Supporting Information

An *o*-Carborane-Based Naphthalene Macrocyclic Arene: Dual-State Emission and C_{60} Recognition

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1. NMR and HR-MS (ESI) Spectra of Compounds

Figure S1. ^{1}H NMR spectrum of **3** (500 MHz, $CDCl_3$).

Figure S2. ^{13}C NMR spectrum of **3** (126 MHz, $CDCl_3$).

Figure S3. ^{1}H NMR spectrum of **4** (500 MHz, $CDCl_3$).

Figure S4. ^{13}C NMR spectrum of **4** (126 MHz, $CDCl_3$)

Figure S5. $^{11}B\{^{1}H\}$ NMR spectrum of **4** (160 MHz, $CDCl_3$)

Figure S6. ^{1}H NMR spectrum of **5** (500 MHz, $CDCl_3$).

Figure S7. ^{13}C NMR spectrum of **5** (126 MHz, $CDCl_3$)

Figure S8. $^{11}B\{^{1}H\}$ NMR spectrum of **5** (160 MHz, $CDCl_3$)

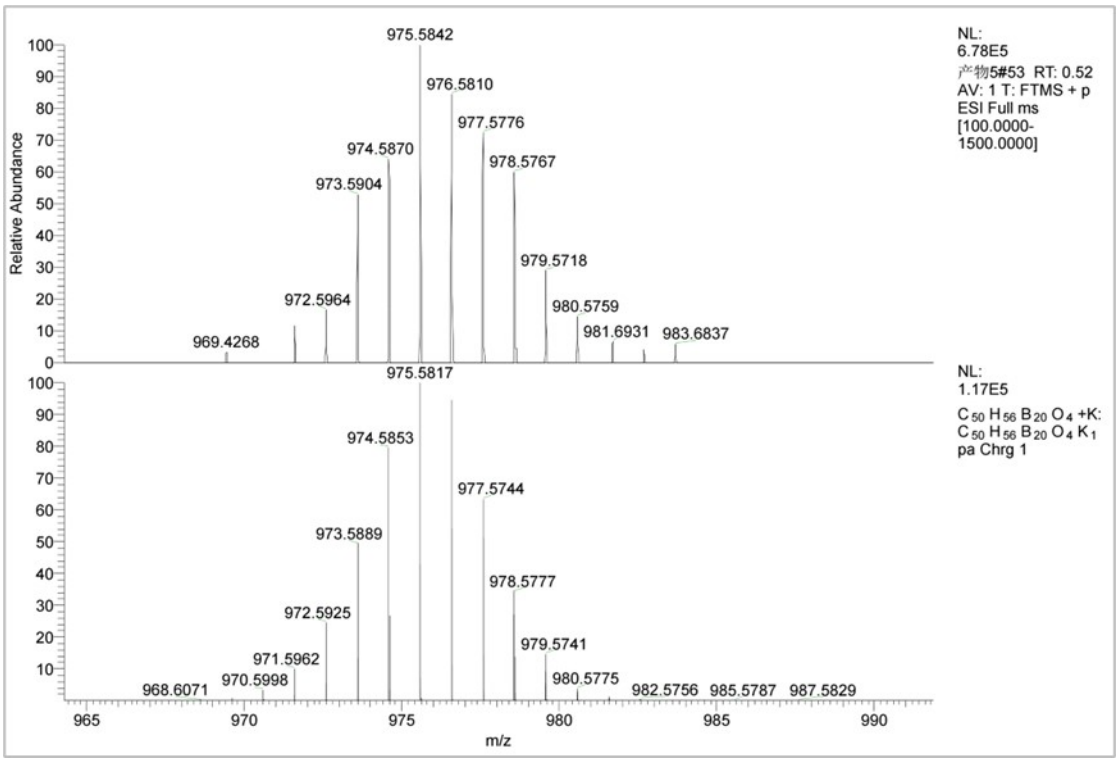

Figure S9. HR-MS (ESI) spectrum of **5**.

2. Crystal Data and Structure Refinement

Table S1. Crystal data and structure refinement for **5**.

Compound	5
Empirical formula	$C_{50}H_{56}B_{20}O_4$
Formula weight	937.15
Temperature/K	293K(2)
Crystal system	monoclinic
Space group	P -1
a/Å	11.3775(6)
b/Å	11.5862(7)
c/Å	25.9327(6)
α/°	91.335(3)
β/°	99.372(3)
γ/°	118.660(6)
Volume/Å^3	2939.3(3)
Z	2
ρ_{calc}g/cm^3	1.059
μ/mm^{-1}	0.448
F(000)	976.0
Crystal size/mm^3	0.11 × 0.11 × 0.25
Radiation	CuKα (λ = 1.54184)
Final R indexes [I>=2σ (I)]	R_1 = 0.0732, wR_2 = 0.2255
Final R indexes [all data]	R_1 = 0.1054, wR_2 = 0.3545
CCDC	2529589

3. Fluorescence Properties

Table S 2. Photophysical Data of Compound **5** in Different Solvents.

Solvents	ε	n	f(ε, n)	λ_a(nm)	λ_f(nm)	$\Delta\lambda$(nm)	ν_a-ν_f(cm^{-1})
MePh	2.38	1.496	0.014	314	569	255	14272
DCM	8.93	1.424	0.217	315	615	300	15486
$CHCl_3$	4.81	1.447	0.148	314	598	284	15125
THF	7.58	1.407	0.209	315	625	310	15746
DMSO	48.9	1.479	0.280	315	646	331	16266
MeCN	37.5	1.344	0.305	315	660	345	16595
MeOH	33.6	1.329	0.309	315	650	335	16361
DMF	36.7	1.4305	0.274	315	685	370	17147

ε: Static dielectric constant of the solvent. n: Refractive index of the solvent at the measurement temperature. f (ε, n): Orientation polarizability (Lippert-Mataga solvent polarity parameter), calculated using the formula $\Delta f = \frac{\epsilon - 1}{2\epsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$.

λ_a: Maximum absorption wavelength. λ_f: Maximum fluorescence emission wavelength. Δλ: Stokes shift.

ν_a-ν_f: Stokes shift, expressed in wavenumbers (cm^{-1}), calculated as ν_a-ν_f = $(\frac{1}{\lambda a} - \frac{1}{\lambda f}) \times 10^7$.

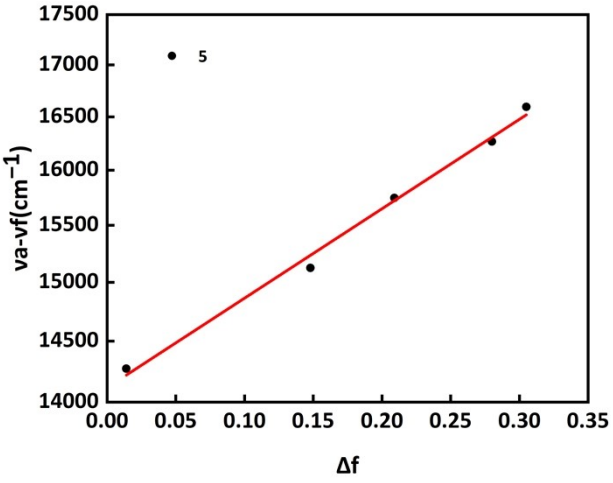

Figure. S10 Solvatochromic Lippert – Mataga models of **5**.

Figure S11. DLS data of **5** in H_2O.

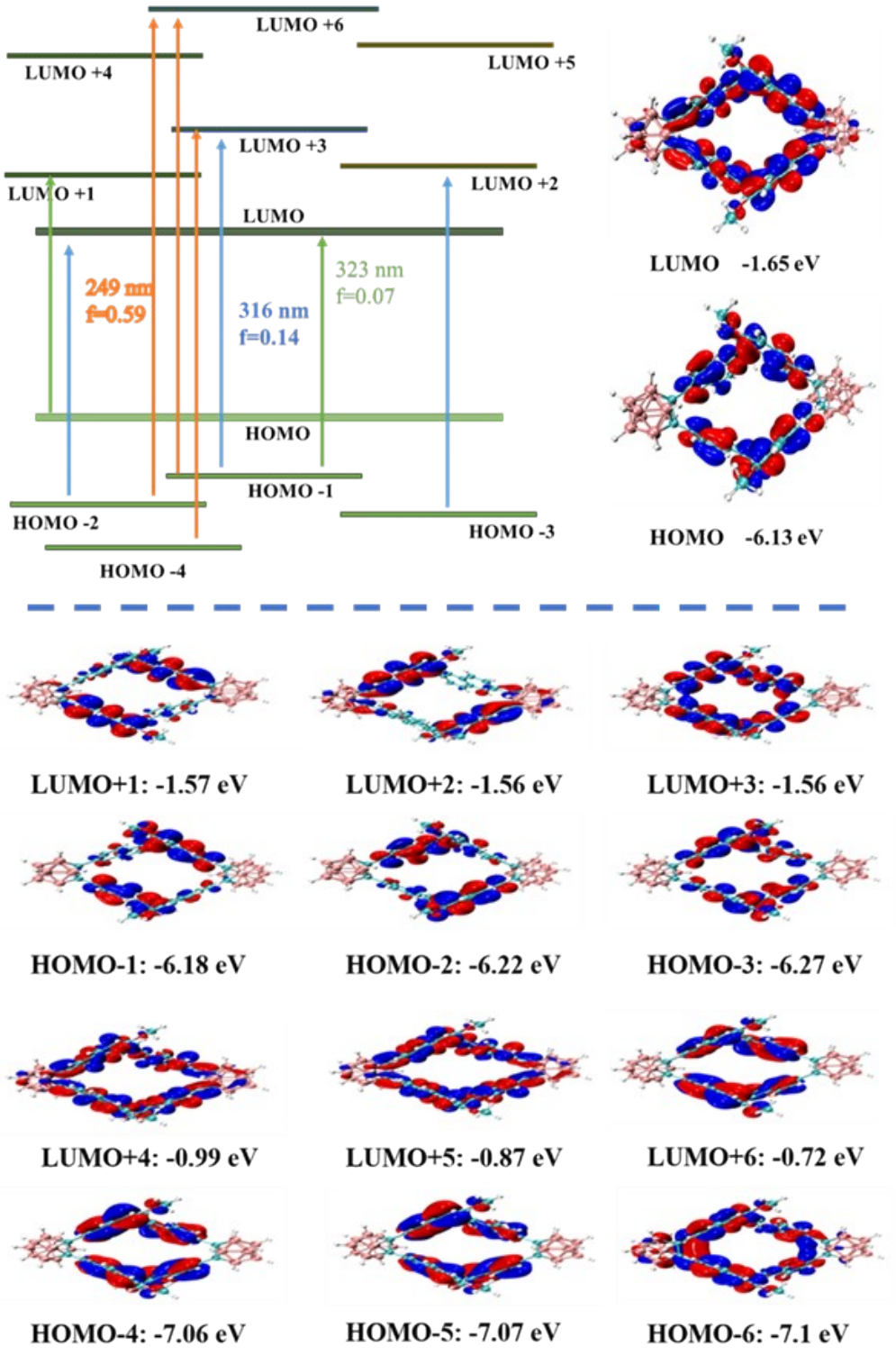

Figure S12. TD-DFT Calculations for Compound **5** at the PBE1PBE Level

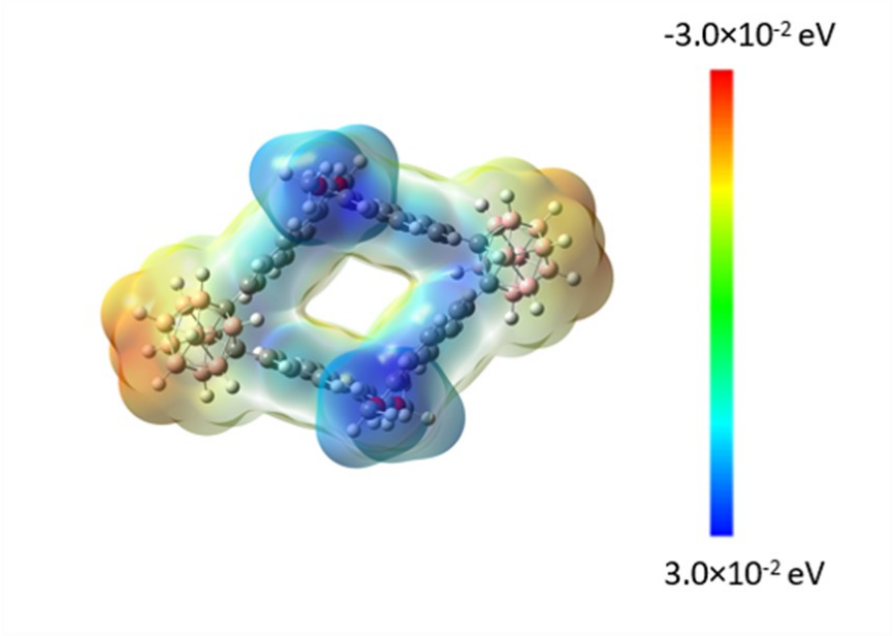

Figure S13. Electrostatic Potential Surface Analysis of **5**

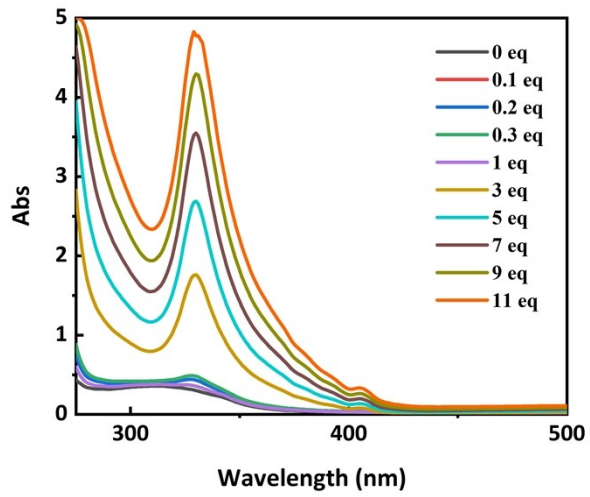

Figure S14. UV-vis titration of **5** (1.0×10^{-5} M) in toluene at 298 K with the C_{60} (0-15 eq).

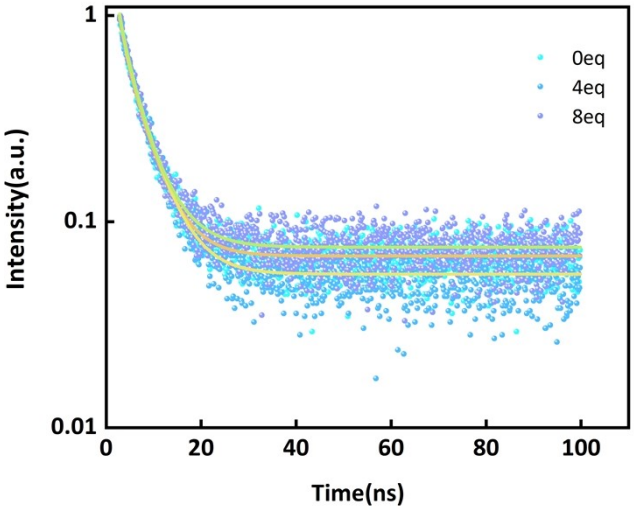

Figure S15. Ffluorescence lifetime curves of **5** (1.0×10^{-5} M) in toluene at 298 K with different equivalents of C_{60} (0-8 eq) excited at 340 nm.