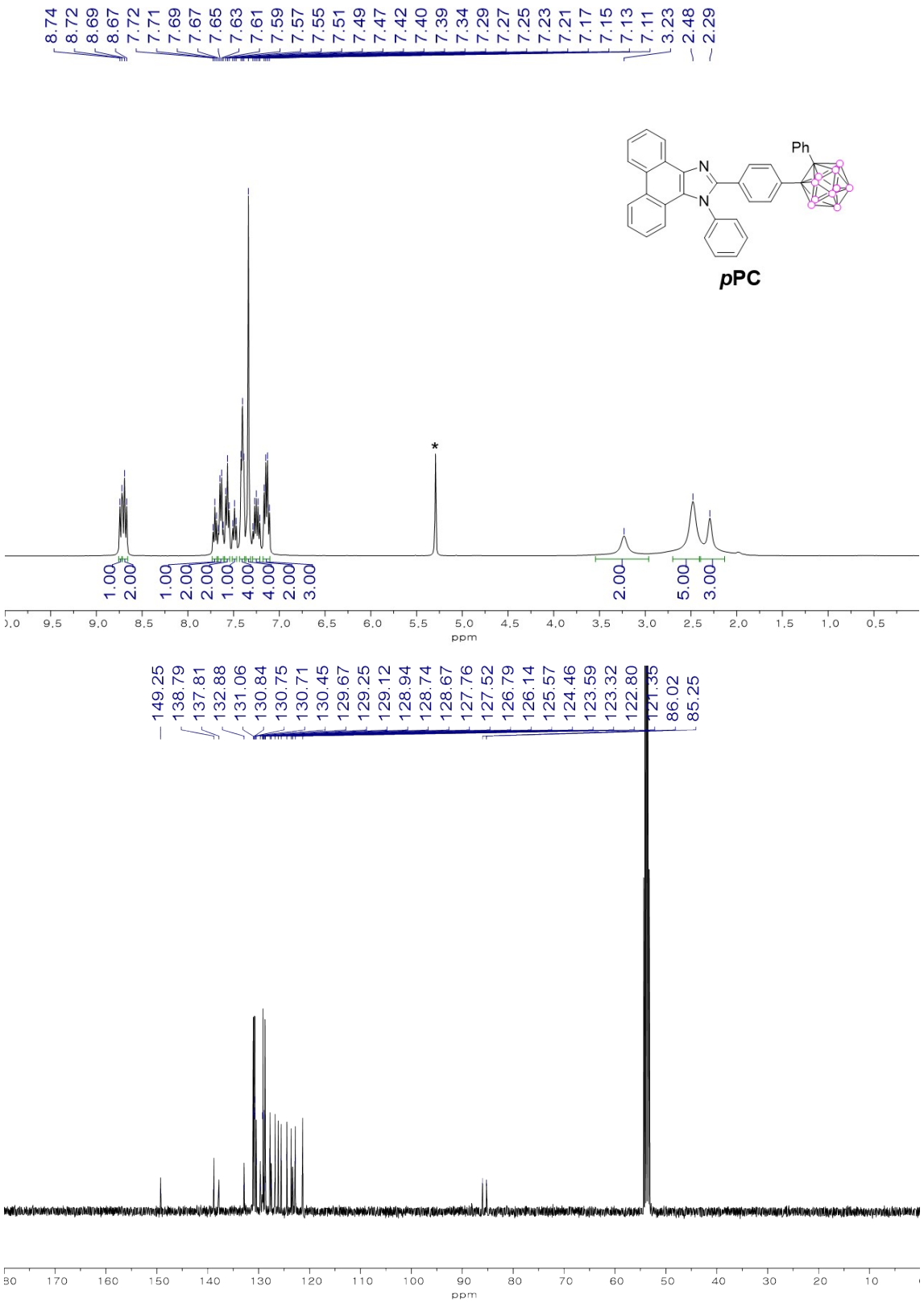

Fig. S14 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of ***p*PC** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

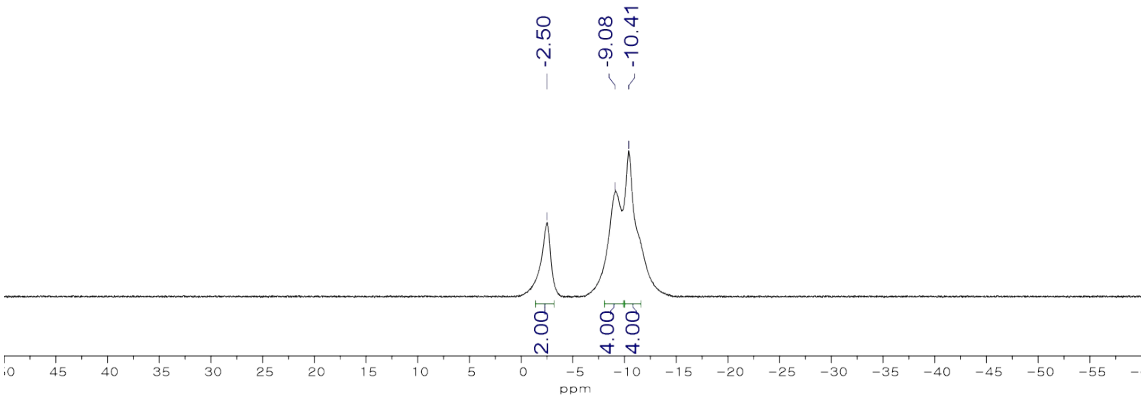

Fig. S15 $^{11}B\{^{1}H\}$ NMR spectra of ***p*PC** in CD_2Cl_2.

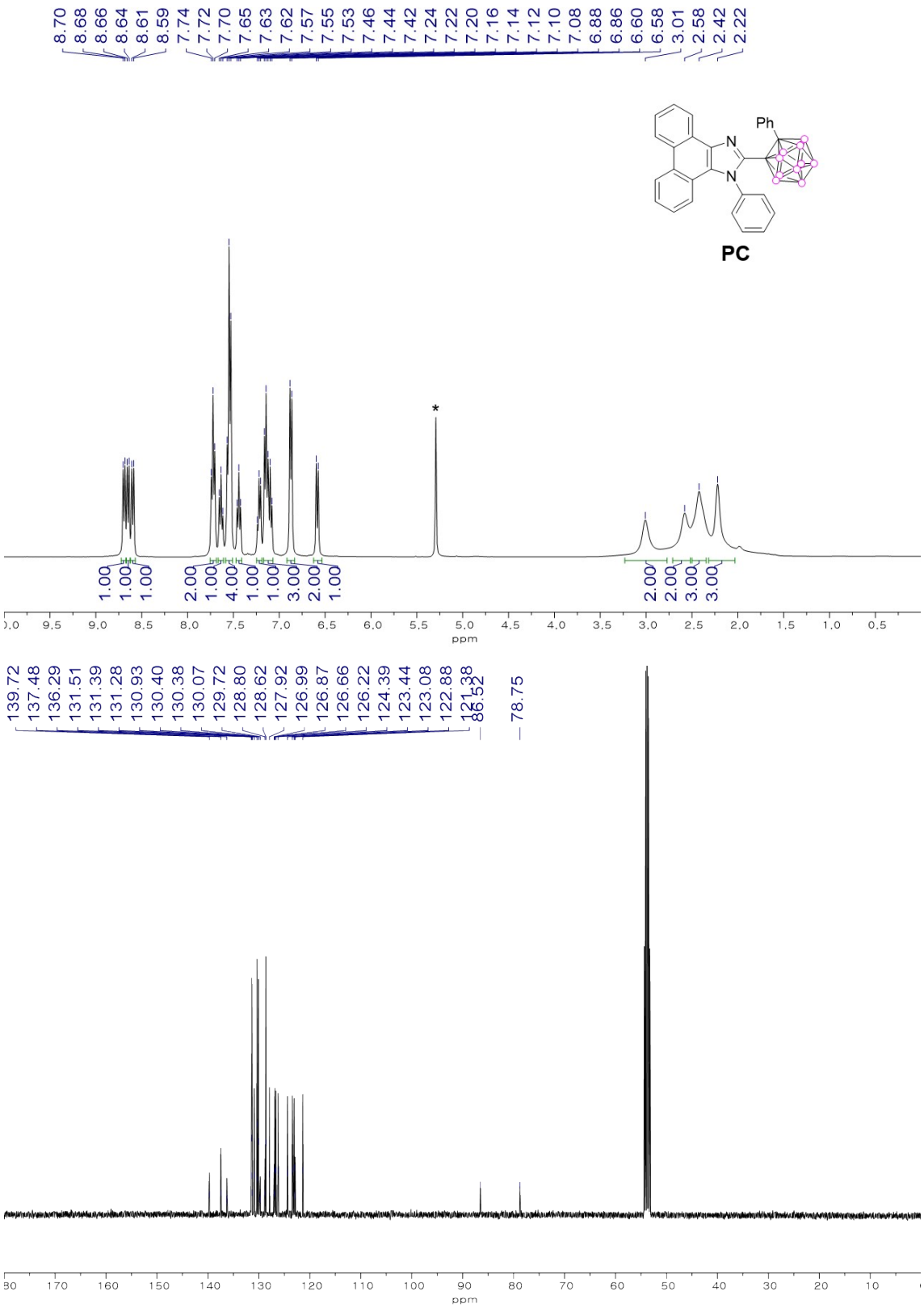

Fig. S16 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **PC** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

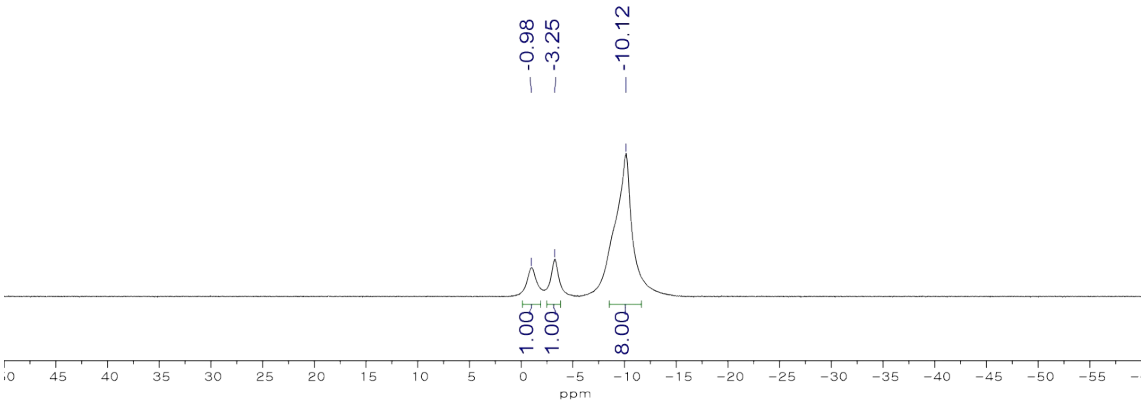

Fig. S17 $^{11}B\{^{1}H\}$ NMR spectra of **PC** in CD_2Cl_2.

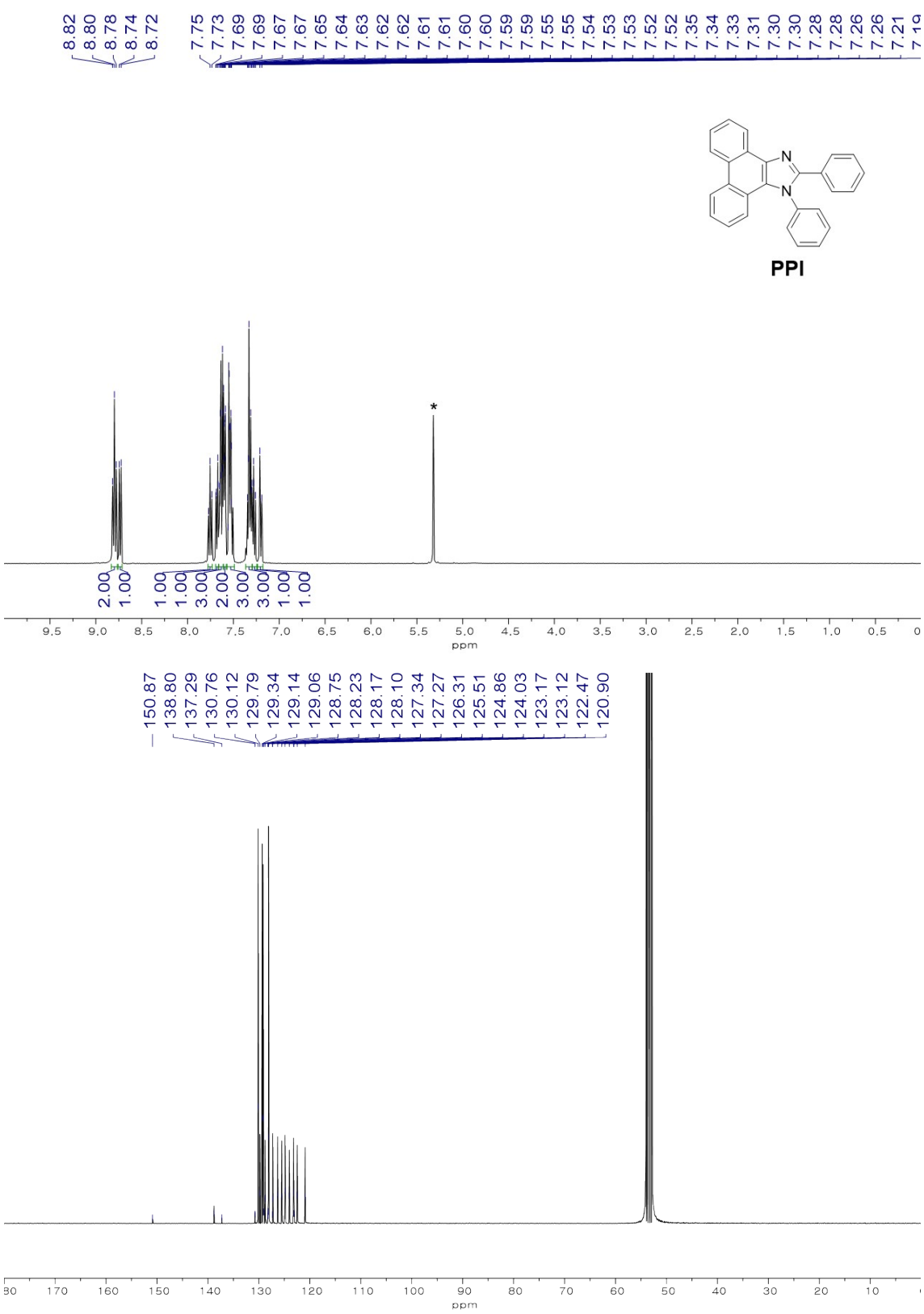

Fig. S18 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **PPI** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

Table S1 Crystallographic data and parameters for **PC**, ***o*PC**, ***m*PC**, and ***p*PC**.

Compound	**PC**	***o*PC**·CH_2Cl_2	***m*PC**·CH_3OH	***p*PC**
Formula	$C_{29}H_{28}B_{10}N_2$	$C_{35}H_{32}B_{10}N_2{\cdot}CH_2Cl_2$	$C_{35}H_{32}B_{10}N_2{\cdot}CH_3OH$	$C_{35}H_{32}B_{10}N_2$
Formula weight	512.63	673.65	620.77	588.72
Crystal system	Triclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	P_{-1}	P21/c	$Pna2_1$	$P2_1/c$
a (Å)	10.754(2)	14.133(3)	17.1475(6)	17.897(4)
b (Å)	16.376(3)	18.494(4)	11.1715(4)	13.095(3)
c (Å)	18.497(4)	13.764(3)	17.1764(6)	13.490(3)
α (°)	64.13(3)	90	90	90
β (°)	73.49(3)	104.15(3)	90	99.45(3)
γ (°)	88.75(3)	90	90	90
V (Å^3)	2790.3(12)	3488.4(13)	3290.4(2)	3118.6(11)
Z	4	4	4	4
ρ_{calc}(g cm^{-3})	1.220	1.283	1.253	1.254
μ (mm^{-1})	0.065	0.217	0.070	0.068
F(000)	1064	1392	1296	1224
T (K)	293(2)	293(2)	173(2)	293(2)
Scan mode	*φ and ω-scan*	*φ and ω-scan*	*φ and ω-scan*	*φ and ω-scan*
hkl range	$-13 < h < 13$, $-21 < k < 21$, $-24 < l < 23$	$-18 < h < 17$, $-24 < k < 24$, $-17 < l < 14$	$-22 < h < 22$, $-13 < k < 14$, $-22 < l < 17$	$-23 < h < 23$, $-17 < k < 17$, $-15 < l < 17$
Measd reflns	26198	34635	32339	30643
Unique reflns [R_{int}]	12680 [0.1592]	8009 [0.2162]	7017 [0.0561]	7143 [0.0307]
Reflns used for refinement	12680	8009	7017	7143
Refined parameters	739	451	446	424
R_1[a] (I > 2σ(I))	0.0789	0.0981	0.0390	0.0481
wR_2[b] all data	0.1718	0.2566	0.0979	0.1396
GOF on F^2	0.926	1.039	1.046	1.009
ρ_{fin} (max/min) (e Å^{-3})	0.212, −0.170	0.413, −0.359	0.232, −0.156	0.373, −0.189

[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 **PC**, ***o*PC**, ***m*PC**, and ***p*PC**.

Compound	**PC**	***o*PC**	***m*PC**	***p*PC**
		length (Å)		
C1–C2	1.721(5)	1.757(5)	1.723(3)	1.7278(16)
C1–C24	1.476(5)	–	–	–
C2–C3	1.477(5)	1.507(6)	1.504(3)	1.5114(15)
C1–C30	–	1.494(6)	1.510(3)	1.5034(16)
		angles (°)		
C24–C1–C2	119.8(3)	–	–	–
C30–C1–C2	–	119.6(4)	117.34(16)	119.59(9)
C1–C2–C3	119.0(3)	117.8(3)	118.93(16)	120.82(9)
C3–N1–C4	105.7(3)	–	–	–
N1–C4–C5	105.8(4)	–	–	–
C4–C5–N2	110.7(4)	–	–	–
C5–N2–C3	106.4(4)	–	–	–
N2–C3–N1	111.4(4)	–	–	–
C9–N1–C10	–	105.8(4)	106.86(17)	106.36(9)
N1–C10–C11	–	104.3(4)	105.06(18)	105.23(10)
C10–C11–N2	–	112.3(4)	111.22(18)	111.18(10)
C11–N2–C9	–	104.7(3)	105.14(18)	105.11(10)
N2–C9–N1	–	112.7(4)	111.72(18)	112.08(10)

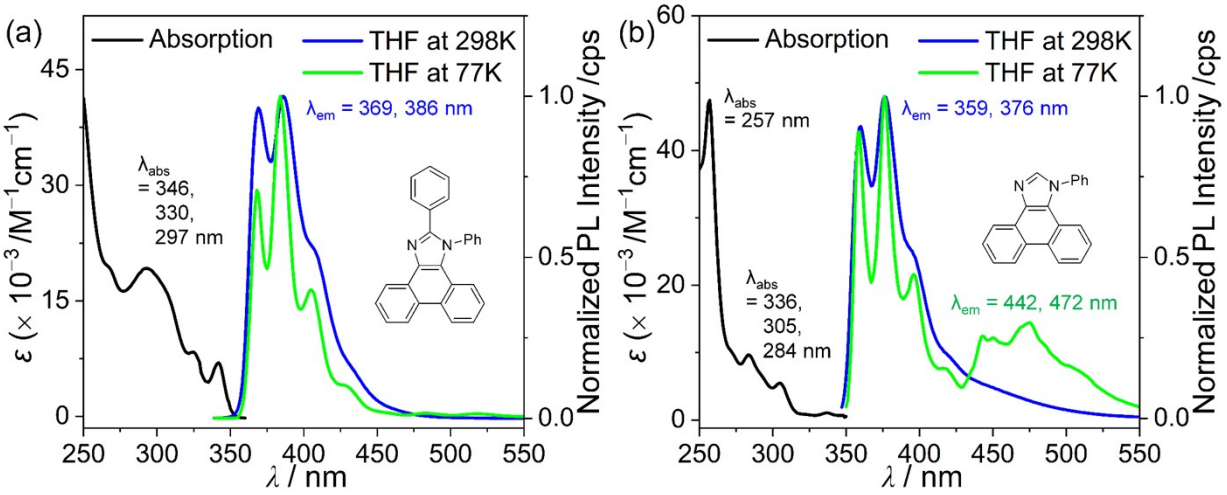

Fig. S19 UV-vis absorption (left side) and PL spectra (right side) for (a) 1,2-diphenyl-1*H*-phenanthro[9,10-*d*]imidazole (**PPI**, λ_{ex} = 329 nm) and (b) 1-phenyl-1*H*-phenanthro[9,10-*d*]imidazole (**PI**, λ_{ex} = 337 nm). Black line: absorption spectra in THF (3.0×10^{-5} M), blue line: PL spectra in THF (3.0×10^{-5} M) at 298 K, and green line: PL spectra in THF (3.0×10^{-5} M) at 77 K.

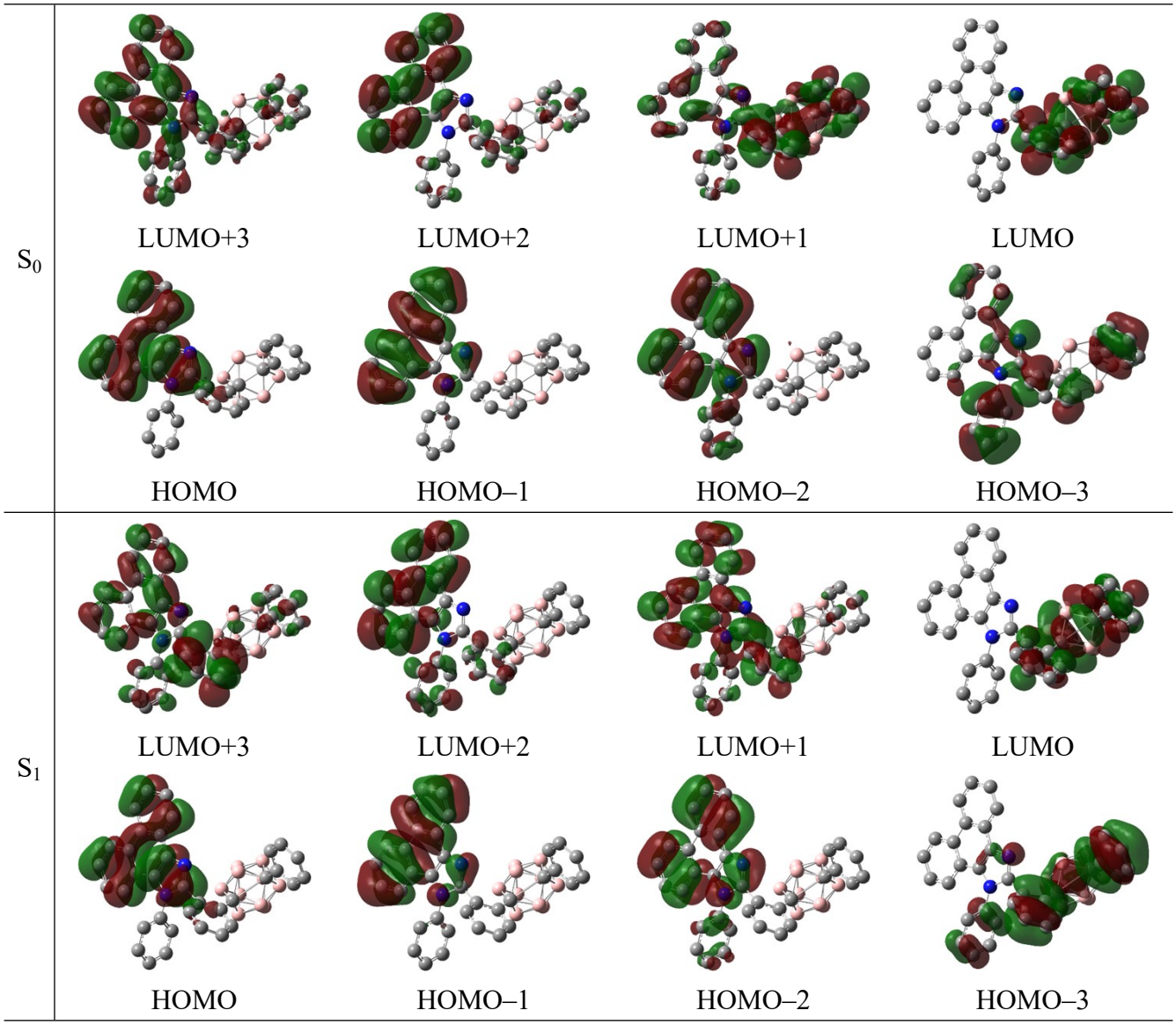

Fig. S20 The selected frontier orbitals of ***o*PC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

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

state	λ_{calc} /nm	f_{calc}	Major contribution
			S_0
1	347.71	0.0692	HOMO → LUMO (96.7%)
2	321.07	0.0385	HOMO−1 → LUMO+3 (10.8%)
□	□	□	HOMO → LUMO+1 (52.5%)
□	□	□	HOMO → LUMO+2 (28.0%)
3	312.27	0.0417	HOMO → LUMO+1 (69.5%)
□	□	□	HOMO → LUMO+2 (21.9%)
4	300.10	0.0106	HOMO−1 → LUMO (12.3%)
□	□	□	HOMO−1 → LUMO+2 (10.5%)
□	□	□	HOMO → LUMO+3 (61.6%)
5	296.41	0.0211	HOMO−1 → LUMO (83.8%)
			HOMO → LUMO+3 (11.4%)
			S_1
1	570.86	0.2153	HOMO → LUMO (99.8%)
2	457.76	0.0002	HOMO−1 → LUMO (99.4%)
3	425.58	0.0003	HOMO−2 → LUMO (98.4%)
4	422.03	0.0088	HOMO−4 → LUMO (10.3%)
□	□	□	HOMO−3 → LUMO (81.1%)
5	413.02	0.0910	HOMO−4 → LUMO (84.3%)
□	□	□	HOMO−3 → LUMO (8.0%)

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

	E (eV)	carborane -phenyl	*o*-carborane	bridged -phenyl	phenanthro -imidazole	*N*-phenyl
			S_0			
LUMO+3	−0.86	3.4	5.0	5.0	79.7	6.9
LUMO+2	−0.97	2.8	2.5	4.2	87.7	2.8
LUMO+1	−1.11	25.4	15.9	33.9	21.2	3.6
LUMO	−1.50	20.8	37.8	37.9	2.6	0.9
HOMO	−5.56	0.0	0.6	2.4	96.7	0.3
HOMO−1	−6.06	0.0	0.1	0.1	99.2	0.6
HOMO−2	−6.74	0.0	0.5	0.6	92.1	6.8
HOMO−3	−7.00	13.9	1.5	26.5	16.4	41.7
			S_1			
LUMO+3	−0.85	5.2	4.2	47.7	36.7	6.2
LUMO+2	−0.90	0.8	0.5	4.7	86.7	7.3
LUMO+1	−1.02	2.4	2.1	16.1	74.7	4.7
LUMO	−3.58	8.7	81.5	9.3	0.3	0.3
HOMO	−5.36	0.0	0.5	2.0	97.2	0.3
HOMO−1	−6.11	0.0	0.1	0.1	99.3	0.5
HOMO−2	−6.72	0.1	0.3	0.3	95.1	4.2
HOMO−3	−7.01	47.5	12.9	25.5	3.8	10.3

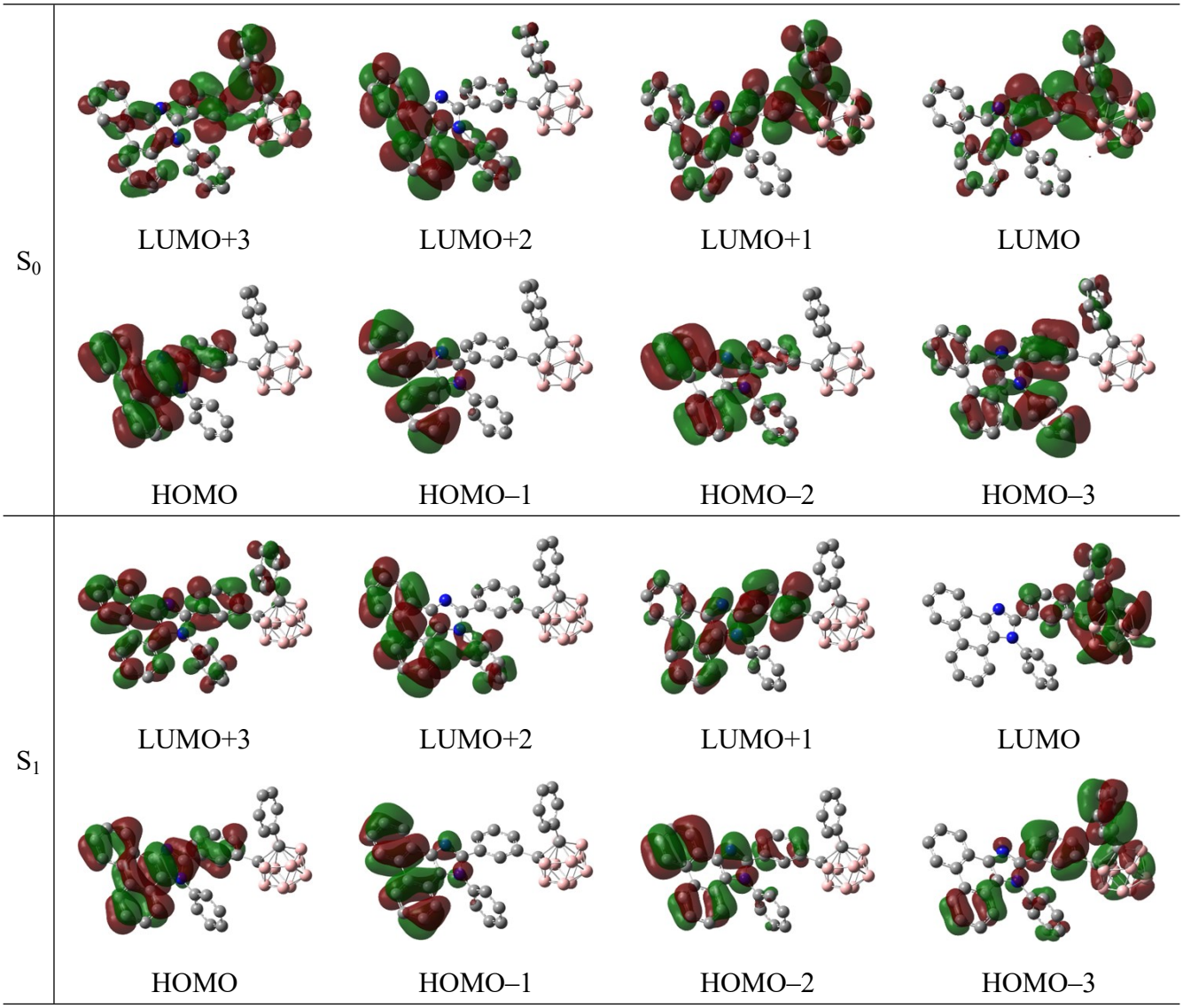

Fig. S21 The selected frontier orbitals of ***m*PC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

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

state	λ_{calc} /nm	f_{calc}	Major contribution
		S_0	
1	346.93	0.3397	HOMO → LUMO (94.4%)
2	333.03	0.1297	HOMO → LUMO+1 (82.4%)
□	□	□	HOMO → LUMO+2 (9.3%)
3	320.71	0.0670	HOMO−1 → LUMO+1 (6.0%)
□	□	□	HOMO → LUMO+1 (11.9%)
□	□	□	HOMO → LUMO+2 (68.9%)
4	301.89	0.0047	HOMO−1 → LUMO (24.1%)
□	□	□	HOMO−1 → LUMO+1 (8.1%)
□	□	□	HOMO → LUMO+3 (19.8%)
□	□	□	HOMO → LUMO+4 (32.8%)
5	297.44	0.0508	HOMO → LUMO+3 (28.4%)
□	□	□	HOMO → LUMO+4 (46.5%)
□	□	□	HOMO → LUMO+5 (17.3%)
		S_1	
1	557.20	0.3067	HOMO → LUMO (99.7%)
2	436.21	0.0024	HOMO−1 → LUMO (99.7%)
3	414.34	0.0826	HOMO−2 → LUMO (94.1%)
4	408.22	0.0005	HOMO−4 → LUMO (21.0%)
□	□	□	HOMO−3 → LUMO (68.7%)
5	401.93	0.0082	HOMO−4 → LUMO (74.9%)
□	□	□	HOMO−3 → LUMO (20.1%)

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

	E (eV)	carborane -phenyl	*o*-carborane	bridged -phenyl	phenanthro -imidazole	*N*-phenyl
			S_0			
LUMO+3	−0.86	32.9	12.6	29.5	21.4	3.5
LUMO+2	−0.99	2.7	1.1	2.0	85.1	9.1
LUMO+1	−1.31	18.9	18.3	30.0	32.1	0.7
LUMO	−1.50	11.7	26.5	44.4	15.9	1.6
HOMO	−5.52	0.0	0.2	9.8	89.7	0.3
HOMO−1	−6.10	0.0	0.0	0.2	99.2	0.6
HOMO−2	−6.76	0.1	0.3	5.3	90.4	3.9
HOMO−3	−7.04	3.8	0.5	21.5	25.0	49.2
			S_1			
LUMO+3	−0.83	6.6	1.9	15.8	69.0	6.6
LUMO+2	−0.95	0.3	0.2	1.2	87.2	11.1
LUMO+1	−1.47	0.6	1.9	43.4	52.8	1.2
LUMO	−3.54	10.8	80.0	9.2	0.0	0.0
HOMO	−5.32	0.0	0.3	12.3	87.1	0.2
HOMO−1	−6.14	0.0	0.0	0.3	99.2	0.5
HOMO−2	−6.73	0.7	0.8	8.3	88.5	1.7
HOMO−3	−7.02	37.5	11.6	31.2	15.6	4.1

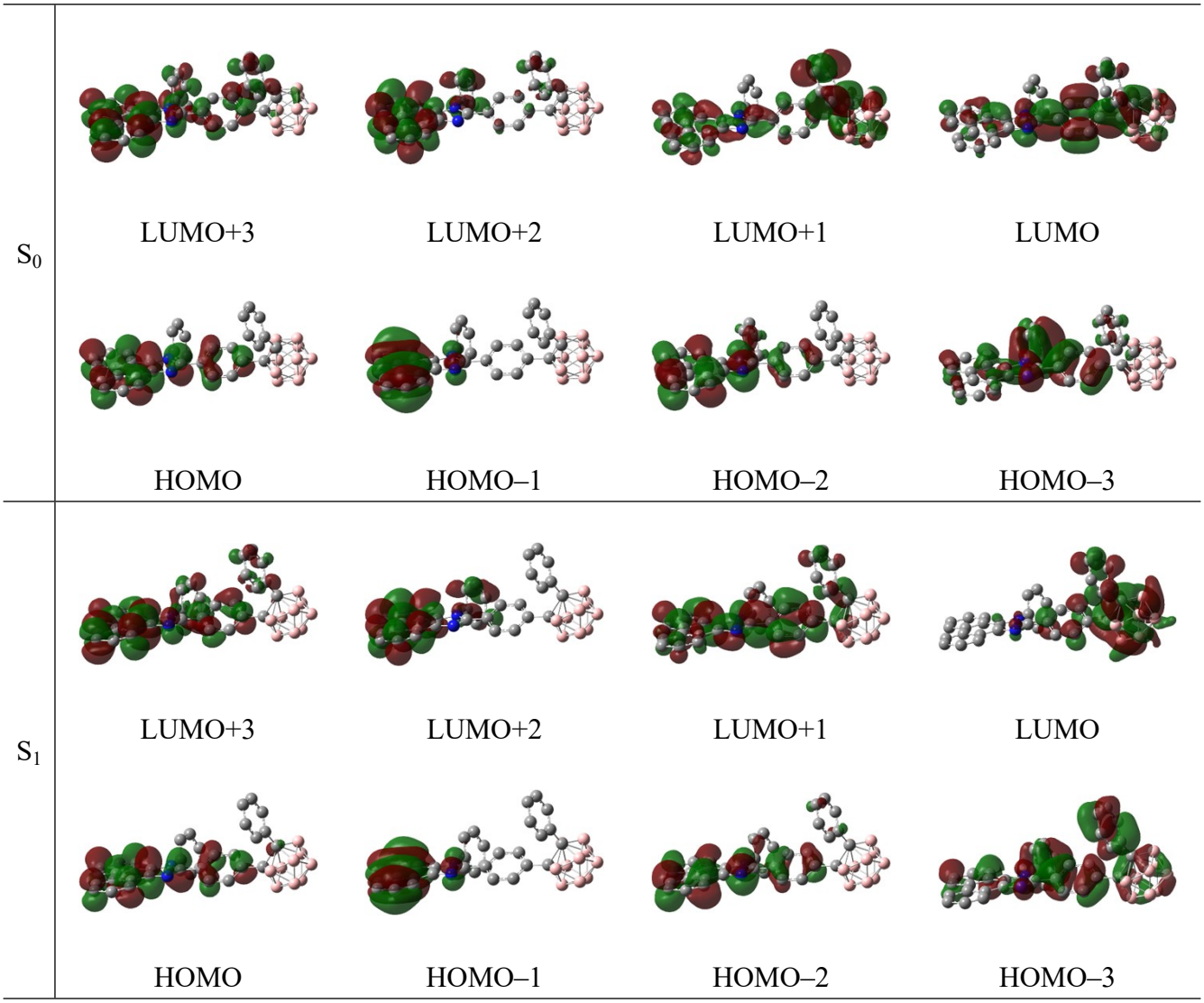

Fig. S22 The selected frontier orbitals of ***p*PC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

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

state	λ_{calc} /nm	f_{calc}	Major contribution
			S_0
1	370.40	0.4775	HOMO → LUMO (98.2%)
2	325.44	0.0012	HOMO−1 → LUMO (25.5%)
□	□	□	HOMO → LUMO+1 (10.1%)
□	□	□	HOMO → LUMO+2 (53.4%)
3	314.08	0.0483	HOMO−1 → LUMO (51.8%)
□	□	□	HOMO → LUMO+1 (27.9%)
□	□	□	HOMO → LUMO+3 (9.1%)
4	305.96	0.0467	HOMO−1 → LUMO (12.2%)
□	□	□	HOMO → LUMO+1 (50.2%)
□	□	□	HOMO → LUMO+2 (30.0%)
5	296.90	0.0542	HOMO → LUMO+2 (23.6%)
□	□	□	HOMO → LUMO+3 (55.6%)
□	□	□	HOMO → LUMO+4 (9.2%)
			S_1
1	543.71	0.4560	HOMO → LUMO (99.8%)
2	415.64	0.0079	HOMO−1 → LUMO (99.6%)
3	394.29	0.1098	HOMO−3 → LUMO (7.7%)
□	□	□	HOMO−2 → LUMO (89.3%)
4	388.00	0.0492	HOMO−3 → LUMO (82.8%)
□	□	□	HOMO−2 → LUMO (7.2%)
5	384.91	0.0032	HOMO−5 → LUMO (37.1%)
□	□	□	HOMO−4 → LUMO (61.0%)

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

	E (eV)	carborane -phenyl	*o*-carborane	bridged -phenyl	phenanthro -imidazole	*N*-phenyl
			S_0			
LUMO+3	−0.82	8.3	3.2	9.4	70.9	8.1
LUMO+2	−0.99	3.9	1.4	1.9	84.4	8.4
LUMO+1	−1.12	46.1	22.2	5.0	26.3	0.6
LUMO	−1.74	5.9	23.4	45.0	24.9	0.8
HOMO	−5.52	0.0	0.9	10.1	88.7	0.3
HOMO−1	−6.11	0.0	0.0	0.2	99.2	0.6
HOMO−2	−6.76	0.1	0.6	6.0	89.9	3.5
HOMO−3	−7.05	2.6	2.5	22.0	25.0	47.9
			S_1			
LUMO+3	−0.86	4.9	1.6	13.6	73.6	6.3
LUMO+2	−0.99	0.1	0.0	0.5	90.2	9.3
LUMO+1	−1.39	5.3	5.1	34.1	53.8	1.6
LUMO	−3.42	8.0	83.1	7.2	1.6	0.1
HOMO	−5.41	0.5	2.6	10.4	86.2	0.3
HOMO−1	−6.17	0.0	0.0	0.3	99.1	0.5
HOMO−2	−6.75	2.2	1.9	10.1	83.9	1.9
HOMO−3	−6.99	25.7	8.3	21.9	27.8	16.4

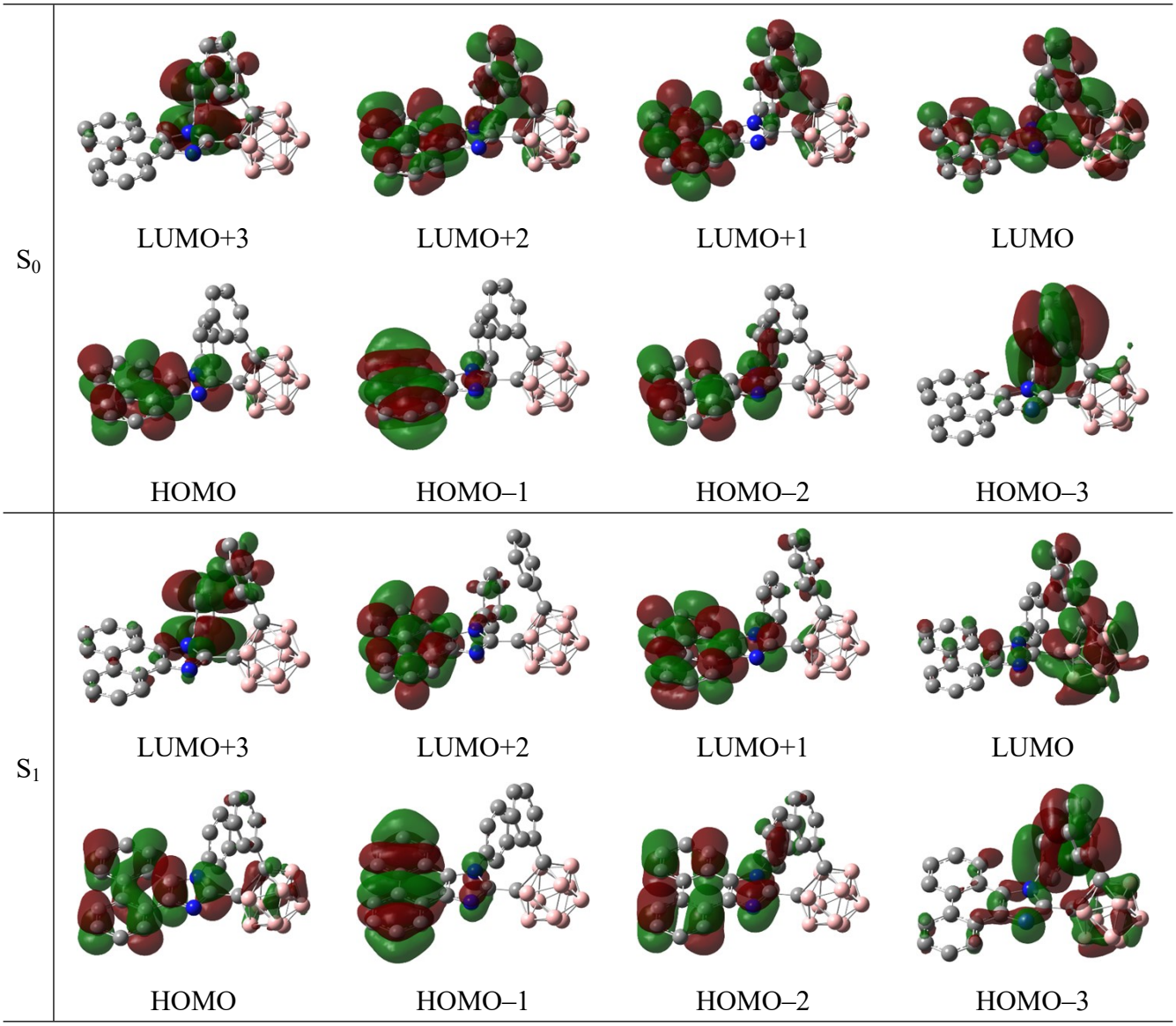

Fig. S23 The selected frontier orbitals of **PC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

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

state	λ_{calc} /nm	f_{calc}	Major contribution
			S_0
1	332.69	0.2617	HOMO → LUMO (93.8%)
2	312.47	0.0167	HOMO−1 → LUMO (32.7%)
□	□	□	HOMO → LUMO+1 (43.5%)
□	□	□	HOMO → LUMO+2 (10.7%)
3	298.62	0.0213	HOMO−1 → LUMO (38.8%)
□	□	□	HOMO → LUMO+1 (39.5%)
□	□	□	HOMO → LUMO+2 (11.2%)
4	287.92	0.0743	HOMO−1 → LUMO (22.5%)
□	□	□	HOMO−1 → LUMO+1 (14.1%)
□	□	□	HOMO → LUMO+2 (58.3%)
5	280.88	0.0029	HOMO → LUMO+3 (95.3%)
			S_1
1	539.77	0.4130	HOMO → LUMO (99.9%)
2	416.15	0.0216	HOMO−1 → LUMO (99.2%)
3	400.28	0.0416	HOMO−2 → LUMO (94.0%)
4	386.67	0.0063	HOMO−4 → LUMO (30.6%)
			HOMO−3 → LUMO (62.4%)
5	376.47	0.0062	HOMO−4 → LUMO (90.0%)

Table S10 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **PC** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

	E (eV)	carborane -phenyl	*o*-carborane	phenanthro -imidazole	*N*-phenyl
			S_0		
LUMO+3	−0.78	6.0	3.8	6.1	84.0
LUMO+2	−0.99	17.1	6.8	72.6	3.4
LUMO+1	−1.08	15.5	6.3	75.2	3.0
LUMO	−1.56	17.4	38.0	43.7	0.9
HOMO	−5.80	0.2	3.5	96.2	0.2
HOMO−1	−6.19	0.0	0.1	99.5	0.4
HOMO−2	−6.91	1.0	0.8	93.9	4.3
HOMO−3	−7.16	67.9	3.8	3.8	24.4
			S_1		
LUMO+3	−0.74	8.8	1.7	6.6	82.9
LUMO+2	−1.07	0.1	0.1	96.3	3.5
LUMO+1	−1.15	3.0	2.3	92.9	1.8
LUMO	−3.45	8.3	83.8	7.7	0.2
HOMO	−5.69	1.1	4.5	94.1	0.2
HOMO−1	−6.27	0.1	0.3	99.2	0.5
HOMO−2	−6.89	1.4	1.5	92.0	5.2
HOMO−3	−7.16	32.2	10.5	11.2	46.1

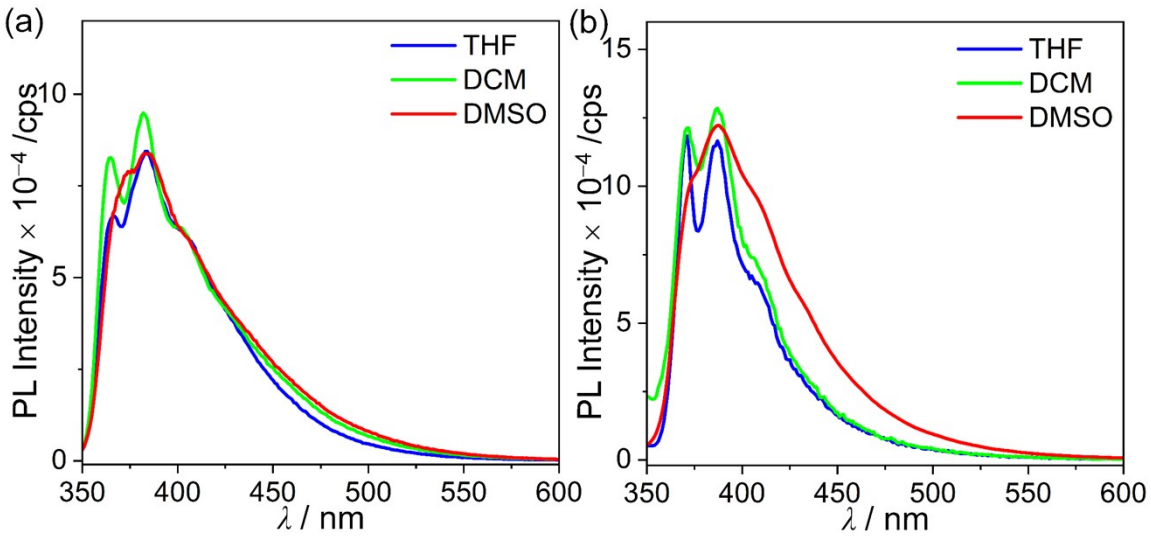

Fig. S24 PL spectra of (a) ***o*PC** (3.0×10^{-5} M, λ_{ex} = 338 nm) and (b) ***m*PC** (λ_{ex} = 342 nm) in various organic solvents.

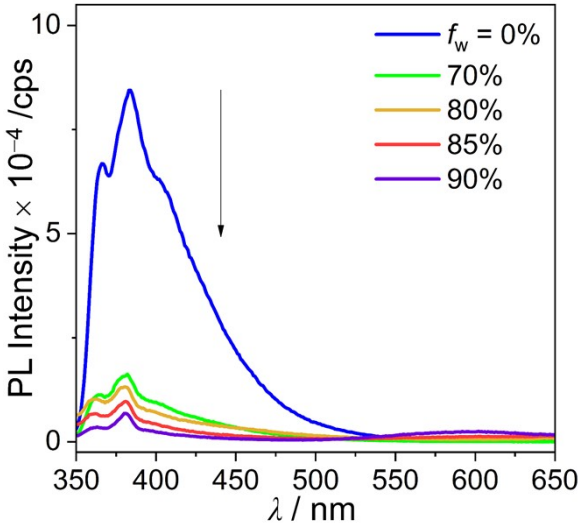

Fig. S25 PL spectra of ***o*PC** (λ_{ex} = 338 nm) in THF/distilled water mixtures (3.0×10^{-5} M).

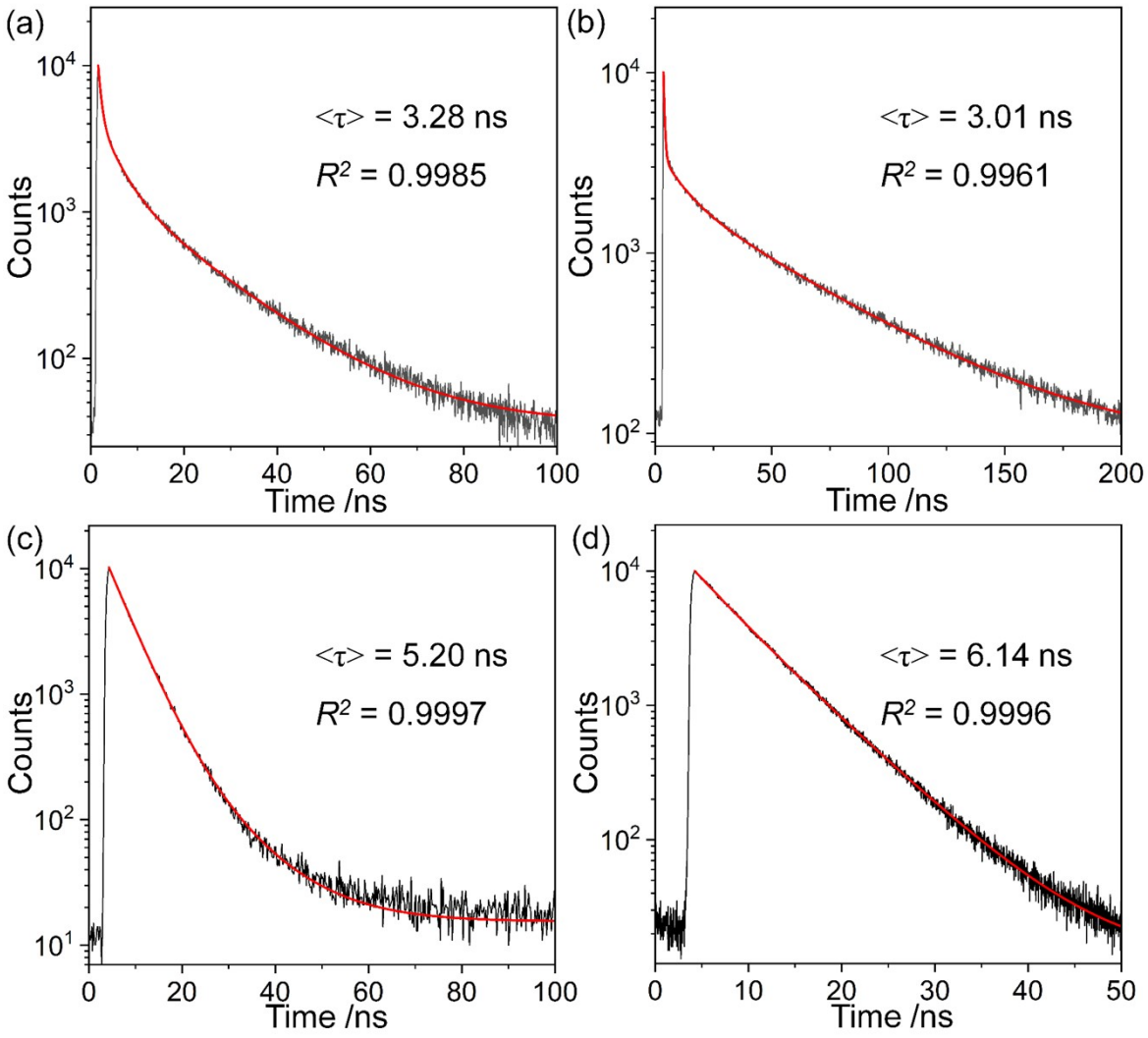

Fig. S26 Emission decay curves for (a) ***o*PC**, (b) ***m*PC**, (c) ***p*PC**, and (d) **PC** in the film state (5 wt% doped in PMMA) detected at each CT based emission maxima at 298 K. Each red-line is its exponential fitting curve for the decay curves.

Table S11 Low-energy electronic transitions (LUMO → HOMO transitions) data (computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$)) of S_1-states as Ψ was varied from 0–360°, and molecular orbital distributions on the *o*-carborane moieties of the LUMO levels (%) and the 1*H*-phenanthro[9,10-*d*]imidazole moiety of the HOMO levels (%) for ***p*PC** and **PC**

***p*PC**				
Ψ /°	HOMO	LUMO	λ_{calc}	$f_{calc.}$
0	72	81.5	896.06	0.0010
30	74.2	83	836.71	0.1279
60	80.3	85.9	673.12	0.3462
90	83.6	86.1	543.91	0.4599
120	80.3	85.3	653.71	0.3811
150	74.4	82.7	875.71	0.1351
180	72.1	81.1	900.62	0.0000
210	74.4	83.2	868.14	0.1254
240	80.1	85.4	620.28	0.3615
270	83.7	86.6	545.89	0.4385
300	80.3	85.1	687.60	0.3773
330	74.7	82.4	819.13	0.1389
360	72	81.5	896.06	0.0010

PC				
Ψ /°	HOMO	LUMO	λ_{calc}	$f_{calc.}$
0	91.1	72.1	992.75	0.0010
30	92.6	82.3	914.68	0.0575
60	94.4	83.7	664.09	0.3735
90	94.7	85	543.88	0.4186
120	94	83.6	653.85	0.0255
150	91.9	81.8	906.35	0.0022
180	91.1	72.2	1090.89	0.0000
210	91.7	81.5	910.39	0.0031
240	93.8	83.5	659.14	0.0336
270	94.8	85.5	525.29	0.4153
300	94.7	84.5	655.62	0.3554
330	92.5	82.8	908.83	0.0548
360	91.5	72.1	992.75	0.0010

Table S12 Cartesian coordinates of the ground state (S_0) fully optimized geometry of ***o*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	3.531624	-0.780142	0.971232
C	2.195008	0.379879	0.859643
C	1.981318	1.096428	-0.467702
C	0.768393	1.076589	-1.210665
C	0.695175	1.791680	-2.417790
H	-0.233521	1.757158	-2.976952
C	1.767938	2.520545	-2.918440
H	1.674192	3.055113	-3.858083
C	2.955204	2.543697	-2.195857
H	3.814366	3.100620	-2.555281
C	3.048447	1.844116	-0.996640
H	3.986434	1.883208	-0.465144
C	-0.482372	0.347149	-0.865431
C	-2.620759	0.030015	-0.325243
C	-2.002806	-1.153754	-0.709582
C	-2.708603	-2.403121	-0.742110
C	-2.080655	-3.597824	-1.150068
H	-1.035613	-3.558641	-1.438718
C	-2.785879	-4.786768	-1.182456
H	-2.297558	-5.703931	-1.498004
C	-4.140075	-4.801416	-0.804843
H	-4.700499	-5.731193	-0.828523
C	-4.767962	-3.634895	-0.400442
H	-5.812514	-3.687394	-0.117153
C	-4.079088	-2.399907	-0.353293
C	-4.719583	-1.150819	0.082120
C	-6.069174	-1.123533	0.500715
H	-6.651563	-2.036909	0.493151
C	-6.682580	0.039918	0.932313
H	-7.721414	0.017428	1.247026
C	-5.958477	1.240825	0.968519
H	-6.430343	2.155136	1.315277
C	-4.635791	1.260459	0.563826
H	-4.085409	2.190565	0.602789
C	-3.992152	0.086338	0.109305
C	-1.761226	2.426929	-0.259764
C	-2.351238	3.197002	-1.267131
H	-2.711924	2.714213	-2.169548
C	-2.478530	4.575016	-1.094893
H	-2.938500	5.173347	-1.874976
C	-2.012967	5.181744	0.074478
H	-2.111243	6.254859	0.205293
C	-1.422311	4.407394	1.074707
H	-1.061505	4.874608	1.985511
C	-1.296919	3.026317	0.912806
H	-0.852216	2.415480	1.689835
C	4.420316	-1.021779	-0.222957
C	4.008053	-1.828273	-1.294261
H	3.020856	-2.271652	-1.295592
C	4.863448	-2.070063	-2.368647
H	4.524275	-2.695516	-3.188342
C	6.144193	-1.517447	-2.389761
H	6.808607	-1.708834	-3.226679
C	6.566778	-0.720477	-1.324873
H	7.562822	-0.289124	-1.325252
C	5.713323	-0.473936	-0.251216
H	6.060618	0.141229	0.570449
N	-1.631658	1.006484	-0.444162
N	-0.686444	-0.939839	-1.048856
B	0.938937	-0.154179	1.882795
H	-0.176047	0.057946	1.577064
B	1.900547	-1.325973	0.945430
H	1.482685	-1.859090	-0.010428
B	1.480608	-1.665806	2.631359
H	0.704039	-2.525165	2.886242
B	1.571302	-0.127040	3.536654
H	0.848676	0.114058	4.446922
B	2.023193	1.151981	2.384261
H	1.681259	2.284446	2.370736
B	3.105565	-2.044740	2.037763
H	3.519753	-3.121276	1.776329
B	2.905047	-1.291315	3.636477
H	3.169183	-1.894181	4.624189
B	3.252395	0.451095	3.460849
H	3.763990	1.109270	4.305044
B	3.633793	0.752278	1.768192
H	4.390735	1.560804	1.376842
B	4.192057	-0.740742	2.545885
H	5.356442	-0.918201	2.645177

Table S13 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of ***o*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	3.813478	-0.683406	1.021368
C	1.967378	0.862356	0.724589
C	1.667081	1.547028	-0.563020
C	0.523077	1.304741	-1.375138
C	0.367107	1.946878	-2.613662
H	-0.510889	1.725545	-3.213248
C	1.306920	2.858617	-3.082964
H	1.169524	3.340454	-4.045175
C	2.410641	3.145270	-2.282231
H	3.152635	3.867847	-2.608714
C	2.578262	2.502284	-1.060035
H	3.450490	2.737305	-0.465786
C	-0.601869	0.414727	-1.008334
C	-2.659403	-0.125062	-0.343819
C	-1.897168	-1.265640	-0.778026
C	-2.438257	-2.575326	-0.760274
C	-1.673778	-3.681941	-1.197306
H	-0.661411	-3.505766	-1.541565
C	-2.219864	-4.953494	-1.178476
H	-1.638974	-5.806116	-1.511312
C	-3.532504	-5.125817	-0.722050
H	-3.971815	-6.117484	-0.701955
C	-4.295040	-4.038288	-0.285800
H	-5.303009	-4.231095	0.058290
C	-3.775697	-2.737921	-0.289390
C	-4.549636	-1.567056	0.175830
C	-5.854429	-1.705013	0.664363
H	-6.322443	-2.680067	0.699997
C	-6.586940	-0.609908	1.122332
H	-7.594385	-0.763936	1.493773
C	-6.032091	0.673907	1.110529
H	-6.600665	1.522159	1.474285
C	-4.747006	0.855534	0.631474
H	-4.315083	1.845851	0.625221
C	-3.988254	-0.243179	0.155087
C	-2.094260	2.340721	-0.317512
C	-2.777114	3.042852	-1.313845
H	-3.093514	2.532052	-2.217217
C	-3.047837	4.397806	-1.125364
H	-3.578807	4.950251	-1.893611
C	-2.632597	5.039231	0.044173
H	-2.842573	6.094481	0.186389
C	-1.945644	4.326716	1.028954
H	-1.620044	4.823980	1.936587
C	-1.671887	2.969148	0.854425
H	-1.142254	2.404994	1.612916
C	4.756856	-1.077311	-0.048529
C	4.495543	-2.185842	-0.876898
H	3.583287	-2.753940	-0.730490
C	5.390628	-2.564664	-1.875764
H	5.164317	-3.425699	-2.498576
C	6.571559	-1.846234	-2.077600
H	7.267956	-2.140930	-2.856946
C	6.846812	-0.745119	-1.262823
H	7.763190	-0.178835	-1.404382
C	5.952959	-0.365380	-0.263436
H	6.182010	0.489419	0.363916
N	-1.818430	0.936828	-0.519789
N	-0.659123	-0.891455	-1.186410
B	0.905524	0.206684	1.771231
H	-0.253694	0.282403	1.540818
B	2.116620	-0.872479	0.841222
H	1.725330	-1.504067	-0.079782
B	1.533781	-1.244283	2.546708
H	0.755761	-2.099617	2.835893
B	1.568080	0.334630	3.409769
H	0.849698	0.602808	4.322938
B	1.978443	1.576780	2.200091
H	1.666651	2.723772	2.245846
B	3.177661	-1.710393	2.122301
H	3.499756	-2.852780	2.052351
B	2.902586	-0.788875	3.618219
H	3.111047	-1.289639	4.679808
B	3.247983	0.933229	3.243555
H	3.744353	1.671247	4.036675
B	3.556953	0.967972	1.438067
H	4.325409	1.761783	1.008987
B	4.254022	-0.345092	2.555433
H	5.410596	-0.422126	2.819529

Table S14 Cartesian coordinates of the ground state (S_0) fully optimized geometry of ***m*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-4.439027	0.463318	-0.683124
C	-3.666550	-0.284855	0.715083
C	-2.469881	0.380990	1.347346
C	-1.175362	0.131335	0.870884
H	-1.038225	-0.522670	0.022946
C	-0.056261	0.728204	1.469812
C	-0.250676	1.594439	2.559544
H	0.612213	2.066814	3.014339
C	-1.530611	1.832136	3.046862
H	-1.671894	2.488081	3.899729
C	-2.637206	1.227661	2.452656
H	-3.624627	1.413294	2.855872
C	1.325036	0.549855	0.984191
C	3.199895	-0.328540	0.148668
C	3.378414	0.993756	0.540459
C	4.634595	1.671313	0.386345
C	4.798302	3.019132	0.766182
H	3.947116	3.542319	1.188878
C	6.015399	3.653400	0.597456
H	6.136405	4.692030	0.890321
C	7.095466	2.945738	0.041304
H	8.053454	3.437871	-0.097145
C	6.947615	1.620383	-0.333451
H	7.803577	1.110599	-0.759400
C	5.718846	0.937445	-0.172780
C	5.538217	-0.472080	-0.547793
C	6.608367	-1.232884	-1.069803
H	7.578063	-0.769894	-1.206295
C	6.466908	-2.566938	-1.410840
H	7.315396	-3.115874	-1.807561
C	5.230497	-3.204835	-1.234759
H	5.113157	-4.253497	-1.490427
C	4.154680	-2.496961	-0.729465
H	3.210636	-3.004927	-0.592518
C	4.271645	-1.130090	-0.384531
C	1.183877	-1.865381	0.266089
C	0.736516	-2.251614	-1.001513
H	0.904837	-1.598091	-1.851382
C	0.088733	-3.477452	-1.156573
H	-0.256491	-3.782158	-2.139312
C	-0.115907	-4.307605	-0.050976
H	-0.621183	-5.260187	-0.174500
C	0.328861	-3.911929	1.212318
H	0.171789	-4.555110	2.072252
C	0.983071	-2.689520	1.375320
H	1.341065	-2.374236	2.349693
C	-3.879579	1.744396	-1.246332
C	-4.314462	2.990843	-0.769760
H	-5.045436	3.045499	0.027033
C	-3.822986	4.172648	-1.322169
H	-4.171988	5.125935	-0.938023
C	-2.894009	4.131189	-2.362261
H	-2.511668	5.052294	-2.790949
C	-2.466472	2.897128	-2.853267
H	-1.752209	2.850652	-3.669204
C	-2.955512	1.713710	-2.302690
H	-2.622076	0.766115	-2.707151
N	1.860541	-0.607924	0.429107
N	2.222100	1.518103	1.057161
B	-4.855978	-1.053348	1.666670
H	-4.688545	-1.050583	2.837260
B	-5.200427	0.493224	0.862553
H	-5.266469	1.510263	1.448439
B	-6.405866	-0.797116	0.839855
H	-7.412031	-0.682084	1.457590
B	-5.535539	-2.345423	0.654116
H	-5.921947	-3.354780	1.144675
B	-3.796248	-1.982664	0.590072
H	-2.894613	-2.617778	1.015564
B	-6.119689	0.168221	-0.621549
H	-6.825367	1.019898	-1.040046
B	-6.311967	-1.594135	-0.755104
H	-7.263075	-2.056891	-1.293528
B	-4.682140	-2.306130	-0.913531
H	-4.451201	-3.274213	-1.559144
B	-3.513428	-0.983834	-0.851429
H	-2.477272	-0.937160	-1.404197
B	-5.058612	-0.759220	-1.698808
H	-5.033029	-0.550682	-2.862501

Table S15 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of ***m*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-4.750571	0.400442	-0.726579
C	-3.451185	-0.346073	1.148863
C	-2.248540	0.343812	1.676862
C	-0.977531	0.088542	1.144630
H	-0.894251	-0.612191	0.327801
C	0.164848	0.756199	1.627833
C	0.031521	1.703527	2.666528
H	0.909128	2.222946	3.029815
C	-1.221006	1.943192	3.212552
H	-1.328410	2.657012	4.023119
C	-2.346678	1.274729	2.727522
H	-3.317972	1.479326	3.163888
C	1.504689	0.576664	1.081001
C	3.311487	-0.277223	0.086399
C	3.548416	1.034681	0.616941
C	4.809739	1.685040	0.483709
C	5.012756	2.985348	0.991155
H	4.188318	3.480968	1.490975
C	6.242167	3.605411	0.842061
H	6.402766	4.605638	1.228870
C	7.275087	2.927000	0.183055
H	8.241739	3.403424	0.057687
C	7.082936	1.639827	-0.319326
H	7.914237	1.161011	-0.820570
C	5.851093	0.980912	-0.183407
C	5.616943	-0.386979	-0.691204
C	6.640591	-1.110150	-1.317171
H	7.619849	-0.667287	-1.442813
C	6.444826	-2.406690	-1.788292
H	7.267174	-2.928622	-2.265874
C	5.202735	-3.034597	-1.644218
H	5.052555	-4.045780	-2.005181
C	4.162466	-2.356748	-1.036372
H	3.206951	-2.846519	-0.926282
C	4.335950	-1.032816	-0.554310
C	1.290660	-1.771277	0.108813
C	0.750505	-1.977445	-1.162920
H	0.845941	-1.209871	-1.923649
C	0.094907	-3.178894	-1.431797
H	-0.330843	-3.348838	-2.414867
C	-0.016769	-4.155058	-0.438053
H	-0.530614	-5.086552	-0.651251
C	0.524966	-3.933056	0.829776
H	0.435355	-4.689423	1.602242
C	1.185104	-2.735978	1.111007
H	1.615488	-2.551279	2.089305
C	-4.452085	1.599805	-1.531471
C	-4.984258	2.859198	-1.189023
H	-5.620603	2.945808	-0.314911
C	-4.710925	3.988707	-1.957375
H	-5.137602	4.946093	-1.671412
C	-3.896332	3.895814	-3.089109
H	-3.683368	4.776938	-3.686883
C	-3.362014	2.654253	-3.443637
H	-2.731304	2.564921	-4.323880
C	-3.633754	1.523359	-2.676609
H	-3.215443	0.565224	-2.965967
N	1.996445	-0.541649	0.385825
N	2.446138	1.514871	1.216985
B	-4.616041	-0.980231	2.103231
H	-4.470147	-0.876511	3.279290
B	-4.952612	0.480270	0.994248
H	-5.038478	1.557079	1.488959
B	-6.203892	-0.815942	1.355168
H	-7.151995	-0.678951	2.063945
B	-5.308127	-2.372432	1.246642
H	-5.617544	-3.355885	1.845280
B	-3.595621	-1.968843	1.012797
H	-2.664127	-2.627178	1.347677
B	-6.238343	-0.052089	-0.235158
H	-7.149490	0.636492	-0.565987
B	-6.258719	-1.827936	-0.128829
H	-7.221513	-2.436519	-0.481021
B	-4.571645	-2.390400	-0.394134
H	-4.327658	-3.404811	-0.970282
B	-3.571004	-0.851387	-0.482920
H	-2.590199	-0.815320	-1.152442
B	-5.212529	-1.040385	-1.332775
H	-5.329820	-1.117893	-2.513607

Table S16 Cartesian coordinates of the ground state (S_0) fully optimized geometry of ***p*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-5.315607	0.514145	0.185902
C	-4.219103	-0.463734	-0.796537
C	-2.731562	-0.300207	-0.636637
C	-2.015610	0.613708	-1.426743
H	-2.531087	1.232176	-2.150675
C	-0.636787	0.728735	-1.310624
H	-0.099379	1.439816	-1.926738
C	0.086460	-0.068778	-0.405548
C	-0.629387	-0.983619	0.383095
H	-0.120250	-1.604897	1.107751
C	-2.011522	-1.097434	0.264292
H	-2.525630	-1.820449	0.884866
C	1.540673	0.147482	-0.322147
C	3.736231	-0.163973	-0.061132
C	3.439740	1.144580	-0.429379
C	4.461053	2.140416	-0.592744
C	4.147666	3.468203	-0.947855
H	3.105813	3.727991	-1.102984
C	5.148564	4.411792	-1.089824
H	4.902504	5.433713	-1.362352
C	6.487627	4.040399	-0.876721
H	7.278847	4.776308	-0.983897
C	6.808127	2.738085	-0.529979
H	7.851736	2.492044	-0.374064
C	5.811697	1.745101	-0.378557
C	6.124615	0.353043	-0.025272
C	7.459216	-0.071802	0.160678
H	8.268095	0.640254	0.051167
C	7.778891	-1.381543	0.474663
H	8.817901	-1.666730	0.607931
C	6.759779	-2.335022	0.611940
H	7.002103	-3.366474	0.848990
C	5.438541	-1.961874	0.441818
H	4.664982	-2.709627	0.544472
C	5.086566	-0.627501	0.131456
C	2.255420	-2.191534	0.302190
C	2.272021	-2.639859	1.626818
H	2.473605	-1.936567	2.428233
C	2.031692	-3.987006	1.897733
H	2.045042	-4.339052	2.924291
C	1.771616	-4.877511	0.852395
H	1.582749	-5.924690	1.066695
C	1.754513	-4.421100	-0.467084
H	1.553433	-5.110748	-1.280610
C	1.999008	-3.075702	-0.747662
H	1.993484	-2.708977	-1.768671
C	-4.748471	1.498563	1.175824
C	-4.529175	1.122972	2.510551
H	-4.747164	0.113251	2.835425
C	-4.042109	2.043956	3.436573
H	-3.879640	1.732459	4.463566
C	-3.769688	3.356091	3.048131
H	-3.389481	4.072279	3.769890
C	-3.997824	3.743299	1.727306
H	-3.800136	4.763621	1.414380
C	-4.485313	2.824808	0.798886
H	-4.668419	3.149567	-0.217661
N	2.498467	-0.803705	0.017504
N	2.091355	1.319604	-0.592226
B	-4.925468	-1.992560	-1.071520
H	-4.189803	-2.916610	-1.131088
B	-4.928262	-0.736352	-2.324190
H	-4.194703	-0.791411	-3.250163
B	-6.397819	-1.688336	-2.019127
H	-6.776337	-2.483175	-2.815120
B	-6.503074	-1.970305	-0.258964
H	-6.953515	-2.957429	0.220615
B	-5.118122	-1.172030	0.492494
H	-4.550594	-1.512415	1.464252
B	-5.123233	0.825231	-1.499444
H	-4.559441	1.798365	-1.841325
B	-6.508112	0.072201	-2.296432
H	-6.961714	0.552955	-3.281467
B	-7.499672	-0.706254	-1.031974
H	-8.681390	-0.785736	-1.108431
B	-6.715933	-0.396089	0.532930
H	-7.223203	-0.214158	1.585533
B	-6.719224	0.860207	-0.719933
H	-7.227915	1.911406	-0.533785

Table S17 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of ***p*PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-5.678444	0.509008	0.212553
C	-4.002859	-0.677574	-0.985777
C	-2.540904	-0.485592	-0.804124
C	-1.826992	0.443321	-1.585490
H	-2.351757	1.032974	-2.328119
C	-0.461214	0.621073	-1.419795
H	0.069992	1.346871	-2.024468
C	0.257933	-0.139731	-0.474745
C	-0.449224	-1.070437	0.309469
H	0.055628	-1.652542	1.068487
C	-1.819513	-1.233623	0.144821
H	-2.341554	-1.951114	0.766852
C	1.689702	0.135332	-0.353352
C	3.883804	-0.107134	-0.010395
C	3.545776	1.203516	-0.465784
C	4.531953	2.212062	-0.651460
C	4.174344	3.509157	-1.082253
H	3.128297	3.719558	-1.274290
C	5.146246	4.480889	-1.247164
H	4.875196	5.478016	-1.576527
C	6.485007	4.162791	-0.981557
H	7.255488	4.916752	-1.105043
C	6.848101	2.884062	-0.558130
H	7.896043	2.691171	-0.366504
C	5.889957	1.872858	-0.382645
C	6.240665	0.506914	0.050622
C	7.573254	0.139468	0.286232
H	8.366233	0.865061	0.158973
C	7.924039	-1.149753	0.678879
H	8.968428	-1.389048	0.849333
C	6.940112	-2.131677	0.847578
H	7.213417	-3.137663	1.146336
C	5.612893	-1.812990	0.630284
H	4.858626	-2.574953	0.759564
C	5.229686	-0.503398	0.236862
C	2.469109	-2.152157	0.425065
C	2.442880	-2.509849	1.775889
H	2.577856	-1.750435	2.539019
C	2.240922	-3.846464	2.119792
H	2.218495	-4.133531	3.165869
C	2.063483	-4.808616	1.121742
H	1.903278	-5.846854	1.393844
C	2.089422	-4.437453	-0.224099
H	1.950237	-5.183551	-0.999353
C	2.294624	-3.103747	-0.580542
H	2.319340	-2.801382	-1.621887
C	-5.386340	1.528004	1.232541
C	-5.247807	1.178526	2.592335
H	-5.351816	0.140029	2.887139
C	-4.987770	2.146520	3.558696
H	-4.889731	1.850753	4.599405
C	-4.854641	3.490380	3.197385
H	-4.649806	4.243904	3.951845
C	-4.990408	3.853697	1.854397
H	-4.894145	4.894974	1.560133
C	-5.250647	2.888569	0.885159
H	-5.356593	3.185014	-0.152647
N	2.678047	-0.771967	0.062382
N	2.213174	1.316811	-0.669096
B	-4.706145	-2.141342	-1.178641
H	-3.994629	-3.093333	-1.155363
B	-4.712266	-0.872941	-2.446503
H	-4.005831	-0.847465	-3.402054
B	-6.138287	-1.906803	-2.206401
H	-6.433403	-2.722992	-3.022448
B	-6.306685	-2.163167	-0.435977
H	-6.708437	-3.185234	0.024703
B	-5.018826	-1.104533	0.327989
H	-4.507151	-1.413531	1.353033
B	-5.025664	0.631052	-1.405123
H	-4.518578	1.658421	-1.714051
B	-6.315572	-0.136712	-2.459424
H	-6.724196	0.324012	-3.478687
B	-7.377434	-1.028394	-1.321553
H	-8.535014	-1.230348	-1.518905
B	-6.810929	-0.654219	0.328475
H	-7.475847	-0.661024	1.313416
B	-6.815317	0.623449	-0.946775
H	-7.483879	1.605912	-0.948875

Table S18 Cartesian coordinates of the ground state (S_0) fully optimized geometry of **PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.978621	-0.842119	0.357535
C	1.891206	-0.486625	-0.992708
C	0.421961	-0.391524	-0.737149
C	-1.661128	0.323888	-0.398652
C	-1.610533	-1.056032	-0.561679
C	-2.783194	-1.883307	-0.502994
C	-2.711905	-3.281127	-0.665112
H	-1.742237	-3.732798	-0.845590
C	-3.856968	-4.053604	-0.593876
H	-3.798762	-5.130545	-0.719027
C	-5.096942	-3.435622	-0.357743
H	-5.999975	-4.035635	-0.299018
C	-5.178500	-2.061722	-0.199436
H	-6.153286	-1.624744	-0.019685
C	-4.029344	-1.239636	-0.267940
C	-4.086942	0.222199	-0.114459
C	-5.317861	0.882014	0.098038
H	-6.231912	0.304363	0.158195
C	-5.404152	2.257217	0.229361
H	-6.370705	2.724397	0.390758
C	-4.244359	3.039723	0.147282
H	-4.303031	4.119646	0.241239
C	-3.016765	2.434751	-0.056752
H	-2.134753	3.054413	-0.122558
C	-2.901976	1.031158	-0.184984
C	0.101814	2.116536	-0.354282
C	0.303776	2.624856	0.931922
H	0.161827	1.980227	1.792504
C	0.692722	3.954649	1.087933
H	0.853244	4.354208	2.084131
C	0.874981	4.768564	-0.033634
H	1.179095	5.803030	0.090992
C	0.660924	4.254321	-1.313983
H	0.794296	4.886399	-2.185919
C	0.266478	2.925326	-1.479399
H	0.078967	2.519227	-2.466982
C	2.421961	-0.862760	1.757753
C	2.669411	0.216994	2.621768
H	3.242680	1.068659	2.276066
C	2.193007	0.202336	3.931452
H	2.399589	1.044541	4.584327
C	1.458946	-0.888484	4.400336
H	1.086743	-0.898982	5.420050
C	1.211565	-1.967031	3.551069
H	0.645831	-2.823060	3.904883
C	1.690329	-1.958084	2.241193
H	1.491763	-2.806968	1.600491
N	-0.338799	0.753691	-0.508881
N	-0.328163	-1.475995	-0.772884
B	4.199652	-1.910621	-0.170126
H	4.594646	-2.695188	0.621959
B	2.532731	-2.085008	-0.756011
H	1.809478	-2.941331	-0.414084
B	3.881969	-2.230117	-1.885347
H	4.139471	-3.283685	-2.365904
B	5.115943	-1.028057	-1.414045
H	6.279603	-1.216070	-1.552806
B	4.507581	-0.176077	0.018924
H	5.129604	0.243174	0.932554
B	2.421844	-1.346600	-2.373510
H	1.587725	-1.740697	-3.110937
B	4.022882	-0.687270	-2.768781
H	4.387024	-0.628388	-3.896893
B	4.385192	0.593661	-1.577393
H	5.012244	1.568248	-1.830676
B	3.024173	0.687184	-0.454574
H	2.647301	1.635543	0.121175
B	2.734953	0.390363	-2.189966
H	2.124871	1.189737	-2.807897

Table S19 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of **PC** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	3.390689	-0.703353	0.364939
C	1.557088	-0.715358	-1.177151
C	0.111467	-0.586498	-0.832238
C	-1.912781	0.241038	-0.346878
C	-1.902105	-1.175780	-0.380604
C	-3.055051	-1.945341	-0.103480
C	-3.009225	-3.363758	-0.119656
H	-2.066561	-3.843416	-0.357218
C	-4.142538	-4.099836	0.167125
H	-4.112021	-5.183852	0.157067
C	-5.335435	-3.427992	0.476184
H	-6.231069	-3.995334	0.707351
C	-5.393392	-2.032221	0.492776
H	-6.339537	-1.567557	0.740553
C	-4.266460	-1.249210	0.202348
C	-4.290128	0.223191	0.196110
C	-5.474507	0.932115	0.448116
H	-6.392469	0.396179	0.654436
C	-5.519218	2.324436	0.434466
H	-6.457685	2.830826	0.634883
C	-4.363240	3.063241	0.158030
H	-4.395549	4.147309	0.139991
C	-3.173086	2.405525	-0.096805
H	-2.287430	2.983703	-0.314758
C	-3.100199	0.987015	-0.082543
C	-0.104570	1.956995	-0.658060
C	0.233341	2.573835	0.549150
H	0.143529	2.023676	1.479648
C	0.694779	3.889313	0.535741
H	0.961389	4.374472	1.469134
C	0.817990	4.576907	-0.674722
H	1.180891	5.599803	-0.682075
C	0.473302	3.951520	-1.874777
H	0.565344	4.485328	-2.814985
C	0.003941	2.636960	-1.871454
H	-0.276842	2.142768	-2.794642
C	3.229347	-0.400665	1.786701
C	3.334699	0.924840	2.265483
H	3.530150	1.728813	1.564690
C	3.200501	1.206801	3.621416
H	3.292440	2.232436	3.966976
C	2.951970	0.179371	4.537510
H	2.845316	0.402192	5.594729
C	2.844585	-1.138007	4.079856
H	2.656595	-1.944136	4.783007
C	2.978353	-1.426487	2.725574
H	2.895454	-2.451891	2.382704
N	-0.610016	0.608078	-0.636901
N	-0.655586	-1.647890	-0.691015
B	4.253260	-1.905340	-0.284012
H	4.870288	-2.586210	0.468717
B	2.415081	-1.971471	-0.412285
H	1.812842	-2.696533	0.303425
B	3.524544	-2.613938	-1.728556
H	3.727037	-3.767808	-1.936189
B	4.801225	-1.372708	-1.908522
H	5.914315	-1.612450	-2.257046
B	4.526825	-0.139556	-0.636584
H	5.357358	0.563109	-0.159629
B	1.980763	-1.920582	-2.218621
H	1.109124	-2.585550	-2.666948
B	3.460629	-1.390480	-3.040941
H	3.635814	-1.646056	-4.190261
B	3.948583	0.160837	-2.277810
H	4.467052	1.041475	-2.887075
B	2.784777	0.411257	-0.880833
H	2.515549	1.504594	-0.531898
B	2.239254	-0.184317	-2.571421
H	1.582479	0.482704	-3.300188