Electronic Supplementary Information

Salen–Al/Carbazole Dyad-Based Guest–Host Assembly: Enhancement of Luminescence Efficiency via Intramolecular Energy Transfer

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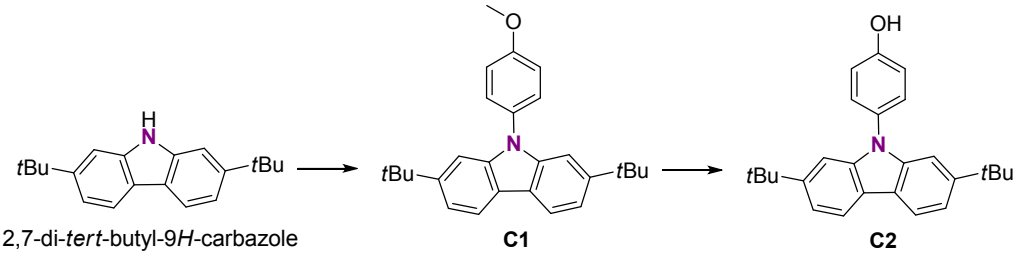
Contents

Experimental section

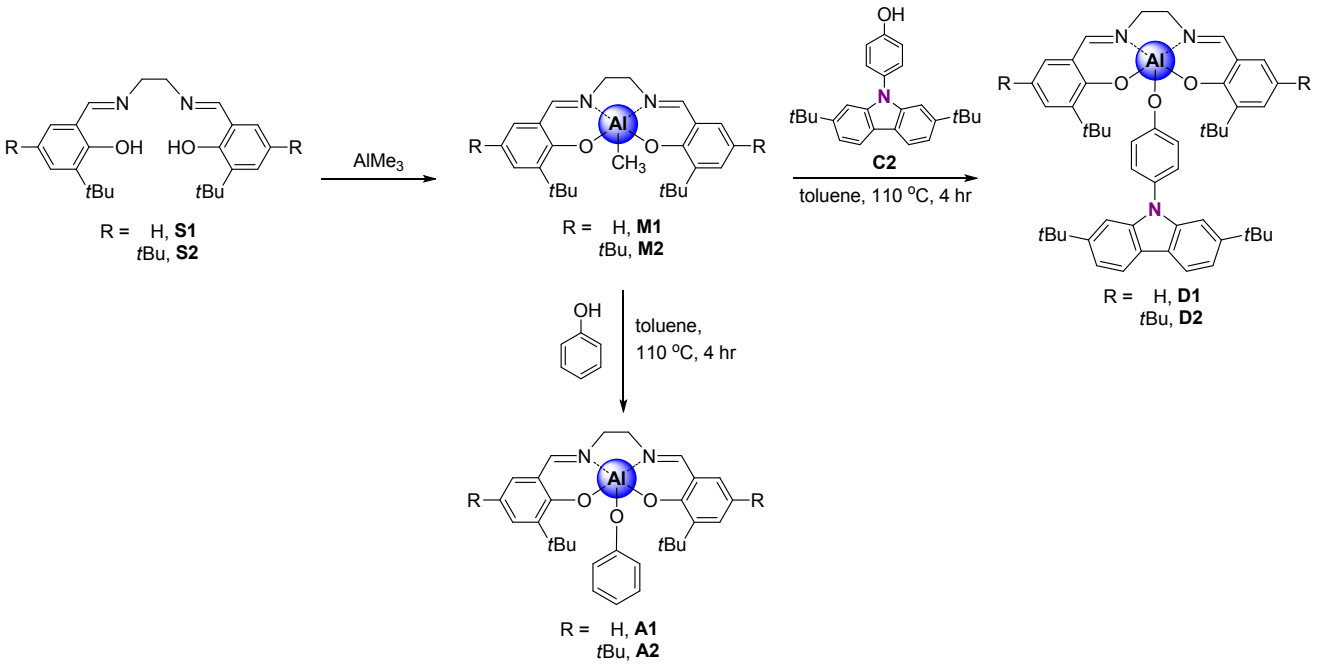
General considerations. All manipulations were carried out under an inert N_2 atmosphere using standard Schlenk and glove box techniques. All anhydrous grade solvents (dichloromethane, dimethylacetamide, toluene) purchased from Aldrich were dried by passing them via an activated alumina column and stored over activated molecular sieves (5Å). Spectrophotometric grade tetrahydrofuran (THF) (Merck) was used as received. Commercial reagents were used without any further purification after purchasing from Aldrich (1-iodo-4-methoxybenzene, cuprous oxide (Cu_2O), boron tribromide (BBr_3), trimethylaluminum ($AlMe_3$, 2.0 M in toluene), 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde, 3-*tert*-butyl-2-hydroxybenzaldehyde). 2,7-di-*tert*-butyl-9*H*-carbazole,[1] salen ligands (**S1** and **S2**),[2] and aluminum mononuclear complexes (**A1** and **A2**)[3] were prepared according to modified literature procedures. Deuterated solvent (chloroform-*d*[1]) from Cambridge Isotope Laboratories were used after drying over activated molecular sieves (5 Å). NMR spectra were recorded on a Bruker Avance 400 spectrometer (400.13 MHz for ^1H and 100.62 MHz for ^{13}C) at ambient temperature. Chemical shifts are given in ppm, and are referenced against external Me_4Si (^1H, ^{13}C). Elemental analyses were performed on an EA3000 (Eurovector). HRMS measurements were measured by using a model of JEOL JMS700. UV/Vis absorption and PL spectra were recorded on a Jasco V-530 and a Fluoromax-4P (HORIBA) spectrophotometer, respectively. Fluorescence decay lifetimes were measured using a time-correlated single-photon counting (TCSPC) spectrometer (FLS920–EDINBURGH Instruments) equipped with a EPL-375ps pulsed semiconductor diode laser as an excitation source and a microchannel plate photomultiplier tube (MCP-PMT, 200−850 nm) as a detector at 298 K.



Synthesis of 2,7-di-*tert*-butyl-9-(4-methoxyphenyl)-9*H*-carbazole (C1). 2,7-di-tert-butyl-9*H*-carbazole (6.3 g, 22.2 mmol) 1-iodo-4-methoxybenzene (5.2 g, 22.1 mmol) and cuprous oxide (6.6 g, 45.8 mmol) were added to dimethylacetamide of 50 mL in a 2-neck Schlenck flask. After being stirred at 170 °C for 24 h, the reaction mixture was cooled to ambient temperature and filtered. The filtrate was concentrated under reduced pressure. And then, the crude product was poured into a mixture solvent of methanol and water (1:1, v/v). The resulting solid was collected by filtration and dried *in vacuo* to afford **C1** as a white solid (5.8 g, 68%). ^1H NMR ($CDCl_3$): δ 7.99 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.8

Hz, 2H), 7.30 (dd, J = 8.0, 8.4 Hz, 2H), 7.14 (d, J = 1.2 Hz, 2H), 7.12 (d, J = 8.8 Hz, 2H), 3.93 (s, 3H, OCH_3), 1.35 (s, 18H, *tert*-butyl). ^{13}C NMR ($CDCl_3$): δ 158.56, 148.98, 141.77, 130.58, 128.60, 120.66, 119.38, 117.50, 115.02, 105.86, 55.53 (OCH_3), 35.13 (*tert*-butyl), 31.76 (*tert*-butyl). HRMS m/z Calcd. for $C_{27}H_{31}NO$: 385.2406. Found: 385.2406.

Synthesis of 4-(2,7-di-*tert*-butyl-9*H*-carbazol-9-yl)phenol (C2). To a solution of **C2** (5.8 g, 15.1 mmol) in dichloromethane (100 mL), a boron tribromide (1.43 mL, 15.1 mmol) was added slowly during 1 h at 0 °C. After being stirred at 0 °C for 30 min, the reaction mixture was allowed to warm up to ambient temperature. Stirring was continued for 10 h, and then saturated NH_4Cl aqueous solution (30 mL) was added to the reaction mixture for quenching the reaction. The resulting mixture was extracted with dichloromethane (30 mL × 3) and the organic phases were dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified by silica-gel column chromatography (hexane/DCM = 10/1, v/v), affording as a white solid **C2** (5.3 g, 80%). ^{1}H NMR ($CDCl_3$): δ 7.99 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 9.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.26 (br s, 2H), 7.05 (d, J = 8.5 Hz, 2H), 1.36 (s, 18H, *tert*-butyl). ^{13}C NMR ($CDCl_3$): δ 154.54, 149.07, 141.76, 130.80, 128.88, 120.68, 119.44, 117.60, 116.62, 105.86, 35.16 (*tert*-butyl), 31.78 (*tert*-butyl). HRMS m/z Calcd. for $C_{26}H_{29}NO$: 371.2249 Found: 371.2250.



Synthesis of D1. The **S1** (0.19 g, 0.5 mmol) was dissolved in toluene (10 mL). $AlMe_3$ (0.28 mL, 0.55 mmol) was added to **S1** in toluene solution at −78 °C. Then, the mixture was slowly heated to 110 °C and refluxed for 1 h. After cooling to ambient temperature, **C2** (0.18 g, 0.5 mmol) in toluene (20 mL) was added to the mixture and it was refluxed for 4 h at 110 °C. After cooling to ambient temperature, all

the volatiles were removed under reduced pressure. The residue was washed with *n*-hexane (50 mL) and the desired **D1** was obtained as a yellow solid (0.25 g, 68%). ^{1}H NMR ($CDCl_3$): δ 8.45 (s, 2H), 7.91 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 7.6 Hz, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 7.6 Hz, 2H), 7.12 (s, 2H), 6.97 (d, J = 8.4 Hz, 2H), 6.75 (dd, J = 7.6 Hz, 2H), 6.53 (d, J = 8.4 Hz, 2H), 4.21 (m, 2H), 3.84 (m, 2H), 1.48 (s, 18H), 1.30 (s, 18H). ^{13}C NMR ($CDCl_3$): δ = 170.02, 165.21, 159.51, 148.51, 142.01, 141.75, 133.03, 131.73, 127.88, 127.21, 120.89, 120.33, 119.23, 119.10, 116.88, 116.72, 106.12, 55.04, 35.41, 35.06, 31.80, 29.61. Anal. Calcd for $C_{50}H_{58}AlN_3O_3$: C, 77.39; H, 7.53; N, 5.41. Found: C, 76.92; H, 7.15; N, 5.25.

Synthesis of D2. This compound was prepared in a manner analogous to the synthesis of **D1** using **S2** (0.25 g, 0.5 mmol). The desired **D2** was obtained as a yellow solid (0.24 g, 64%). ^{1}H NMR ($CDCl_3$): δ 8.45 (s, 2H), 7.91 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 2.4 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 7.14 (s, 2H), 7.07 (d, J = 2.4 Hz, 2H), 6.98 (d, J = 8.8 Hz, 2H), 6.54 (d, J = 8.4 Hz, 2H) 4.19 (m, 2H), 3.79 (m, 2H), 1.48 (s, 18H), 1.30 (s, 18H), 1.29 (s, 18H). ^{13}C NMR ($CDCl_3$): δ = 170.20, 163.39, 159.79, 148.49, 142.09, 141.07, 138.54, 131.15, 127.89, 127.15, 127.00, 120.92, 120.32, 119.09, 118.26, 116.83, 106.16, 55.04, 35.59, 35.07, 34.01, 31.81, 31.35, 29.67. Anal. Calcd for $C_{58}H_{74}AlN_3O_3$: C, 78.43; H, 8.40; N, 4.73. Found: C, 78.01; H, 8.11; N, 4.27.

Synthesis of A1. This compound was prepared in a manner analogous to the synthesis of **D1** but with phenol (0.38 g, 1.0 mmol) as an ancillary ligand. The desired **A1** was obtained as a yellow solid (0.59 g, 68%). ^{1}H NMR ($CDCl_3$): δ 8.31 (s, 2H), 7.46 (d, J = 7.6 Hz, 2H), 7.08 (d, J = 7.6 Hz, 2H), 6.85 (m, 2H), 6.72 (m, 2H), 6.51 (m, 1H), 6.34 (d, J = 8.4 Hz, 2H), 4.00 (m, 2H), 3.67 (m, 2H), 1.48 (s, 18H). ^{13}C NMR ($CDCl_3$): δ = 169.84, 165.12, 160.22, 141.70, 132.78, 131.66, 128.68, 119.73, 119.26, 117.09, 116.49, 54.90, 35.38, 29.59.

Synthesis of A2. This compound was prepared in a manner analogous to the synthesis of **D2** but with phenol (0.54 g, 1.5 mmol) as an ancillary ligand. The desired **A2** was obtained as a yellow solid (0.59 g, 64%). ^{1}H NMR ($CDCl_3$): δ 8.34 (s, 2H), 7.53 (d, J = 2.4 Hz, 2H), 7.01 (d, J = 2.4 Hz, 2H), 6.85 (m, 2H), 6.50 (m, 2H), 6.37 (d, J = 7.6 Hz, 2H), 4.01 (m, 2H), 3.69 (m, 2H), 1.49 (s, 18H), 1.30 (s, 18H). ^{13}C NMR ($CDCl_3$): δ = 169.99, 163.33, 160.46, 141.01, 138.33, 130.90, 128.60, 127.04, 119.80, 118.32, 116.86, 55.00, 35.58, 33.99, 31.36, 29.69.

X-ray crystallography. Single crystals suitable for X-ray diffraction study were grown from THF/MeOH solution of **D1**, respectively. Single crystal of **D1** was coated with Paratone oil and mounted onto a glass capillary. The crystallographic measurements were performed on a Bruker D8QUEST CCD area detector diffractometer with a graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). The structure was solved by direct methods and all non-hydrogen atoms were subjected to

anisotropic refinement by a full-matrix least-squares method on F^2 by using the SHELXTL/PC package, resulting in X-ray crystallographic data of **D1** in CIF format (CCDC 1819002). Hydrogen atoms were placed at their geometrically calculated positions and refined riding on the corresponding carbon atoms with isotropic thermal parameters. The detailed crystallographic data are given in Table S1 and S2.

UV/Vis absorption and photoluminescence (PL) measurements. The solution UV/Vis absorption and PL measurements were performed in degassed tetrahydrofuran with a 1-cm quartz cuvette (5.0×10^{-5} M). PL measurements were also carried out in the film state (5 wt% doped on PMMA) for **D1** and **D2** on 1.5 × 1.5 cm quartz plates (thickness = 1 mm) at ambient temperature. The solution quantum efficiencies were measured with reference to that of quinine sulfate (0.5 M H_2SO_4, $\Phi = 0.55$).[4] The absolute photoluminescence quantum yields (PLQYs) of **A1**, **A2**, **D1**, and **D2** in the film state were obtained with an absolute PL quantum yield spectrophotometer (Quantaurus-QY C11347-11, Hamamatsu Photonics), equipped with a 3.3 inch integrating sphere at 298 K.

Theoretical calculations. The optimized structure at ground and first excited state of **D1** and **D2** were obtained using the density functional theory (DFT) method with the B3LYP functional[5] and 6-31G(d)[6] basis sets. Time-dependent density functional theory (TD-DFT)[7] measurements using the hybrid B3LYP functional (TD-B3LYP) were used to obtain the electronic transition energies which also included an account of electron correlation. All the calculations for **D1** and **D2** were performed in THF solution. Solvent effects were evaluated with the conductor-like polarizable continuum model (CPCM).[8] All calculations were carried out using the GAUSSIAN 09 program.[9] The GaussSum 3.0 was used to calculate the percent contribution of a group in a molecule to each molecular orbital.[10]

Reference

1. A. W. Freeman, M. Urvoy and M. E. Criswell, *J. Org. Chem.*, 2005, **70**, 5014.
2. S. J. Dzugan and V. L. Goedken, *Inorg. Chem.*, 1986, **25**, 2858.
3. K. Y. Hwang, M. H. Lee, H. Jang, Y. Sung, J. S. Lee, S. H. Kim and Y. Do, *Dalton Trans.*, 2008, 1818; K. Y. Hwang, H. Kim, Y. S. Lee, M. H. Lee and Y. Do, *Chem. Eur. J.*, 2009, **15**, 6478; D. A. Atwood, M. S. Hill, J. A. Jegier and D. Rutherford, *Organometallics*, 1997, **16**, 2659.
4. W. H. Melhuish, *J. Phys. Chem.*, 1961, **65**, 229.
5. P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623; C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter*, 1988, **37**, 785.
6. J. S. Binkley, J. A. Pople and W. J. Hehre, *J. Am. Chem. Soc.*, 1980, **102**, 939.
7. E. Runge and E. K. U. Gross, *Phys. Rev. Lett.*, 1984, **52**, 997.
8. M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669; V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995.

9. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09 Revision D.01, Gaussian. Inc.*, Wallingford, CT, 2013.
10. N. M. O'Boyle, A. L. Tenderholt and K. M. Langner, *J. Comp. Chem.*, 2008, **29**, 839.

^{1}H and ^{13}C NMR Spectra

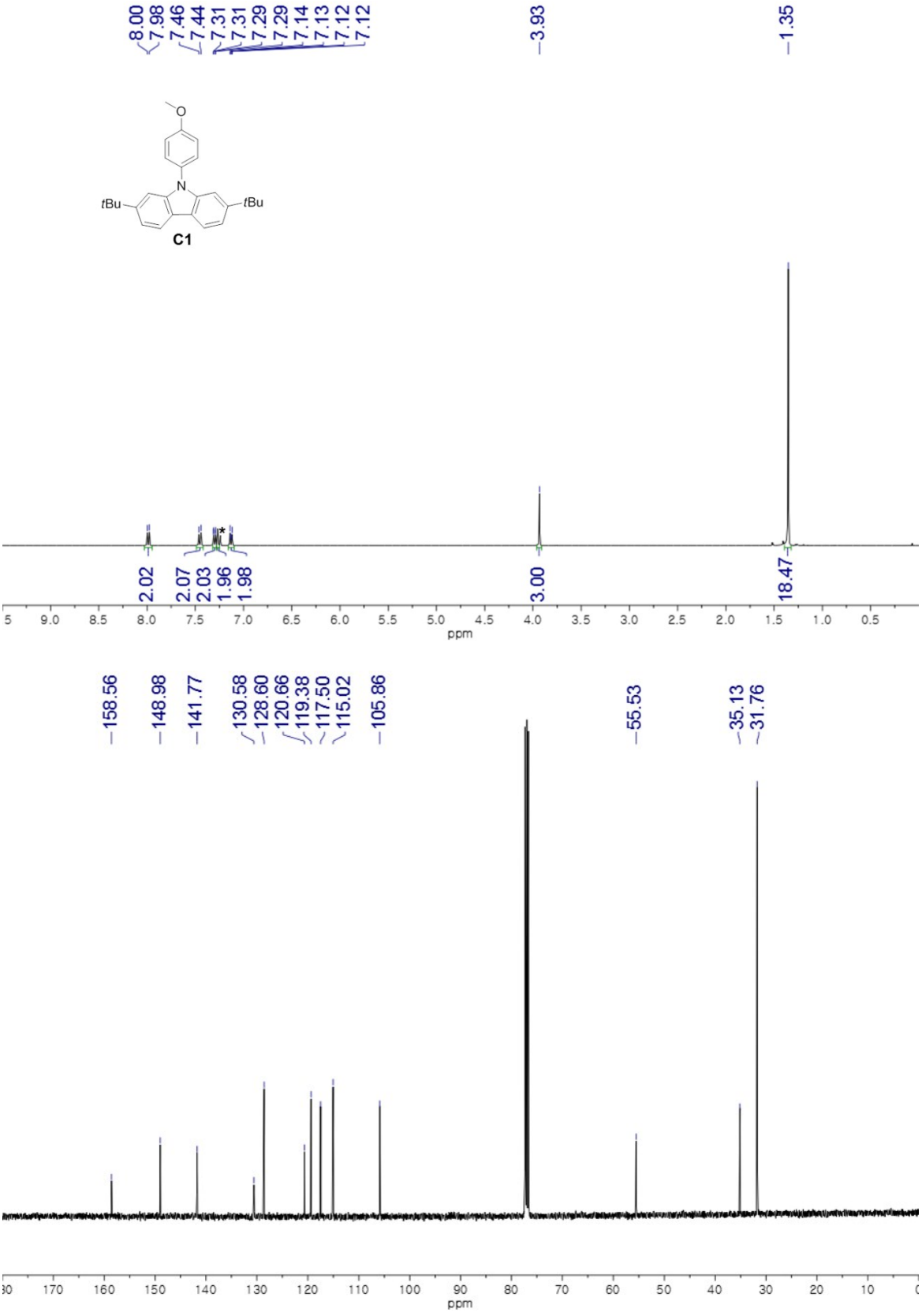


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **C1** (∗ from residual $CHCl_3$ in $CDCl_3$).

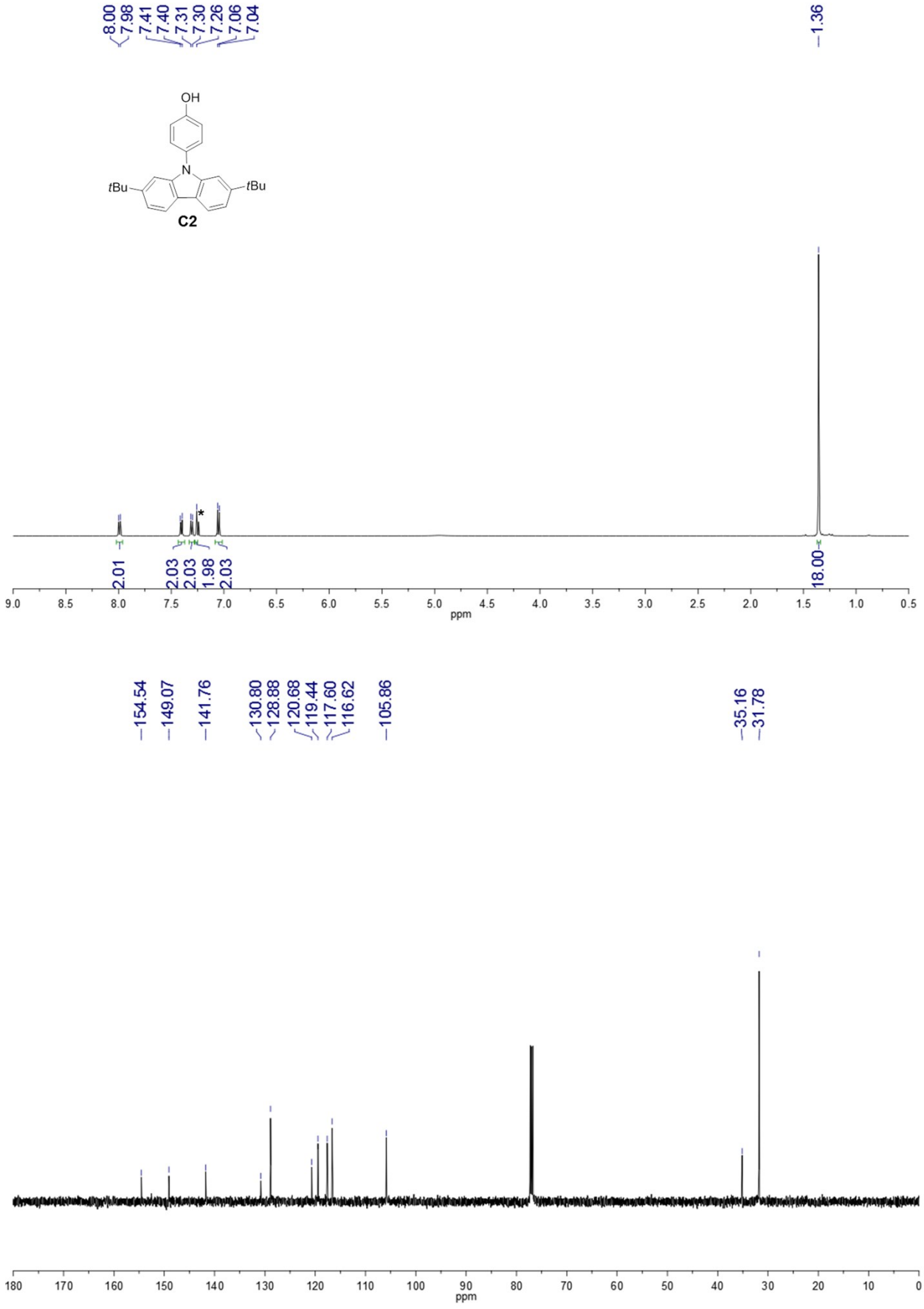


Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **C2** (* from residual $CHCl_3$ in $CDCl_3$).

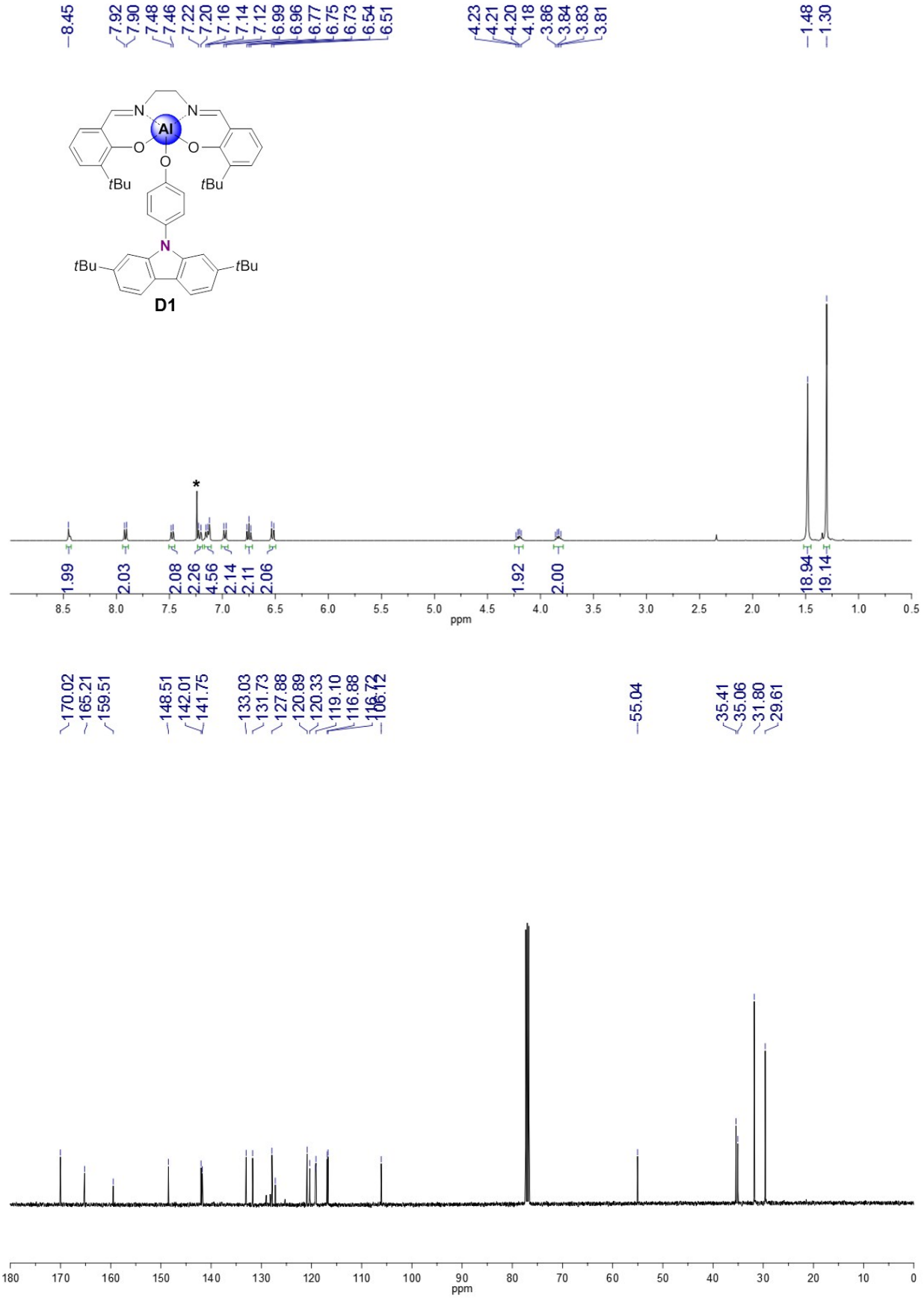


Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **D1** (∗ from residual $CHCl_3$ in $CDCl_3$).

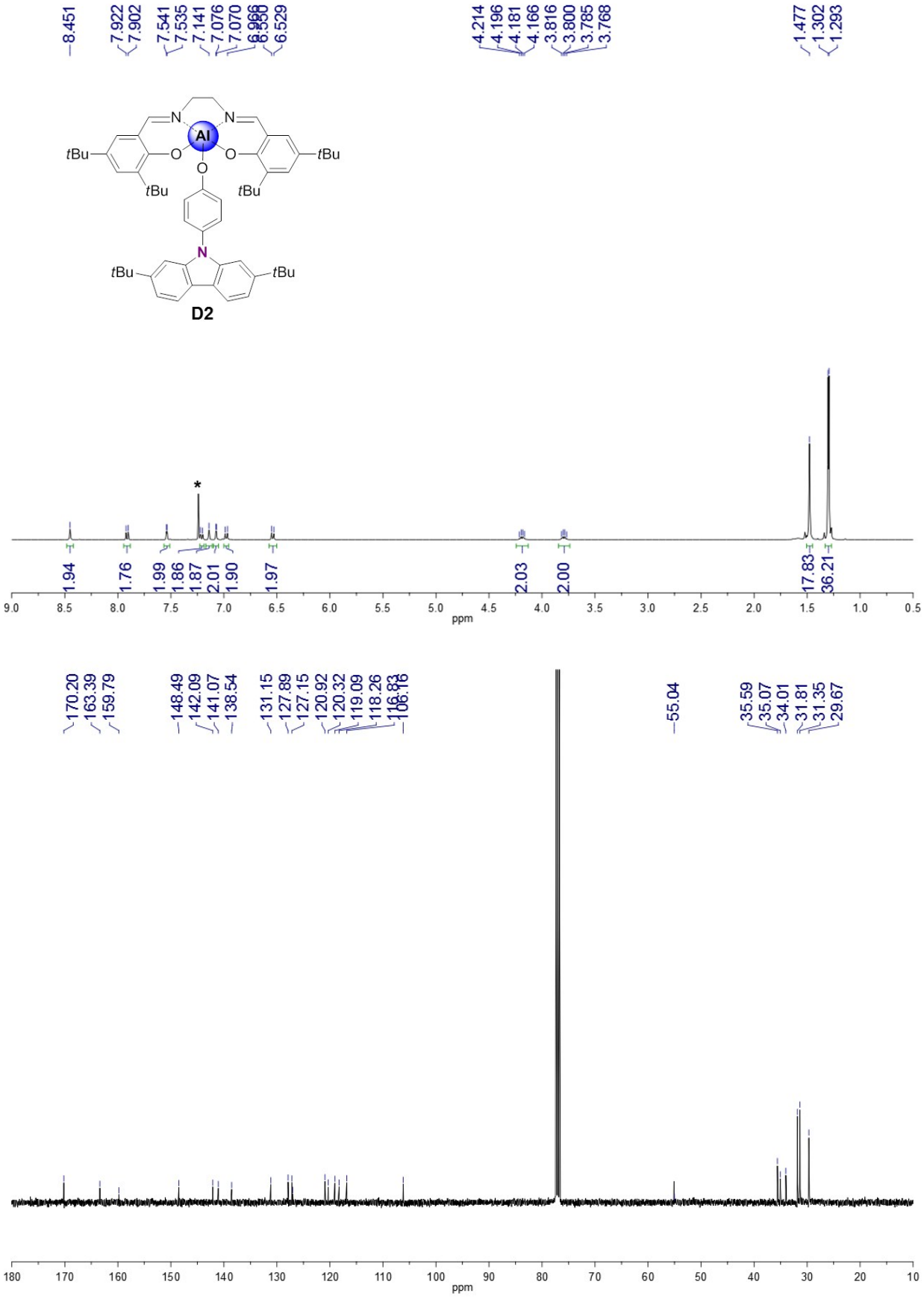


Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **D2** (∗ from residual $CHCl_3$ in $CDCl_3$).

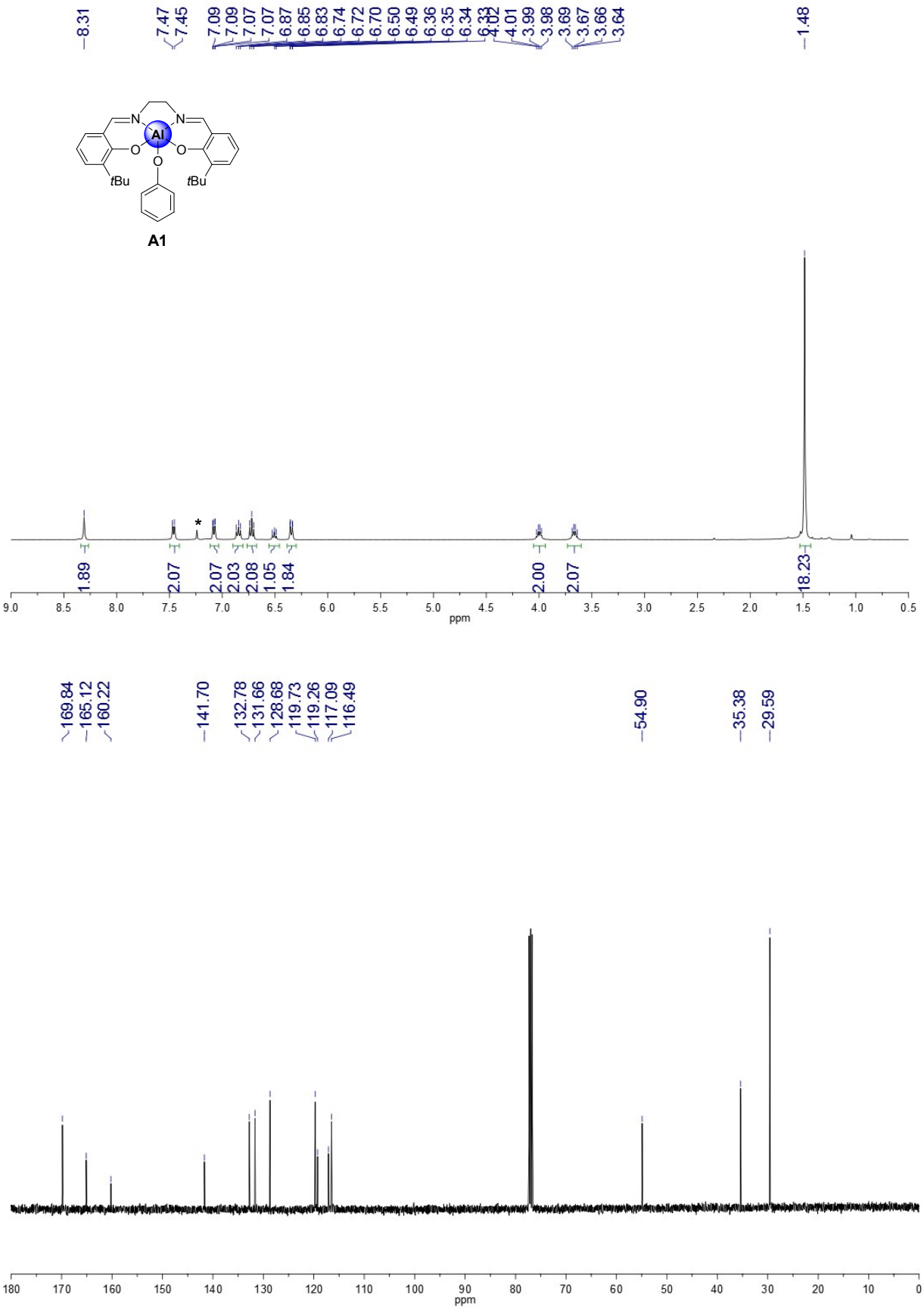


Fig. S5 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **A1** (∗ from residual $CHCl_3$ in $CDCl_3$).

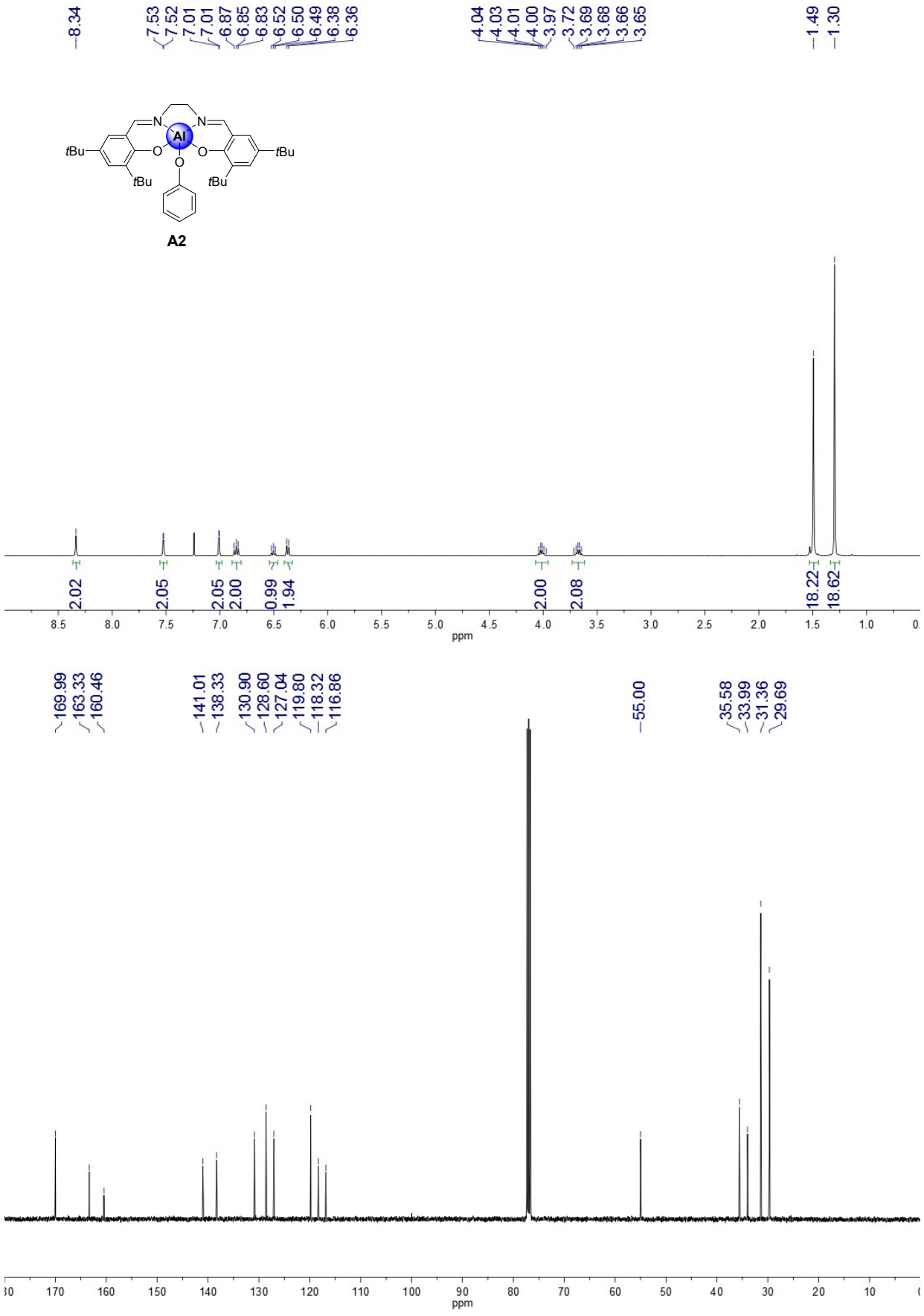


Fig. S6 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **A2** (∗ from residual $CHCl_3$ in $CDCl_3$).

Table S1 Crystallographic data and parameters for **D1**

Compound	**D1**
Formula	$C_{50}H_{58}AlN_3O_3$
Formula weight	775.97
Crystal system	Monoclinic
Space group	P21/c
a (Å)	9.9221(3)
b (Å)	22.0031(6)
c (Å)	20.2879(5)
β (°)	101.0014(17)
V (Å^3)	4347.8(2)
Z	4
ρ_{calc}(g cm^{-3})	1.185
μ (mm^{-1})	0.092
F(000)	1664
T (K)	296(2)
Scan mode	*multi-scan*
hkl range	$-11< h <11$, $-26 < k < 26$, $-23 < l < 24$
Measd reflns	49274
Unique reflns [R_{int}]	7953 [0.2016]
Reflns used for refinement	7953
Refined parameters	526
R_1[a] (I > 2σ(I))	0.0864
wR_2[b] all data	0.2320
GOF on F^2	0.983
ρ_{fin} (max/min) (e Å^{-3})	0.266, −0.372

[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 (deg) for **D1**

Compound	**D1**
	lengths
Al–O1	1.781(3)
Al–O2	1.795(3)
Al–O3	1.759(3)
Al–N1	1.987(4)
Al–N2	1.988(4)
	angles
O1–Al–O2	91.85(15)
O1–Al–O3	114.16(16)
O2–Al–O3	102.80(15)
O1–Al–N1	88.41(16)
O2–Al–N1	163.35(16)
O3–Al–N1	92.24(16)
O1–Al–N2	135.39(16)
O2–Al–N2	88.89(16)
O3–Al–N2	109.08(16)
N1–Al–N2	79.34(16)

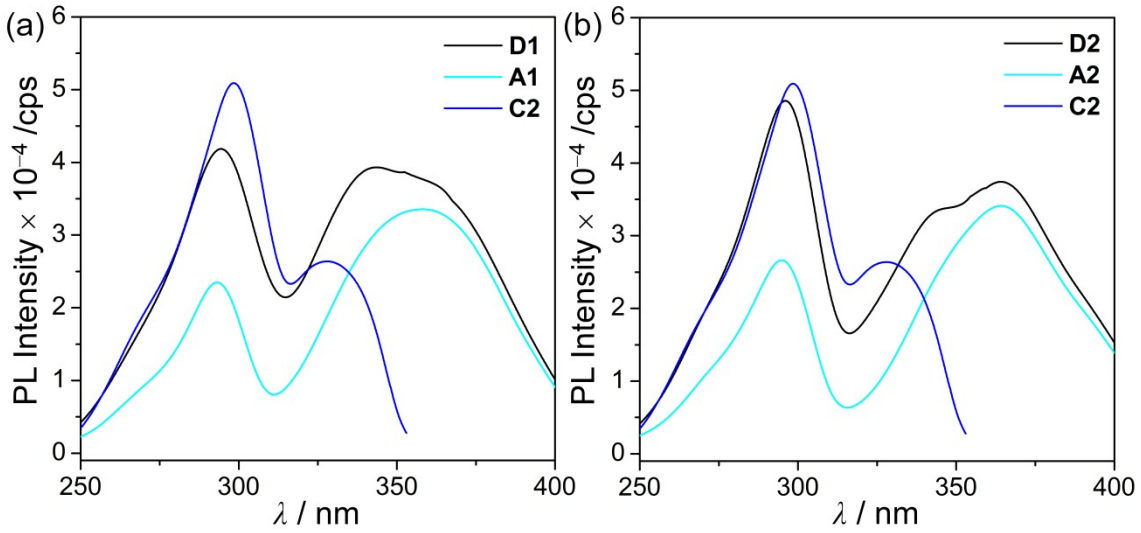


Fig. S7 Excitation graphs in THF (5.0×10^{-5} M) for (a) **D1**, **A1**, and **C2** and (b) **D2**, **A2**, and **C2** at room temperature.

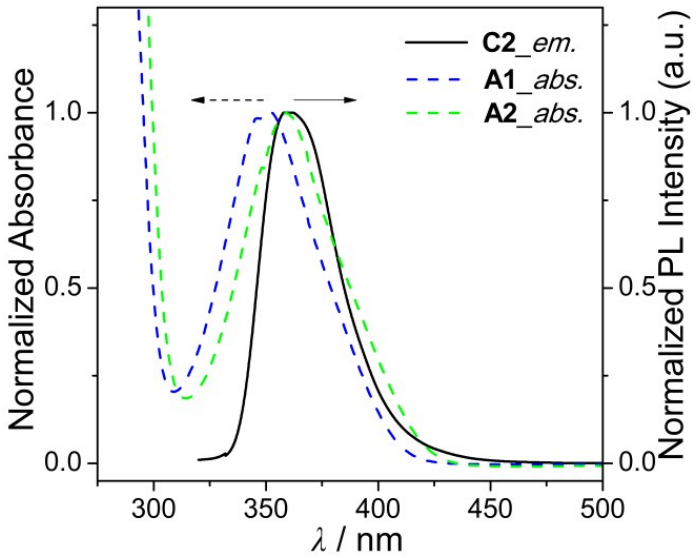


Fig. S8 Comparison of the absorption spectra of monomeric complexes (**A1** and **A2**) and the emission spectra of **C2** (5.0×10^{-5} M, THF).

Emission decay curves in THF solution

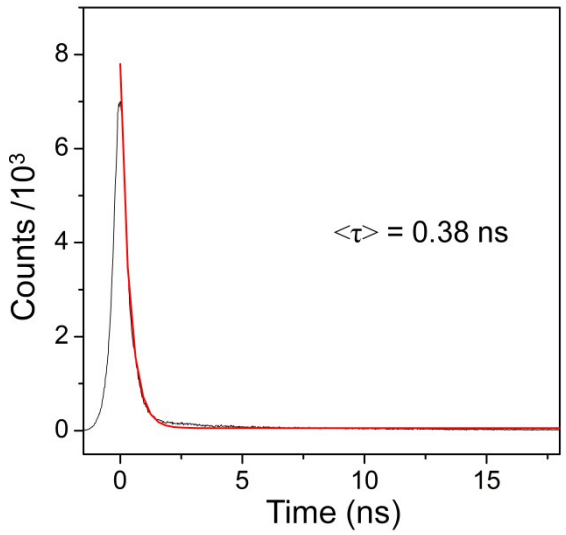


Fig. S9 Emission decay curve detected at 380 nm of THF (3.0×10^{-5} M) solution of **C2** at 298 K (black line). The red-line corresponds to the single-exponential fitting curve ($R^2 = 0.9943$) for the experimental curve.

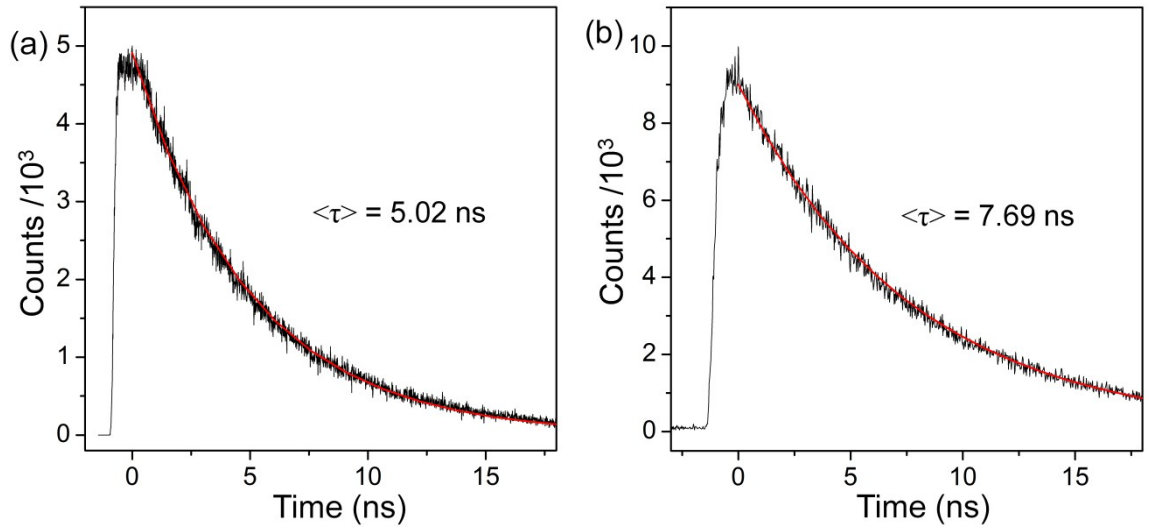


Fig. S10 Emission decay curves detected at (a) 400 nm and (b) 450 nm of THF (5.0×10^{-5} M) solution of **D1** at 298 K (black line). The red-line corresponds to the single-exponential fitting curve ($R^2 = 0.9972$ and 0.9958) for the experimental curve.

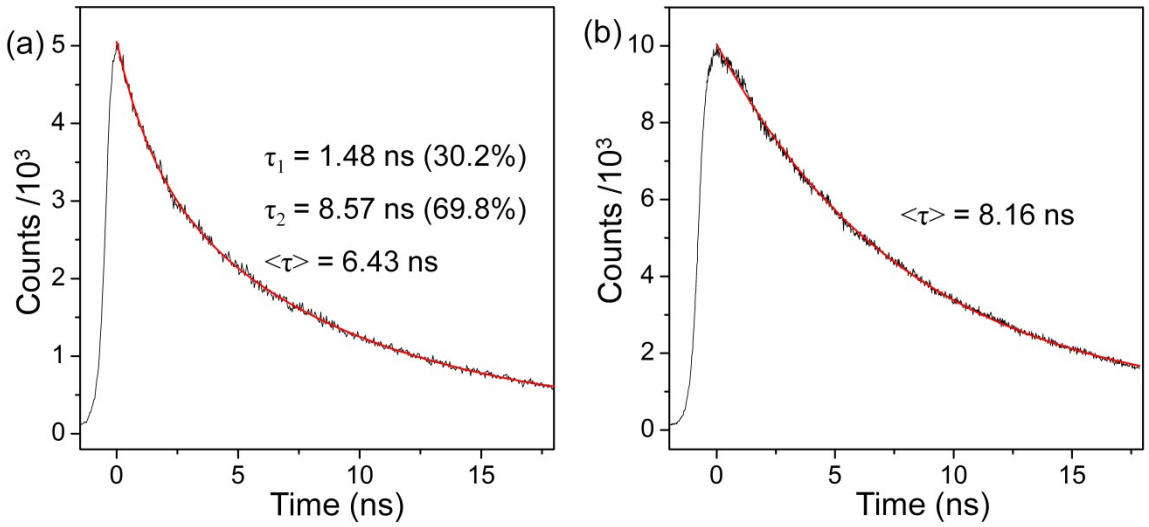


Fig. S11 Emission decay curves detected at (a) 380 nm and (b) 460 nm of THF (5.0×10^{-5} M) solution of **D2** at 298 K (black line). The red-line corresponds to the double or single-exponential fitting curve (R^2 = 0.9984 and 0.9987) for the experimental curve.

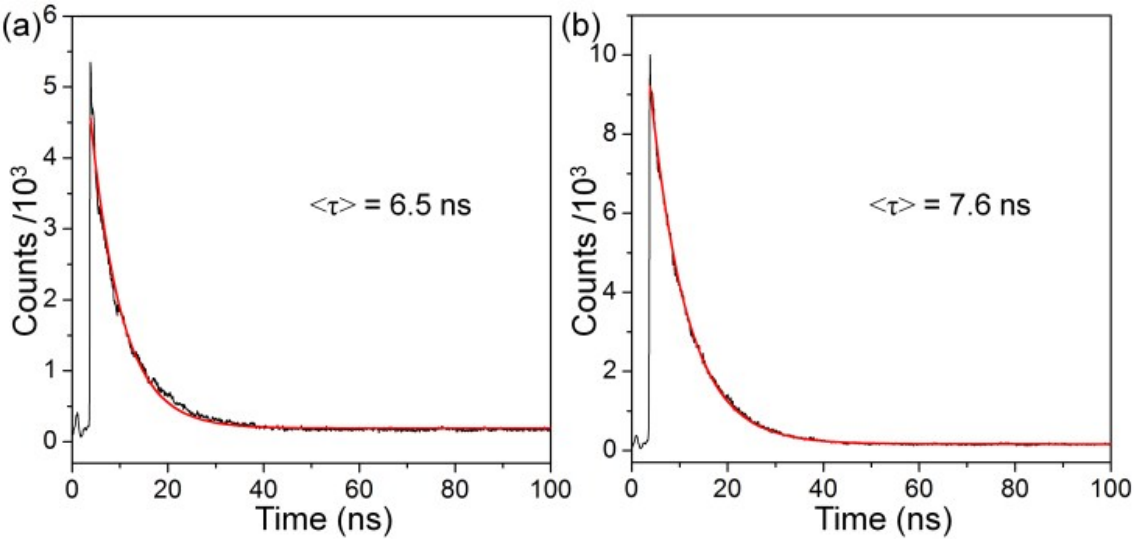


Fig. S12. Emission decay curves detected at (a) 380 nm and (b) 460 nm of THF (5.0×10^{-5} M) solution of an equimolar mixture, **A1+C2** at 298 K (black line). The red-line corresponds to the double or single-exponential fitting curve (R^2 = 0.9907 and 0.9986) for the experimental curve.

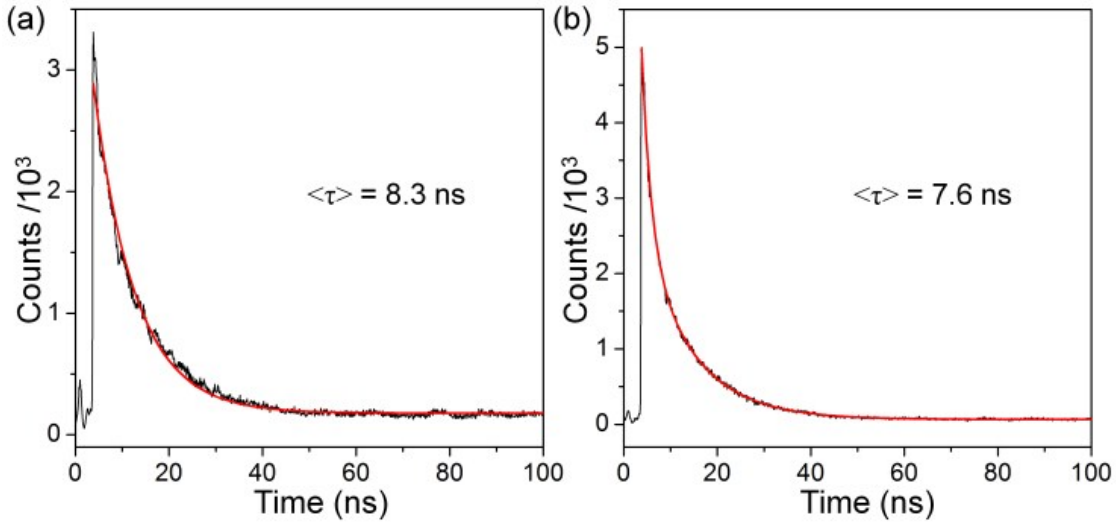
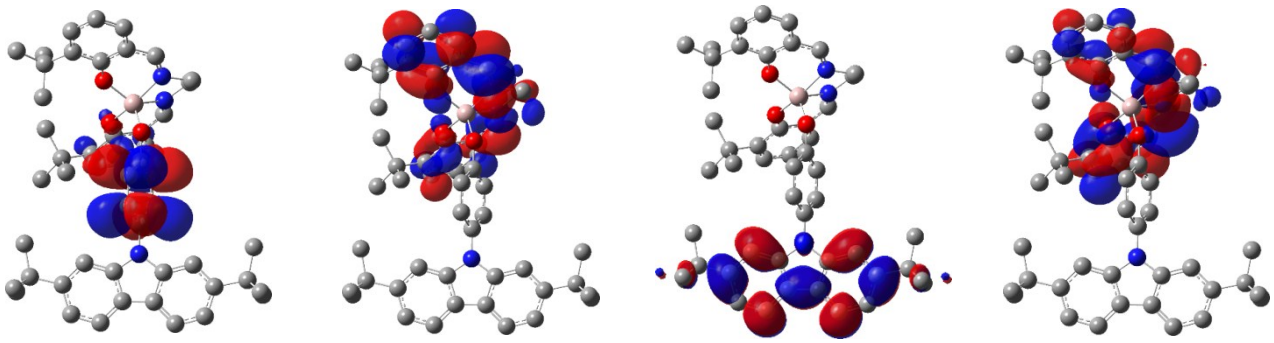


Fig. S13 Emission decay curve detected at (a) 380 nm and (b) 460 nm of THF (5.0×10^{-5} M) solution of an equimolar mixture, **A2+C2** at 298 K (black line). The red-line corresponds to the double or single-exponential fitting curve (R^2 = 0.9913 and 0.9987) for the experimental curve.

Theoretical calculation results for D1 and D2



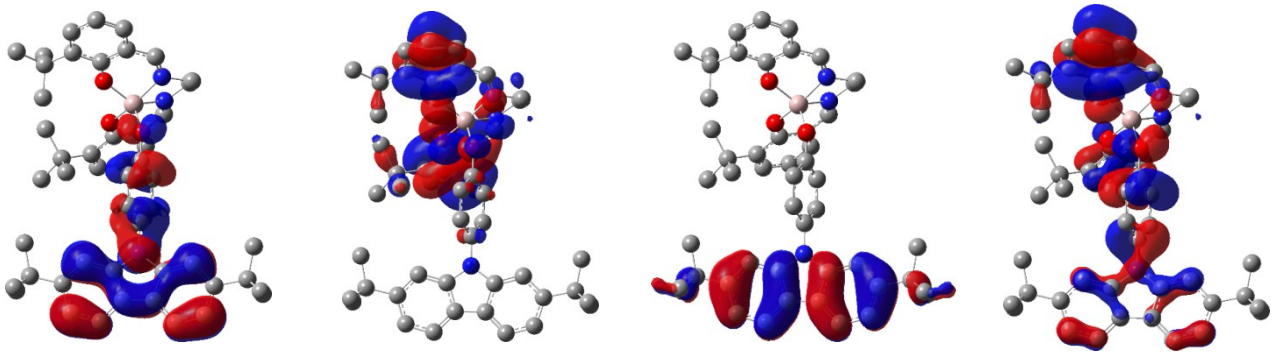


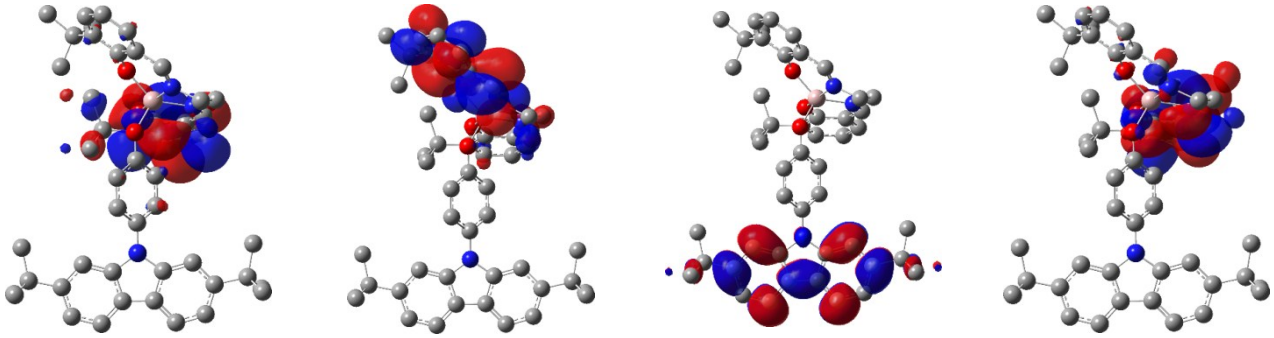
Fig. S14 Frontier molecular orbitals of **D1** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the ground state (S_0) optimized geometries.

Table S3 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **D1** from TD-B3LYP/6-31G(d) calculations in THF at the ground state (S_0) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	425.50	0.0011	HOMO → LUMO (96.5%)
2	376.59	0.0046	HOMO−3 → LUMO+1 (2.7%)
			HOMO−2 → LUMO (46.6%)
			HOMO → LUMO+1 (48.9%)
3	375.71	0.0313	HOMO−1 → LUMO (70.6%)
			HOMO → LUMO+1 (27.2%)
4	372.57	0.0000	HOMO−1 → LUMO (99.6%)
5	358.30	0.0293	HOMO−3 → LUMO (96.6%)
6	342.73	0.0207	HOMO−4 → LUMO (97.1%)
7	335.32	0.0823	HOMO−3 → LUMO+1 (4.5%)
			HOMO−2 → LUMO+1 (92.0%)

Table S4 Molecular orbital energies (in eV) and distributions (in %) of **D1** at the ground state (S_0) optimized geometries

	E (eV)	salen-Al	bridged phenoxy	carbazole
LUMO+4	0.12	77.4	18.9	3.7
LUMO+3	−0.05	6.7	91.1	2.2
LUMO+2	−0.61	99.8	0.2	0.0
LUMO+1	−1.56	0.0	0.3	99.7
LUMO	−1.91	99.4	0.6	0.0
HOMO	−5.22	0.8	23.5	75.7
HOMO−1	−5.54	94.6	4.1	1.4
HOMO−2	−5.76	0.0	0.0	100.0
HOMO−3	−5.86	51.9	34.6	13.5
HOMO−4	−6.04	53.8	36.4	9.8



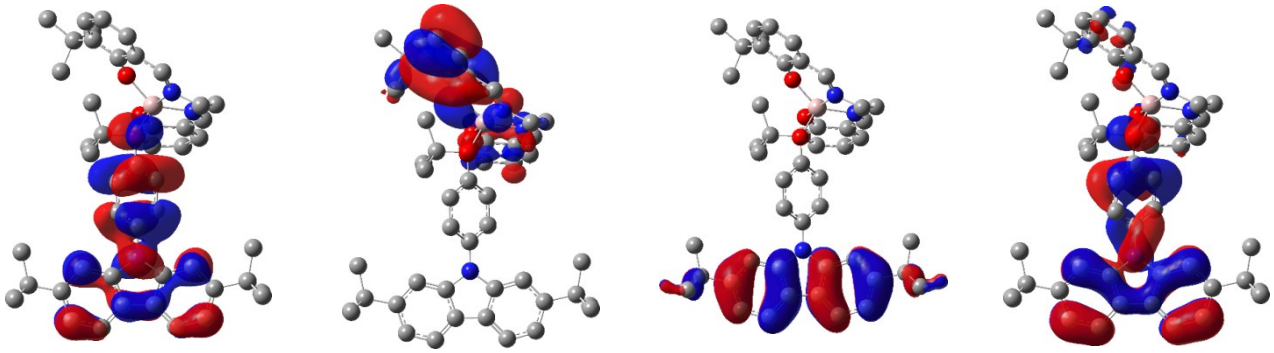


Fig. S15 Frontier molecular orbitals of **D1** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the first excited state (S_1) optimized geometries.

Table S5 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **D1** 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	736.53	0.0039	HOMO → LUMO (99.3%)
2	492.50	0.0000	HOMO → LUMO+1 (99.0%)
3	458.81	0.0501	HOMO−1 → LUMO (99.9%)
4	435.65	0.0149	HOMO−2 → LUMO (98.9%)
5	413.83	0.0074	HOMO−3 → LUMO (98.2%)
6	393.31	0.0387	HOMO−4 → LUMO (96.8%)
7	364.65	0.0255	HOMO → LUMO+2 (98.5%)
8	356.89	0.0928	HOMO−2 → LUMO+1 (93.0%)

Table S6 Molecular orbital energies (in eV) and distributions (in %) of **D1** at the first excited state (S_1) optimized geometries

	E (eV)	salen-Al	bridged phenoxy	carbazole
LUMO+4	0.16	52.9	25.3	21.8
LUMO+3	−0.03	98.2	1.6	0.2
LUMO+2	−0.62	99.4	0.5	0.1
LUMO+1	−1.55	0.0	0.9	99.1
LUMO	−2.45	99.5	0.5	0.0
HOMO	−4.62	1.3	59.5	39.2
HOMO−1	−5.59	98.1	0.9	1.1
HOMO−2	−5.81	0.0	0.0	100.0
HOMO−3	−5.87	6.0	36.2	57.8
HOMO−4	−6.14	93.6	4.7	1.6

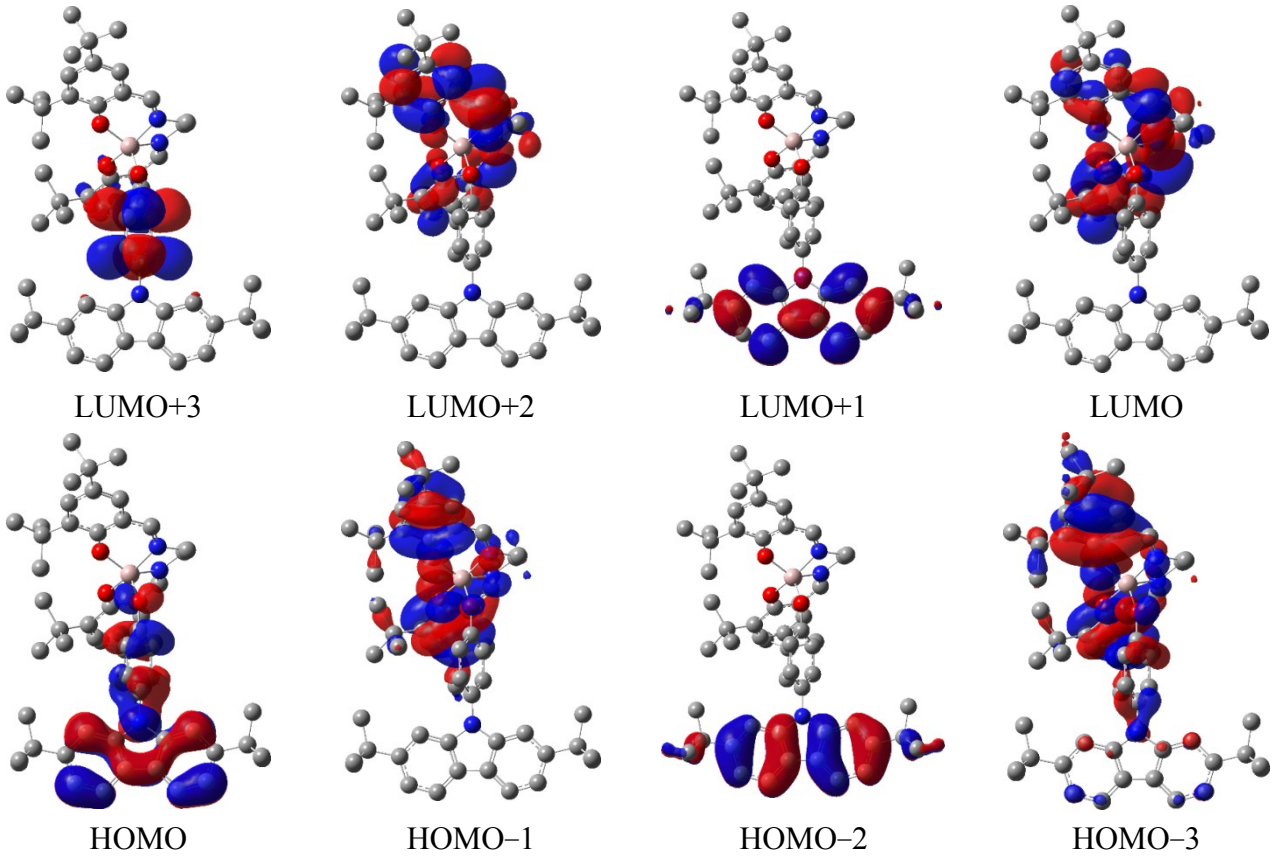


Fig. S16 Frontier molecular orbitals of **D2** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the ground state (S_0) optimized geometries.

Table S7 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **D2** from TD-B3LYP/6-31G(d) calculations in THF at the ground state (S_0) optimized geometries

state	λ (nm)	f_{calc}	contribution
1	423.41	0.0027	HOMO → LUMO (96.5%)
2	384.98	0.0351	HOMO−1 → LUMO (97.7%)
3	374.84	0.0130	HOMO → LUMO+1 (96.0%)
4	366.93	0.0000	HOMO−1 → LUMO (99.6%)
5	361.78	0.0628	HOMO−3 → LUMO (97.5%)
6	342.97	0.0796	HOMO−2 → LUMO+1 (93.2%)
7	341.22	0.0323	HOMO−4 → LUMO (94.9%)

Table S8 Molecular orbital energies (in eV) and distributions (in %) of **D2** at the ground state (S_0) optimized geometries

	E (eV)	salen-Al	bridged phenoxy	carbazole
LUMO+4	0.17	24.5	58.7	16.8
LUMO+3	−0.04	4.1	93.7	2.2
LUMO+2	−0.61	99.8	0.2	0.0
LUMO+1	−1.51	0.0	0.3	99.6
LUMO	−1.86	99.4	0.6	0.0
HOMO	−5.19	1.1	26.3	72.6
HOMO−1	−5.54	97.7	1.6	0.7
HOMO−2	−5.62	0.0	0.0	100.0
HOMO−3	−5.77	83.4	10.3	6.3
HOMO−4	−5.99	19.2	60.0	20.9

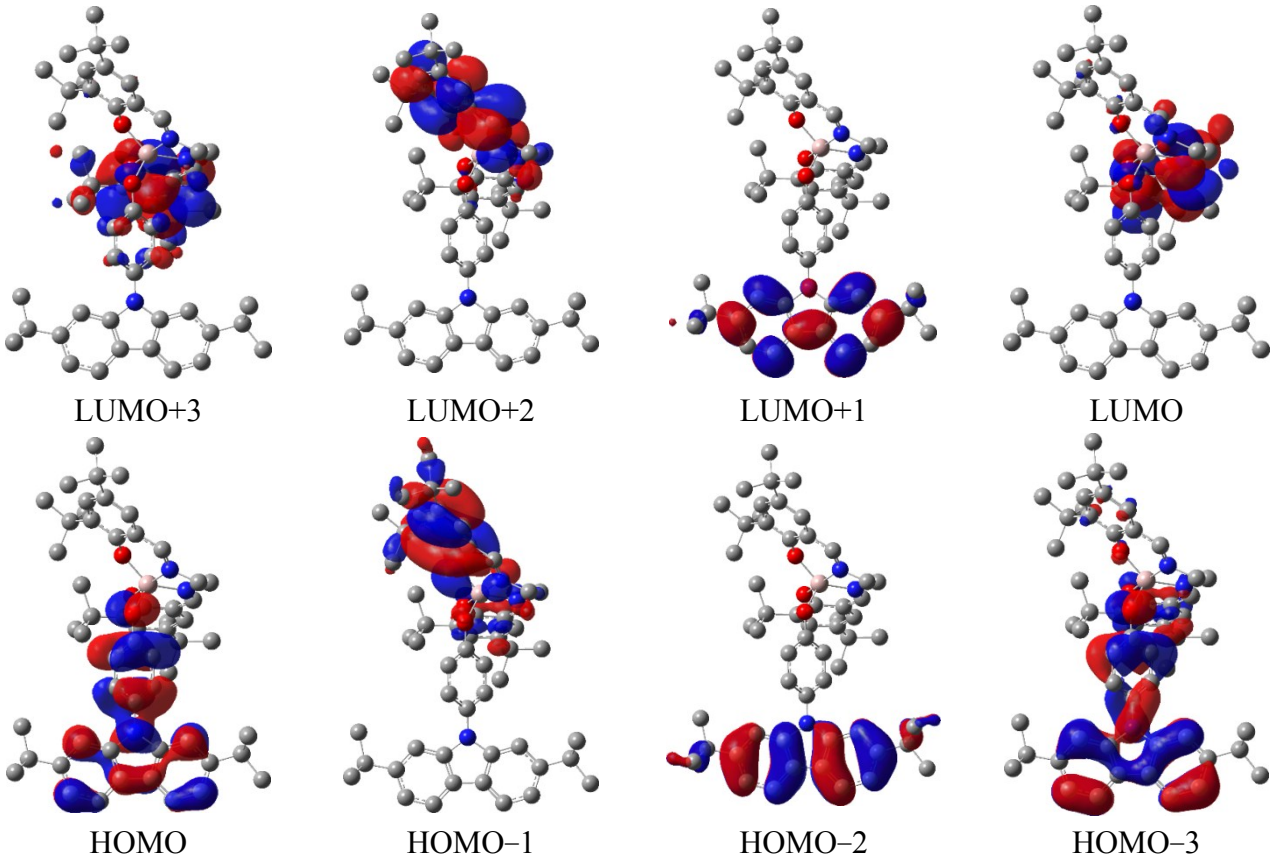


Fig. S17 Frontier molecular orbitals of **D2** from B3LYP/6-31G(d) calculations (Isovalue = 0.04) with in THF at the first excited state (S_1) optimized geometries.

Table S9 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for **D2** 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	719.33	0.0028	HOMO → LUMO (99.2%)
2	497.86	0.0194	HOMO → LUMO+1 (98.9%)
3	477.66	0.0490	HOMO−1 → LUMO (98.9%)
4	430.15	0.0004	HOMO−2 → LUMO (98.6%)
5	410.33	0.0236	HOMO−4 → LUMO (7.1%)
			HOMO−3 → LUMO (90.6%)
6	398.70	0.0318	HOMO−4 → LUMO (90.4%)
			HOMO−3 → LUMO (7.3%)
7	370.62	0.0285	HOMO → LUMO+2 (98.6%)
8	354.08	0.0956	HOMO−2 → LUMO+1 (94.8%)

Table S10 Molecular orbital energies (in eV) and distributions (in %) of **D2** at the first excited state (S_1) optimized geometries

	E (eV)	salen-Al	bridged phenoxy	carbazole
LUMO+4	0.17	3.3	25.8	71.0
LUMO+3	0.06	95.3	4.1	0.5
LUMO+2	−0.67	99.4	0.5	0.1
LUMO+1	−1.52	0.0	0.8	99.2
LUMO	−2.39	99.5	0.5	0.0
HOMO	−4.61	1.3	59.6	39.1
HOMO−1	−5.60	99.4	0.3	0.3
HOMO−2	−5.66	0.1	0.8	99.0
HOMO−3	−5.85	12.5	32.5	55.0
HOMO−4	−6.01	86.3	7.7	6.1

Table S11 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **D1** from B3LYP calculations (in Å)

Atom	x	y	z
Al	-3.062902	-1.450508	0.269955
N	-2.968342	-2.790004	1.761603
N	-3.848019	-3.073563	-0.632094
O	-2.643885	-0.128966	1.475588
O	-4.394659	-0.456808	-0.468851
O	-1.615994	-1.494337	-0.773255
C	-2.117427	-0.104495	2.679995
C	-1.647224	1.124428	3.257185
C	-1.105338	1.063322	4.538999
H	-0.735356	1.974282	4.994613
C	-1.005625	-0.120543	5.295863
C	-1.466063	-1.297513	4.754365
H	-1.410996	-2.230361	5.310595
C	-2.018651	-1.309205	3.451060
C	-2.486605	-2.563459	2.949916
H	-2.423660	-3.406604	3.644107
C	-3.428620	-4.152927	1.445108
H	-4.475163	-4.254538	1.758106
H	-2.835220	-4.907589	1.971568
C	-3.334752	-4.320074	-0.074155
H	-2.286109	-4.435250	-0.373323
H	-3.897612	-5.194377	-0.418393
C	-4.732541	-3.080673	-1.574589
H	-5.041956	-4.041750	-1.997236
C	-5.369050	-1.909212	-2.110587
C	-6.231797	-2.086916	-3.214109
H	-6.348789	-3.083053	-3.634500
C	-6.905972	-1.009579	-3.745684
C	-6.735642	0.255465	-3.157836
H	-7.283618	1.083534	-3.591585
C	-5.911880	0.494003	-2.057151
C	-5.190106	-0.619968	-1.516209
C	-0.341569	-1.092262	-0.705483
C	0.238731	-0.442304	-1.813252
H	-0.377204	-0.258786	-2.688956
C	1.574933	-0.053407	-1.796627
H	2.011402	0.433750	-2.664106
C	1.801609	-0.929186	0.441916
H	2.410277	-1.108177	1.323897
C	0.470176	-1.337916	0.420205
H	0.045526	-1.844170	1.281775
H	-7.565413	-1.127855	-4.599862
H	-0.573630	-0.092697	6.291273
C	2.368038	-0.287412	-0.666043
C	4.198473	1.438305	-0.669109
C	4.842490	-0.730399	-0.587525
C	3.459864	2.626202	-0.710336
C	5.614532	1.433872	-0.626869
C	4.872741	-2.129210	-0.565539
C	6.026141	0.047999	-0.574924
C	4.137331	3.849708	-0.718710
H	2.378132	2.580714	-0.736003
C	6.288436	2.662243	-0.635989
C	6.107865	-2.783472	-0.520626
H	3.942371	-2.683262	-0.585101
C	7.261016	-0.612208	-0.527597
C	5.554648	3.841627	-0.682476
H	7.374707	2.696639	-0.605135
C	7.290320	-2.001396	-0.499351
H	8.189562	-0.046657	-0.515787
H	6.092450	4.785063	-0.690407
H	8.255617	-2.497365	-0.462297
N	3.736343	0.120330	-0.644378
C	-5.790149	1.906302	-1.448597
C	-4.319299	2.384865	-1.504113
H	-3.661939	1.724453	-0.938089
H	-3.967117	2.423206	-2.542417
H	-4.238071	3.395566	-1.085544
C	-6.636613	2.945922	-2.212217
H	-6.324598	3.046436	-3.258322
H	-7.706225	2.706742	-2.193305
H	-6.511672	3.925139	-1.736631
C	-6.297946	1.885497	0.013508
H	-7.358325	1.606344	0.047505
H	-5.734140	1.176686	0.621519
H	-6.198700	2.881766	0.461893
C	-1.745259	2.463713	2.497845
C	-1.157260	3.637364	3.308101
H	-1.250845	4.557321	2.720294
H	-1.687987	3.797518	4.253804
H	-0.092897	3.496265	3.529964
C	-0.961246	2.389516	1.165643
H	0.102005	2.195803	1.352723
H	-1.342990	1.601602	0.515885
H	-1.040399	3.346589	0.634999
C	-3.231390	2.790190	2.220427
H	-3.787181	2.891562	3.160803
H	-3.311856	3.740663	1.678082
H	-3.702363	2.011695	1.619838
C	6.219172	-4.320246	-0.496059
C	7.027899	-4.799431	-1.725546
H	7.122022	-5.892286	-1.716649
H	6.530007	-4.509311	-2.658165
H	8.038331	-4.377759	-1.739258
C	6.944652	-4.764983	0.796583
H	6.385427	-4.451651	1.685961
H	7.040004	-5.857493	0.822955
H	7.951536	-4.340486	0.866300
C	4.842665	-5.011123	-0.531954
H	4.226740	-4.739278	0.332914
H	4.284272	-4.761860	-1.441535
H	4.976882	-6.098619	-0.513677
C	3.392019	5.198052	-0.764006
C	1.862405	5.024005	-0.808500
H	1.541215	4.467158	-1.696136
H	1.484666	4.501758	0.077691
H	1.381254	6.008042	-0.842825
C	3.744805	6.024825	0.495885
H	4.819533	6.221954	0.566862
H	3.228074	6.992252	0.472920
H	3.438492	5.498031	1.407219
C	3.821012	5.984193	-2.026290
H	4.898088	6.180557	-2.039306
H	3.569277	5.428498	-2.937155
H	3.304629	6.951204	-2.064816

Table S12 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **D1** from B3LYP calculations (in Å)

Atom	x	y	z
Al	-3.003266	-1.155365	-0.378438
N	-2.555104	-2.963562	-0.013065
N	-3.400471	-1.978685	-2.198194
O	-2.731450	-0.624103	1.328527
O	-4.486196	-0.114793	-0.606895
O	-1.628692	-0.120536	-1.174200
C	-2.251682	-1.239062	2.426858
C	-1.984717	-0.503137	3.608749
C	-1.519506	-1.200799	4.742616
H	-1.310712	-0.661253	5.657654
C	-1.318632	-2.587362	4.729225
C	-1.559625	-3.307143	3.575146
H	-1.396733	-4.383216	3.549536
C	-2.015656	-2.663832	2.389676
C	-2.207011	-3.441329	1.223166
H	-2.025087	-4.512414	1.303406
C	-2.678002	-3.953756	-1.074632
H	-3.630043	-4.505899	-1.006726
H	-1.868917	-4.696946	-1.030227
C	-2.625292	-3.197477	-2.407543
H	-1.588190	-2.917327	-2.632673
H	-3.013798	-3.794234	-3.241507
C	-4.298733	-1.610856	-3.049716
H	-4.419454	-2.188328	-3.972621
C	-5.194019	-0.498317	-2.867918
C	-6.045580	-0.167666	-3.943101
H	-5.963891	-0.731905	-4.869491
C	-6.961507	0.854693	-3.814941
C	-7.041955	1.543263	-2.593358
H	-7.775112	2.337789	-2.517022
C	-6.239142	1.255072	-1.488324
C	-5.271263	0.205070	-1.624211
C	-0.355986	-0.029368	-0.999677
C	0.376876	0.956877	-1.743173
H	-0.173855	1.573651	-2.444809
C	1.733322	1.093101	-1.597739
H	2.274803	1.809861	-2.203263
C	1.742214	-0.744482	0.023424
H	2.276100	-1.355757	0.741072
C	0.381140	-0.876212	-0.103959
H	-0.153782	-1.599556	0.497554
H	-7.618245	1.124529	-4.636376
H	-0.966706	-3.091968	5.626227
C	2.451032	0.241940	-0.712274
C	4.540882	1.596251	-0.495894
C	4.759427	-0.686956	-0.472193
C	4.050737	2.903696	-0.452494
C	5.913115	1.306565	-0.353069
C	4.545558	-2.063092	-0.583139
C	6.051975	-0.139078	-0.342427
C	4.955461	3.966537	-0.327482
H	2.987287	3.091995	-0.495533
C	6.815262	2.362446	-0.221441
C	5.641916	-2.932088	-0.500433
H	3.550220	-2.451629	-0.746036
C	7.145752	-1.001486	-0.267305
C	6.332474	3.669096	-0.223603
H	7.878489	2.172348	-0.108029
C	6.929521	-2.376080	-0.333190
H	8.154127	-0.610534	-0.168427
H	7.046113	4.480723	-0.124432
H	7.789288	-3.034955	-0.267619
N	3.824819	0.374589	-0.569602
C	-6.387570	2.048707	-0.173638
C	-5.062882	2.781429	0.146701
H	-4.235048	2.079247	0.248297
H	-4.819868	3.497710	-0.648121
H	-5.158855	3.340951	1.085372
C	-7.493778	3.120354	-0.259342
H	-7.285896	3.870853	-1.030926
H	-8.479254	2.684081	-0.460290
H	-7.556484	3.645327	0.700548
C	-6.769687	1.091048	0.981199
H	-7.734638	0.610379	0.777119
H	-6.017985	0.313821	1.121848
H	-6.867096	1.653091	1.918425
C	-2.204372	1.025681	3.673951
C	-1.795663	1.624580	5.036614
H	-1.959503	2.708676	5.017369
H	-2.389520	1.217816	5.863191
H	-0.736282	1.454680	5.262253
C	-1.355505	1.740657	2.595605
H	-0.286149	1.564283	2.768768
H	-1.606369	1.382681	1.596590
H	-1.525728	2.824886	2.633834
C	-3.702033	1.347564	3.465027
H	-4.306515	0.892494	4.260073
H	-3.869264	2.432603	3.496995
H	-4.053369	0.970824	2.504131
C	5.480765	-4.461350	-0.591189
C	6.302285	-4.996327	-1.788775
H	6.198307	-6.085480	-1.859744
H	5.951695	-4.559606	-2.731024
H	7.368856	-4.770020	-1.688610
C	5.999612	-5.106026	0.716777
H	5.424915	-4.754864	1.581495
H	5.902137	-6.196799	0.663862
H	7.054635	-4.874261	0.896656
C	4.013573	-4.887100	-0.787578
H	3.378754	-4.563864	0.045337
H	3.592346	-4.488552	-1.717762
H	3.954579	-5.979498	-0.841591
C	4.490506	5.434701	-0.290950
C	2.960861	5.570425	-0.410031
H	2.585267	5.157230	-1.353185
H	2.439725	5.073492	0.416238
H	2.685517	6.630242	-0.381710
C	4.928961	6.080559	1.045437
H	6.016377	6.061838	1.172245
H	4.607351	7.128213	1.080171
H	4.480477	5.558848	1.898647
C	5.136374	6.203638	-1.468693
H	6.230096	6.183279	-1.420220
H	4.833259	5.774137	-2.430464
H	4.821238	7.253688	-1.450660

Table S13 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of **D2** from B3LYP calculations (in Å)

Atom	x	y	z
Al	-2.476990	-0.240316	-1.390845
N	-2.103861	-1.150304	-3.137939
N	-3.513358	0.939633	-2.654197
O	-1.736724	-1.679038	-0.519509
O	-3.899667	-0.196423	-0.260214
O	-1.305129	1.060190	-1.037401
C	-0.945331	-2.665877	-0.878457
C	-0.294448	-3.492100	0.098962
C	0.526804	-4.512315	-0.368979
H	1.027321	-5.130580	0.365947
C	0.766970	-4.816580	-1.733618
C	0.121709	-4.024725	-2.659762
H	0.245306	-4.193272	-3.724945
C	-0.722101	-2.957849	-2.259784
C	-1.349339	-2.200937	-3.296286
H	-1.165359	-2.546654	-4.317794
C	-2.686116	-0.523257	-4.336550
H	-3.640183	-1.014155	-4.565878
H	-2.026002	-0.628196	-5.203961
C	-2.942458	0.947956	-3.996818
H	-1.993318	1.496722	-3.974551
H	-3.605511	1.420364	-4.729694
C	-4.589361	1.604308	-2.383578
H	-5.025875	2.236073	-3.163691
C	-5.284095	1.562127	-1.127120
C	-6.385104	2.435126	-0.967581
H	-6.608347	3.114004	-1.784788
C	-7.148394	2.431240	0.184051
C	-6.781603	1.491194	1.176072
H	-7.378109	1.471214	2.079727
C	-5.722567	0.591310	1.080177
C	-4.923949	0.631075	-0.108230
C	-0.026784	1.146065	-0.652044
C	0.331801	2.052247	0.366115
H	-0.450380	2.641615	0.836000
C	1.659220	2.203729	0.756286
H	1.920329	2.918794	1.531398
C	2.323102	0.533991	-0.855958
H	3.099561	-0.065199	-1.323273
C	0.998443	0.396986	-1.263834
H	0.746526	-0.299991	-2.057267
C	2.667794	1.441079	0.153489
C	4.545232	1.296623	1.822659
C	5.076712	2.038447	-0.249274
C	3.878314	0.808212	2.951962
C	5.937622	1.558513	1.826647
C	5.036360	2.466523	-1.580906
C	6.277228	2.032578	0.502769
C	4.603213	0.579097	4.125820
H	2.813327	0.618305	2.901769
C	6.659678	1.325120	3.004395
C	6.217550	2.892891	-2.195986
H	4.093545	2.462371	-2.113468
C	7.458617	2.458179	-0.118809
C	5.995631	0.845937	4.127261
H	7.729578	1.514676	3.043034
C	7.419130	2.876246	-1.443726
H	8.398621	2.465710	0.427524
H	6.569433	0.673404	5.032845
H	8.343686	3.201669	-1.911234
N	4.028791	1.589077	0.557807
C	-5.427065	-0.409938	2.216940
C	-4.002702	-0.175035	2.774967
H	-3.243460	-0.311510	2.004483
H	-3.911721	0.840344	3.180189
H	-3.798851	-0.880595	3.589927
C	-6.409012	-0.263983	3.398044
H	-6.354556	0.727283	3.863027
H	-7.447720	-0.448720	3.100296
H	-6.152480	-1.001315	4.166987
C	-5.564640	-1.856481	1.683076
H	-6.590251	-2.044379	1.341902
H	-4.883491	-2.040690	0.851109
H	-5.339851	-2.575028	2.481026
C	-0.502407	-3.268052	1.611724
C	0.314186	-4.257149	2.468652
H	0.124417	-4.050435	3.527837
H	0.032271	-5.300069	2.282996
H	1.393225	-4.156735	2.302653
C	-0.058984	-1.841063	2.013797
H	1.006251	-1.691802	1.798874
H	-0.625640	-1.077623	1.480298
H	-0.208248	-1.695943	3.091163
C	-1.995284	-3.476716	1.960770
H	-2.308350	-4.501013	1.723064
H	-2.155985	-3.317809	3.034476
H	-2.632196	-2.782078	1.412240
C	6.249050	3.379319	-3.657893
C	6.754994	4.841146	-3.705403
H	6.788392	5.198295	-4.742078
H	6.089538	5.503601	-3.139620
H	7.761905	4.939086	-3.286395
C	7.204388	2.481933	-4.480814
H	6.865057	1.439490	-4.472753
H	7.239180	2.819698	-5.523942
H	8.226264	2.505517	-4.088359
C	4.860365	3.333554	-4.323450
H	4.455399	2.315533	-4.352724
H	4.138298	3.974239	-3.804574
H	4.935798	3.689531	-5.357164
C	3.935349	0.053473	5.411228
C	2.422255	-0.176835	5.237360
H	1.896761	0.748731	4.976063
H	2.208141	-0.921620	4.462450
H	1.996074	-0.545258	6.177319
C	4.582227	-1.292371	5.818134
H	5.656539	-1.189726	6.003602
H	4.119970	-1.674482	6.736712
H	4.447060	-2.044484	5.032055
C	4.134869	1.080712	6.551821
H	5.194873	1.259939	6.759617
H	3.675172	2.042479	6.295720
H	3.669755	0.717543	7.476500
C	-8.344884	3.369121	0.419469
C	-8.582434	4.313002	-0.774273
H	-7.715598	4.956676	-0.963505
H	-8.804926	3.759250	-1.693725
H	-9.438837	4.963561	-0.564748
C	-9.628492	2.531795	0.634009
H	-9.542285	1.864758	1.498494
H	10.488186	3.190649	0.807350
H	-9.844841	1.915246	-0.246228
C	-8.085207	4.235384	1.675037
H	-7.944543	3.622561	2.571921
H	-7.188434	4.852494	1.545855
H	-8.935021	4.903996	1.859210
C	1.706562	-5.976137	-2.106591
C	1.167189	-7.297993	-1.509898
H	1.834615	-8.130428	-1.764019
H	1.092882	-7.254517	-0.418028
H	0.171261	-7.527748	-1.906185
C	3.119808	-5.698912	-1.540251
H	3.799262	-6.522676	-1.791027
H	3.535424	-4.775525	-1.960208
H	3.110347	-5.596602	-0.449733
C	1.826264	-6.153050	-3.632038
H	2.231536	-5.256931	-4.115936
H	2.504220	-6.984592	-3.854581
H	0.858191	-6.382911	-4.091996

Table S14 Cartesian coordinates of the first singlet excited state (S_1) fully optimized geometry in THF of **D2** from B3LYP calculations (in Å)

Atom	x	y	z
Al	-2.373170	-0.861318	-0.823621
N	-1.735249	-2.305084	-1.879059
N	-3.073421	-0.282788	-2.643943
O	-1.792683	-1.589136	0.726304
O	-3.937837	-0.253911	-0.106279
O	-1.261618	0.675786	-0.777972
C	-1.062921	-2.684051	1.016485
C	-0.620246	-2.933754	2.338774
C	0.108400	-4.110395	2.593567
H	0.442714	-4.302725	3.604500
C	0.423420	-5.060563	1.598945
C	-0.000121	-4.793573	0.307827
H	0.220249	-5.482741	-0.502211
C	-0.732810	-3.617492	-0.028469
C	-1.098258	-3.411812	-1.379513
H	-0.822693	-4.185755	-2.095126
C	-2.010945	-2.311743	-3.309511
H	-2.891403	-2.930486	-3.550678
H	-1.164697	-2.716499	-3.883225
C	-2.282808	-0.861213	-3.726019
H	-1.334404	-0.313294	-3.799151
H	-2.797425	-0.795078	-4.692253
C	-4.145319	0.393170	-2.896178
H	-4.410785	0.590481	-3.940445
C	-5.052256	0.893274	-1.897518
C	-6.117320	1.708701	-2.341909
H	-6.161494	1.939383	-3.401953
C	-7.068075	2.199961	-1.466595
C	-6.924167	1.823511	-0.111089
H	-7.664377	2.195906	0.586336
C	-5.911445	1.009903	0.393536
C	-4.922827	0.527042	-0.525125
C	0.010798	0.858336	-0.706069
C	0.511810	2.187720	-0.495707
H	-0.208809	2.995139	-0.426981
C	1.858035	2.433596	-0.412753
H	2.218887	3.448683	-0.297485
C	2.314253	0.053108	-0.778501
H	3.022213	-0.765270	-0.832910
C	0.966876	-0.205104	-0.839944
H	0.608905	-1.219629	-0.959009
C	2.793217	1.371676	-0.557735
C	4.797497	2.484509	0.438840
C	5.152044	1.058557	-1.322479
C	4.248031	3.186620	1.514533
C	6.184751	2.464326	0.188382
C	5.005513	0.228504	-2.430629
C	6.410894	1.566107	-0.930773
C	5.093069	3.943642	2.336625
H	3.188506	3.131121	1.721442
C	7.028839	3.212906	1.008884
C	6.147755	-0.168142	-3.149096
H	4.023482	-0.097129	-2.749948
C	7.542336	1.180515	-1.643425
C	6.477795	3.947272	2.056381
H	8.102249	3.216340	0.843943
C	7.402388	0.312837	-2.730288
H	8.524321	1.555507	-1.370165
H	7.146472	4.526544	2.684902
H	8.296683	0.022841	-3.268179
N	4.156099	1.621789	-0.484781
C	-5.860110	0.650417	1.893929
C	-4.542946	1.176363	2.513009
H	-3.672451	0.735520	2.026599
H	-4.483788	2.267872	2.417679
H	-4.504000	0.930239	3.581364
C	-7.022073	1.279248	2.690492
H	-7.005397	2.374916	2.654730
H	-8.001469	0.938153	2.335198
H	-6.933496	0.984228	3.742188
C	-5.963042	-0.884049	2.069553
H	-6.919640	-1.252161	1.678063
H	-5.154130	-1.399119	1.550388
H	-5.914026	-1.145553	3.134038
C	-0.931583	-1.948210	3.488562
C	-0.320167	-2.388327	4.835400
H	-0.567343	-1.644443	5.602283
H	-0.714552	-3.353044	5.174941
H	0.772583	-2.463993	4.789094
C	-0.350211	-0.550006	3.167589
H	0.743195	-0.598917	3.084502
H	-0.749058	-0.162975	2.229177
H	-0.592397	0.158070	3.971402
C	-2.461271	-1.851307	3.692230
H	-2.871955	-2.828274	3.977811
H	-2.697581	-1.141262	4.496227
H	-2.957760	-1.520521	2.779491
C	5.980088	-1.098063	-4.366834
C	5.077166	-0.410136	-5.419020
H	4.946291	-1.065448	-6.288208
H	4.082097	-0.183578	-5.021686
H	5.523992	0.528891	-5.765344
C	7.325997	-1.433198	-5.036961
H	8.006379	-1.951868	-4.352258
H	7.151403	-2.094205	-5.892879
H	7.831473	-0.535461	-5.410307
C	5.322323	-2.424109	-3.914984
H	5.943568	-2.937225	-3.171972
H	4.333898	-2.260848	-3.472621
H	5.196312	-3.093971	-4.773727
C	4.558246	4.752669	3.533453
C	3.030468	4.632534	3.688425
H	2.499104	5.008800	2.806666
H	2.716825	3.597272	3.864449
H	2.703249	5.226199	4.548751
C	5.217157	4.238801	4.836245
H	6.307481	4.335294	4.809979
H	4.852007	4.814253	5.695125
H	4.976097	3.183343	5.007333
C	4.907164	6.247804	3.336645
H	5.987461	6.409972	3.262578
H	4.443306	6.642127	2.425199
H	4.539497	6.834745	4.186615
C	-8.236900	3.103978	-1.895386
C	-8.222277	3.388785	-3.409124
H	-7.303713	3.900631	-3.718553
H	-8.315890	2.468669	-3.997469
H	-9.066484	4.036605	-3.670858
C	-9.580994	2.420686	-1.547684
H	-9.673660	2.223484	-0.474345
H	-10.421604	3.061210	-1.841689
H	-9.681287	1.464582	-2.074550
C	-8.146755	4.457491	-1.150481
H	-8.185064	4.328843	-0.063395
H	-7.212496	4.976874	-1.394192
H	-8.982242	5.107676	-1.438005
C	1.212420	-6.328665	1.980056
C	0.422290	-7.135766	3.037840
H	0.976782	-8.036645	3.330902
H	0.238068	-6.547312	3.942827
H	-0.550067	-7.450419	2.640254
C	2.587082	-5.932965	2.569950
H	3.157000	-6.826297	2.856250
H	3.179437	-5.373995	1.835495
H	2.480136	-5.304784	3.460464
C	1.463490	-7.251440	0.772090
H	2.052378	-6.752137	-0.006034
H	2.021397	-8.139156	1.092795
H	0.525268	-7.593331	0.320254