Electronic Supplementary Information

Salen-Indium/Triarylborane Triads: Synthesis and Ratiometric Emission-Colour Changes by Fluoride Ion Binding

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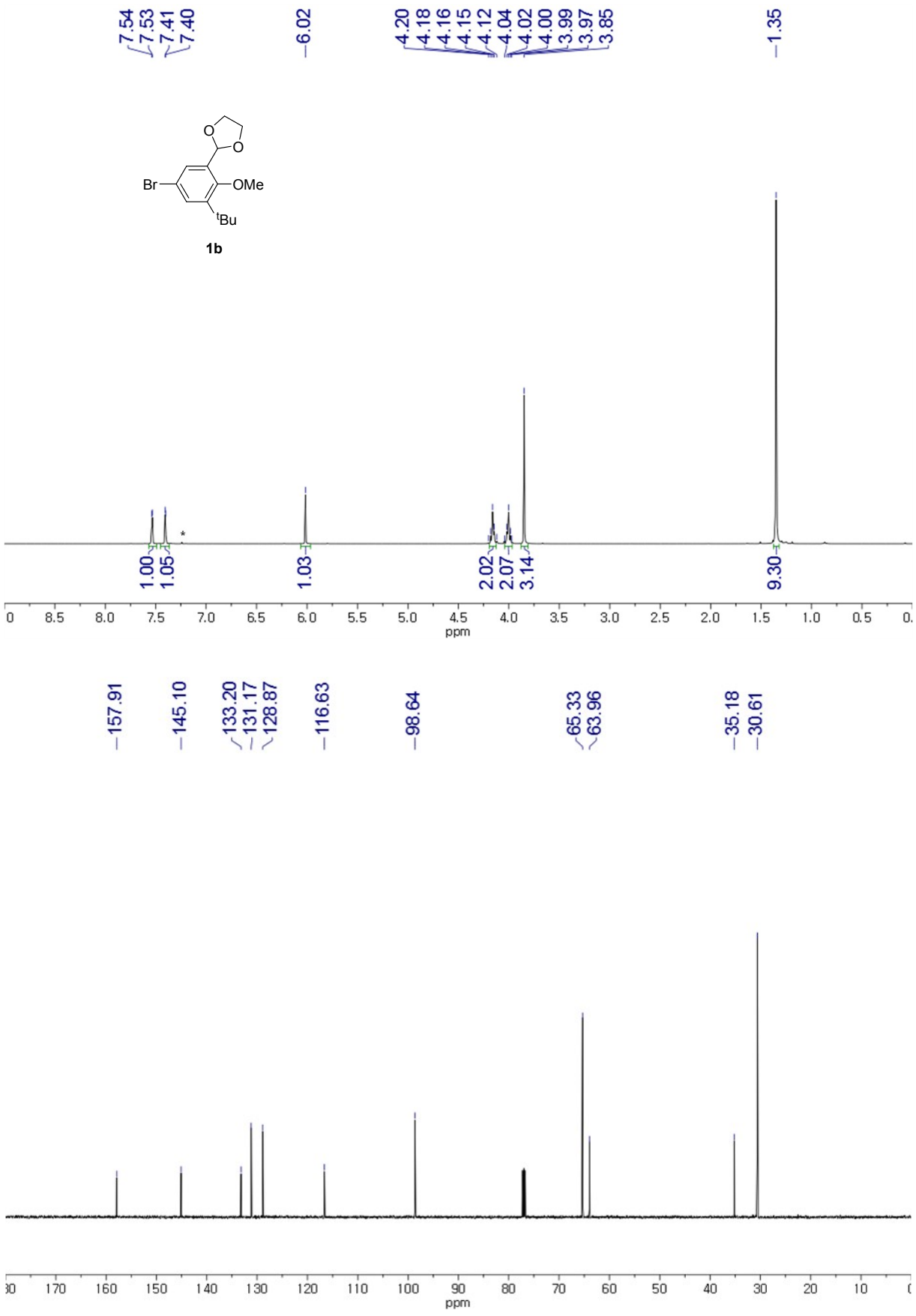

Figure S1. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1b** (∗ from residual $CHCl_3$ in $CDCl_3$).

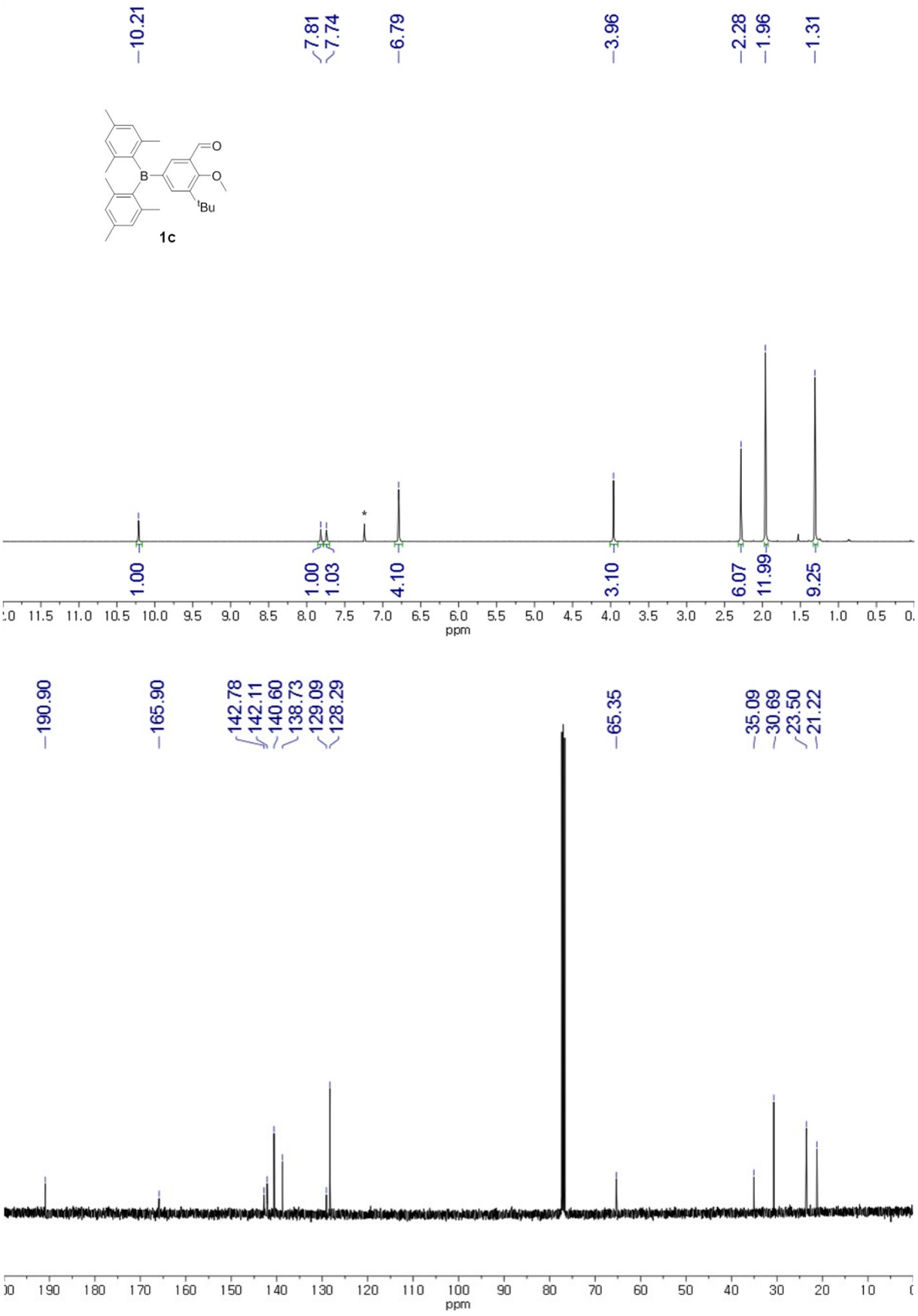

Figure S2. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1c** (∗ from residual $CHCl_3$ in $CDCl_3$).

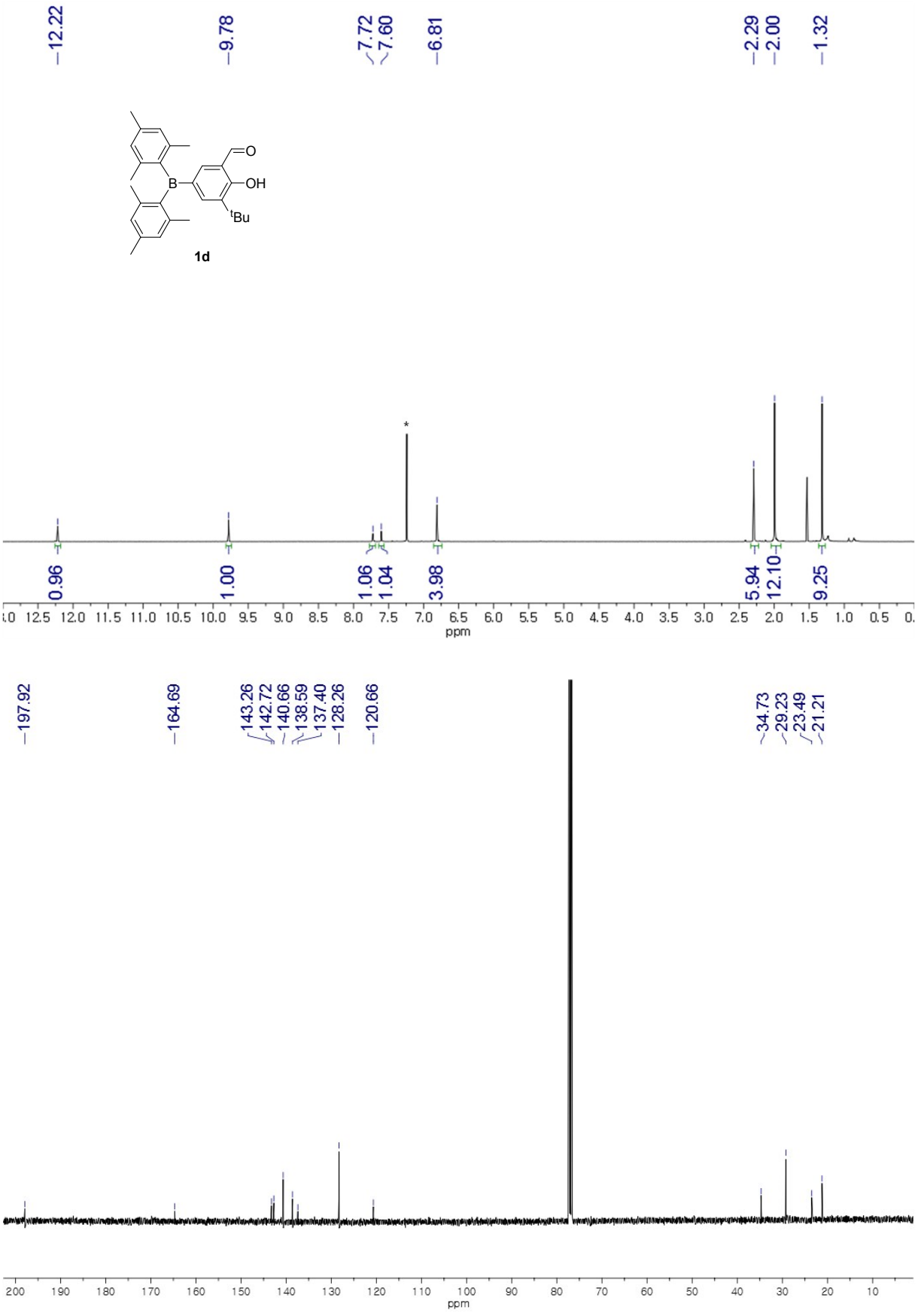

Figure S3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1d** (∗ from residual $CHCl_3$ in $CDCl_3$).

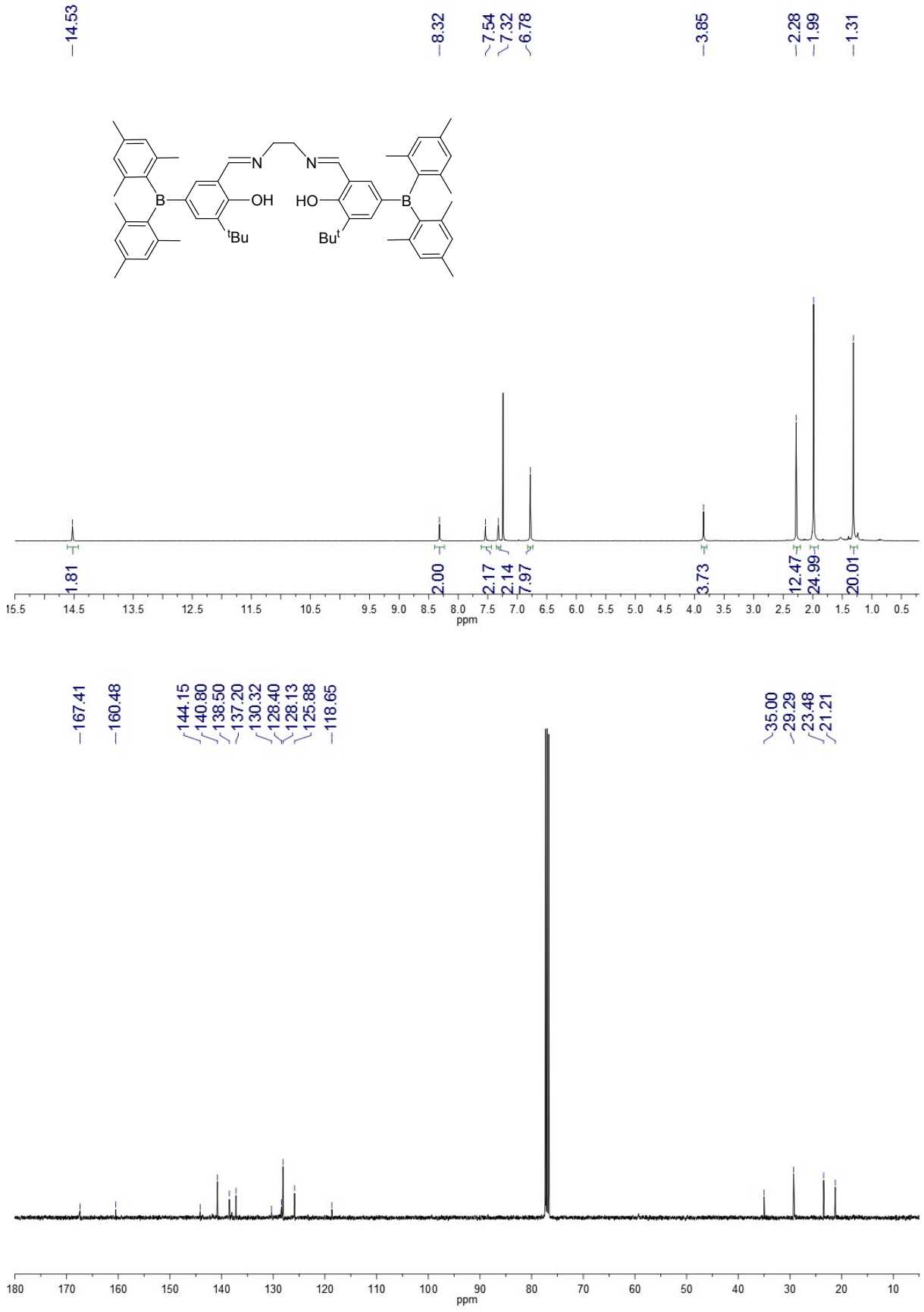

Figure S4. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1e** (∗ from residual $CHCl_3$ in $CDCl_3$).

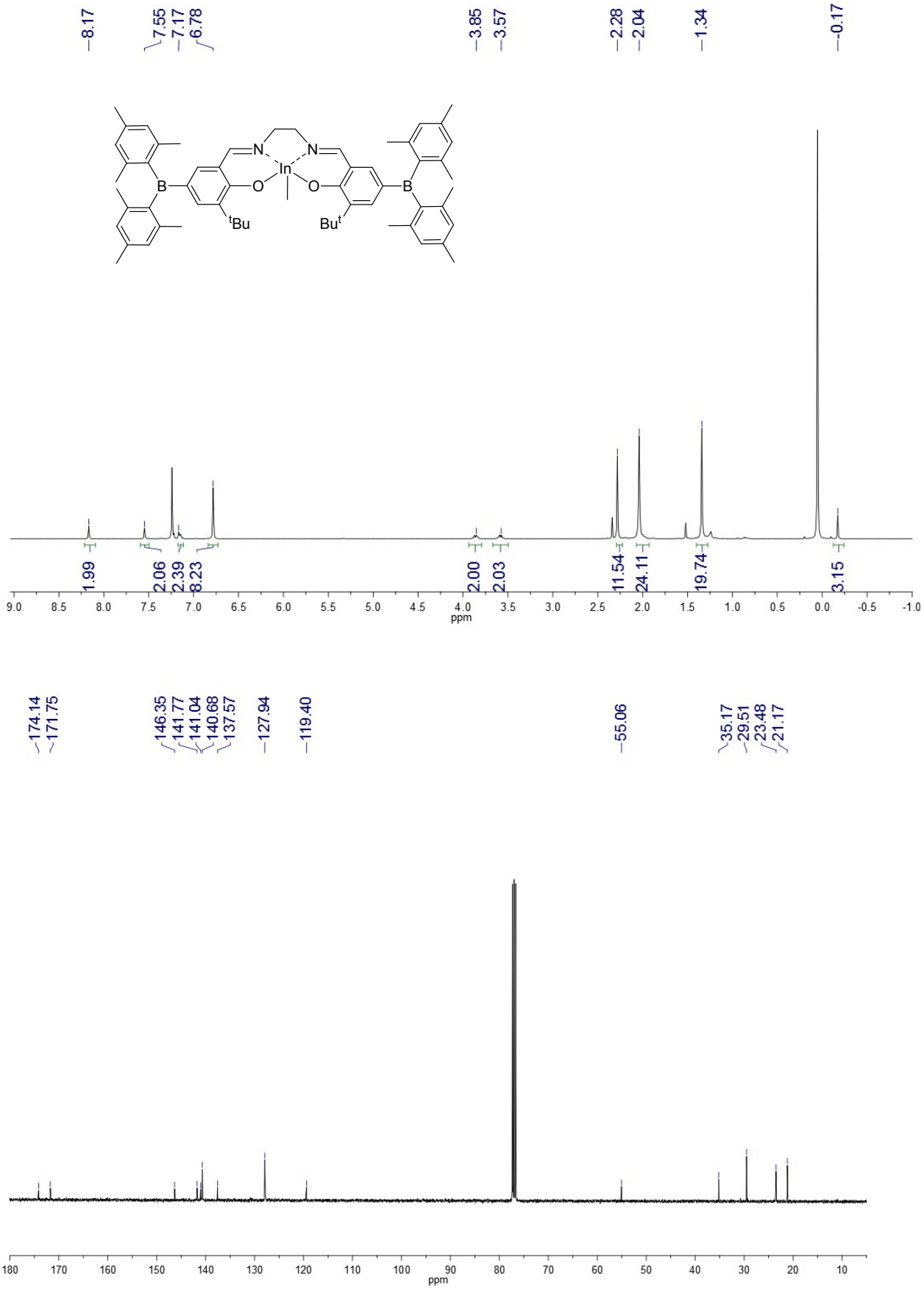

Figure S5. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1** (∗ from residual $CHCl_3$ in $CDCl_3$).

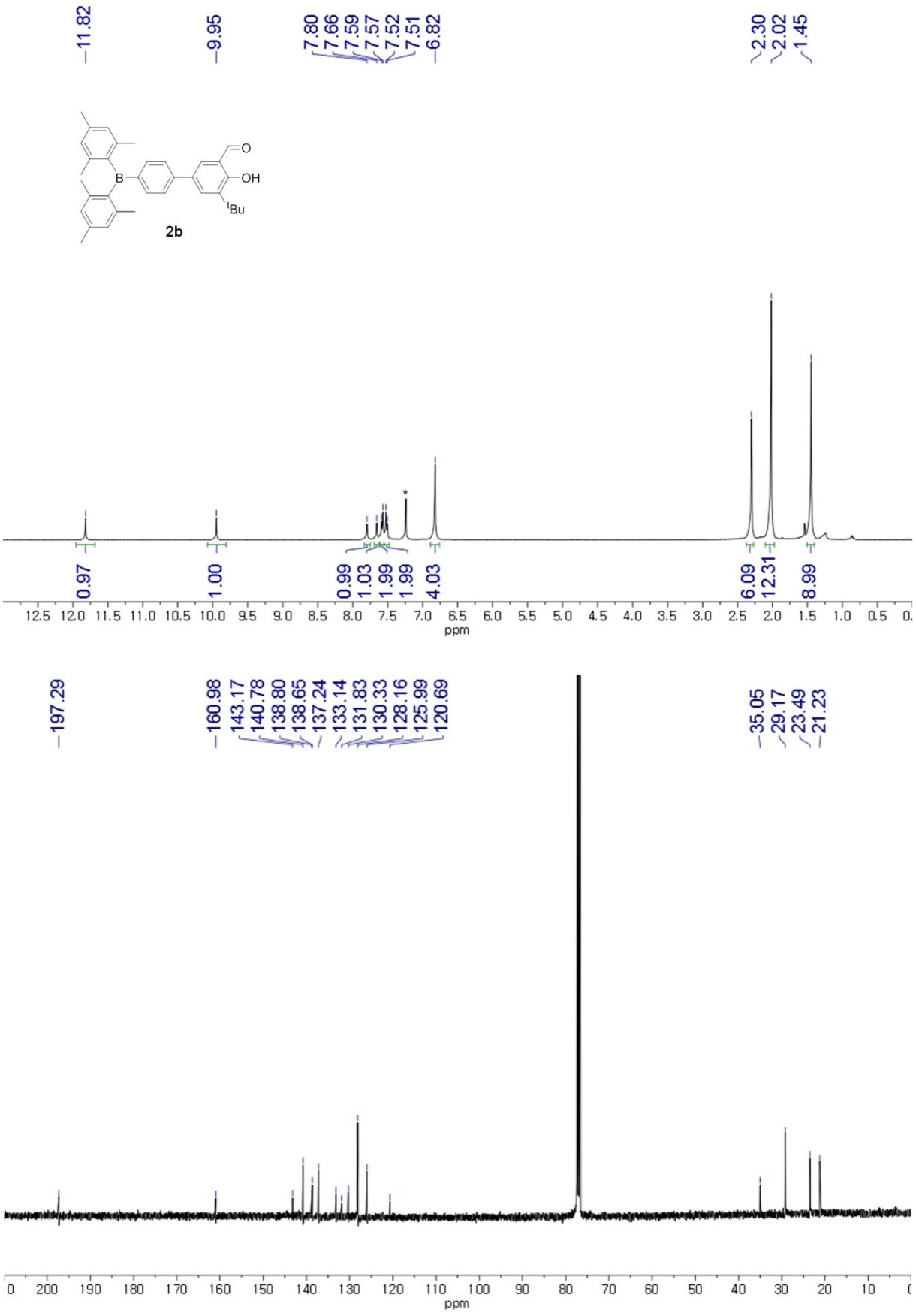

Figure S6. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2b** (∗ from residual $CHCl_3$ in $CDCl_3$).

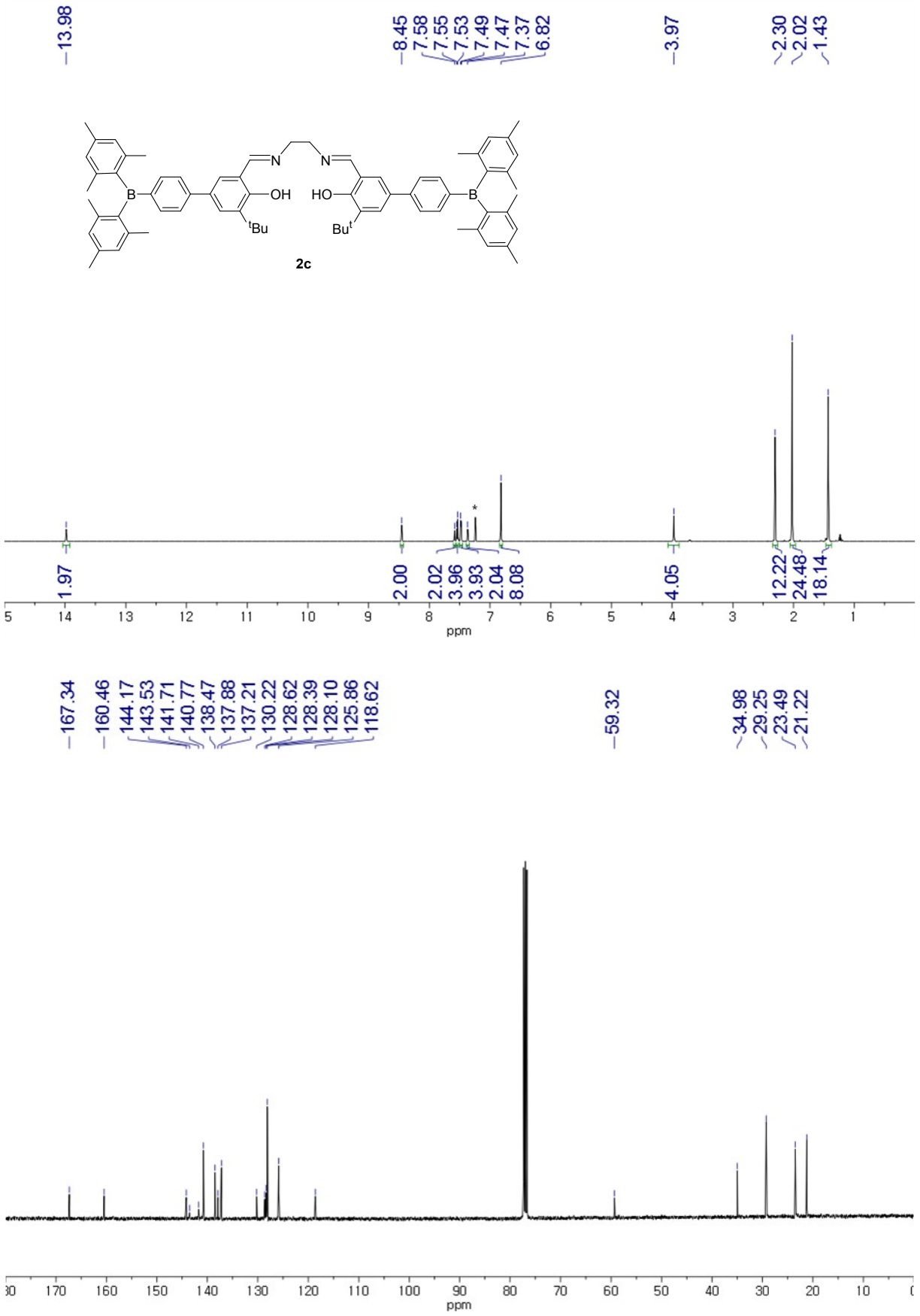

Figure S7. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2c** (∗ from residual $CHCl_3$ in $CDCl_3$).

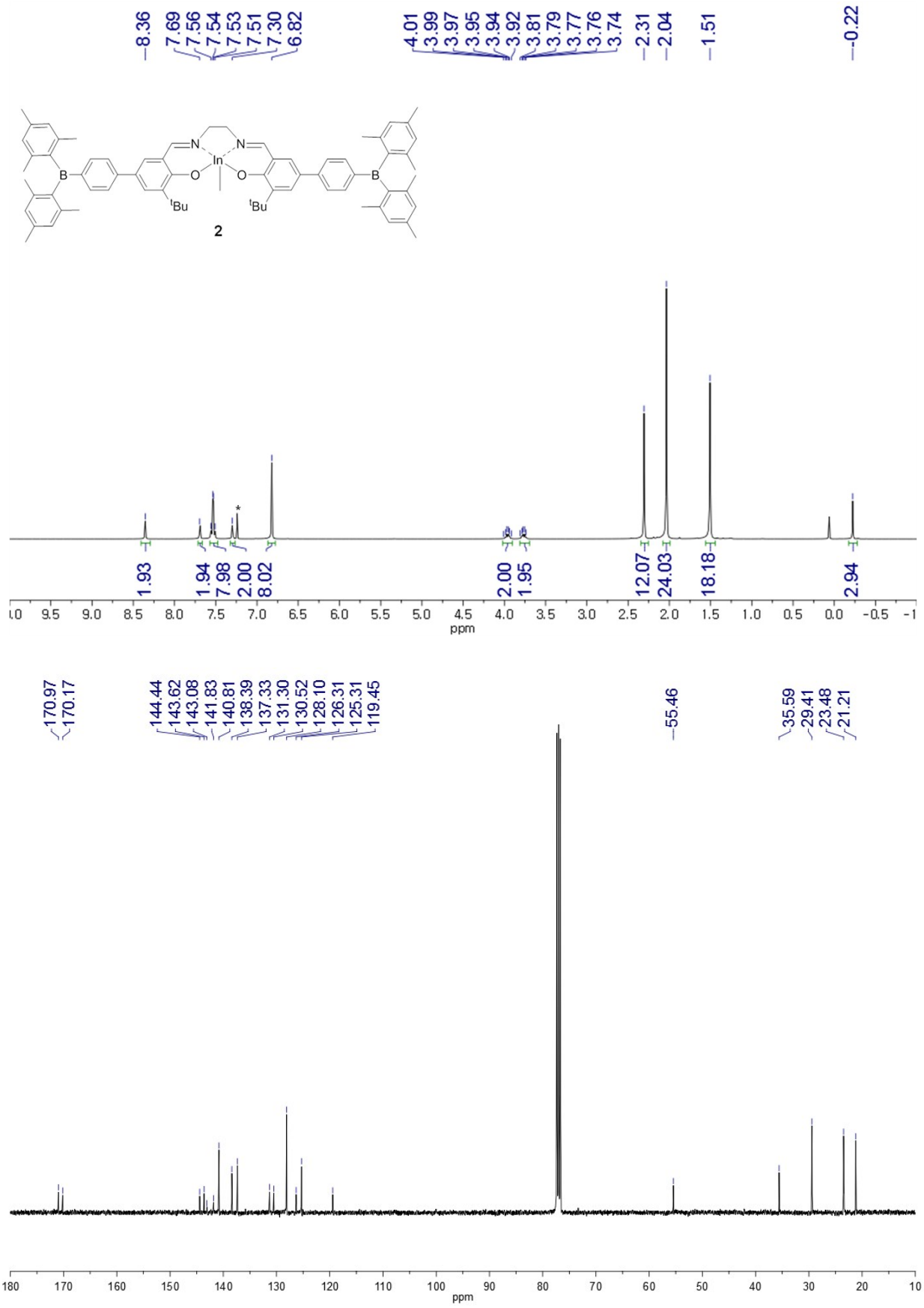

Figure S8. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2** (∗ from residual $CHCl_3$ in $CDCl_3$).

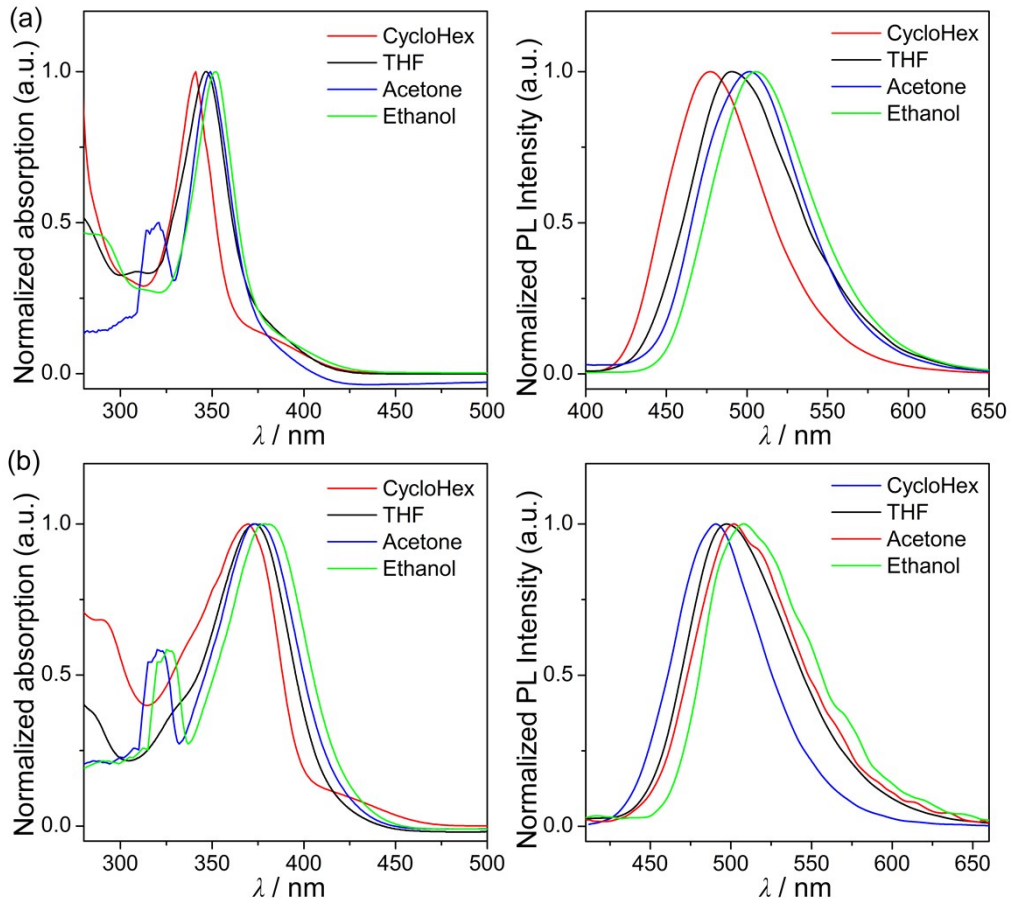

Figure S9. The UV–vis absorption (left) and PL emission (right) spectra of (a) **1** (λ_{ex}= 369 nm) and (b) **2** (λ_{ex} = 374 nm) in various organic solvents at 298 K (2.0×10^{-5} M).

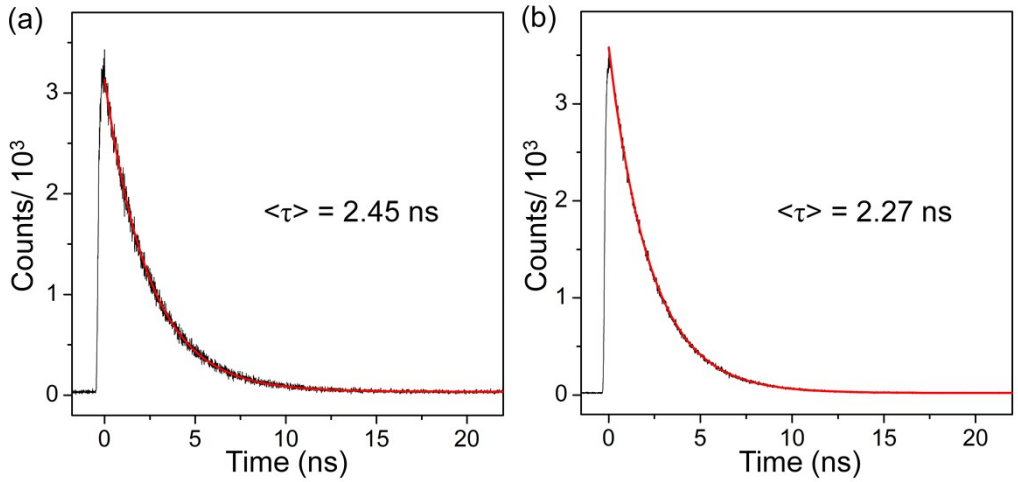

Figure S10. Emission decay curve detected at 500 nm of (a) **1** and (b) **2** in THF (5.0×10^{-5} M) at 298 K (black line). The red-line corresponds to the single-exponential fitting curve (R^2 = 0.9972 and 0.9994) for the experimental curve.

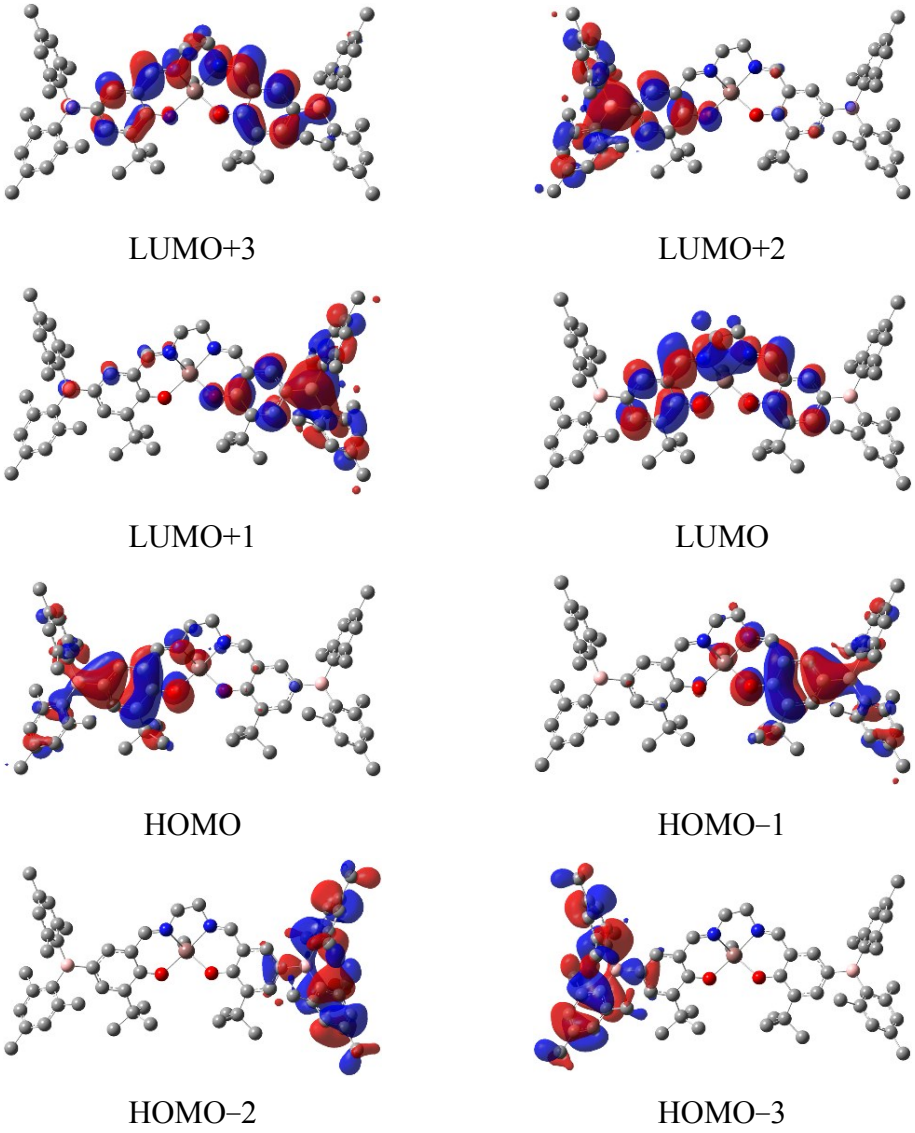

Figure S11. Frontier molecular orbitals of **1** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the ground state (S_0) optimized geometries.

Table S1. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **1** from TD-B3LYP/6-31G(d) calculations in THF at the ground state (S_0) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	368.76	0.1284	HOMO → LUMO (88.8%)
2	358.65	0.0810	HOMO−1 → LUMO (86.8%)
3	339.80	0.9037	HOMO−1 → LUMO+1 (44.7%)
			HOMO−1 → LUMO+3 (11.9%)
4	335.50	0.0853	HOMO−1 → LUMO+1 (13.7%)
			HOMO → LUMO+2 (37.5%)
			HOMO → LUMO+3 (18.3%)
5	330.86	0.0527	HOMO−1 → LUMO+1 (13.2%)
			HOMO−1 → LUMO+3 (48.1%)
			HOMO → LUMO+3 (15.3%)

Table S2. Molecular orbital energies (in eV) and distributions (in %) of **1** at the ground state (S_0) optimized geometries

	E (eV)	salen moiety	In-CH_3	imine bridge	$B(Mes)_2$
LUMO+4	−0.04	1.8	0.0	0.0	98.2
LUMO+3	−1.42	68.2	0.1	23.7	8.0
LUMO+2	−1.44	32.8	0.3	0.4	66.5
LUMO+1	−1.49	32.8	0.4	0.8	66.0
LUMO	−1.72	74.6	1.1	23.5	0.7
HOMO	−5.66	77.6	2.6	5.5	14.3
HOMO−1	−5.70	77.3	3.3	4.4	15.0
HOMO−2	−6.08	4.9	0.0	0.0	95.1
HOMO−3	−6.09	5.0	0.0	0.1	94.9
HOMO−4	−6.17	3.1	0.1	0.1	96.8

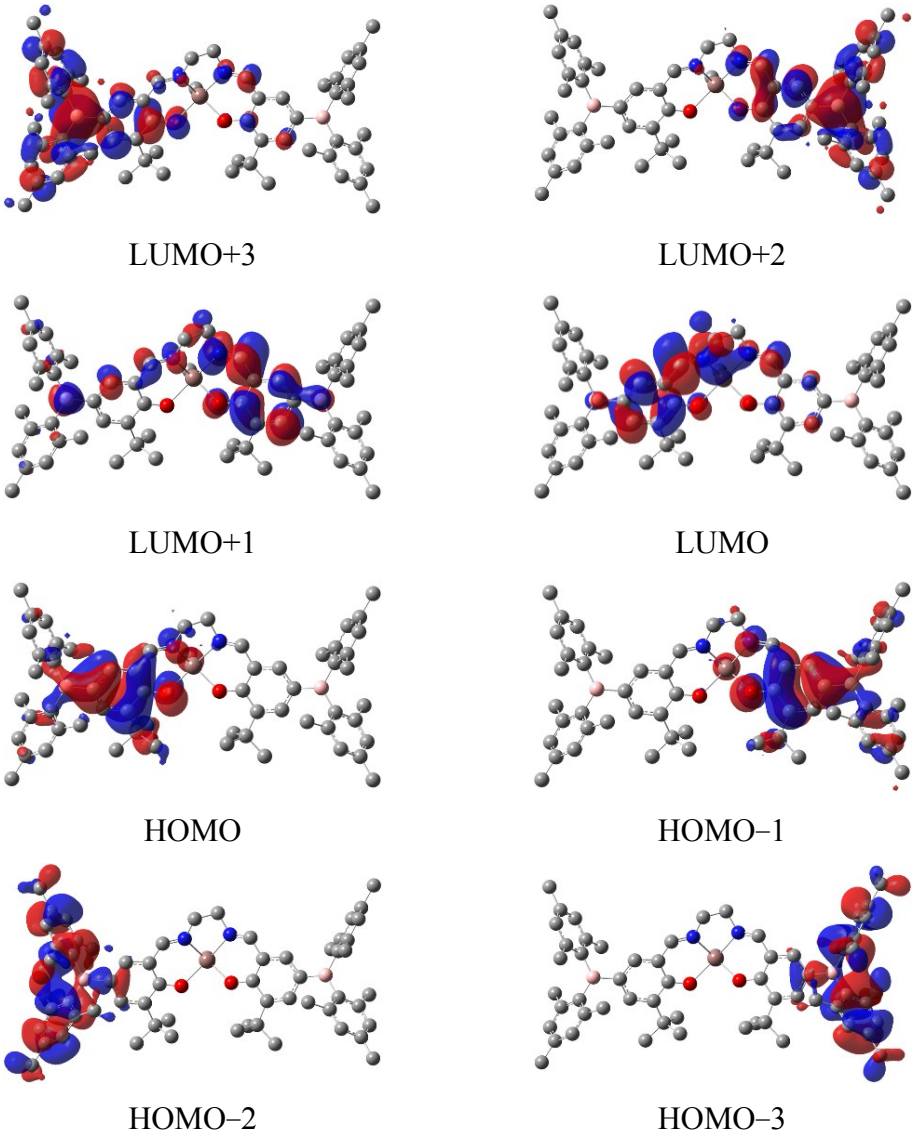

Figure S12. Frontier molecular orbitals of **1** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the first excited state (S_1) optimized geometries.

Table S3. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **1** from TD-B3LYP/6-31G(d) calculations in THF at the first excited state (S_1) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	450.41	0.0953	HOMO → LUMO (98.1%)
2	389.32	0.0277	HOMO–1 → LUMO (96.6%)
3	367.95	0.2035	HOMO → LUMO+1 (80.9%)
			HOMO → LUMO+3 (15.5%)
4	360.84	0.3111	HOMO → LUMO+1 (15.6%)
			HOMO → LUMO+3 (77.8%)
5	353.07	0.0298	HOMO–2 → LUMO (92.8%)

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

	E (eV)	salen moiety	In-CH_3	imine bridge	$B(Mes)_2$
LUMO+4	−0.05	1.8	0.0	0.0	98.2
LUMO+3	−1.44	30.0	0.2	1.9	67.9
LUMO+2	−1.48	30.3	0.3	3.4	66.0
LUMO+1	−1.53	68.3	0.2	19.4	11.9
LUMO	−2.02	71.5	1.4	24.2	3.0
HOMO	−5.37	73.9	2.4	3.8	19.9
HOMO−1	−5.70	78.1	2.8	4.4	14.8
HOMO−2	−6.04	5.0	0.0	0.1	95.0
HOMO−3	−6.08	4.9	0.0	0.0	95.1
HOMO−4	−6.17	2.9	0.1	0.1	96.9

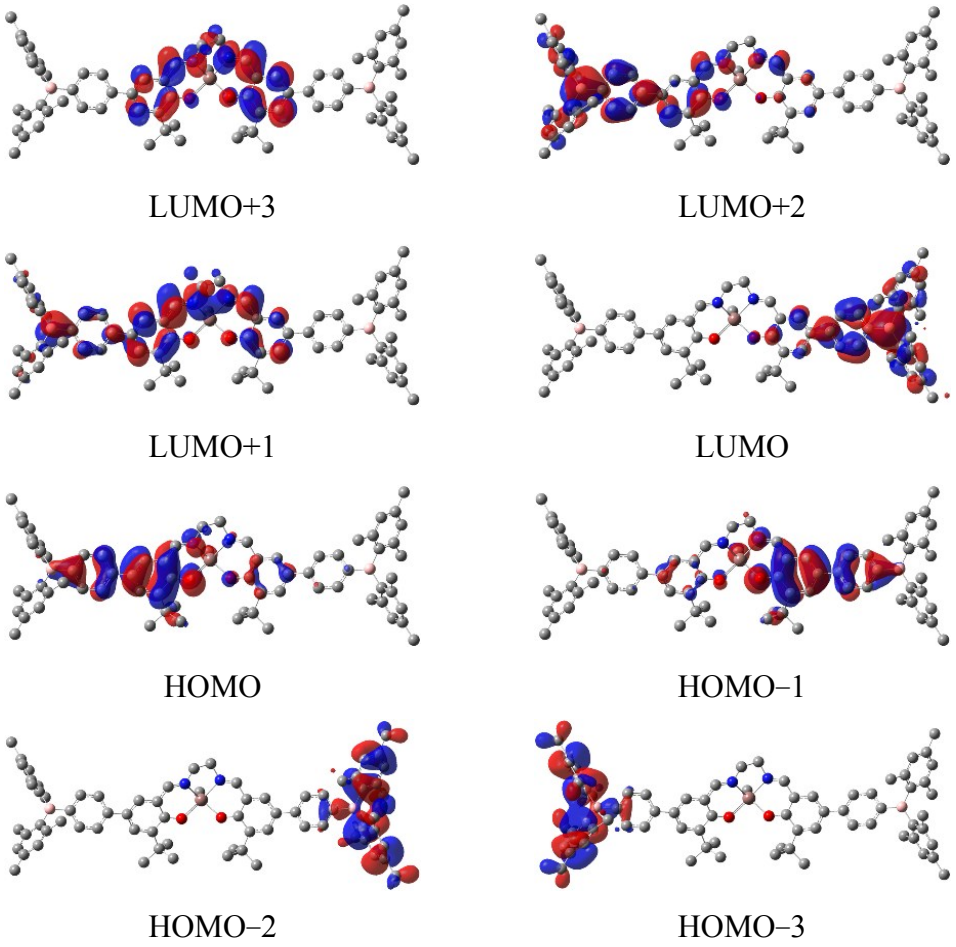

Figure S13. Frontier molecular orbitals of **2** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the ground state (S_0) optimized geometries.

Table S5. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **2** from TD-B3LYP/6-31G(d) calculations in THF at the ground state (S_0) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	397.97	0.3850	HOMO → LUMO+1 (89.8%)
2	387.14	0.2711	HOMO−1 → LUMO (30.2%)
			HOMO−1 → LUMO+1 (46.1%)
			HOMO−1 → LUMO+2 (13.8%)
3	384.07	1.0953	HOMO−1 → LUMO (20.0%)
			HOMO−1 → LUMO+1 (20.7%)
			HOMO → LUMO+2 (50.6%)
4	379.70	0.0802	HOMO−1 → LUMO (32.5%)
			HOMO−1 → LUMO+1 (13.3%)
			HOMO → LUMO+2 (40.5%)
5	362.68	0.0044	HOMO−1 → LUMO (10.0%)
			HOMO → LUMO (86.8%)

Table S6. Molecular orbital energies (in eV) and distributions (in %) of **2** at the ground state (S_0) optimized geometries

	E (eV)	salen + Ph of C5	In-CH_3	imine bridge	B$(Mes)_2$
LUMO+4	−0.31	34.3	0.5	0.0	65.2
LUMO+3	−1.46	75.4	0.1	23.8	0.7
LUMO+2	−1.72	23.8	0.2	3.8	72.2
LUMO+1	−1.75	72.2	0.9	23.6	3.3
LUMO	−1.76	8.1	0.1	0.2	91.5
HOMO	−5.39	72.5	1.6	5.0	21.0
HOMO−1	−5.44	72.3	3.0	4.1	20.6
HOMO−2	−6.12	0.1	0.0	0.0	99.9
HOMO−3	−6.13	0.1	0.0	0.0	100.0
HOMO−4	−6.18	2.0	0.2	0.2	97.6

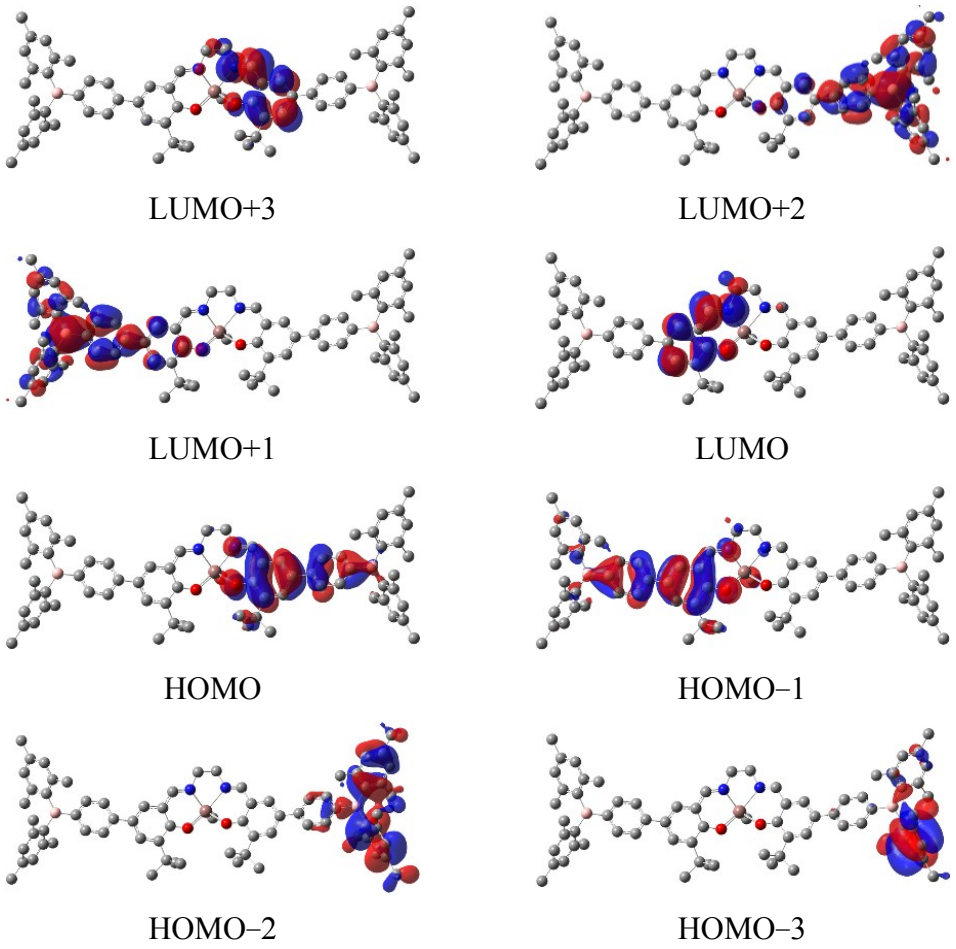

Figure S14. Frontier molecular orbitals of **2** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the first excited state (S_1) optimized geometries.

Table S7. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **2** from TD-B3LYP/6-31G(d) calculations in THF at the first excited state (S_1) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	595.22	0.0038	HOMO → LUMO (99.6%)
2	442.45	0.1323	HOMO–1 → LUMO (94.1%)
3	435.21	0.3738	HOMO → LUMO+1 (53.1%)
			HOMO → LUMO+2 (43.0%)
4	433.93	0.3682	HOMO → LUMO+1 (46.1%)
			HOMO → LUMO+2 (52.1%)
5	383.18	0.1072	HOMO → LUMO+3 (95.7%)

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

	E (eV)	salen + Ph of C5	In-CH_3	imine bridge	$B(Mes)_2$
LUMO+4	–0.41	40.1	0.3	0.0	59.6
LUMO+3	–1.16	74.4	0.3	24.3	1.0
LUMO+2	–1.65	7.1	0.1	0.3	92.6
LUMO+1	–1.83	10.3	0.1	0.0	89.6
LUMO	–2.39	76.2	1.0	22.2	0.6
HOMO	–4.91	74.8	1.1	4.1	20.0
HOMO–1	–5.70	66.6	3.2	5.2	24.9
HOMO–2	–6.04	0.1	0.0	0.0	99.9
HOMO–3	–6.16	0.0	0.0	0.0	100.0
HOMO–4	–6.18	1.4	0.1	0.0	98.5

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

Atom	x	y	z
N	-1.220405	2.213522	0.162517
N	1.402843	2.430724	-0.331615
O	-1.491205	-0.441667	-0.824462
O	1.476640	-0.375269	-0.738333
C	-2.759046	-0.312667	-0.552543
C	-3.676285	-1.393636	-0.828781
C	-5.010599	-1.213186	-0.495872
H	-5.706427	-2.017883	-0.703144
C	-5.563198	-0.037164	0.091431
C	-4.657542	0.992889	0.346400
H	-5.014056	1.915506	0.799542
C	-3.286450	0.889612	0.049000
C	-2.470962	2.014968	0.437034
H	-2.988844	2.767050	1.043837
C	-0.535567	3.364657	0.768071
H	-0.239156	3.094059	1.789450
H	-1.194231	4.239693	0.824745
C	0.730002	3.690699	-0.041901
H	0.448852	4.162378	-0.992368
H	1.370730	4.387331	0.512312
C	2.632307	2.228586	0.004520
H	3.195275	3.060324	0.445143
C	3.366158	0.990162	-0.132959
C	4.742535	1.057648	0.143247
H	5.164048	2.025862	0.405709
C	5.576582	-0.060112	0.100390
C	4.940842	-1.290348	-0.231362
H	5.577917	-2.166498	-0.262062
C	3.592436	-1.443758	-0.522447
C	2.754689	-0.269394	-0.483467
C	-3.181414	-2.702733	-1.482129
C	-2.142410	-3.393074	-0.565342
H	-1.783715	-4.318209	-1.034267
H	-2.594791	-3.659769	0.397945
H	-1.284383	-2.746112	-0.377268
C	-4.329663	-3.708027	-1.710134
H	-3.923957	-4.613661	-2.175059
H	-5.100877	-3.310733	-2.380310
H	-4.810962	-4.007232	-0.771863
C	-2.553307	-2.406945	-2.866512
H	-1.701743	-1.730042	-2.783356
H	-3.293271	-1.952850	-3.537129
H	-2.209919	-3.340625	-3.329723
C	3.000246	-2.826762	-0.873254
C	1.930904	-3.222671	0.174137
H	1.505678	-4.203142	-0.074750
H	1.120074	-2.493572	0.210813
H	2.378491	-3.295578	1.173130
C	2.373325	-2.802761	-2.288949
H	1.972437	-3.793493	-2.537379
H	3.129194	-2.549045	-3.042458
H	1.562028	-2.076581	-2.356166
C	4.072607	-3.936538	-0.871733
H	4.547590	-4.054821	0.109103
H	4.859173	-3.755315	-1.613636
H	3.597241	-4.891464	-1.123385
In	-0.008846	0.951127	-1.254791
C	-0.167690	1.441717	-3.338288
H	-0.113516	0.537140	-3.954528
H	-1.121049	1.936329	-3.557005
H	0.640353	2.112485	-3.651162
B	-7.073458	0.091542	0.441689
B	7.096591	0.038230	0.411031
C	-7.963963	-1.222743	0.551788
C	-9.112953	-1.405400	-0.266615
C	-7.632322	-2.264156	1.460125
C	-9.869149	-2.578729	-0.173938
C	-8.431470	-3.412804	1.542025
C	-9.552963	-3.596174	0.731580
H	-10.733907	-2.699562	-0.824297
H	-8.164572	-4.186882	2.259896
C	-7.686687	1.540650	0.686762
C	-8.249400	1.899041	1.946646
C	-7.672135	2.532864	-0.327344
C	-8.753773	3.184223	2.157531
C	-8.199385	3.810355	-0.079290
C	-8.744023	4.161285	1.153855
H	-9.165276	3.433364	3.134466
H	-8.182889	4.547514	-0.881075
C	7.903612	-1.277579	0.797867
C	7.520522	-2.064253	1.919322
C	9.028944	-1.712138	0.044649
C	8.250114	-3.209842	2.262684
C	9.715980	-2.876918	0.405966
C	9.346662	-3.643759	1.514331
H	7.951233	-3.777391	3.142689
H	10.570242	-3.189487	-0.192283
C	7.804432	1.462765	0.330587
C	7.800807	2.210772	-0.877910
C	8.454642	2.038113	1.457224
C	8.438286	3.457366	-0.941026
C	9.058563	3.296537	1.360293
C	9.071509	4.024167	0.166408
H	8.437301	3.999695	-1.885397
H	9.537495	3.718490	2.242417
C	-6.428420	-2.197943	2.384255
H	-6.589861	-2.825098	3.267675
H	-5.521167	-2.562743	1.887315
H	-6.211910	-1.183751	2.729115
C	-10.412055	-4.833900	0.847295
H	-11.275251	-4.658998	1.503881
H	-10.807440	-5.139900	-0.127691
H	-9.849366	-5.674330	1.267296
C	-9.543779	-0.369186	-1.286159
H	-10.433104	-0.705813	-1.828545
H	-9.780022	0.590275	-0.814499
H	-8.761065	-0.174345	-2.029040
C	7.134469	1.715017	-2.150334
H	6.079676	2.013744	-2.192225
H	7.628211	2.139307	-3.031370
H	7.156223	0.626678	-2.245996
C	8.480321	1.348257	2.806624
H	9.118695	1.892808	3.509736
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H	8.852480	0.321936	2.735197
C	9.771376	5.360259	0.073488
H	10.849269	5.234008	-0.096527
H	9.379627	5.960784	-0.754266
H	9.658142	5.937150	0.998175
C	-8.276463	0.932397	3.113474
H	-8.707149	-0.034045	2.835246
H	-7.266723	0.736094	3.497297
H	-8.863208	1.339873	3.943056
C	-7.165007	2.277464	-1.735639
H	-6.650760	1.321128	-1.837279
H	-7.997111	2.285715	-2.451891
H	-6.469401	3.065394	-2.049549
C	-9.317547	5.536935	1.403210
H	-9.093130	6.219305	0.577093
H	-10.409040	5.499301	1.515969
H	-8.918004	5.976913	2.324938
C	6.336992	-1.710639	2.803525
H	6.202509	-0.632447	2.923051
H	5.398682	-2.100557	2.390319
H	6.460278	-2.145880	3.801052
C	9.505134	-0.972298	-1.189632
H	8.777136	-1.041998	-2.008131
H	9.665195	0.091924	-0.994200
H	10.445392	-1.395010	-1.557986
C	10.095092	-4.904884	1.878534
H	9.657564	-5.783197	1.384564
H	11.144865	-4.850981	1.570460
H	10.063901	-5.092619	2.957245

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

Atom	x	y	z
N	-1.169104	2.302381	0.351859
N	1.449486	2.563238	-0.113988
O	-1.495065	-0.329690	-0.766496
O	1.438456	-0.214723	-0.675103
C	-2.753064	-0.225611	-0.497464
C	-3.666232	-1.275837	-0.918410
C	-5.020825	-1.171698	-0.542552
H	-5.708233	-1.958625	-0.823265
C	-5.534081	-0.081518	0.163599
C	-4.605259	0.957742	0.541154
H	-4.997280	1.812294	1.088636
C	-3.254388	0.921733	0.258797
C	-2.411580	1.997862	0.761971
H	-2.877298	2.645334	1.506030
C	-0.487049	3.366439	1.079356
H	-0.196428	3.019572	2.084779
H	-1.145269	4.238199	1.216187
C	0.787269	3.784956	0.324391
H	0.518861	4.377988	-0.559195
H	1.433694	4.396029	0.966850
C	2.675531	2.304027	0.206642
H	3.252493	3.078588	0.725719
C	3.379243	1.064711	-0.040417
C	4.761990	1.076143	0.209470
H	5.214732	2.012974	0.528465
C	5.564850	-0.058587	0.075769
C	4.891100	-1.246632	-0.327198
H	5.502545	-2.135346	-0.430876
C	3.533065	-1.343411	-0.597804
C	2.726711	-0.154977	-0.456137
C	-3.158084	-2.487319	-1.711900
C	-2.115944	-3.272671	-0.871469
H	-1.777027	-4.149159	-1.436988
H	-2.562737	-3.628624	0.064547
H	-1.249269	-2.656143	-0.631702
C	-4.294200	-3.469643	-2.068182
H	-3.874710	-4.300941	-2.645177
H	-5.069883	-2.999812	-2.683454
H	-4.770270	-3.895752	-1.178034
C	-2.518115	-2.021476	-3.046715
H	-1.670085	-1.357332	-2.876845
H	-3.254960	-1.497659	-3.667073
H	-2.167857	-2.896185	-3.607703
C	2.894545	-2.684666	-1.022339
C	1.851983	-3.125345	0.034435
H	1.387260	-4.072895	-0.266571
H	1.067194	-2.376857	0.154365
H	2.333196	-3.282819	1.007821
C	2.220015	-2.548550	-2.409397
H	1.778841	-3.508015	-2.707698
H	2.957351	-2.268259	-3.171941
H	1.431538	-1.794793	-2.397930
C	3.937165	-3.816791	-1.134289
H	4.436836	-4.017262	-0.179568
H	4.706109	-3.599037	-1.884721
H	3.430686	-4.739526	-1.439870
In	-0.008581	1.201111	-1.091905
C	-0.245701	1.628553	-3.185547
H	-0.085952	0.725141	-3.783745
H	-1.253100	2.003294	-3.396712
H	0.476538	2.385838	-3.509976
B	-7.072524	0.015378	0.461071
B	7.087592	-0.025362	0.378867
C	-7.882009	-1.331798	0.651530
C	-9.027896	-1.624752	-0.140837
C	-7.475808	-2.298930	1.610907
C	-9.703932	-2.838153	0.021781
C	-8.197241	-3.489544	1.761694
C	-9.312378	-3.784844	0.974362
H	-10.564472	-3.048653	-0.610900
H	-7.878643	-4.205985	2.517115
C	-7.752457	1.440760	0.559293
C	-8.535038	1.808905	1.690394
C	-7.604073	2.401087	-0.482111
C	-9.106656	3.084070	1.765334
C	-8.216094	3.654955	-0.379406
C	-8.963916	4.025317	0.741726
H	-9.686157	3.347789	2.648258
H	-8.106417	4.361906	-1.199819
C	7.856675	-1.388621	0.671577
C	7.459637	-2.230809	1.746779
C	8.962315	-1.809423	-0.117581
C	8.158634	-3.415603	2.013213
C	9.618549	-3.012786	0.165974
C	9.236397	-3.834318	1.230058
H	7.849750	-4.027321	2.859527
H	10.458270	-3.312445	-0.459001
C	7.842371	1.377381	0.393579
C	7.863431	2.204556	-0.761859
C	8.514636	1.852962	1.553465
C	8.548140	3.427621	-0.744852
C	9.165854	3.091082	1.537920
C	9.205111	3.895069	0.394439
H	8.566159	4.031285	-1.651027
H	9.661199	3.434979	2.444540
C	-6.279711	-2.093268	2.524136
H	-6.401907	-2.664146	3.450906
H	-5.350105	-2.433381	2.051767
H	-6.130636	-1.044826	2.798524
C	-10.089554	-5.066199	1.164047
H	-10.972117	-4.904179	1.797636
H	-10.449665	-5.461618	0.207790
H	-9.479417	-5.837169	1.645949
C	-9.532085	-0.675473	-1.210493
H	-10.420283	-1.084900	-1.701989
H	-9.794928	0.303194	-0.797417
H	-8.779229	-0.502328	-1.989598
C	7.172149	1.822132	-2.059688
H	6.125539	2.150941	-2.066803
H	7.668901	2.296787	-2.912932
H	7.162823	0.743501	-2.234817
C	8.513244	1.076877	2.855510
H	9.174767	1.547607	3.589900
H	7.510487	1.039017	3.300579
H	8.841246	0.042353	2.717382
C	9.955596	5.206658	0.387941
H	11.034476	5.047414	0.256633
H	9.620110	5.856063	-0.427464
H	9.824964	5.748045	1.331838
C	-8.759065	0.872496	2.862389
H	-9.308804	-0.026555	2.566590
H	-7.815284	0.536783	3.307929
H	-9.331330	1.373102	3.649843
C	-6.823544	2.104104	-1.747747
H	-5.745177	2.053469	-1.554241
H	-7.109762	1.148254	-2.199755
H	-6.987293	2.886835	-2.495327
C	-9.579073	5.400315	0.852694
H	-9.810676	5.816580	-0.133474
H	-10.501887	5.380661	1.442448
H	-8.893713	6.101719	1.347881
C	6.293150	-1.898973	2.661343
H	6.194328	-0.827353	2.852662
H	5.340605	-2.229892	2.229930
H	6.407639	-2.403158	3.627005
C	9.448931	-1.009129	-1.309272
H	8.704777	-0.993019	-2.115858
H	9.657968	0.032116	-1.046700
H	10.363953	-1.444845	-1.723317
C	9.951450	-5.135728	1.510237
H	9.504919	-5.964565	0.944071
H	11.007601	-5.082524	1.224261
H	9.897111	-5.402864	2.571059

Table S11. Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **2** from B3LYP calculations (in Å)

Atom	x	y	z
N	-1.242990	2.050307	-0.238527
N	1.379943	2.315744	-0.716434
O	-1.487782	-0.564102	-1.333588
O	1.473980	-0.473759	-1.200845
C	-2.760389	-0.451742	-1.058448
C	-3.670580	-1.523952	-1.380499
C	-5.011743	-1.364407	-1.058778
H	-5.705473	-2.150708	-1.329899
C	-5.555502	-0.220495	-0.420939
C	-4.672164	0.798914	-0.101513
H	-5.027153	1.682684	0.422689
C	-3.297879	0.716197	-0.410619
C	-2.491624	1.828882	0.028443
H	-3.014447	2.550082	0.667698
C	-0.570655	3.182871	0.414017
H	-0.271070	2.874725	1.423831
H	-1.238651	4.047878	0.505851
C	0.691193	3.555304	-0.381724
H	0.404147	4.057699	-1.314597
H	1.321976	4.239863	0.198569
C	2.610573	2.116046	-0.382842
H	3.162169	2.938581	0.088685
C	3.356336	0.889803	-0.559520
C	4.733867	0.965508	-0.269627
H	5.140412	1.924172	0.043003
C	5.559508	-0.146121	-0.347047
C	4.950624	-1.373015	-0.707069
H	5.597181	-2.238370	-0.782685
C	3.599593	-1.526975	-0.992554
C	2.753988	-0.361171	-0.936784
C	-3.168881	-2.804140	-2.083332
C	-2.124825	-3.520058	-1.191784
H	-1.761776	-4.425624	-1.694168
H	-2.574529	-3.823434	-0.238274
H	-1.271115	-2.874206	-0.982208
C	-4.308959	-3.809301	-2.348711
H	-3.895014	-4.696401	-2.840962
H	-5.080185	-3.397055	-3.009949
H	-4.791288	-4.142547	-1.422312
C	-2.542407	-2.451359	-3.454965
H	-1.698680	-1.768503	-3.344942
H	-3.286552	-1.981750	-4.110047
H	-2.187932	-3.363889	-3.950722
C	3.020928	-2.909347	-1.366920
C	1.949867	-3.325277	-0.328689
H	1.529325	-4.303221	-0.594693
H	1.137086	-2.598972	-0.284020
H	2.394633	-3.412293	0.670354
C	2.399332	-2.868607	-2.784395
H	2.004337	-3.857775	-3.047866
H	3.156668	-2.600654	-3.531441
H	1.585074	-2.145140	-2.843085
C	4.099602	-4.012851	-1.375113
H	4.574392	-4.136817	-0.394748
H	4.884941	-3.822249	-2.116118
H	3.629528	-4.968125	-1.634810
In	-0.013739	0.849156	-1.697632
C	-0.153319	1.423943	-3.762115
H	-0.137677	0.541750	-4.412178
H	-1.085057	1.966213	-3.960803
H	0.681929	2.071558	-4.051787
C	7.009358	-0.062417	-0.056819
C	7.702480	-1.136255	0.536914
C	7.746904	1.099073	-0.361602
C	9.066578	-1.052643	0.796694
H	7.161394	-2.036283	0.815388
C	9.104131	1.184482	-0.070501
H	7.251631	1.933855	-0.850024
C	9.815950	0.110168	0.509144
H	9.566525	-1.902984	1.253425
H	9.636481	2.100164	-0.313897
C	-6.999203	-0.128479	-0.105821
C	-7.666141	1.113281	-0.103983
C	-7.758420	-1.273931	0.206883
C	-9.021769	1.200169	0.191961
H	-7.119829	2.014621	-0.367836
C	-9.111195	-1.175952	0.515500
H	-7.275525	-2.246636	0.237628
C	-9.794081	0.061476	0.516484
H	-9.502313	2.174559	0.167682
H	-9.657879	-2.080561	0.768280
B	11.349192	0.206605	0.819874
B	-11.320781	0.167835	0.857543
C	12.187942	-1.131730	0.987368
C	12.905787	-1.403386	2.185300
C	12.231417	-2.109530	-0.042804
C	13.612633	-2.601908	2.328973
C	12.975526	-3.284366	0.129095
C	13.671033	-3.556289	1.308592
H	14.138078	-2.793173	3.263128
H	13.008056	-4.008423	-0.683523
C	12.014528	1.643471	0.948365
C	13.057424	2.050616	0.065467
C	11.572551	2.581697	1.916387
C	13.600053	3.333989	0.157852
C	12.152339	3.858280	1.984293
C	13.163977	4.259691	1.114670
H	14.385327	3.622927	-0.538996
H	11.799301	4.553438	2.744800
C	-12.115490	1.470346	0.416028
C	-12.725356	2.311154	1.392762
C	-12.210402	1.867803	-0.942001
C	-13.373473	3.486179	1.007123
C	-12.884602	3.049158	-1.290084
C	-13.470410	3.876730	-0.335042
H	-13.815050	4.118858	1.775503
H	-12.949355	3.323910	-2.342001
C	-12.025441	-1.024348	1.634493
C	-13.117032	-1.726307	1.042638
C	-11.584021	-1.456440	2.911188
C	-13.703152	-2.806829	1.704162
C	-12.210583	-2.538651	3.550020
C	-13.268207	-3.231899	2.966583
H	-14.523182	-3.336439	1.221709
H	-11.855601	-2.841952	4.533924
C	11.502381	-1.943904	-1.365088
H	12.005630	-2.513568	-2.153713
H	10.471853	-2.313531	-1.301458
H	11.443819	-0.902581	-1.691876
C	14.481342	-4.821518	1.468522
H	14.127739	-5.611103	0.797200
H	15.540839	-4.646707	1.237067
H	14.435645	-5.199548	2.495926
C	12.905145	-0.441334	3.357257
H	13.496481	-0.841985	4.186758
H	13.324577	0.532446	3.084113
H	11.892545	-0.257880	3.736047
C	10.526933	2.257369	2.967455
H	9.992442	1.328209	2.764855
H	10.993088	2.161691	3.957030
H	9.784852	3.061198	3.042781
C	13.579100	1.143476	-1.031152
H	13.864111	0.158933	-0.648923
H	12.825254	0.978758	-1.812053
H	14.454560	1.585935	-1.517115
C	13.776542	5.638608	1.194910
H	14.851643	5.586000	1.408691
H	13.667441	6.180087	0.246835
H	13.307596	6.239034	1.980869
C	-11.669703	1.034723	-2.089717
H	-12.492144	0.568942	-2.648641
H	-11.117143	1.660354	-2.800781
H	-11.003439	0.236163	-1.760232
C	-12.659894	1.994045	2.873888
H	-13.189217	2.754835	3.456382
H	-13.108228	1.021766	3.102690
H	-11.626347	1.962902	3.239974
C	-14.188534	5.148454	-0.722609
H	-15.250403	5.106900	-0.448112
H	-13.762251	6.020149	-0.210626
H	-14.128781	5.328585	-1.800662
C	-10.486694	-0.756474	3.691855
H	-9.911766	-0.054783	3.086152
H	-10.912363	-0.194693	4.533862
H	-9.785491	-1.483705	4.118184
C	-13.653891	-1.361979	-0.327482
H	-14.028244	-0.333403	-0.357309
H	-12.883703	-1.443519	-1.103761
H	-14.475005	-2.027939	-0.611200
C	-13.930560	-4.398349	3.662144
H	-14.989132	-4.192542	3.866211
H	-13.896808	-5.303965	3.043700
H	-13.443717	-4.624096	4.616234

Table S12. Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **2** from B3LYP calculations (in Å)

Atom	x	y	z
N	-1.209116	1.924379	-1.499086
N	1.452865	1.983495	-1.767805
O	-1.441859	-0.964232	-1.376511
O	1.496030	-0.757959	-1.140954
C	-2.747208	-0.754842	-1.146503
C	-3.630573	-1.864767	-1.042426
C	-4.980417	-1.639005	-0.726198
H	-5.662299	-2.477201	-0.675920
C	-5.504335	-0.345532	-0.520094
C	-4.641288	0.737732	-0.652796
H	-5.011181	1.745690	-0.477831
C	-3.263616	0.591541	-0.970075
C	-2.493646	1.785903	-1.052197
H	-3.010246	2.706910	-0.774893
C	-0.572923	3.206938	-1.259956
H	-0.391545	3.370360	-0.183640
H	-1.196027	4.047154	-1.606814
C	0.778401	3.259110	-1.991591
H	0.610523	3.354894	-3.071969
H	1.383814	4.110383	-1.656025
C	2.641298	1.940998	-1.301401
H	3.190785	2.871369	-1.114201
C	3.370781	0.713064	-0.975365
C	4.712469	0.846663	-0.685062
H	5.155813	1.836354	-0.714880
C	5.511595	-0.261015	-0.311639
C	4.886541	-1.532116	-0.222036
H	5.511523	-2.373507	0.041546
C	3.550392	-1.752159	-0.487494
C	2.730204	-0.600935	-0.892521
C	-3.120885	-3.308944	-1.265837
C	-2.064659	-3.667631	-0.193822
H	-1.680633	-4.683629	-0.358202
H	-2.509153	-3.636520	0.809099
H	-1.229121	-2.967363	-0.223139
C	-4.247041	-4.359499	-1.159992
H	-3.825678	-5.356854	-1.334063
H	-5.033972	-4.199023	-1.906341
H	-4.713973	-4.368724	-0.168293
C	-2.506723	-3.451246	-2.679612
H	-1.679769	-2.753648	-2.819821
H	-3.263110	-3.252543	-3.449579
H	-2.134350	-4.472988	-2.833086
C	2.925431	-3.149095	-0.362238
C	1.834318	-3.124721	0.739691
H	1.394006	-4.123652	0.835832
H	1.036505	-2.419100	0.504893
H	2.268570	-2.853089	1.709037
C	2.312263	-3.592158	-1.715903
H	1.908977	-4.605917	-1.613393
H	3.077105	-3.612700	-2.501208
H	1.504067	-2.932847	-2.033747
C	3.968352	-4.212203	0.041003
H	4.424532	-3.998810	1.014366
H	4.766289	-4.314462	-0.703543
H	3.468338	-5.182874	0.120836
In	-0.115465	0.298110	-2.234931
C	0.298127	-0.142114	-4.295201
H	0.719691	-1.147388	-4.406700
H	-0.618617	-0.096440	-4.894179
H	1.013082	0.573118	-4.717271
C	6.938331	-0.093421	-0.016216
C	7.603812	-0.956044	0.882868
C	7.688700	0.938490	-0.622825
C	8.956529	-0.792005	1.152484
H	7.051569	-1.737868	1.393875
C	9.038447	1.097180	-0.335466
H	7.218281	1.598839	-1.344260
C	9.715482	0.238353	0.556833
H	9.439588	-1.471388	1.848993
H	9.588286	1.900516	-0.817455
C	-6.930946	-0.149139	-0.174670
C	-7.635507	1.005960	-0.575367
C	-7.644961	-1.108256	0.574327
C	-8.967416	1.197344	-0.226901
H	-7.130489	1.751399	-1.183153
C	-8.985675	-0.924246	0.892861
H	-7.129614	-1.997345	0.926512
C	-9.696692	0.238479	0.514553
H	-9.468950	2.105917	-0.550472
H	-9.498305	-1.690620	1.468625
B	11.252801	0.422730	0.874757
B	-11.197168	0.451740	0.899341
C	12.102197	-0.856624	1.247609
C	12.841934	-0.920220	2.460918
C	12.135920	-1.990275	0.389180
C	13.560097	-2.076775	2.785817
C	12.891561	-3.114972	0.737714
C	13.608143	-3.184843	1.935581
H	14.102907	-2.109591	3.728635
H	12.919304	-3.961708	0.053818
C	11.865428	1.877966	0.801685
C	12.989541	2.161982	-0.024099
C	11.298232	2.950620	1.542338
C	13.488503	3.466202	-0.105877
C	11.848973	4.234788	1.456376
C	12.940049	4.519582	0.632334
H	14.335524	3.664010	-0.760234
H	11.411015	5.035225	2.050210
C	-12.070931	-0.804448	1.332151
C	-12.275921	-1.908589	0.465861
C	-12.649061	-0.873125	2.633313
C	-13.026819	-3.015666	0.892602
C	-13.376800	-1.998404	3.025445
C	-13.585375	-3.085655	2.166755
H	-13.174522	-3.844987	0.202111
H	-13.791942	-2.031506	4.031588
C	-11.809393	1.918632	0.851202
C	-11.276674	2.978836	1.629406
C	-12.901568	2.222363	-0.012841
C	-11.819732	4.270065	1.536618
C	-13.404247	3.523262	-0.087027
C	-12.881782	4.568168	0.685792
H	-11.393502	5.061870	2.151258
H	-14.226607	3.730626	-0.769970
C	11.392155	-2.037083	-0.934155
H	11.859607	-2.760207	-1.610484
H	10.348611	-2.345240	-0.797490
H	11.373383	-1.070763	-1.446708
C	14.430058	-4.403702	2.282990
H	13.959794	-5.322134	1.914991
H	15.429281	-4.349246	1.830107
H	14.568292	-4.498476	3.365025
C	12.850812	0.218410	3.462513
H	13.500768	-0.018650	4.310567
H	13.204360	1.152680	3.016293
H	11.849750	0.415235	3.866250
C	10.109518	2.767202	2.469857
H	9.159788	2.829687	1.925081
H	10.117868	1.802219	2.985310
H	10.098141	3.550108	3.235211
C	13.663953	1.097581	-0.868281
H	14.055466	0.279600	-0.255653
H	12.975322	0.651115	-1.595954
H	14.498404	1.525897	-1.432223
C	13.528743	5.909006	0.563265
H	14.390999	6.007355	1.236548
H	13.881564	6.144588	-0.446793
H	12.797414	6.668980	0.857398
C	-12.464188	0.238087	3.647704
H	-12.853152	1.193376	3.280221
H	-12.981683	0.000055	4.582605
H	-11.406342	0.396687	3.890419
C	-11.772178	-1.944853	-0.965393
H	-11.294745	-2.906833	-1.187122
H	-12.606032	-1.834044	-1.671186
H	-11.049798	-1.156817	-1.181876
C	-14.394381	-4.282055	2.611325
H	-15.451187	-4.019545	2.751588
H	-14.348250	-5.091186	1.875420
H	-14.034807	-4.675128	3.570092
C	-13.529303	1.172216	-0.908278
H	-12.804430	0.750668	-1.615273
H	-13.934516	0.334895	-0.330641
H	-14.346171	1.603122	-1.495995
C	-10.161864	2.786865	2.641473
H	-10.558003	2.832401	3.664657
H	-9.646235	1.832312	2.530219
H	-9.414237	3.584344	2.555049
C	-13.464600	5.960079	0.606331
H	-14.439671	6.012540	1.108880
H	-12.808670	6.696100	1.082431
H	-13.625140	6.268939	-0.433323

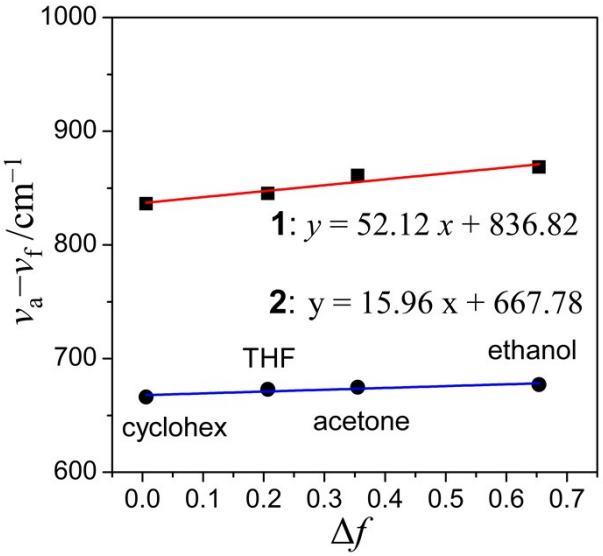

Figure S15. Lippert–Mataga plots for **1** and **2** in solvents with different polarity (ν_a: absorbance wavenumber, ν_b: fluorescence wavenumber, Δf : orientation polarizability, the red-line is the linear fitting for **1** and the blue-line is for **2**).

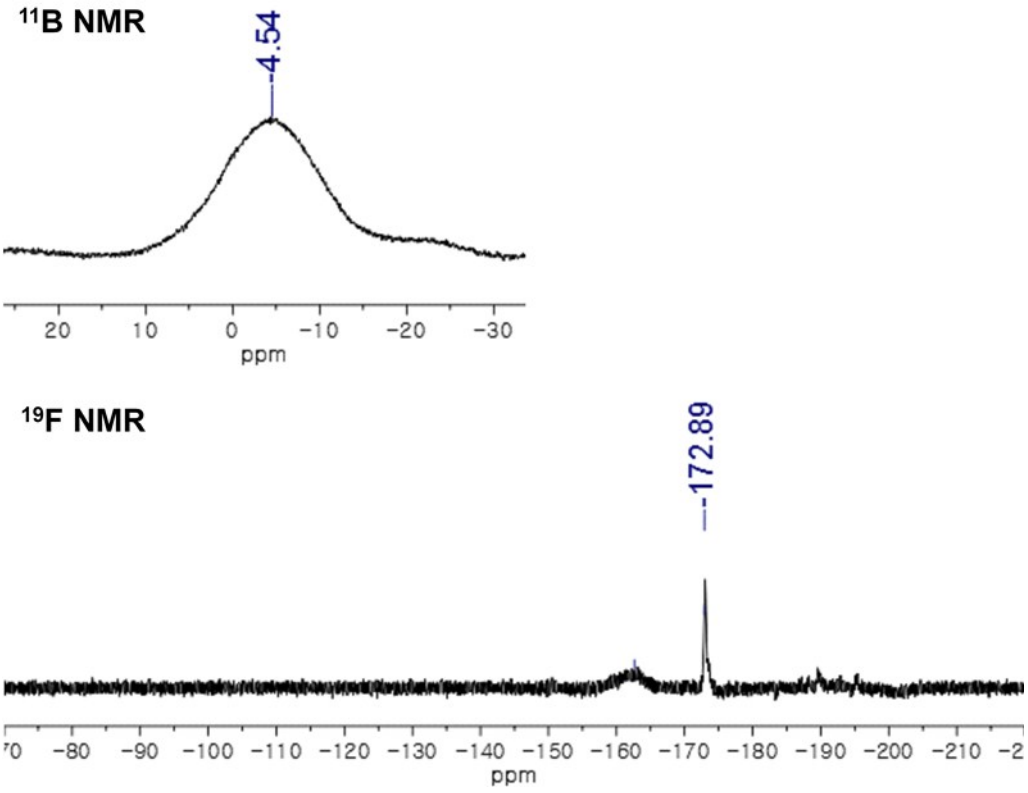

Figure S16. ^{11}B and ^{19}F NMR spectra of **1** with 1.0 equiv. of TBAF in THF-d^8.