Electronic Supplementary Information

Planarity of *N*-Aryl in Appended 1,2,4-Triazole-based *o*-Carboranyl Luminophores: Key Factor to Control Intramolecular Charge Transfer

Mingi Kim,[a]‡ Chan Hee Ryu,[a]‡ Ju Hyun Hong,[a] Ji Hye Lee,[a] Hyonseok Hwang,[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
† The first and second authors contributed equally to this work.

Contents

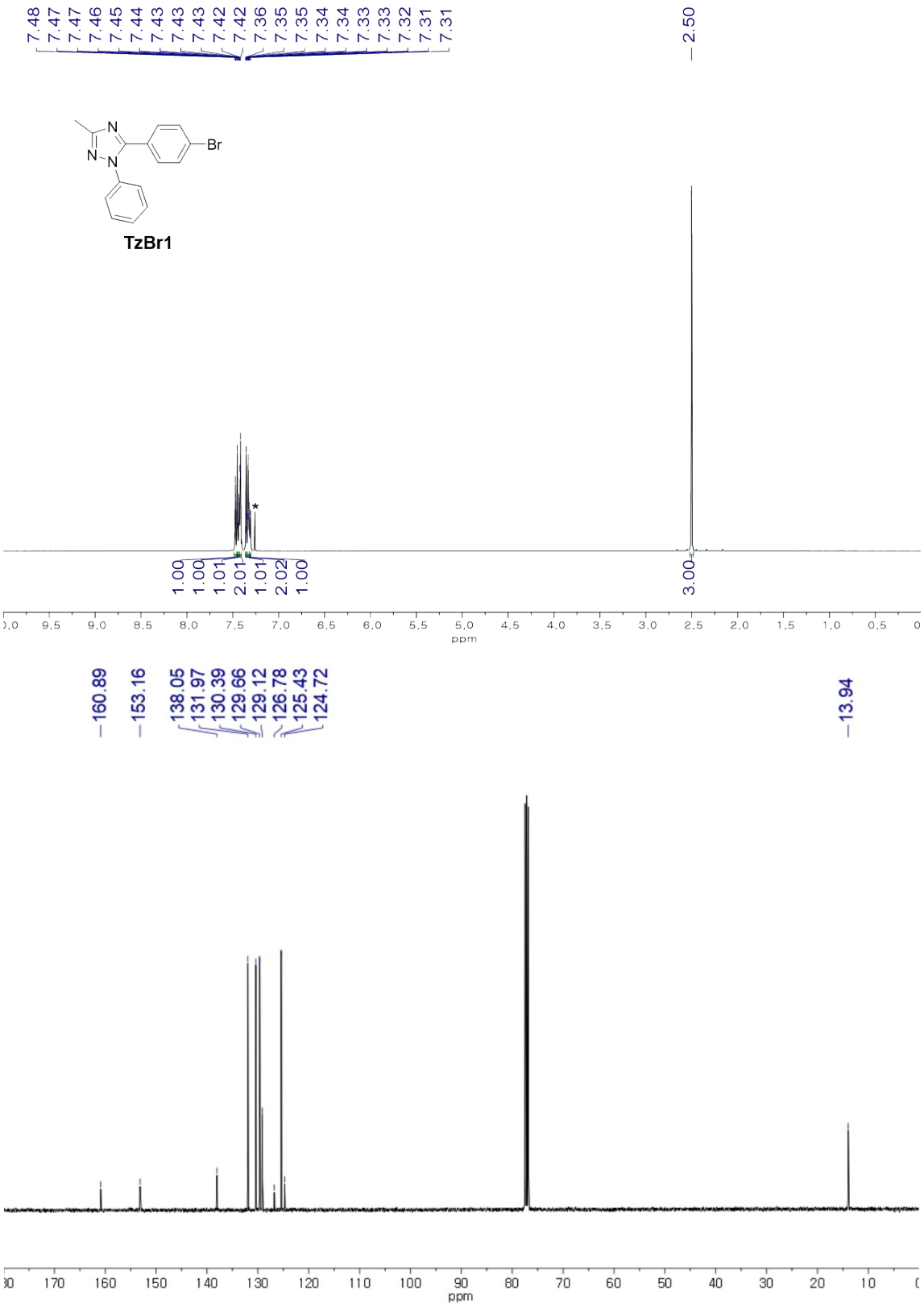


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **TzBr1** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

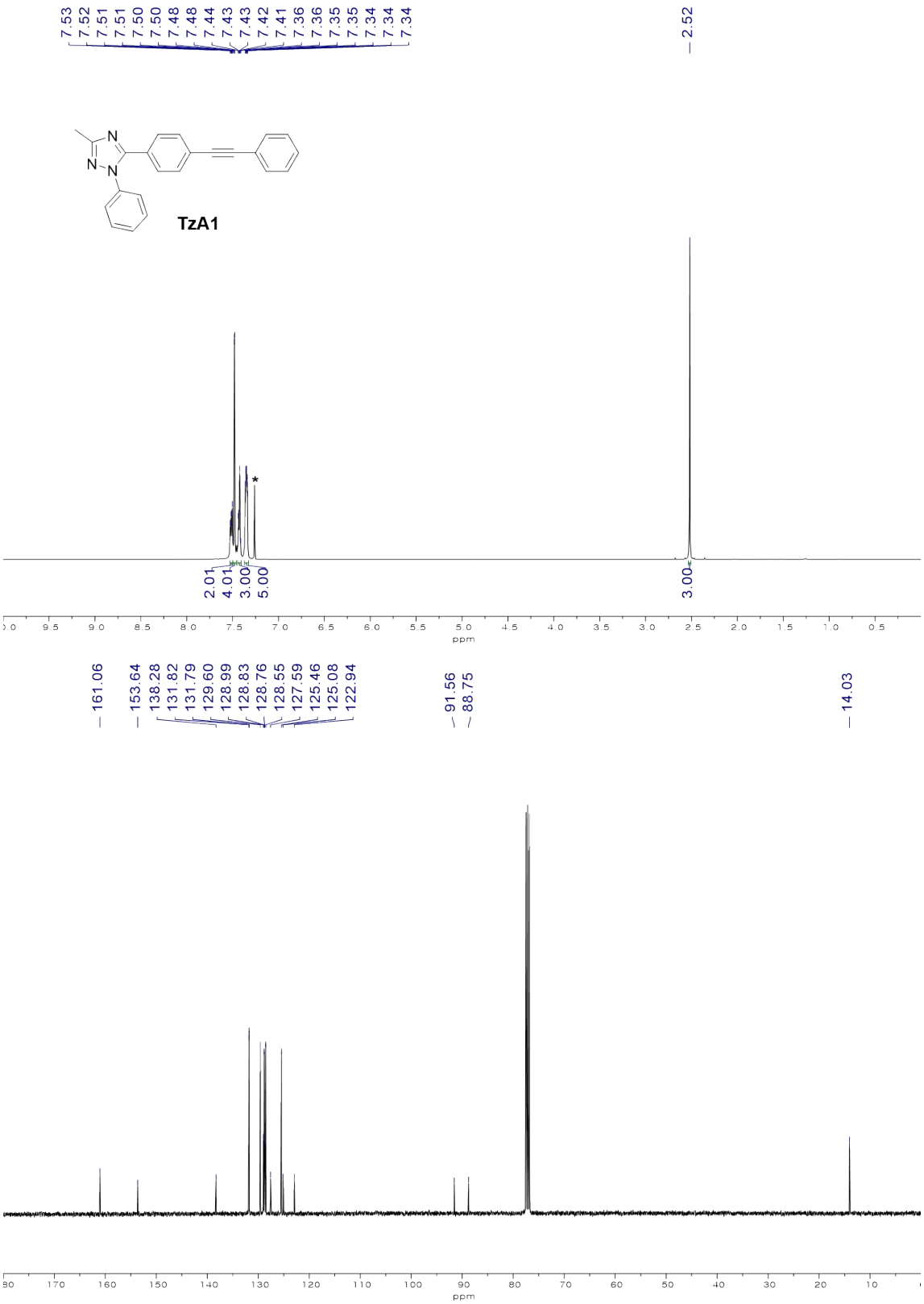


Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **TzA1** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

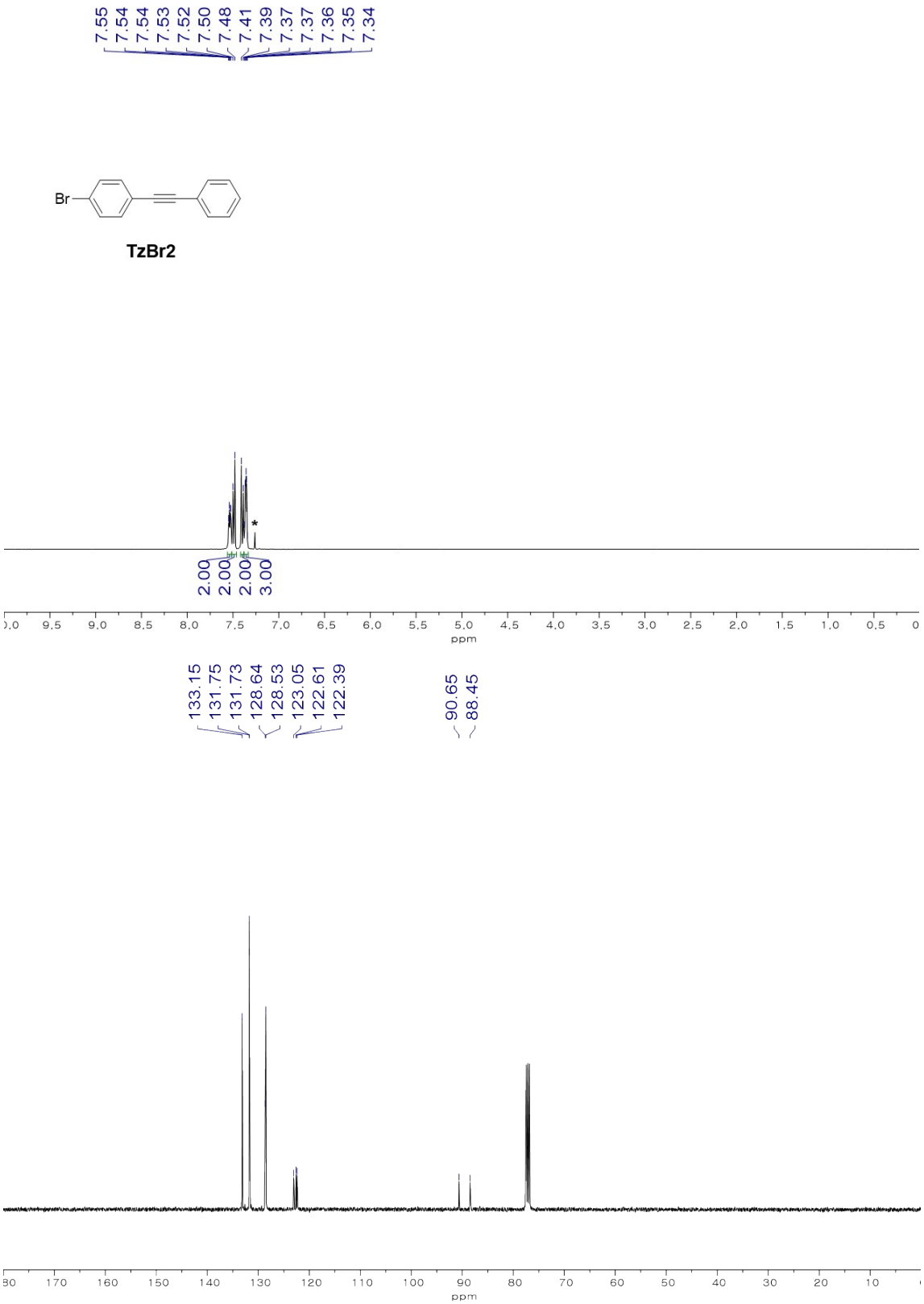


Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **TzBr2** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

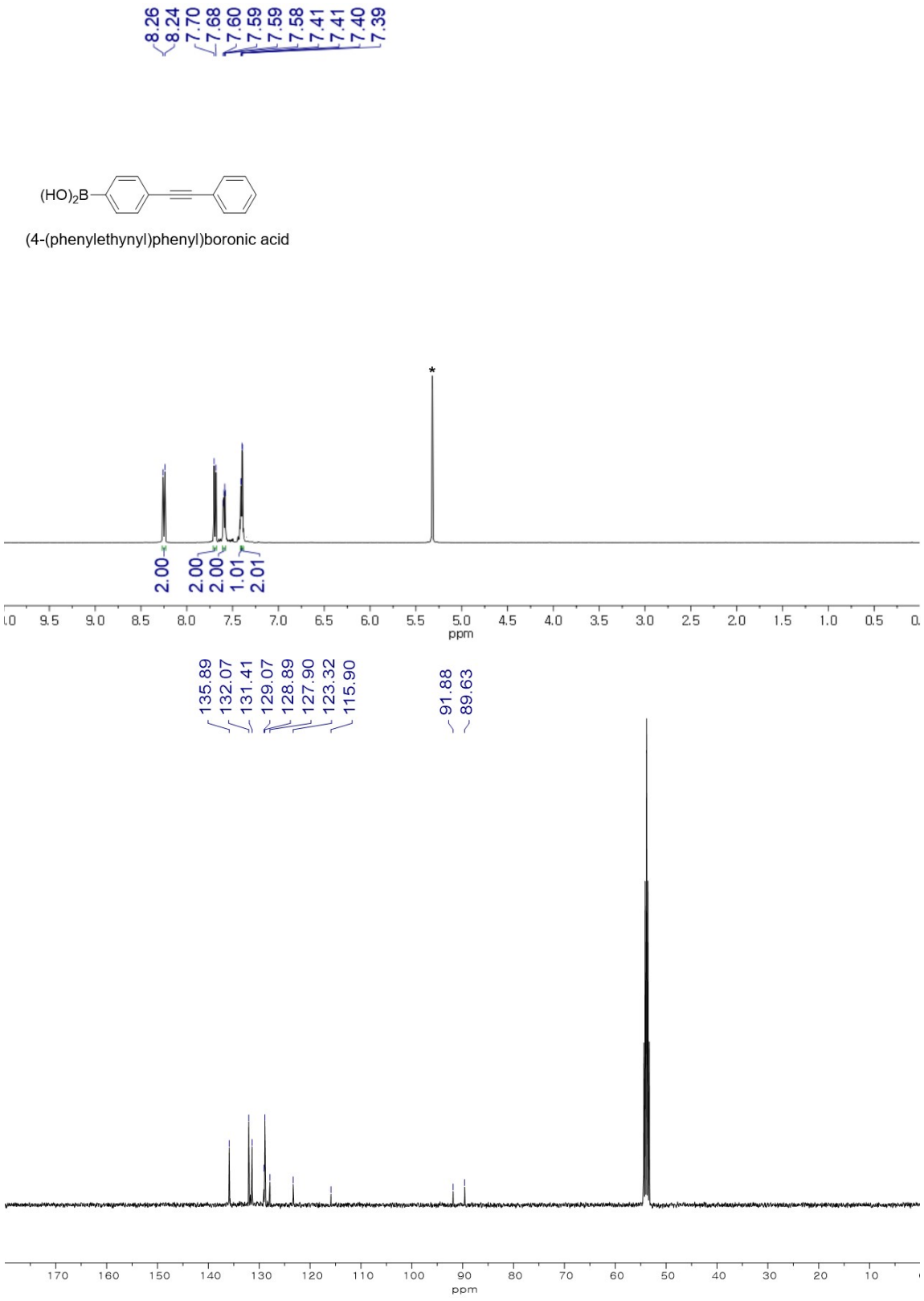


Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of (4-(phenylethynyl)phenyl)boronic acid in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

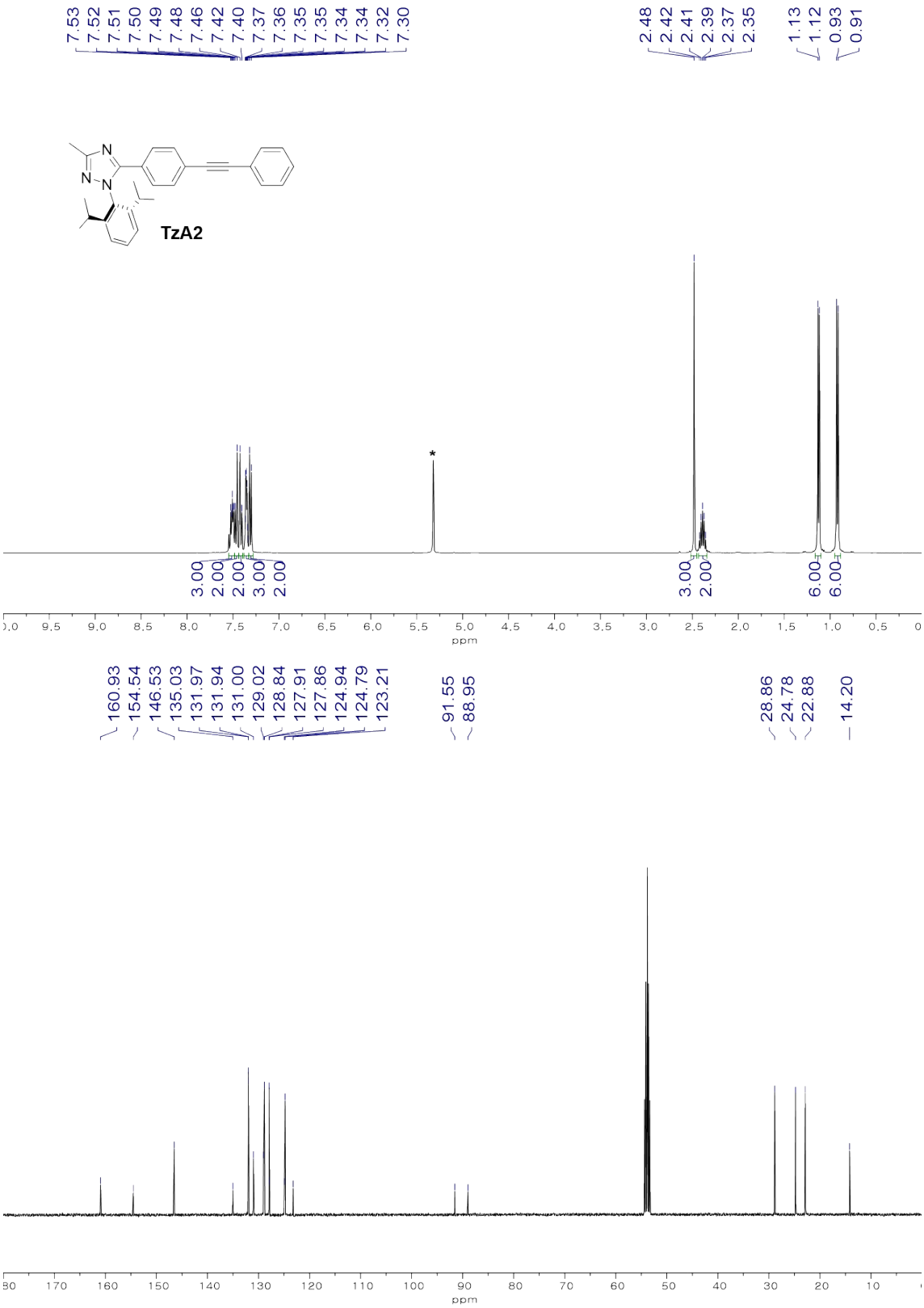


Fig. S5 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **TzA2** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

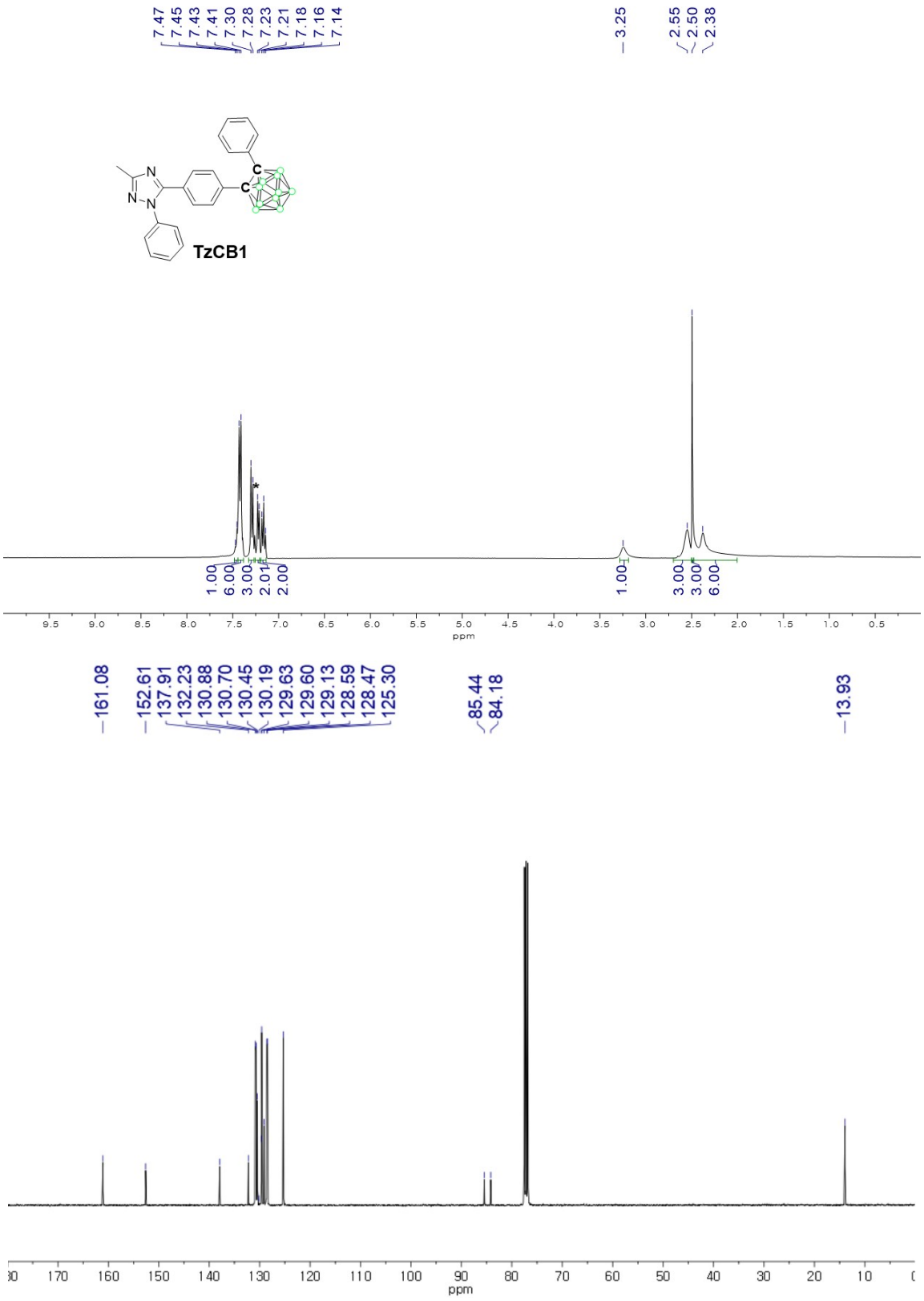


Fig. S6 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **TzCB1** in $CDCl_3$ (* from residual $CHCl_3$ in $CDCl_3$).

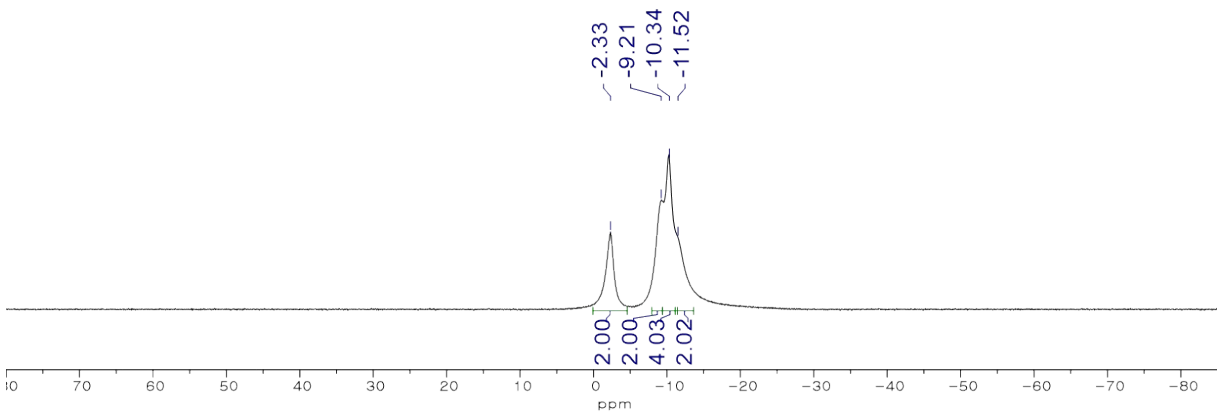
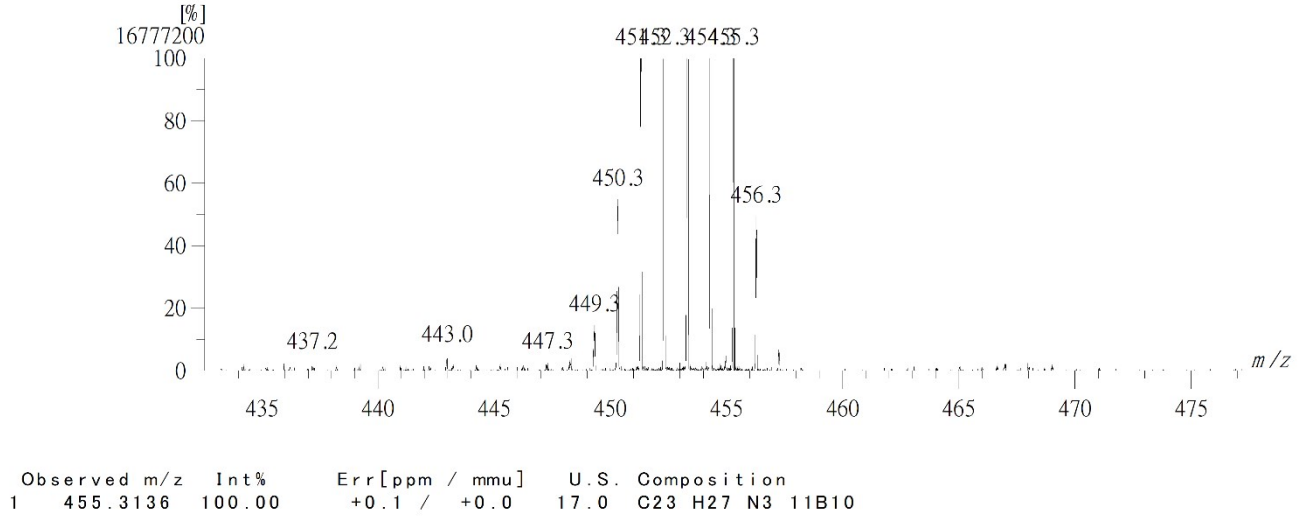


Fig. S7 $^{11}B\{^{1}H\}$NMR spectra of **TzCB1** in $CDCl_3$.



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	455.3136	100.00	+0.1 / +0.0	17.0	C23 H27 N3 11B10

Fig. S8 HR-mass spectrum for **TzCB1** (Calcd for $C_{23}H_{27}B_{10}N_3$: 455.3136. Found: 455.3136).

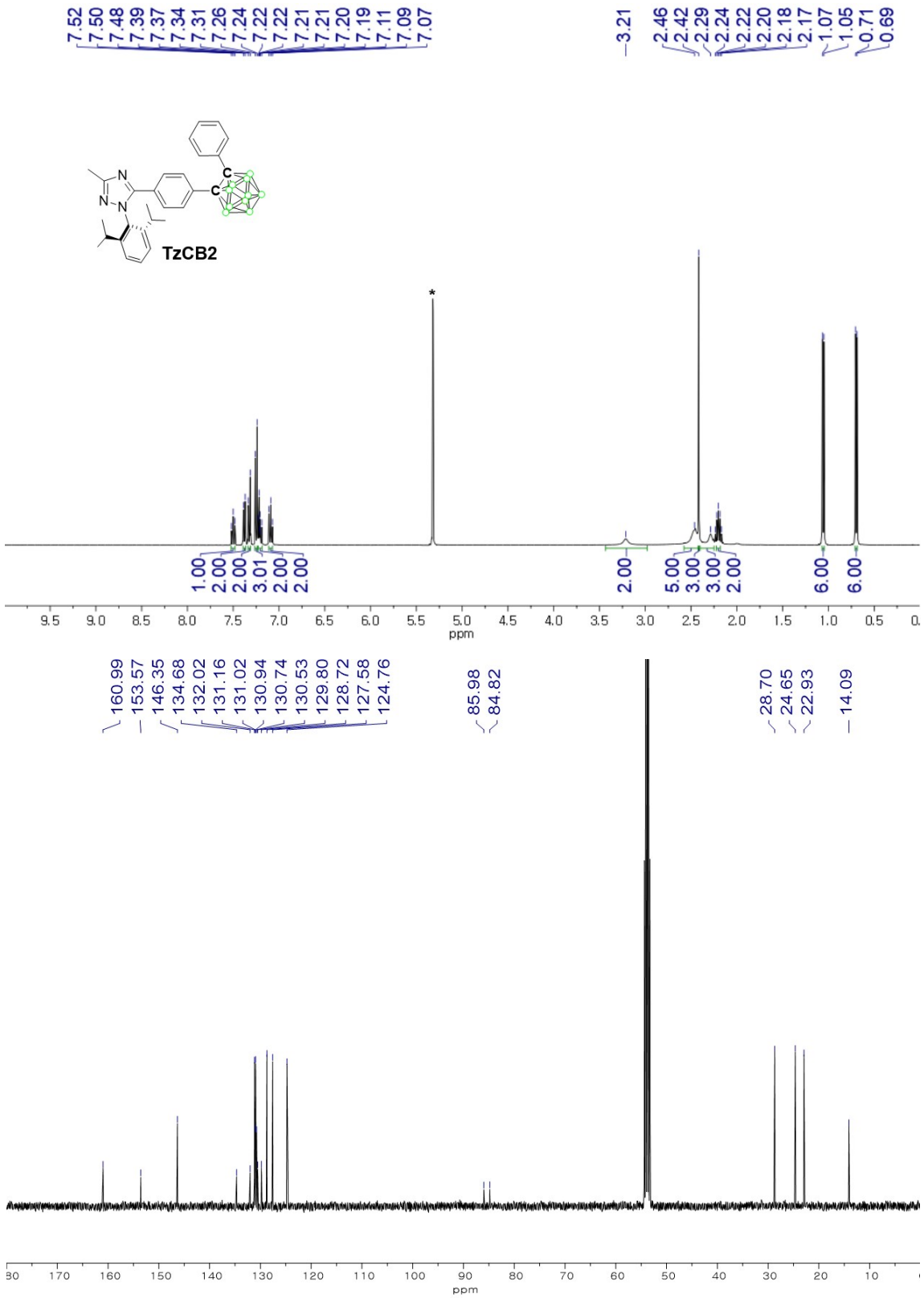


Fig. S9 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of **TzCB2** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).

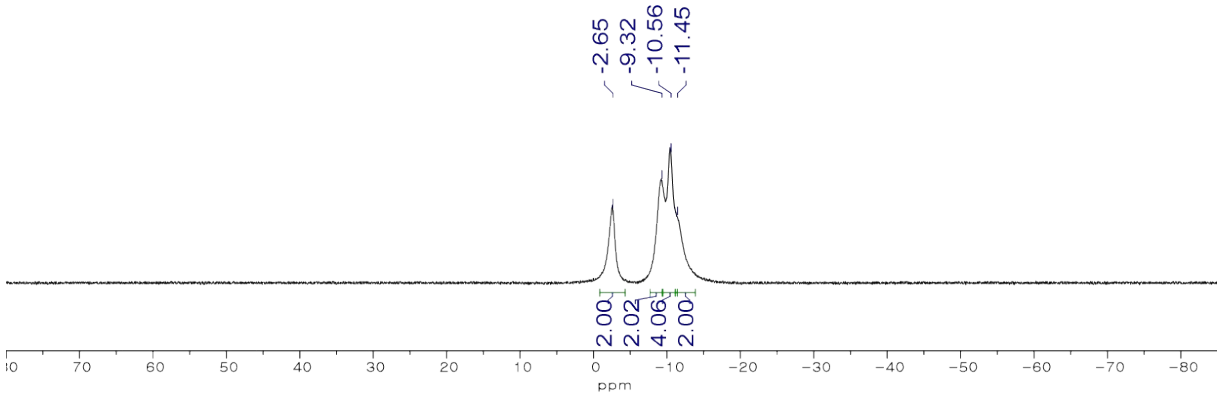
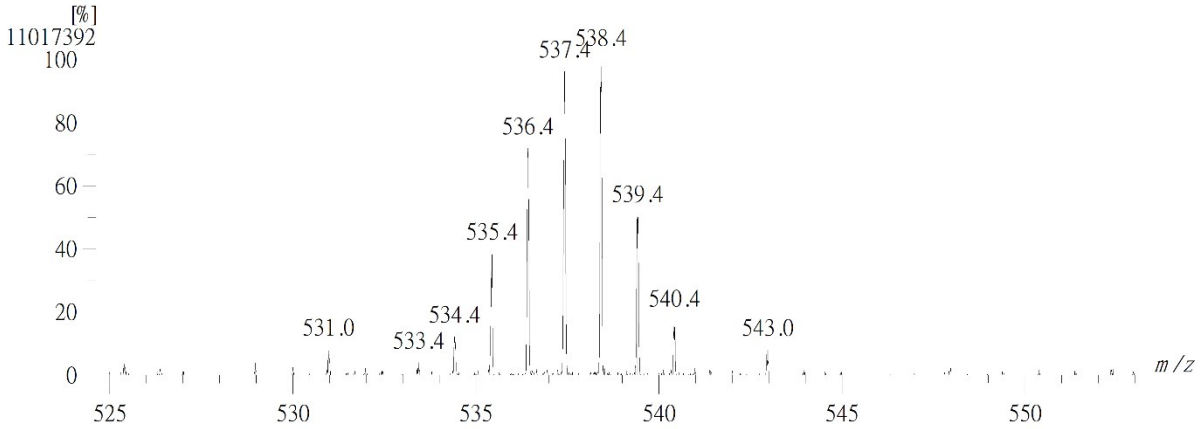


Fig. S10 $^{11}B\{^{1}H\}$NMR spectra of **TzCB2** in CD_2Cl_2.



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	539.4072	50.45	-0.5 / -0.3	17.0	C29 H39 N3 11B10

Fig. S11 HR-mass spectrum for **TzCB2** (Calcd for $C_{29}H_{39}B_{10}N_3$: 539.4075. Found: 539.4072).

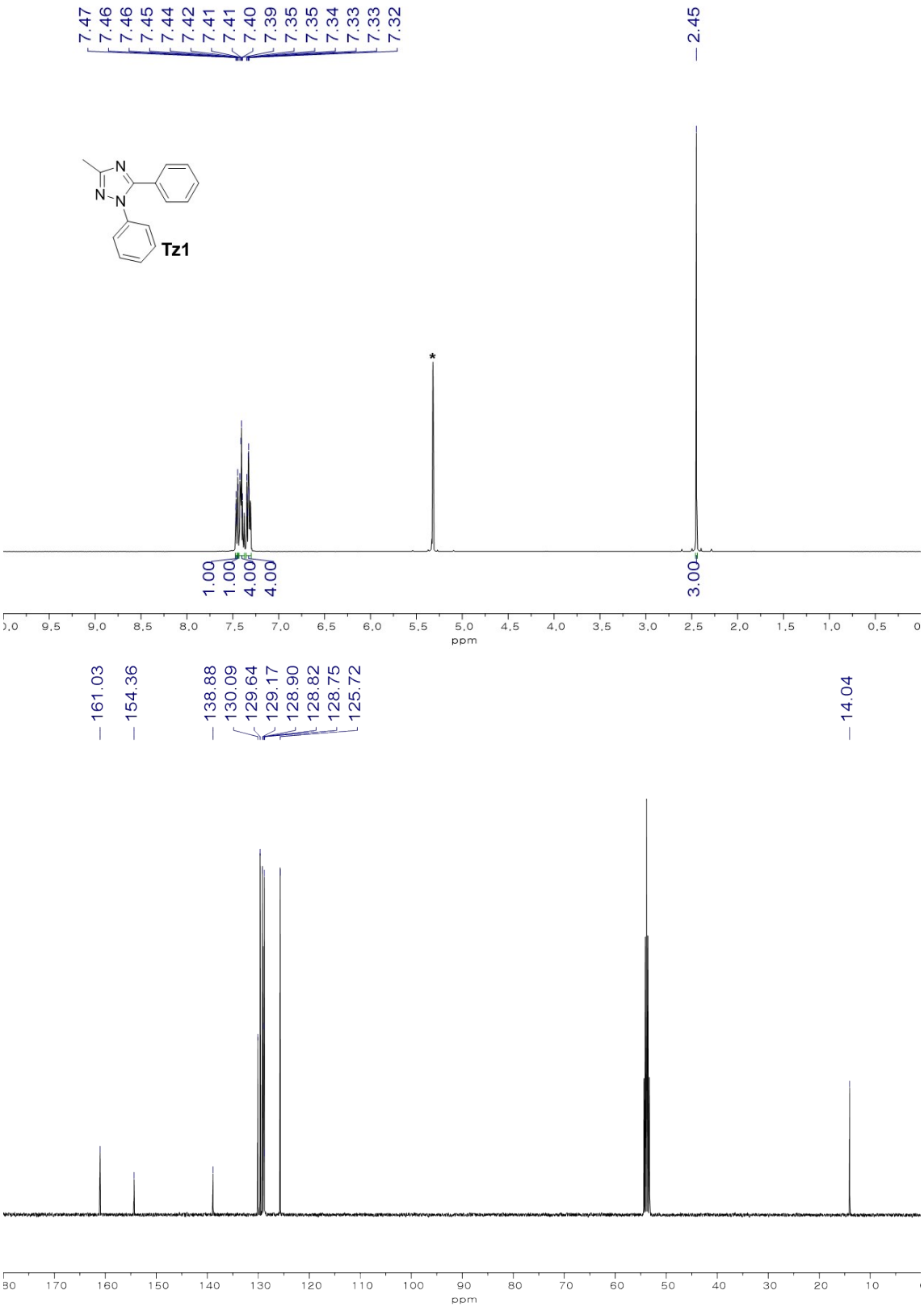
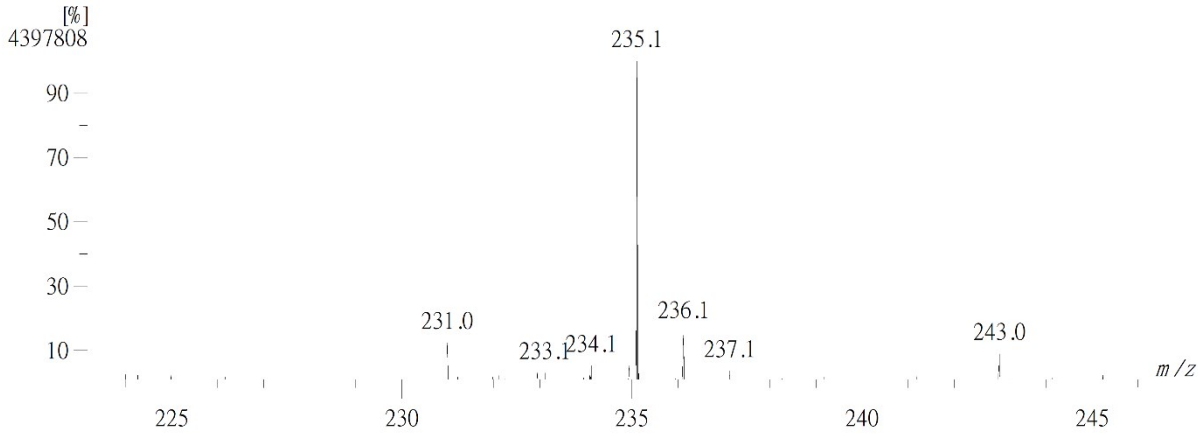


Fig. S12 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **Tz1** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	235.1108	100.00	-0.6 / -0.1	11.0	C15 H13 N3

Fig. S13 HR-mass spectrum for **Tz1** (Calcd for $C_{15}H_{13}N_3$: 235.1109. Found: 235.1108).

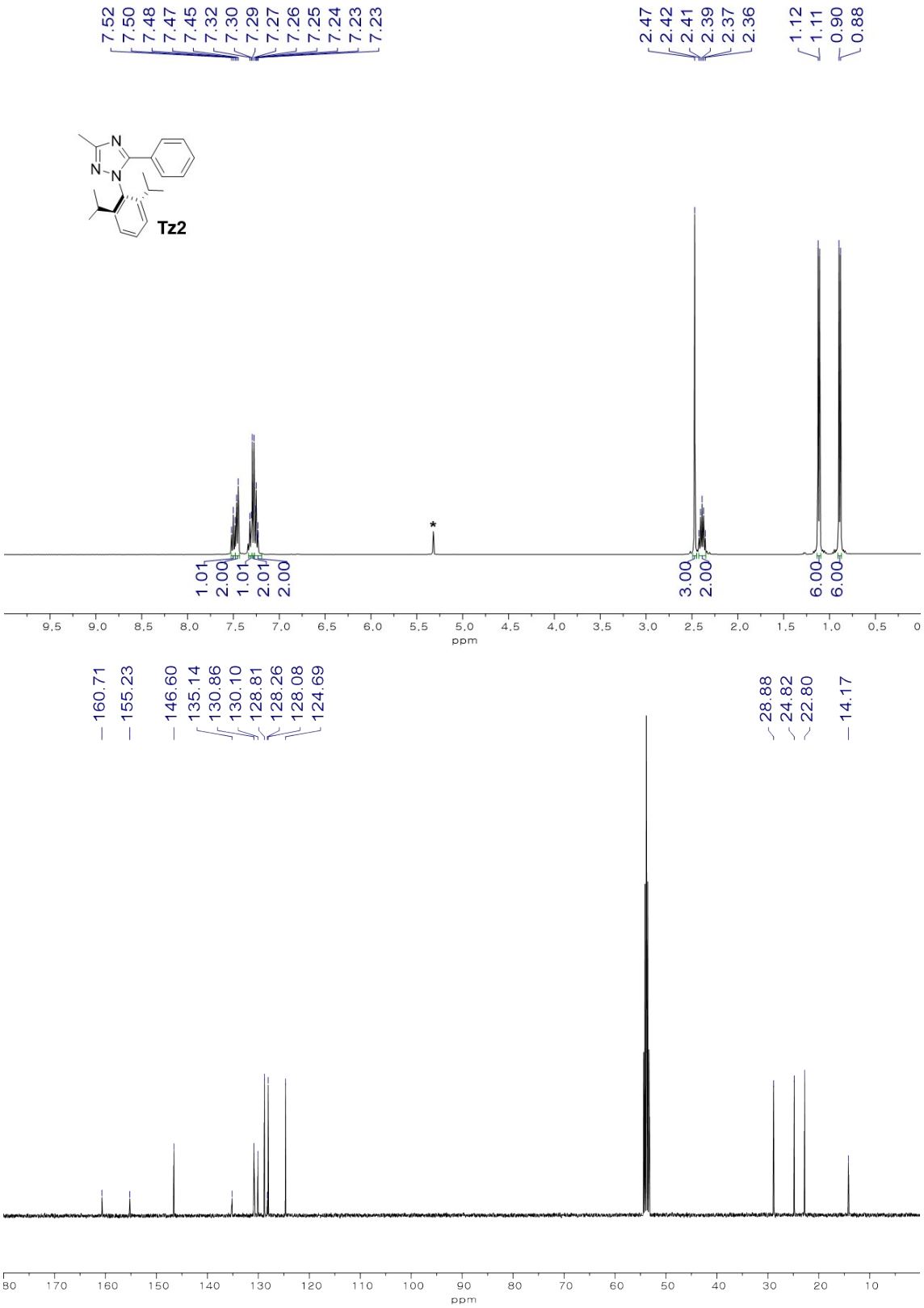
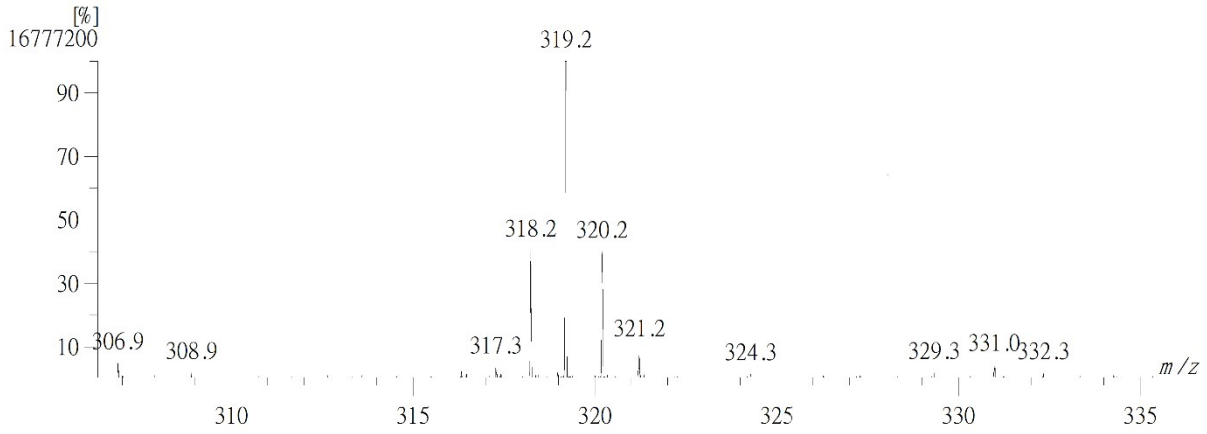


Fig. S14 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **Tz2** in CD_2Cl_2 (* from residual CH_2Cl_2 in CD_2Cl_2).



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	319.2044	100.00	-1.4 / -0.4	11.0	C21 H25 N3

Fig. S15 HR-mass spectrum for **Tz2** (Calcd for $C_{21}H_{25}N_3$ $[M + Na]^+$: 319.2048. Found: 319.2044).

Table S1 Crystallographic data and parameters for **TzCB1** and **TzCB2**

Compound	(**TzCB1**)$_2$·CH_2Cl_2	**TzCB2**
Formula	$(C_{23}H_{27}B_{10}N_3)_2$·$CH_2Cl_2$	$C_{29}H_{39}B_{10}N_3$
Formula weight	992.07	537.73
Crystal system	Triclinic	Monoclinic
Space group	P_{-1}	$P2_1/c$
a (Å)	10.774(2)	30.1062(10)
b (Å)	14.422(3)	9.6045(3)
c (Å)	18.462(4)	22.5622(8)
α (°)	89.83(3)	90
β (°)	80.11(3)	102.4101(12)
γ (°)	73.51(3)	90
V (Å^3)	2706.6(10)	6371.5(4)
Z	2	8
ρ_{calc}(g cm^{-3})	1.217	1.121
μ (mm^{-1})	0.161	0.061
F(000)	1028	2272
T (K)	293(2)	173(2)
Scan mode	*multi-scan*	*multi-scan*
hkl range	$-13 < h < 13$, $-18 < k < 18$, $-23 < l < 23$	$-39 < h < 39$, $-12 < k < 12$, $-29 < l < 29$
Measd reflns	28767	139629
Unique reflns [R_{int}]	12310 [0.0390]	14607 [0.0491]
Reflns used for refinement	12310	14607
Refined parameters	678	767
R_1[a] (I > 2σ(I))	0.0773	0.0511
wR_2[b] all data	0.2574	0.1331
GOF on F^2	1.044	1.022
ρ_{fin} (max/min) (e Å^{-3})	0.781, −0.629	0.261, −0.226

[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 **TzCB1** and **TzCB2**

Compound	**TzCB1**	**TzCB2**
	lengths (Å)	
C1–C2	1.709(4)	1.728(2)
C1–C18	1.512(4)	1.501(2)
C2–C3	1.506(3)	1.504(2)
C6–C9	1.471(3)	1.472(2)
C9–N1	1.354(3)	1.350(2)
C9–N3	1.326(4)	1.3314(19)
C12–N1	1.424(4)	1.4406(19)
N1–N2	1.373(3)	1.3713(17)
	angles (°)	
C2–C1–C18	117.1(2)	117.07(12)
C1–C2–C3	121.9(2)	118.51(11)
C5–C6–C9	123.0(2)	124.55(14)
C6–C9–N1	126.8(3)	126.93(13)
C6–C9–N3	123.5(3)	123.28(14)
N1–C9–N3	109.7(2)	109.79(13)
C9–N1–C12	132.8(2)	132.29(12)
C9–N1–N2	109.2(2)	109.56(12)
C12–N1–N2	117.9(2)	118.09(12)

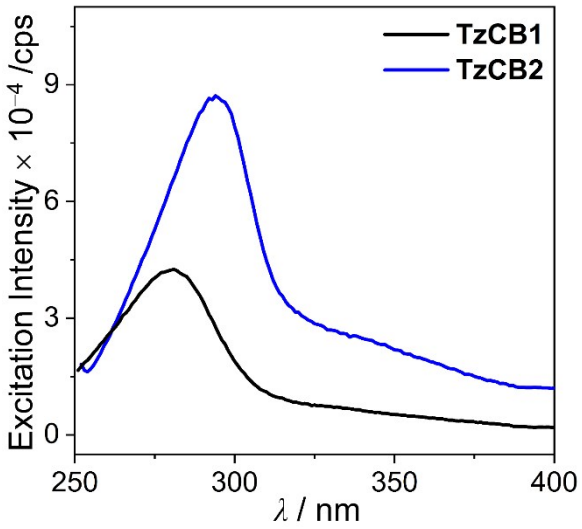


Fig. S16 Excitation graphs of **TzCB1** and **TzCB2** in THF (5.0×10^{-5} M).

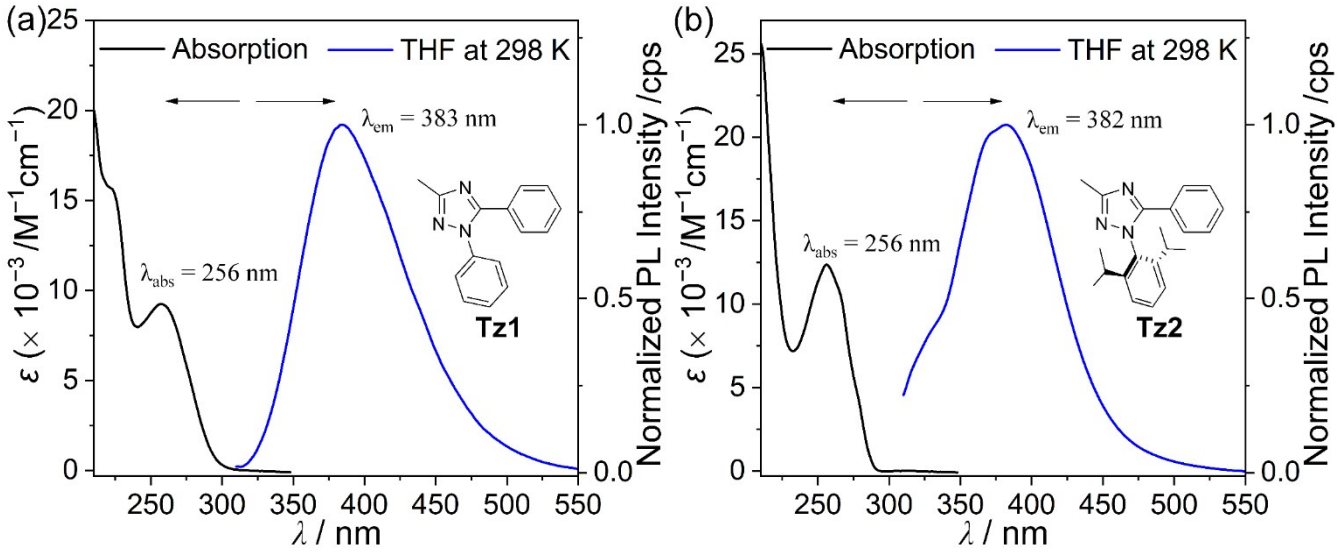


Fig. S17 UV-vis absorption and PL spectra for (a) **Tz1** (λ_{ex} = 281 nm) and (b) **Tz2** (λ_{ex} = 294 nm) in THF (5.0×10^{-5} M).

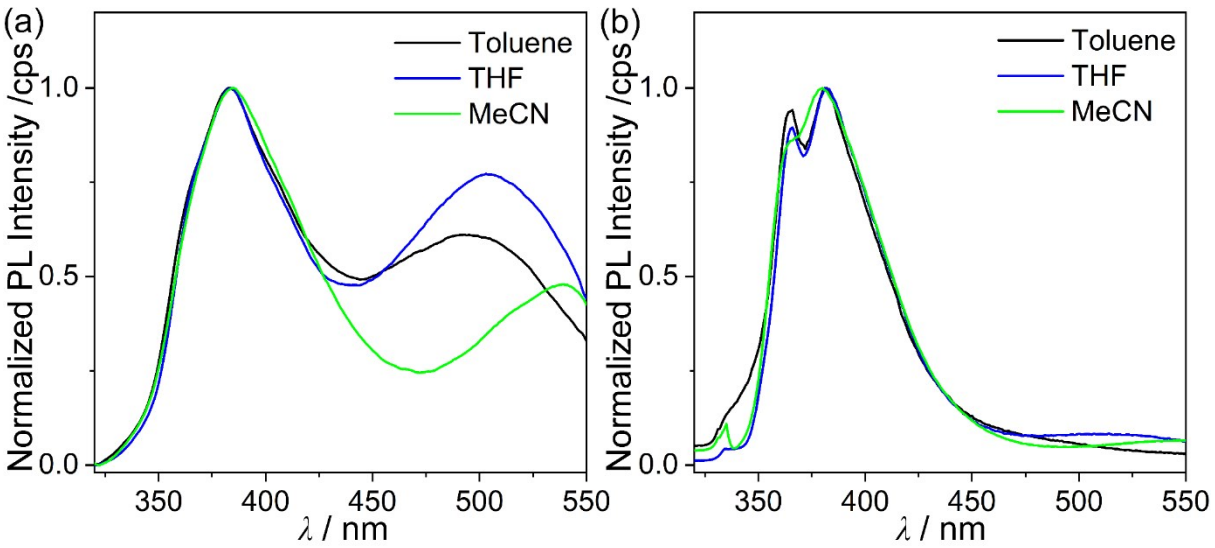


Fig. S18 PL spectra of (a) **TzCB1** (λ_{ex} = 281 nm) and (b) **TzCB2** (λ_{ex} = 294 nm) in various organic solvents (5.0×10^{-5} M).

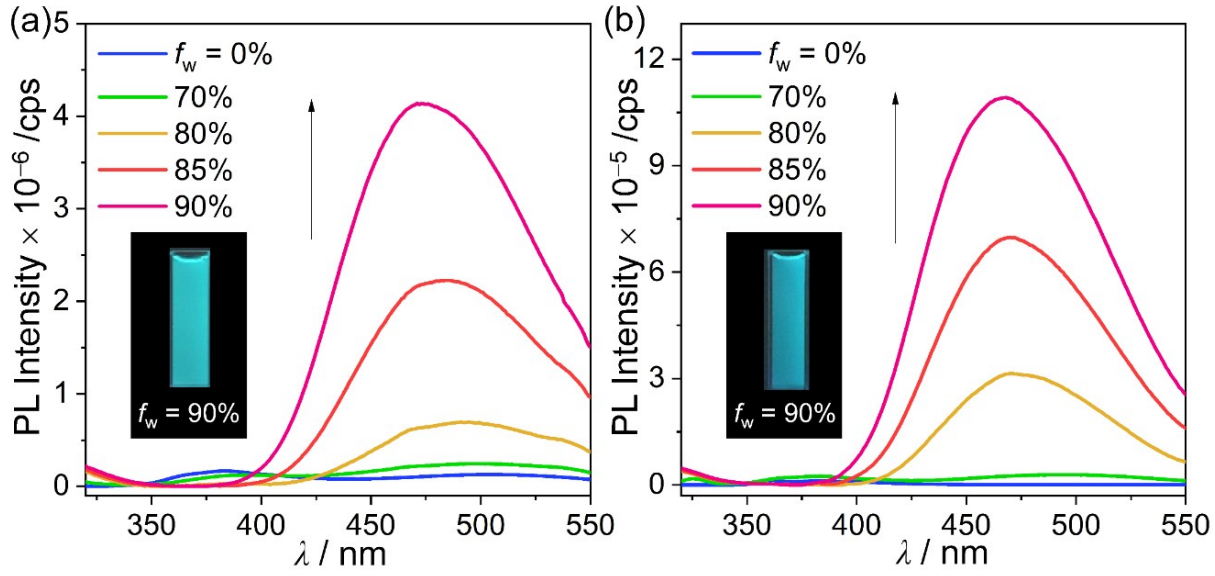


Fig. S19 PL spectra of (a) **TzCB1** and (b) **TzCB2** in THF–distilled water mixtures (water fraction f_w = 5.0×10^{-5} M; λ_{ex} = 281 nm for **TzCB1** and 294 nm for **TzCB2**). Inset figures show the emission color in each state under irradiation by a hand-held UV lamp (λ_{ex} = 265 nm).

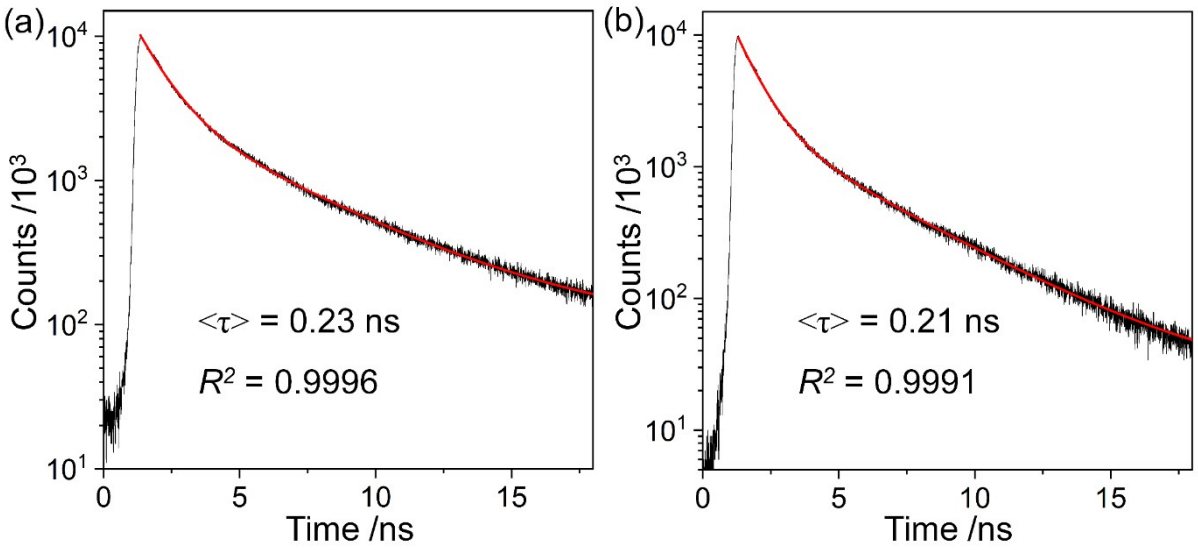


Fig. S20 Emission decay curves for (a) **TzCB1**and (b) **TzCB2** in the film state (5 wt% doped in PMMA) detected at 467 nm at 298 K. Each red-line is its single exponential fitting curve.

Theoretical calculation results for TzCB1 and TzCB2

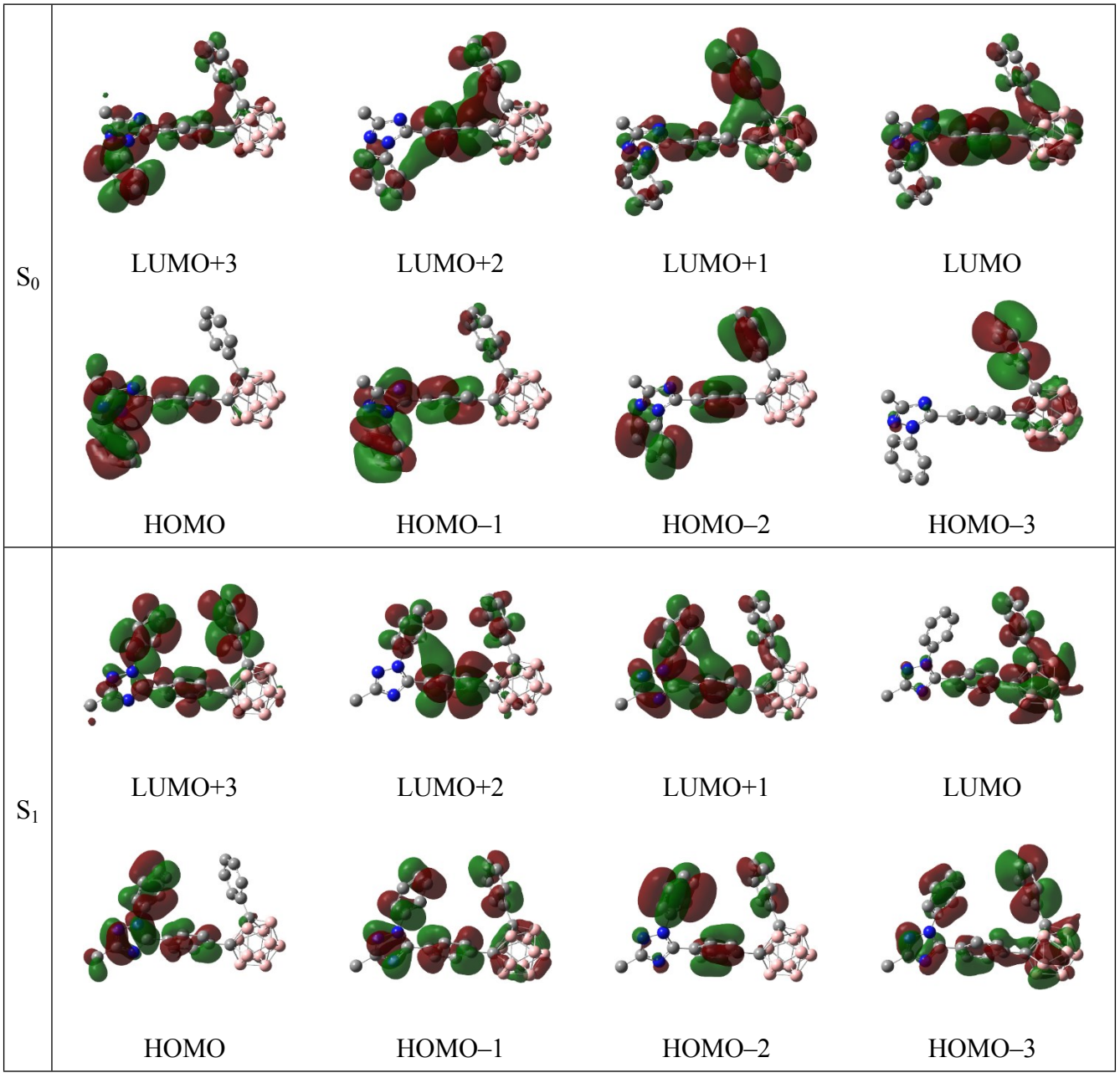


Fig. S21 The selected frontier orbitals of **TzCB1** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S3 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **TzCB1** 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	280.32	0.4540	HOMO → LUMO (97.3%)
2	264.91	0.0321	HOMO−5 → LUMO (11.9%)
			HOMO−2 → LUMO (16.1%)
			HOMO−1 → LUMO (44.2%)
			HOMO → LUMO+1 (19.2%)
3	260.69	0.0483	HOMO−2 → LUMO (67.9%)
			HOMO−1 → LUMO (12.4%)
			HOMO → LUMO+1 (9.6%)
4	256.55	0.0202	HOMO−4 → LUMO (40.1%)
			HOMO−3 → LUMO (52.4%)
5	256.10	0.0611	HOMO−4 → LUMO (39.3%)
			HOMO−3 → LUMO (32.6%)
			HOMO−2 → LUMO (12.7%)
			S_1
1	478.36	0.2172	HOMO → LUMO (99.6%)
2	415.43	0.0885	HOMO−1 → LUMO (97.3%)
3	394.37	0.0027	HOMO−2 → LUMO (97.2%)
4	390.72	0.0084	HOMO−5 → LUMO (9.2%)
			HOMO−3 → LUMO (82.6%)
5	378.21	0.2927	HOMO → LUMO+1 (88.7%)
			HOMO−2 → LUMO (7.3%)

Table S4 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **TzCB1** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

	E (eV)	*N*-phenyl	triazole +bridged phenyl	carborane	carborane -phenyl
			S_0		
LUMO+3	−0.59	70.9	17.2	5.4	6.6
LUMO+2	−0.83	10.8	60.4	8.9	19.9
LUMO+1	−1.12	5.4	14.9	24.8	55.0
LUMO	−1.78	3.7	62.9	28.1	5.3
HOMO	−6.50	25.2	72.3	2.4	0.1
HOMO−1	−7.07	43.7	49.4	2.9	4.0
HOMO−2	−7.15	49.9	20.1	0.5	29.5
HOMO−3	−7.19	0.9	2.0	10.2	86.9
			S_1		
LUMO+3	−0.59	34.7	23.3	5.4	36.6
LUMO+2	−0.76	15.6	68.8	6.9	8.7
LUMO+1	−1.59	31.2	60.5	5.2	3.1
LUMO	−3.52	0.5	14.8	72.0	12.7
HOMO	−6.13	40.3	56.4	2.5	0.8
HOMO−1	−6.94	29.1	48.8	7.3	14.8
HOMO−2	−7.16	70.9	17.2	2.5	9.4
HOMO−3	−7.24	9.3	21.2	15.0	54.5

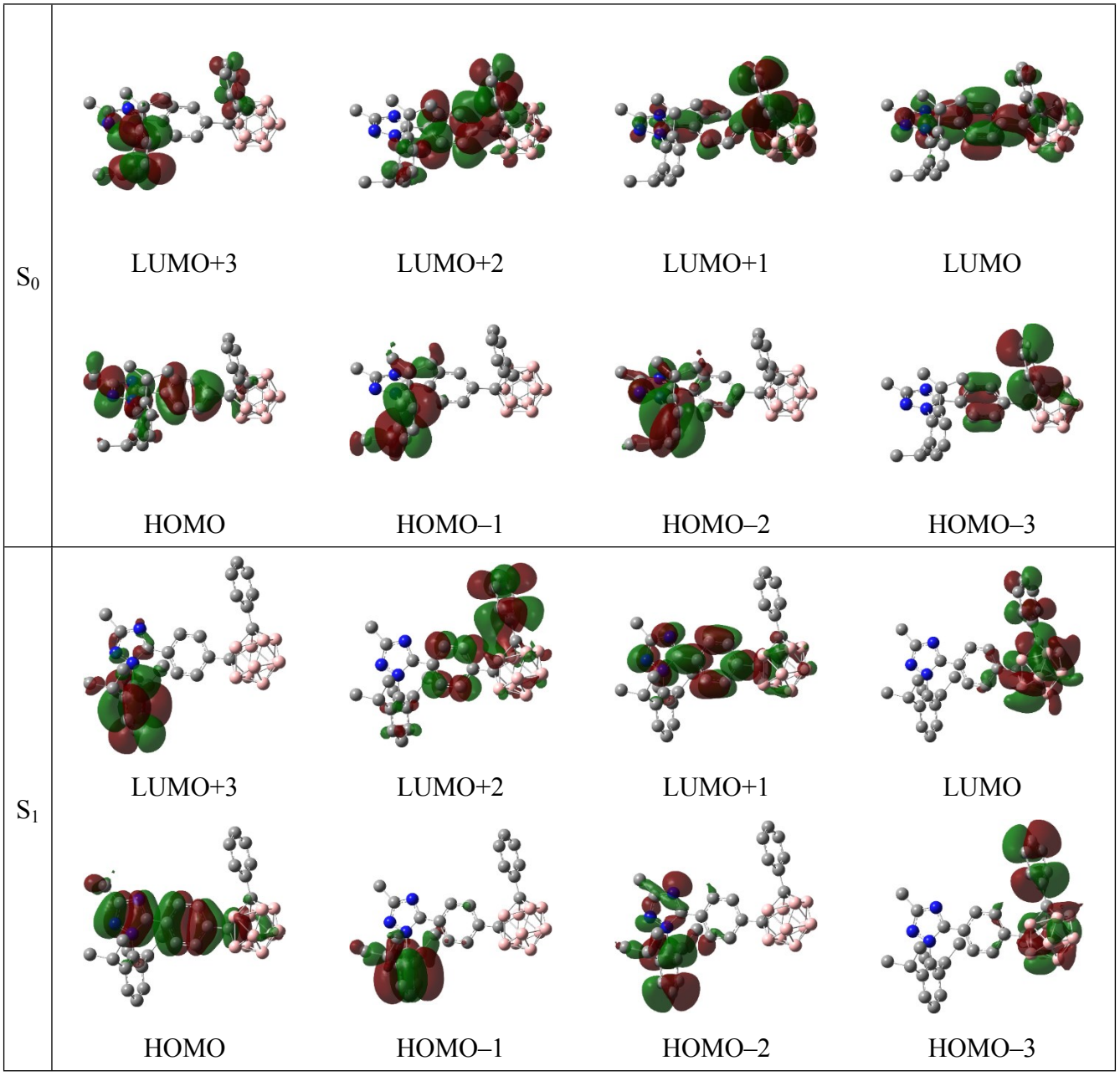


Fig. S22 The selected frontier orbitals of **TzCB2** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S5 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **TzCB2** 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	289.63	0.6102	HOMO → LUMO (94.7%)
2	283.49	0.0041	HOMO−1 → LUMO (98.1%)
3	272.79	0.0890	HOMO−2 → LUMO (91.4%)
4	263.76	0.0062	HOMO−5 → LUMO (7.3%)
			HOMO−4 → LUMO (27.3%)
			HOMO−3 → LUMO (34.3%)
			HOMO → LUMO+2 (22.9%)
5	257.39	0.0553	HOMO−4 → LUMO (71.3%)
			HOMO−3 → LUMO (26.1%)
			S_1
1	488.40	0.3010	HOMO → LUMO (97.0%)
2	425.61	0.0010	HOMO−1 → LUMO (96.6%)
3	394.36	0.0125	HOMO−2 → LUMO (99.8%)
4	393.64	0.0035	HOMO−4 → LUMO (11.5%)
			HOMO−3 → LUMO (76.5%)
5	363.62	0. 3931	HOMO → LUMO+1 (93.7%)

Table S6 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of **TzCB2** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

	E (eV)	*N*-phenyl	triazole +bridged phenyl	carborane	carborane -phenyl
			S_0		
LUMO+3	−0.57	87.0	5.3	1.0	6.7
LUMO+2	−0.82	8.3	58.6	9.4	23.7
LUMO+1	−1.11	0.4	16.2	24.6	58.8
LUMO	−1.80	1.0	65.8	28.0	5.2
HOMO	−6.56	5.1	91.0	3.7	0.2
HOMO−1	−6.73	98.6	1.3	0.0	0.1
HOMO−2	−6.99	81.6	18.0	0.3	0.1
HOMO−3	−7.20	0.5	9.3	3.9	86.2
			S_1		
LUMO+3	−0.58	94.8	4.4	0.1	0.7
LUMO+2	−0.65	3.6	20.0	9.3	67.1
LUMO+1	−1.56	1.4	89.0	9.5	0.2
LUMO	−3.80	0.0	2.2	63.9	33.8
HOMO	−5.97	1.8	90.8	7.4	0.1
HOMO−1	−6.74	98.2	1.8	0.0	0.0
HOMO−2	−6.93	82.9	16.7	0.1	0.3
HOMO−3	−7.27	0.3	1.0	18.5	80.2

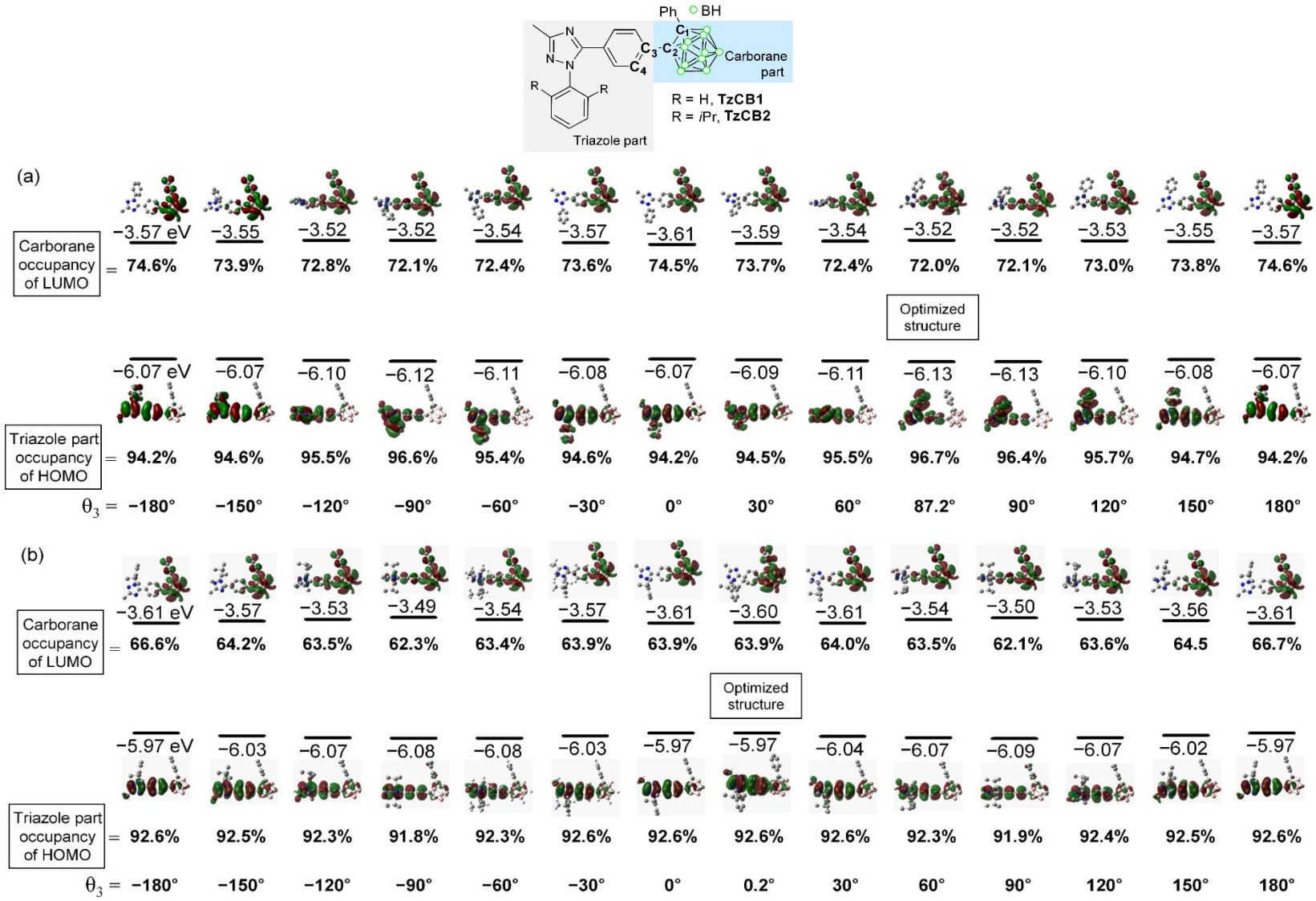


Fig. S23 Low-energy electronic transitions (HOMO → LUMO transitions) of S_1 states as θ_3 (the dihedral angle of C1-C2-C3-C4 atoms) was varied over 0–180° in 30° increments. Molecular orbital distributions on the *o*-carborane moiety of the LUMO level and the appended triazole moiety of the HOMO level (%) are identified for (a) **TzCB1** and (b) **TzCB2**.

Table S7 Cartesian coordinates of the ground state (S_0) fully optimized geometry of **TzCB1** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	2.341919	-0.910124	0.517781
C	3.604895	0.088792	-0.200519
B	3.520689	-0.136537	1.508688
H	3.195727	0.765721	2.188379
B	2.999580	-1.807376	1.812663
H	2.288047	-2.011117	2.735080
B	2.694973	-2.555192	0.232767
H	1.773966	-3.277675	0.064772
B	3.035303	-1.326654	-1.005298
H	2.384477	-1.208836	-1.977252
B	4.222281	-2.590612	-0.670599
H	4.432703	-3.436734	-1.474906
B	4.215413	-2.885128	1.090882
H	4.423035	-3.956364	1.557583
B	4.718752	-1.373884	1.897897
H	5.287008	-1.344467	2.938681
B	5.067948	-0.173895	0.637059
H	5.793724	0.753170	0.746413
B	4.763302	-0.922003	-0.942507
H	5.277579	-0.511191	-1.924882
B	5.488389	-1.879669	0.368142
H	6.624499	-2.217609	0.309158
C	0.922039	-0.407420	0.544181
C	0.021275	-0.760863	-0.471911
H	0.348321	-1.373217	-1.302604
C	-1.303408	-0.337883	-0.435139
H	-1.965842	-0.613559	-1.246909
C	-1.770709	0.449888	0.627140
C	-0.872185	0.805613	1.644245
H	-1.220705	1.418950	2.467199
C	0.450267	0.378708	1.606729
H	1.110795	0.655125	2.418457
C	-3.146076	0.969611	0.693332
N	-4.275730	0.372883	0.208308
N	-5.346478	1.201418	0.406078
C	-4.806797	2.252864	1.009562
N	-3.461599	2.153806	1.210115
C	-4.494602	-0.929675	-0.339766
C	-4.046091	-2.062916	0.343706
C	-4.280068	-3.325323	-0.201656
H	-3.931516	-4.207751	0.325422
C	-4.972567	-3.454644	-1.407496
H	-5.157793	-4.439542	-1.824449
C	-5.432393	-2.315660	-2.073021
H	-5.975184	-2.411647	-3.008042
C	-5.192457	-1.047753	-1.544479
C	-5.612650	3.439807	1.425650
H	-5.254476	4.345254	0.925799
H	-5.527554	3.605246	2.504072
H	-6.663827	3.290763	1.173519
C	3.252882	1.439810	-0.768019
C	2.881785	1.578127	-2.114619
C	3.349197	2.594184	0.024970
C	2.595372	2.834459	-2.646441
H	2.824505	0.708242	-2.756745
C	3.062440	3.848987	-0.510008
H	3.658359	2.520353	1.060117
C	2.679558	3.974020	-1.845858
H	2.309720	2.918957	-3.690160
H	3.142655	4.728539	0.120852
H	2.455707	4.951683	-2.261158
H	-3.528931	-1.955940	1.290846
H	-5.541255	-0.153996	-2.049404

Table S8 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of **TzCB1** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-2.233588	-1.424155	-0.429692
C	-3.707683	0.364434	0.115900
B	-3.019961	-0.226043	-1.374991
H	-2.344056	0.523154	-2.000006
B	-2.945828	-2.040154	-1.767611
H	-2.230807	-2.483242	-2.607335
B	-3.174457	-2.726400	-0.123165
H	-2.634614	-3.696830	0.300814
B	-3.331565	-1.164471	0.867450
H	-2.889628	-1.139909	1.968708
B	-4.765528	-2.226876	0.449576
H	-5.339735	-2.929949	1.220085
B	-4.527891	-2.681400	-1.273543
H	-4.942395	-3.689890	-1.753084
B	-4.401384	-1.129319	-2.171979
H	-4.709985	-1.029574	-3.317714
B	-4.794761	0.206357	-1.087139
H	-5.290150	1.204534	-1.499719
B	-5.024102	-0.483819	0.563544
H	-5.696679	-0.019637	1.426168
B	-5.617330	-1.361075	-0.871575
H	-6.788556	-1.448785	-1.070995
C	-0.773383	-1.397282	-0.208017
C	0.102135	-0.876337	-1.182434
H	-0.299351	-0.518176	-2.122725
C	1.470393	-0.823132	-0.966535
H	2.117045	-0.453862	-1.754483
C	2.020987	-1.298158	0.245619
C	1.158472	-1.870002	1.205244
H	1.576316	-2.259565	2.126909
C	-0.206736	-1.907161	0.984972
H	-0.856277	-2.329751	1.742280
C	3.448056	-1.303242	0.503620
N	4.387292	-0.323500	0.059468
N	5.631291	-0.745336	0.351649
C	5.429874	-1.901112	0.996273
N	4.114028	-2.259018	1.109067
C	4.196006	0.931804	-0.518127
C	3.048266	1.704913	-0.207097
C	2.912332	2.963609	-0.769382
H	2.046905	3.567648	-0.523179
C	3.897512	3.462127	-1.631199
H	3.781671	4.446177	-2.071607
C	5.044196	2.698335	-1.921713
H	5.799432	3.090849	-2.592939
C	5.206069	1.444094	-1.365579
C	6.543933	-2.714757	1.538407
H	6.529947	-3.712270	1.086725
H	6.418035	-2.849675	2.617456
H	7.503413	-2.238480	1.338081
C	-3.267212	1.637828	0.708815
C	-3.206873	1.807796	2.107895
C	-2.905465	2.732911	-0.103671
C	-2.804684	3.017985	2.666925
H	-3.484712	0.983381	2.755474
C	-2.504210	3.941911	0.458817
H	-2.949226	2.630906	-1.182548
C	-2.448134	4.093030	1.847442
H	-2.771553	3.123400	3.747593
H	-2.237128	4.771422	-0.189894
H	-2.134770	5.036139	2.284861
H	2.317860	1.336654	0.499603
H	6.073185	0.833687	-1.581546

Table S9 Cartesian coordinates of the ground state (S_0) fully optimized geometry of **TzCB2** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	3.204781	-1.212659	-0.022527
C	4.238845	0.209968	0.105694
B	3.799483	-0.692876	1.509279
H	3.051958	-0.218648	2.282704
B	3.757086	-2.410991	1.060080
H	2.934350	-3.098472	1.559109
B	4.105015	-2.505923	-0.677302
H	3.523268	-3.260169	-1.377988
B	4.352795	-0.844206	-1.255181
H	3.964689	-0.471011	-2.300271
B	5.745706	-1.886185	-0.950816
H	6.401467	-2.282007	-1.856528
B	5.385351	-2.857529	0.504045
H	5.786830	-3.965398	0.644905
B	5.180402	-1.730988	1.874404
H	5.430234	-2.014264	2.998876
B	5.450589	-0.083587	1.270184
H	5.804494	0.841335	1.916416
B	5.798747	-0.179105	-0.467012
H	6.392720	0.680227	-1.021174
B	6.427666	-1.425422	0.633775
H	7.588940	-1.489527	0.870007
C	1.741291	-1.039209	-0.331583
C	0.799728	-0.873085	0.693251
H	1.116269	-0.853621	1.728197
C	-0.557480	-0.745430	0.411562
H	-1.247567	-0.623406	1.235502
C	-1.021255	-0.785495	-0.912810
C	-0.079358	-0.976078	-1.938831
H	-0.425319	-1.029834	-2.963962
C	1.274107	-1.100327	-1.654218
H	1.966676	-1.254594	-2.472022
C	-2.438343	-0.682406	-1.301840
N	-3.492179	-0.240113	-0.551947
N	-4.643742	-0.357338	-1.277433
C	-4.227606	-0.854520	-2.436395
N	-2.884813	-1.065770	-2.497553
C	-3.549137	0.301433	0.783120
C	-3.251495	1.668418	0.987094
C	-3.276432	2.137512	2.309556
H	-3.046509	3.182908	2.495027
C	-3.594943	1.306386	3.376226
H	-3.601248	1.696629	4.389526
C	-3.928426	-0.022443	3.136751
H	-4.205948	-0.664850	3.967489
C	-3.927700	-0.558723	1.841834
C	-5.160226	-1.150442	-3.565481
H	-5.112021	-2.208612	-3.840170
H	-4.890134	-0.568581	-4.452168
H	-6.185418	-0.905679	-3.282885
C	-2.899764	2.713694	-0.082480
H	-3.165359	3.666197	0.392121
C	-4.416571	-2.006908	1.709546
H	-4.318295	-2.419879	2.720830
C	3.643777	1.581222	-0.086765
C	3.612607	2.177221	-1.357214
C	3.163767	2.312640	1.011026
C	3.096621	3.461058	-1.526707
H	3.999677	1.646716	-2.218059
C	2.648891	3.596585	0.838412
H	3.199753	1.888314	2.006577
C	2.608258	4.174112	-0.431332
H	3.081820	3.902986	-2.517924
H	2.285097	4.145623	1.701182
H	2.208053	5.174360	-0.564508
C	-3.620471	-2.952165	0.792516
H	-3.812765	-2.773808	-0.267373
H	-2.542890	-2.883115	0.967699
H	-3.922506	-3.983168	1.004534
C	-5.921370	-2.041243	1.364390
H	-6.101032	-1.620576	0.371924
H	-6.285426	-3.074479	1.376786
H	-6.504654	-1.467300	2.091302
C	-1.385195	2.788922	-0.363681
H	-0.808227	2.877070	0.561783
H	-1.027727	1.906847	-0.899968
H	-1.167263	3.665778	-0.982749
C	-3.699938	2.666411	-1.395495
H	-3.361662	1.873924	-2.066609
H	-4.768665	2.525161	-1.215527
H	-3.566496	3.616834	-1.923059

Table S10 Cartesian coordinates of the first excited state (S_1) fully optimized geometry of **TzCB2** in THF from B3LYP calculations (in Å)

Atom	X	Y	Z
C	-2.766899	-1.355105	-0.002731
C	-4.917771	-0.138760	0.000341
B	-3.933775	-0.959002	-1.178280
H	-3.551976	-0.325907	-2.107845
B	-3.123450	-2.684629	-0.894170
H	-2.271409	-3.120928	-1.598092
B	-3.122419	-2.686792	0.885874
H	-2.269500	-3.124780	1.587683
B	-3.932412	-0.961969	1.175390
H	-3.549309	-0.331441	2.106162
B	-4.797766	-2.583208	1.424780
H	-5.067275	-3.055932	2.483727
B	-4.357060	-3.587021	-0.004546
H	-4.349504	-4.777844	-0.006079
B	-4.799461	-2.579542	-1.430756
H	-5.070373	-3.049501	-2.490574
B	-5.762285	-1.189893	-0.902441
H	-6.598871	-0.739130	-1.615195
B	-5.761376	-1.192275	0.901235
H	-6.597171	-0.743386	1.616096
B	-5.887797	-2.720698	-0.002517
H	-6.915631	-3.322605	-0.002696
C	-1.454938	-0.707080	-0.002650
C	-0.255480	-1.474102	-0.004818
H	-0.325734	-2.554828	-0.006592
C	0.981044	-0.873721	-0.004804
H	1.868477	-1.489498	-0.006725
C	1.087533	0.547618	-0.002365
C	-0.113753	1.322155	-0.000418
H	-0.030337	2.401219	0.001364
C	-1.342792	0.711081	-0.000419
H	-2.243516	1.312932	0.001366
C	2.323980	1.274275	-0.002524
N	3.626090	0.785486	-0.001178
N	4.480235	1.804205	0.000264
C	3.683471	2.910414	-0.001813
N	2.380851	2.621029	-0.002198
C	4.123789	-0.577401	0.003301
C	4.359412	-1.208491	-1.238884
C	4.757988	-2.551958	-1.195031
H	4.936563	-3.072624	-2.130731
C	4.936179	-3.222258	0.010076
H	5.233818	-4.266100	0.012750
C	4.753132	-2.547208	1.211741
H	4.927977	-3.064173	2.150195
C	4.354509	-1.203492	1.248857
C	4.252808	4.285331	-0.022724
H	3.513995	4.999631	0.341706
H	4.528816	4.565767	-1.045092
H	5.153520	4.337771	0.592345
C	4.323312	-0.548522	-2.623093
H	4.365667	-1.389864	-3.323695
C	4.314374	-0.538279	2.630397
H	4.349723	-1.377161	3.334330
C	-5.092316	1.324361	0.002247
C	-5.178967	2.044495	1.211303
C	-5.181611	2.047301	-1.204942
C	-5.353641	3.426630	1.211040
H	-5.116268	1.510407	2.153506
C	-5.356275	3.429427	-1.201093
H	-5.120989	1.515397	-2.148515
C	-5.442342	4.128488	0.005883
H	-5.423102	3.957295	2.156270
H	-5.427798	3.962284	-2.144936
H	-5.578130	5.205668	0.007281
C	3.055661	0.263922	3.005333
H	3.015014	1.246066	2.527583
H	2.137069	-0.280391	2.768469
H	3.062731	0.442299	4.084975
C	5.594417	0.290903	2.871861
H	5.609353	0.660356	3.902493
H	6.491137	-0.315735	2.714655
H	5.646973	1.151462	2.199228
C	3.062440	0.246233	-3.006803
H	2.145404	-0.301703	-2.772213
H	3.014529	1.229714	-2.532486
H	3.073630	0.420950	-4.087004
C	5.600576	0.285552	-2.862132
H	5.646206	1.149410	-2.193216
H	6.499333	-0.316220	-2.698003
H	5.618682	0.650366	-3.894371

Table S11 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 0°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	-2.332534	-1.509581	-0.276997
C	-3.588720	0.475119	0.107833
B	-3.100675	-0.375103	-1.324284
H	-2.422733	0.207509	-2.105088
B	-3.218546	-2.223183	-1.450073
H	-2.628264	-2.851895	-2.268517
B	-3.359782	-2.645355	0.291177
H	-2.878595	-3.600165	0.811211
B	-3.294231	-0.952592	1.047843
H	-2.754212	-0.819977	2.096614
B	-4.844228	-1.912493	0.901836
H	-5.406108	-2.443300	1.808038
B	-4.801353	-2.625767	-0.747795
H	-5.344865	-3.645025	-1.040002
B	-4.618997	-1.236142	-1.872713
H	-5.016964	-1.269797	-2.994858
B	-4.798565	0.270204	-0.968498
H	-5.236450	1.248347	-1.482598
B	-4.940751	-0.153995	0.772583
H	-5.488886	0.496636	1.602609
B	-5.732136	-1.159409	-0.465413
H	-6.919624	-1.162074	-0.563543
C	-0.865753	-1.563984	-0.158959
C	-0.032838	-1.207644	-1.239972
H	-0.477976	-0.942785	-2.191511
C	1.347301	-1.174491	-1.105080
H	1.962046	-0.893686	-1.954757
C	1.948583	-1.514196	0.122440
C	1.136040	-1.940657	1.187155
H	1.593354	-2.232690	2.126622
C	-0.244142	-1.953182	1.048754
H	-0.858675	-2.256255	1.888306
C	3.400358	-1.491702	0.282165
N	4.271687	-0.421113	-0.126585
N	5.563974	-0.837386	0.035460
C	5.445242	-2.046349	0.549003
N	4.136107	-2.472802	0.715586
C	4.033089	0.918800	-0.363899
C	2.736341	1.498276	-0.220239
C	2.558687	2.837600	-0.499700
H	1.578564	3.281376	-0.372109
C	3.639912	3.626033	-0.928458
H	3.488640	4.676610	-1.147807
C	4.925378	3.059744	-1.064350
H	5.753203	3.674110	-1.397692
C	5.131770	1.728549	-0.786220
C	6.607741	-2.893048	0.906695
H	6.564624	-3.835289	0.350750
H	6.568812	-3.146289	1.971011
H	7.543264	-2.379906	0.685398
C	-2.977333	1.767718	0.470753
C	-2.775516	2.125648	1.819515
C	-2.578831	2.689042	-0.519174
C	-2.199190	3.346849	2.161113
H	-3.079396	1.438748	2.601908
C	-2.002506	3.910200	-0.175113
H	-2.730485	2.443489	-1.564604
C	-1.804830	4.247147	1.167184
H	-2.059652	3.597845	3.208858
H	-1.713348	4.604748	-0.959048
H	-1.358058	5.199966	1.434847
H	1.911771	0.911587	0.149832
H	6.104470	1.271095	-0.895113

Table S12 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 30°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	-2.233784	-1.424322	-0.429606
C	-3.707594	0.364631	0.115543
B	-3.020072	-0.226315	-1.375205
H	-2.344080	0.522594	-2.000458
B	-2.946176	-2.040523	-1.767342
H	-2.231279	-2.483912	-2.607006
B	-3.174811	-2.726366	-0.122721
H	-2.635104	-3.696765	0.301482
B	-3.331662	-1.164133	0.867486
H	-2.889696	-1.139341	1.968724
B	-4.765788	-2.226444	0.449973
H	-5.340041	-2.929224	1.220707
B	-4.528308	-2.681443	-1.273031
H	-4.942982	-3.689993	-1.752288
B	-4.401652	-1.129618	-2.171870
H	-4.710276	-1.030141	-3.317618
B	-4.794802	0.206404	-1.087364
H	-5.290088	1.204529	-1.500172
B	-5.024107	-0.483314	0.563509
H	-5.696564	-0.018835	1.426058
B	-5.617551	-1.360869	-0.871343
H	-6.788794	-1.448484	-1.070673
C	-0.773589	-1.397495	-0.207980
C	0.101943	-0.876753	-1.182497
H	-0.299542	-0.518710	-2.122832
C	1.470203	-0.823540	-0.966613
H	2.116876	-0.454359	-1.754595
C	2.020791	-1.298387	0.245600
C	1.158276	-1.870003	1.205346
H	1.576112	-2.259418	2.127077
C	-0.206944	-1.907153	0.985102
H	-0.856487	-2.329574	1.742500
C	3.447892	-1.303535	0.503490
N	4.387228	-0.323885	0.059219
N	5.631231	-0.745974	0.351136
C	5.429748	-1.901835	0.995522
N	4.113858	-2.259578	1.108487
C	4.196055	0.931849	-0.517387
C	3.047849	1.704456	-0.206682
C	2.911962	2.963476	-0.768228
H	2.046194	3.567102	-0.522229
C	3.897617	3.462866	-1.629003
H	3.781814	4.447182	-2.068819
C	5.044742	2.699590	-1.919199
H	5.800356	3.092771	-2.589603
C	5.206568	1.445027	-1.363821
C	6.543794	-2.715837	1.537146
H	6.529562	-3.713200	1.085133
H	6.418090	-2.851094	2.616174
H	7.503301	-2.239638	1.336777
C	-3.266895	1.638113	0.708106
C	-3.206424	1.808419	2.107137
C	-2.905009	2.732926	-0.104679
C	-2.804001	3.018684	2.665835
H	-3.484340	0.984204	2.754940
C	-2.503518	3.942004	0.457476
H	-2.948846	2.630648	-1.183528
C	-2.447335	4.093466	1.846058
H	-2.770776	3.124369	3.746475
H	-2.236336	4.771307	-0.191461
H	-2.133793	5.036635	2.283221
H	2.317064	1.335617	0.499300
H	6.073992	0.835012	-1.579626

Table S13 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 60°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	2.205840	-1.321521	0.543273
C	3.789013	0.336664	-0.112460
B	2.981690	-0.064331	1.398370
H	2.305907	0.777148	1.891704
B	2.803660	-1.820068	1.984638
H	2.019270	-2.130440	2.821568
B	3.087751	-2.698306	0.444117
H	2.521298	-3.683566	0.096899
B	3.368275	-1.265778	-0.705480
H	2.988524	-1.346639	-1.826690
B	4.729065	-2.330415	-0.086775
H	5.313596	-3.135138	-0.740443
B	4.377535	-2.577252	1.659746
H	4.719987	-3.539236	2.272019
B	4.275607	-0.927303	2.370281
H	4.528587	-0.707631	3.512410
B	4.783215	0.263364	1.170512
H	5.302788	1.278098	1.504593
B	5.069794	-0.623482	-0.384419
H	5.811063	-0.295728	-1.252907
B	5.545144	-1.354592	1.177112
H	6.699634	-1.460078	1.449771
C	0.753433	-1.275248	0.248636
C	-0.150056	-0.648144	1.136619
H	0.223005	-0.220919	2.059352
C	-1.502893	-0.581512	0.859986
H	-2.166533	-0.129596	1.585019
C	-2.019454	-1.152248	-0.331503
C	-1.123855	-1.830028	-1.200371
H	-1.515598	-2.286436	-2.101596
C	0.225679	-1.881917	-0.917706
H	0.895374	-2.387291	-1.602837
C	-3.414202	-1.144446	-0.689206
N	-4.406787	-0.249058	-0.240667
N	-5.590291	-0.625001	-0.717223
C	-5.299791	-1.708718	-1.487686
N	-3.993557	-2.028477	-1.500994
C	-4.324595	0.861063	0.647522
C	-3.480293	1.936684	0.333168
C	-3.462861	3.044296	1.174994
H	-2.817940	3.884190	0.941019
C	-4.284177	3.080426	2.306179
H	-4.263958	3.945720	2.960332
C	-5.137221	2.008795	2.596139
H	-5.773337	2.040835	3.474015
C	-5.172135	0.896249	1.762359
C	-6.351253	-2.435710	-2.241810
H	-6.414001	-3.471957	-1.893267
H	-6.098359	-2.467273	-3.305944
H	-7.320245	-1.954208	-2.110763
C	3.437209	1.544490	-0.867616
C	3.461287	1.553361	-2.279564
C	3.078765	2.739208	-0.205525
C	3.144032	2.704858	-2.993538
H	3.737793	0.649823	-2.811792
C	2.762769	3.888395	-0.923916
H	3.057830	2.759920	0.878574
C	2.790124	3.879596	-2.322172
H	3.174328	2.687128	-4.079158
H	2.495542	4.796476	-0.391106
H	2.541672	4.776670	-2.881069
H	-2.866735	1.904713	-0.559785
H	-5.825927	0.056425	1.966960

Table S14 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 90°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	2.163393	-1.315514	-0.305587
C	3.889483	0.269906	0.153879
B	2.955155	-0.869141	1.131832
H	2.304546	-0.414765	2.013980
B	2.630152	-2.614819	0.578523
H	1.773980	-3.278756	1.066497
B	2.951663	-2.456243	-1.180513
H	2.342920	-2.998425	-2.044869
B	3.394610	-0.651564	-1.272526
H	3.082071	-0.030176	-2.233617
B	4.643095	-1.993070	-1.375546
H	5.215644	-2.314459	-2.367940
B	4.168315	-3.178450	-0.107187
H	4.410516	-4.342323	-0.168193
B	4.129509	-2.247273	1.432467
H	4.326434	-2.753734	2.491122
B	4.783702	-0.629586	1.163814
H	5.346239	-0.054002	2.037389
B	5.109503	-0.468621	-0.617672
H	5.924513	0.231910	-1.123532
B	5.439072	-2.011457	0.231140
H	6.565713	-2.354826	0.406095
C	0.731314	-0.992798	-0.537013
C	-0.191031	-0.960722	0.538655
H	0.157279	-1.180173	1.540323
C	-1.520458	-0.647018	0.340579
H	-2.185412	-0.626370	1.191936
C	-2.003025	-0.359773	-0.963962
C	-1.082219	-0.413292	-2.050194
H	-1.445701	-0.201829	-3.048034
C	0.243610	-0.726876	-1.838592
H	0.924672	-0.762468	-2.679900
C	-3.364328	-0.026826	-1.281848
N	-4.452360	0.097279	-0.413920
N	-5.542211	0.415802	-1.105692
C	-5.102501	0.482735	-2.397623
N	-3.798961	0.222563	-2.530012
C	-4.557269	-0.055198	1.016594
C	-4.355809	1.058683	1.832283
C	-4.479599	0.909121	3.213660
H	-4.324185	1.765773	3.860927
C	-4.805407	-0.335144	3.758632
H	-4.899561	-0.445662	4.834049
C	-5.014478	-1.436891	2.925665
H	-5.273677	-2.401331	3.349481
C	-4.894195	-1.302923	1.542340
C	-6.021306	0.817265	-3.516793
H	-6.046640	-0.001902	-4.242189
H	-5.666149	1.708157	-4.043749
H	-7.029250	0.997413	-3.142848
C	3.661172	1.713762	0.243747
C	3.770701	2.541201	-0.896342
C	3.340100	2.325060	1.476563
C	3.571567	3.914909	-0.804317
H	4.020264	2.096596	-1.853485
C	3.141945	3.699272	1.562823
H	3.254673	1.712091	2.367122
C	3.253383	4.503881	0.423961
H	3.665975	4.530609	-1.694084
H	2.900910	4.146501	2.522843
H	3.096408	5.575950	0.493092
H	-4.106370	2.017341	1.390639
H	-5.055240	-2.146439	0.879980

Table S15 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 120°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	2.083261	-1.060379	-0.736849
C	3.930815	0.094151	0.234804
B	2.926975	-1.263648	0.732250
H	2.322197	-1.147077	1.746423
B	2.461503	-2.627182	-0.441878
H	1.561989	-3.371149	-0.218751
B	2.779243	-1.817273	-2.012530
H	2.124503	-1.938798	-2.996759
B	3.361929	-0.155991	-1.412416
H	3.091877	0.810618	-2.045348
B	4.499785	-1.433156	-2.077725
H	5.034610	-1.381551	-3.139667
B	3.944967	-2.983111	-1.351350
H	4.093441	-4.044929	-1.869098
B	3.992231	-2.726745	0.428504
H	4.156746	-3.619759	1.198000
B	4.771462	-1.182356	0.781795
H	5.385220	-1.029568	1.787354
B	5.092088	-0.363858	-0.804497
H	5.953910	0.423141	-1.025901
B	5.306939	-2.131768	-0.636374
H	6.403635	-2.595670	-0.653248
C	0.682678	-0.572467	-0.769570
C	-0.224128	-0.894320	0.266716
H	0.118058	-1.487213	1.105946
C	-1.530656	-0.443663	0.245974
H	-2.176461	-0.666830	1.084530
C	-1.998844	0.349623	-0.833438
C	-1.086513	0.690581	-1.867497
H	-1.435171	1.303147	-2.690280
C	0.212246	0.225847	-1.840706
H	0.885360	0.477675	-2.651108
C	-3.334138	0.878666	-0.930594
N	-4.493365	0.405973	-0.285810
N	-5.512652	1.216154	-0.555791
C	-4.976494	2.142833	-1.397750
N	-3.671753	1.949167	-1.652372
C	-4.681983	-0.690029	0.607114
C	-5.169411	-0.434985	1.894679
C	-5.355036	-1.504995	2.764509
H	-5.722684	-1.322089	3.768417
C	-5.059658	-2.808849	2.350348
H	-5.206833	-3.638149	3.034264
C	-4.574976	-3.048647	1.060947
H	-4.355708	-4.060833	0.739096
C	-4.377596	-1.989418	0.179700
C	-5.792788	3.242026	-1.971358
H	-5.729513	3.228389	-3.063549
H	-5.406675	4.210580	-1.636477
H	-6.834294	3.146840	-1.664452
C	3.819837	1.402474	0.889190
C	3.981412	2.599411	0.157452
C	3.563310	1.504154	2.274208
C	3.892734	3.838620	0.784202
H	4.183794	2.548369	-0.906740
C	3.475683	2.745657	2.896444
H	3.439740	0.599492	2.859428
C	3.636875	3.921536	2.156634
H	4.025008	4.744765	0.200104
H	3.282005	2.797191	3.963993
H	3.566040	4.889421	2.643448
H	-5.386197	0.583341	2.196076
H	-4.015594	-2.159944	-0.827718

Table S16 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 150°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	-2.226967	-1.416226	0.442549
C	-3.712380	0.358547	-0.118204
B	-3.331974	-1.179598	-0.851607
H	-2.896378	-1.167295	-1.955552
B	-3.162196	-2.727774	0.158578
H	-2.619543	-3.700650	-0.256020
B	-2.927985	-2.018909	1.792616
H	-2.205785	-2.447132	2.633853
B	-3.012742	-0.210312	1.376845
H	-2.336746	0.550106	1.987997
B	-4.385684	-1.109729	2.193074
H	-4.688656	-0.996225	3.338977
B	-4.509538	-2.674032	1.315743
H	-4.916719	-3.678044	1.810600
B	-4.758756	-2.243187	-0.411829
H	-5.333992	-2.958545	-1.170070
B	-5.025745	-0.502890	-0.547653
H	-5.705312	-0.053899	-1.412783
B	-4.790759	0.210168	1.093373
H	-5.288744	1.210978	1.496214
B	-5.607281	-1.364170	0.902432
H	-6.777049	-1.454176	1.109022
C	-0.767434	-1.386555	0.213634
C	-0.204556	-1.907834	-0.976543
H	-0.856315	-2.340156	-1.726379
C	1.159168	-1.869061	-1.203087
H	1.574389	-2.266575	-2.122462
C	2.024945	-1.284320	-0.253106
C	1.477747	-0.798635	0.957052
H	2.126444	-0.422001	1.739506
C	0.110792	-0.853271	1.179078
H	-0.287721	-0.487500	2.117683
C	3.449122	-1.287775	-0.520668
N	4.391418	-0.311354	-0.080313
N	5.631006	-0.728660	-0.386485
C	5.424665	-1.882651	-1.038168
N	4.110335	-2.239646	-1.140974
C	4.203127	0.932974	0.527076
C	5.195884	1.407805	1.413226
C	5.034468	2.649501	1.999113
H	5.776772	3.014142	2.699942
C	3.905173	3.434507	1.700455
H	3.789549	4.407898	2.164159
C	2.935996	2.970745	0.802419
H	2.082877	3.590663	0.552453
C	3.071892	1.725073	0.210249
C	6.536092	-2.689006	-1.596595
H	6.401076	-2.816185	-2.675481
H	6.529531	-3.689931	-1.152356
H	7.495905	-2.211284	-1.401348
C	-3.280951	1.625659	-0.729882
C	-2.920698	2.733199	0.066449
C	-3.228158	1.777315	-2.131495
C	-2.528254	3.936522	-0.513915
H	-2.958676	2.645200	1.146776
C	-2.834698	2.981926	-2.708313
H	-3.504972	0.943018	-2.766723
C	-2.479589	4.069446	-1.904730
H	-2.262062	4.775852	0.122389
H	-2.807163	3.073265	-3.790407
H	-2.172869	5.008172	-2.356052
H	6.050209	0.781193	1.634505
H	2.353617	1.381584	-0.521463

Table S17 Cartesian coordinates of the first excited state (S_1) geometry for **TzCB1** at $\Psi_1 = 180°$ in THF from B3LYP calculations (in Å).

Atom	X	Y	Z
C	-2.328424	-1.502663	-0.286042
C	-3.603668	0.468152	0.107246
B	-3.098727	-0.365813	-1.329002
H	-2.419982	0.228958	-2.099923
B	-3.200536	-2.213630	-1.471146
H	-2.599446	-2.830189	-2.290922
B	-3.349633	-2.652331	0.265386
H	-2.863429	-3.607300	0.780356
B	-3.302690	-0.965711	1.037014
H	-2.770986	-0.837430	2.090532
B	-4.844031	-1.937198	0.872355
H	-5.407489	-2.480144	1.770308
B	-4.784463	-2.635693	-0.783003
H	-5.317322	-3.656907	-1.087634
B	-4.606360	-1.234908	-1.894743
H	-4.996646	-1.262132	-3.019721
B	-4.804214	0.262019	-0.979024
H	-5.247001	1.240800	-1.487608
B	-4.954007	-0.178576	0.757745
H	-5.513007	0.459968	1.589868
B	-5.729133	-1.179707	-0.494166
H	-6.915898	-1.190997	-0.599941
C	-0.861802	-1.549425	-0.160823
C	-0.025649	-1.187806	-1.237546
H	-0.467814	-0.921556	-2.190098
C	1.353962	-1.153960	-1.098065
H	1.970792	-0.873414	-1.946261
C	1.951886	-1.496988	0.130623
C	1.135379	-1.926393	1.191725
H	1.589986	-2.220333	2.131868
C	-0.243971	-1.940318	1.048496
H	-0.861139	-2.246622	1.884921
C	3.402046	-1.479318	0.296677
N	4.282737	-0.427995	-0.138302
N	5.570329	-0.848921	0.036799
C	5.440934	-2.042011	0.586523
N	4.129285	-2.453120	0.762159
C	4.051150	0.903845	-0.425858
C	5.159333	1.701912	-0.842038
C	4.970116	3.038417	-1.108070
H	5.804183	3.643255	-1.443344
C	3.696185	3.624439	-0.948924
H	3.558502	4.678614	-1.159917
C	2.611452	2.852460	-0.501151
H	1.643609	3.313281	-0.343963
C	2.772330	1.508496	-0.232678
C	6.596784	-2.885193	0.972926
H	6.548357	-3.843839	0.446196
H	6.553932	-3.105298	2.044446
H	7.536350	-2.385608	0.738138
C	-3.007121	1.763134	0.485564
C	-2.817907	2.111061	1.838764
C	-2.612091	2.697379	-0.493630
C	-2.257365	3.335461	2.194846
H	-3.119325	1.413970	2.613049
C	-2.051633	3.921640	-0.135002
H	-2.754128	2.459378	-1.542151
C	-1.866679	4.248807	1.211452
H	-2.127325	3.578669	3.245642
H	-1.764390	4.626005	-0.910824
H	-1.431880	5.203918	1.490428
H	6.124576	1.231653	-0.962746
H	1.947939	0.934525	0.157554