

The role of water in THF/water mixtures on CMC, aggregation sizes, and fluorescence quenching of a new calix[4]resorcinarene macrocycle.

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TABLE OF CONTENTS

Materials and Methods.....	S2
Compounds (a) and C1 synthesis reaction	S6
Compound (a) ESI-MS spectra.....	S8
Compound (a) ¹ H NMR spectra	S8
Compound C1 ESI-MS spectra	S9
Compound C1 ¹ H NMR spectra	S9
Absorption spectra at several concentrations in THF/H ₂ O solutions	S10
Absorbance vs. concentration of C1 at 355 and 600 nm	S11
Chemometric analysis of absorption spectra	S12
DLS measurement.....	S15
Normalized luminescence spectra.....	S17
Chemometric analysis of luminescence spectra	S17
AFM measurement.....	S18
DFTBA optimized structures as models of C1	S20
Calculated electronic transitions	S21
NTO analysis of electronic transitions.....	S67
References.....	S87

MATERIALS AND METHODS

1. Materials and Instrumentation

All the necessary chemicals, including 4-hydroxybenzaldehyde, potassium carbonate (K₂CO₃), resorcinol, 1-hexadecanoyl chloride, and acetone, were obtained from Wako Pure Chemical Industries in Osaka, Japan. Distilled water was used to prepare all the solutions, and analytical grade solvents were used in this research without any further purification. Commercial-grade solvents (n-hexane, ethyl acetate, dichloromethane) were employed to purify the compounds through silica gel chromatography after distillation. UV-visible analysis was performed using a Cary-60 spectrophotometer, while ¹H-NMR spectroscopy

was carried out using a Bruker AVANCE III spectrometer. Molecular mass was determined by ESI-MS (Bruker Compass Data Analysis 4.2).

2. Atomic Force Microscopy

The formation of **C1** macrocycle aggregates from neat THF or TFH/H₂O solutions was observed using Atomic Force Microscopy (AFM). The concentration of the macrocycle was kept at 4×10^{-8} M in all experiments, and a 10 ml sample was spotted onto freshly cleaved muscovite mica in a stepwise manner. The sample was then dried under N₂. All images were captured in ambient conditions with a MultiMode Scanning Probe Microscope (Veeco, Santa Barbara, CA, USA) equipped with a Nanoscope V controller (Veeco, Santa Barbara, CA). The measurements were obtained in tapping mode using probes doped with silicon nitride (RTESP, Veeco) with a tip radius of 8-12 nm, 271-311 kHz, and a force constant of 20-80 N/m. The typical scan rates ranged from 1-1.5 Hz.

3. Steady-state and time-resolved emission experiments

In this study, fluorescence measurements were conducted using single-photon-counting equipment, FL3 TCSPC-SP (Horiba Jobin Yvon), at room temperature. The emission spectra were adjusted for source intensity (lamp and grating) using standard correction curves. Fluorescence quantum yields were measured using an Edinburgh Spectrofluorometer FS5 with SC-30 integrating sphere cassette. For time-resolved fluorescence experiments, a NanoLED excitation source (maxima at 295 nm) was used. The emitted photons were detected by a TBX-04 detector, which was connected to a TBX-PS power supply and counted by a FluoroHub-B module. The DataStation measurement control software application was used to control the module. The counting time window for the measurements reported in this study was 0 - 200 ns. The decay curve was measured at 320, 330, and 340 nm for a given solution. Lifetime analysis was performed using the commercial DAS6 Fluorescence Decay Analysis software. The quality of the fit was assessed by minimizing the reduced chi-squared function (χ^2) and visual inspection of the weighted residuals and their autocorrelation. A fit calculation (up to 2 exponentials) was performed on the separate 320, 330, and 340 nm fluorescence decay curves. For samples with lifetimes in the ns order, an instrument response function calibration (IRF) was performed using a diluted Ludox® dispersion.

4. Dynamic Light Scattering

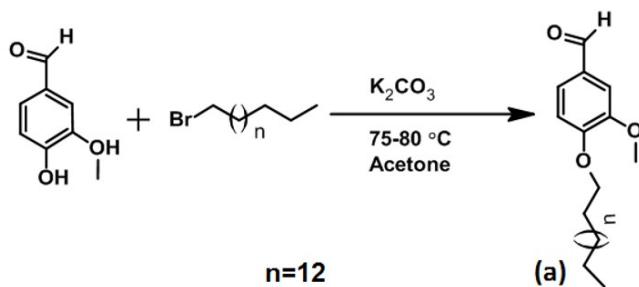
The size of the particles of **C1** was measured using Dynamic Light Scattering (DLS) in neat THF, as well as in THF/H₂O mixtures containing different percentages of water (53/47 and 5/95 v/v) at 25°C. The concentration range for DLS measurements of **C1** was between 0.5mM and 1.5mM. The Zetasizer Nano equipment (Nano ZSizer-ZEN3600, Malvern, UK) was used for the measurements.

5. Synthesis of compound C1

The compound **C1** (2, 4, 6, 8-tetrakis (4-hexadecyloxy)-3-methoxyphenyl)-1, 3, 5, 7 (1, 3)-tetrabenzenacyclooctaphan-1⁴, 1⁶, 3⁴, 3⁶, 5⁴, 5⁶, 7⁴, 7⁶-octaol), was synthesized through a reaction between compound (**a**) and resorcinol (see **Scheme S1**). Compound (**a**) was prepared by reacting 4-hydroxy-3-methoxybenzaldehyde with 1-bromohexadecane in the presence of K₂CO₃ in acetone at 80°C involving a bimolecular nucleophilic substitution reaction. The progress of the reaction was monitored using the TLC technique with the solvent system consisting of n-hexane and ethyl acetate (9:1, v/v). After the reaction was completed, it was stopped and cooled to room temperature. The salt-added water was removed, and the resulting mixture was extracted with ethyl acetate. The extract was then purified through column chromatography using n-hexane and ethyl acetate in a 98:2 ratio (v/v). ESI-MS technique was used to determine the molecular mass (**Figures S1**) which observed at 376.9 *m/z* in agreement with the molecular formula C₂₄H₄₀O₃. Further characterization was performed by ¹H-NMR, FTIR, and their melting point. The ¹H-NMR of (**a**) was performed at 400 MHz in CDCl₃ (**Figure S2**). A triplet of 3H proton of CH₃ appeared at δ = 0.87 ppm with coupling constant 7.4 Hz, a multiplet of 26H of CH₂ at δ = 1.23 ppm, a triplet with 2H of methylene at δ = 1.42 ppm with coupling constant 8.0 Hz, a triplet of 2H of CH₂ at δ = 1.59 ppm with coupling constant 8.0 Hz, a singlet of 3H of OCH₃ at δ = 3.90 ppm, a triplet of 2H of CH₂ at δ = 4.05 ppm with coupling constant 8.0 Hz, a doublet of 1H of benzene at δ = 6.92 ppm with coupling constant 8.0 Hz, a quartet of 2H of CH of aromatic ring at δ = 7.38 ppm with coupling constant 8.0 Hz. FT-IR (KBr, cm⁻¹): 2917.4 (C-H, CH₃), 2847.8 (C-H, CH₂), 1679.0 (aromatic aldehyde, CHO), 1590.2 (C=C, aromatic group), 1272.4 (ether, -O-CH₃, -O-CH₂).¹Yield: 1640 mg, 87.2 %, M.P.: 68.2 - 70.1 °C.

The compound **C1** was obtained by cyclizing compound (**a**) and resorcinol in the presence of sulfuric acid as a catalyst and acetic acid as a solvent. The reaction mixture was heated at 80°C for 18 hours. A brown precipitate was formed, which was filtered, and various spectroscopic techniques were utilized for the characterization of the synthesized compound. ESI-MS technique was used to determine the molecular mass (**Figures S3**). For compound **C1** the mass was observed at 1872.3 m/z , in agreement with the formula $C_{120}H_{176}O_{16}$. The 1H -NMR were performed at 400 MHz in pyridine (**Figure S4**) and a triplet of 8H of terminal methyl group appeared at $\delta = 0.84$ ppm with coupling constant 7.2 Hz, a multiplet of 104H of methylene appeared at $\delta = 1.26$ ppm, a triplet of 8H of CH_2 appeared at $\delta = 1.52$ ppm with coupling constant 7.2 Hz, a singlet of 12H of OCH_3 appeared at $\delta = 3.68$ ppm, a quartet of 8H of CH_2 appeared at $\delta = 4.04$ ppm with coupling constant 8.0 Hz, a triplet of 8H of ArCH with coupling constant 3.6 Hz appeared at $\delta = 6.78$ ppm, a triplet of 8H of ArCH appeared at $\delta = 6.81$ ppm with coupling constant 5.2 Hz, a triplet of 8H of ArCH appeared at $\delta = 6.92$ ppm with coupling constant 2.4 Hz, a singlet of 8H of OH appeared at $\delta = 8.69$ ppm. FT-IR (KBr, cm^{-1}): 3449.4 (resorcinol, OH), 2922.9 (C-H, CH_3), 2852.2 (C-H, CH_2), 1611.2 (C=C, aromatic group), 1513.1 (C=C, aromatic group), 1261.8 (ether, -O- CH_3 , -O- CH_2).¹ Yield: 1670 mg, 89 %. M.P. 170-174 °C.

First step



Second step

6. Theoretical calculations

Density functional theory (DFT) calculations were carried out using Gaussian 16 program package.² The structures of the compounds in their ground state were optimized with DFTBA in a vacuum as implemented in the Gaussian 16. DFTBA is a version of the density-functional-based tight-binding semi-empirical calculation that uses analytic expressions for the

Scheme S1. The schematic illustration shows the synthesis of a functionalized calix4resorcinarene macrocycle through a two-step reaction.

matrix elements rather than tabulated ones. No symmetry constraints were utilized in the full optimization of the structures of the compounds in their ground state. Time-dependent DFT calculations, (TD-DFT), were used to locate the lowest-energy 40 vertical excitations of singlet spin multiplicity, starting from the ground-state minimum-energy geometry of each compound. We screened several functionals to predict the electronic structure accurately. The screening process involved the use of various hybrid functionals such as PBE0, B3LYP, CAM-B3LYP, and MN-15 in TD-DFT calculations. These calculations were combined with the polarizable continuum model (PCM) to simulate THF solvation effects. The aim was to obtain a good fit of the experimental absorption spectra with the calculated one. The 6-31G(d,p) basis set was used for all the atoms. After analyzing the results, it was found that the B3LYP hybrid functional gave the most accurate results in reproducing the experimental absorption spectra of the compounds. As a result, all TD-DFT calculations reported below were carried out with the B3LYP functional. The nature of the transitions was assessed with the help of Natural Transition Orbital (NTO) analysis to obtain a more compact orbital representation for the associated electronic transition density matrix. All the pictures showing molecular geometries and orbitals were created using GaussView 6.³ The output files from Gaussian 16 were analyzed with GaussSum.⁴

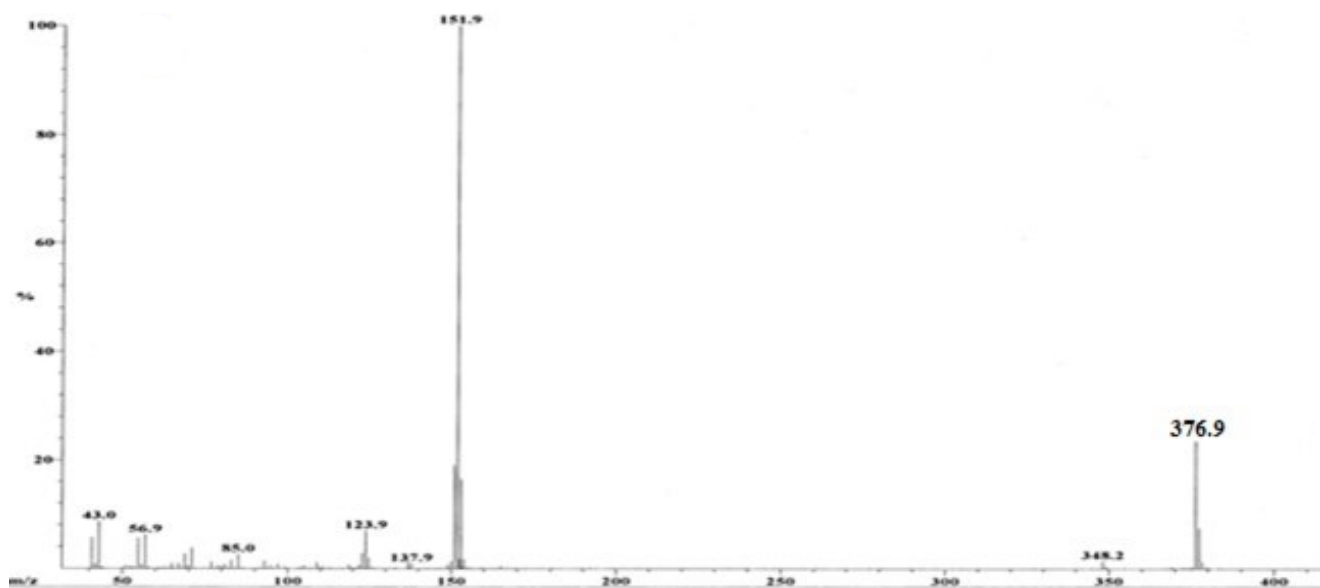


Figure S1. ESI-MS spectra of compound (a)

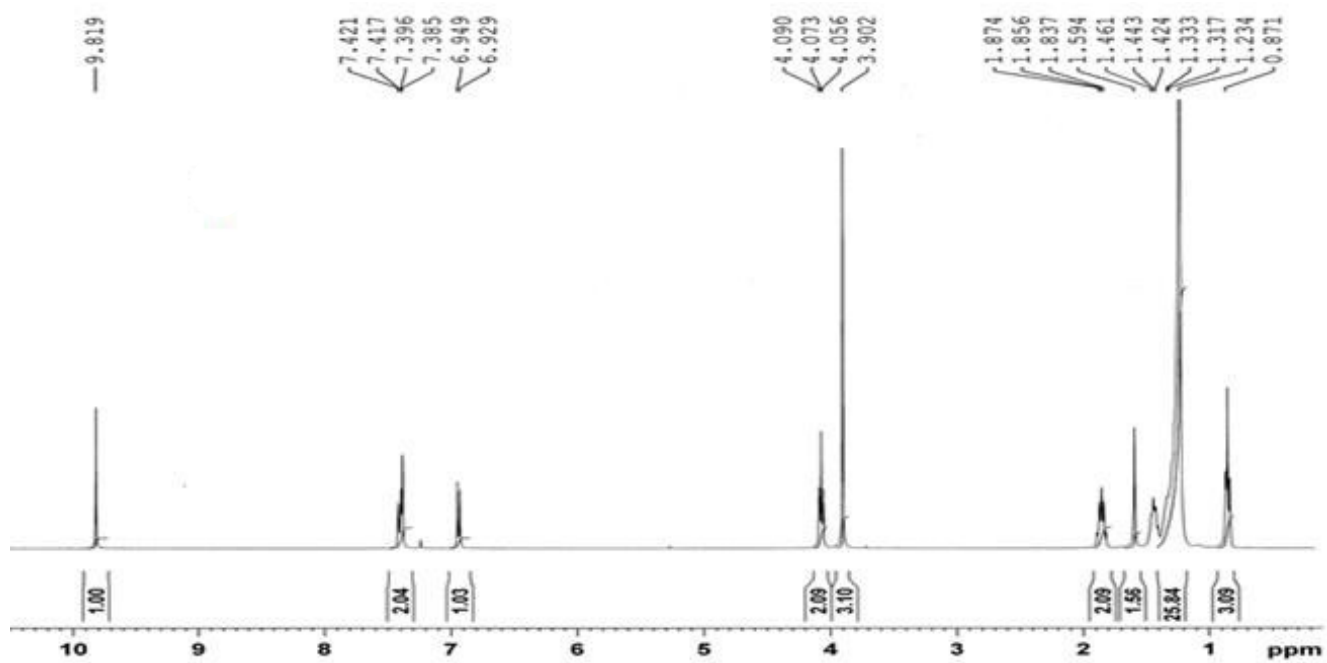


Figure S2. ¹H NMR spectra of compound (a)

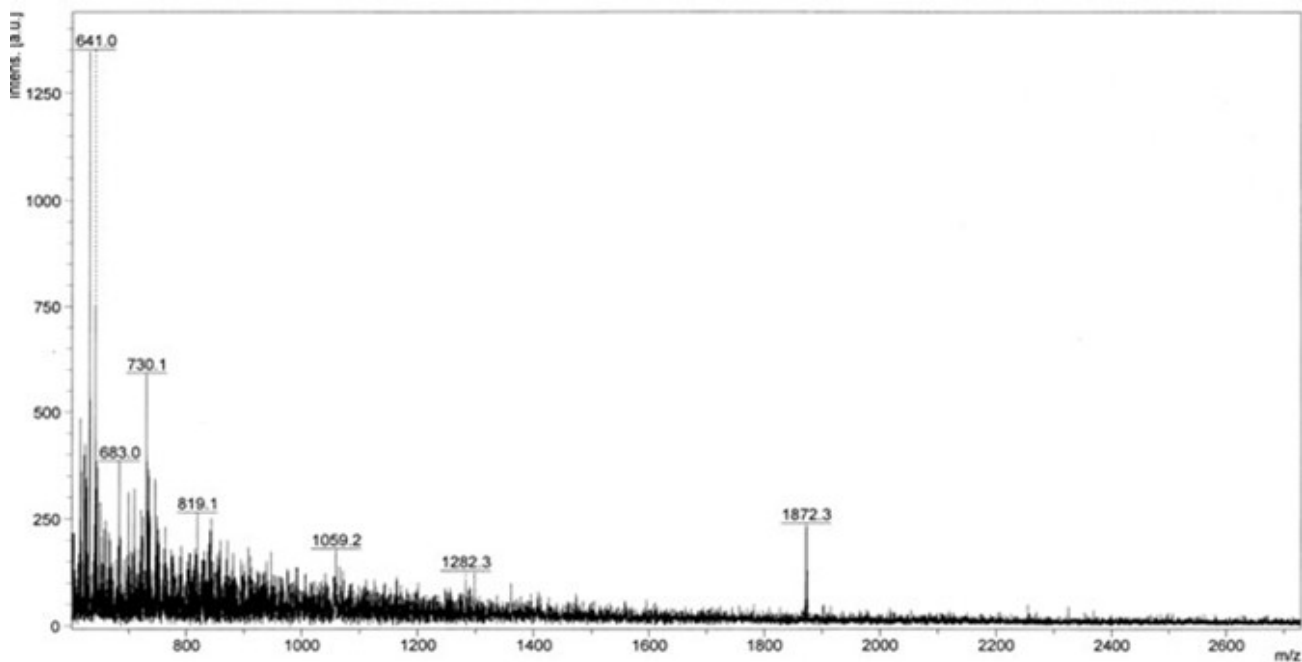
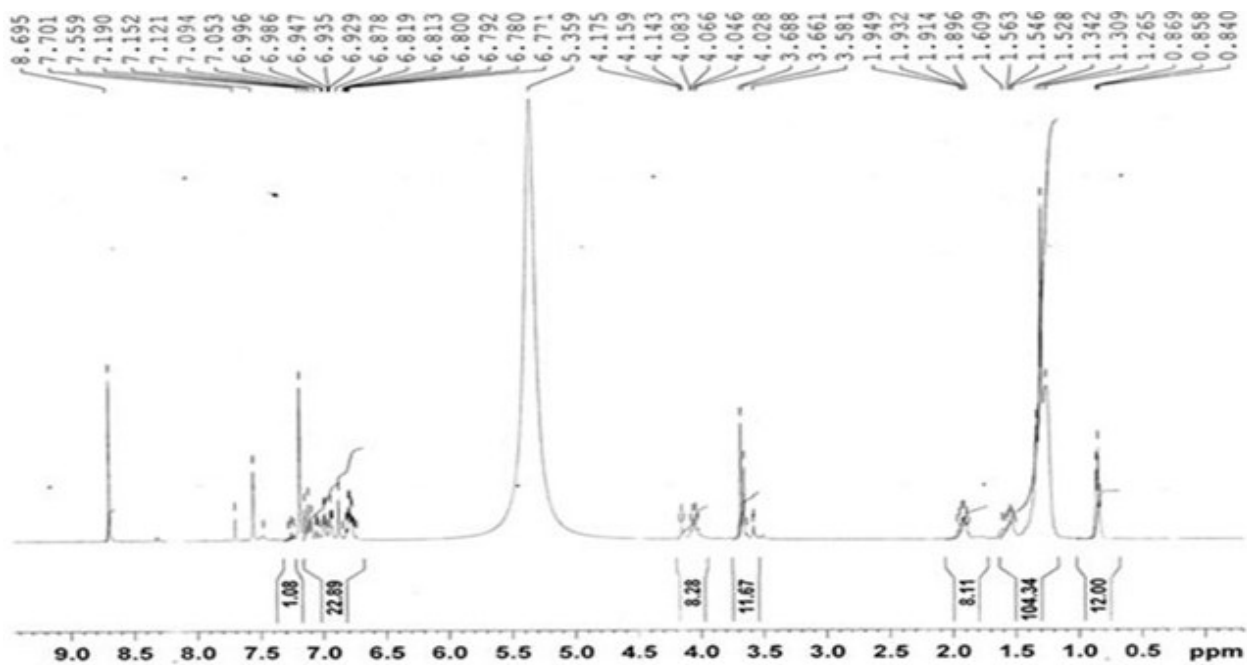
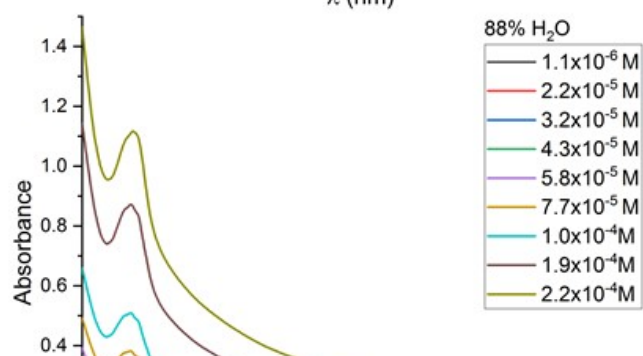
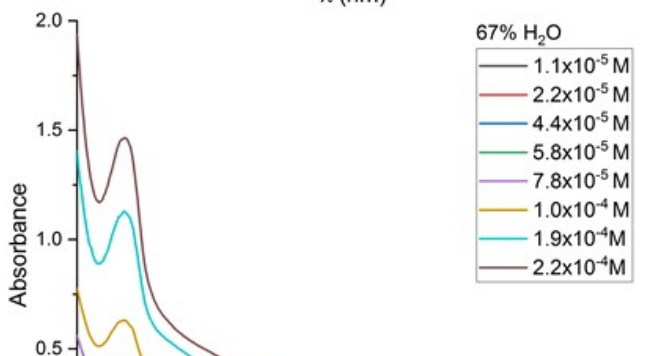
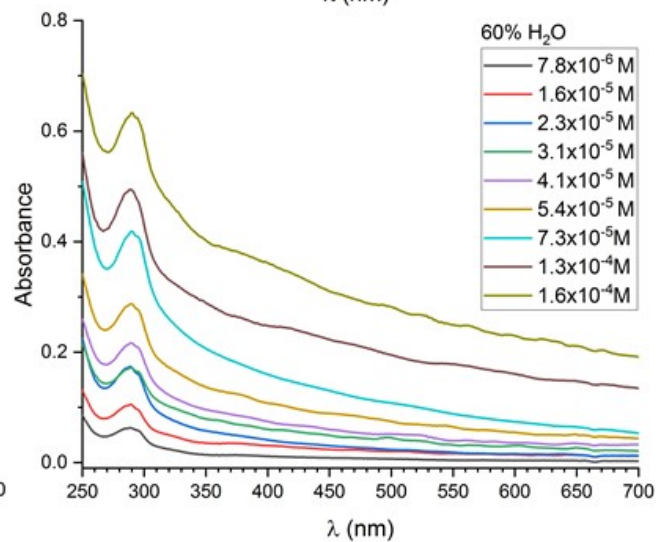
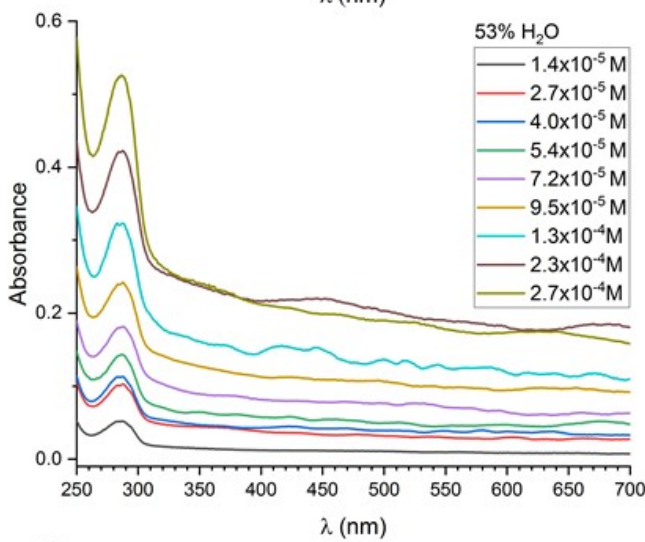
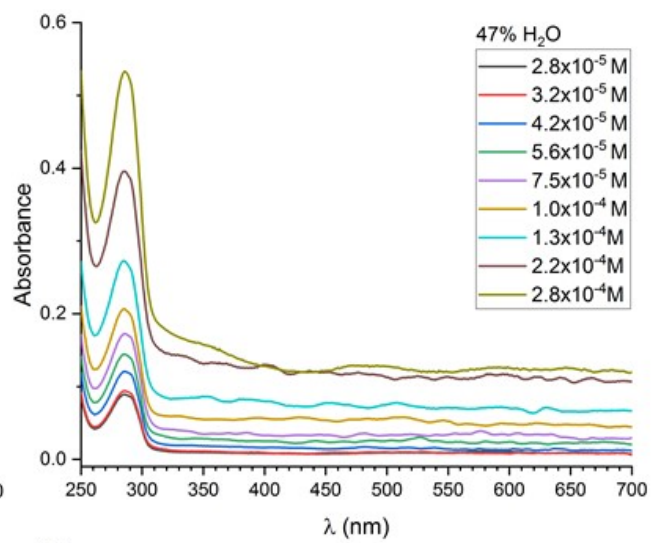
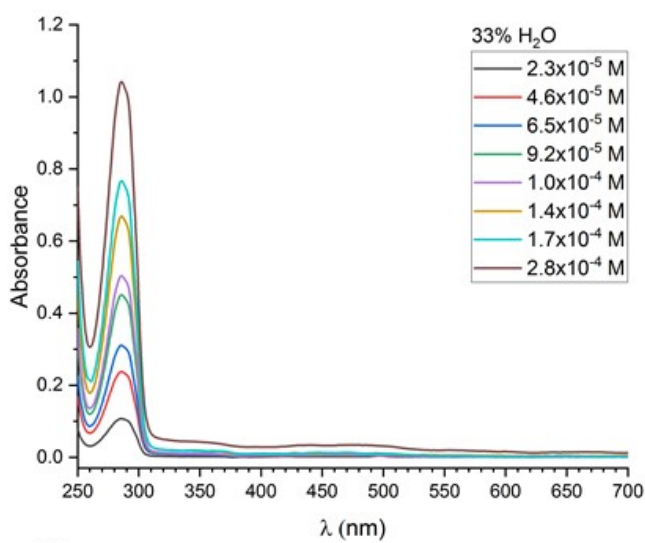


Figure S3. ESI-MS spectra of compound C1





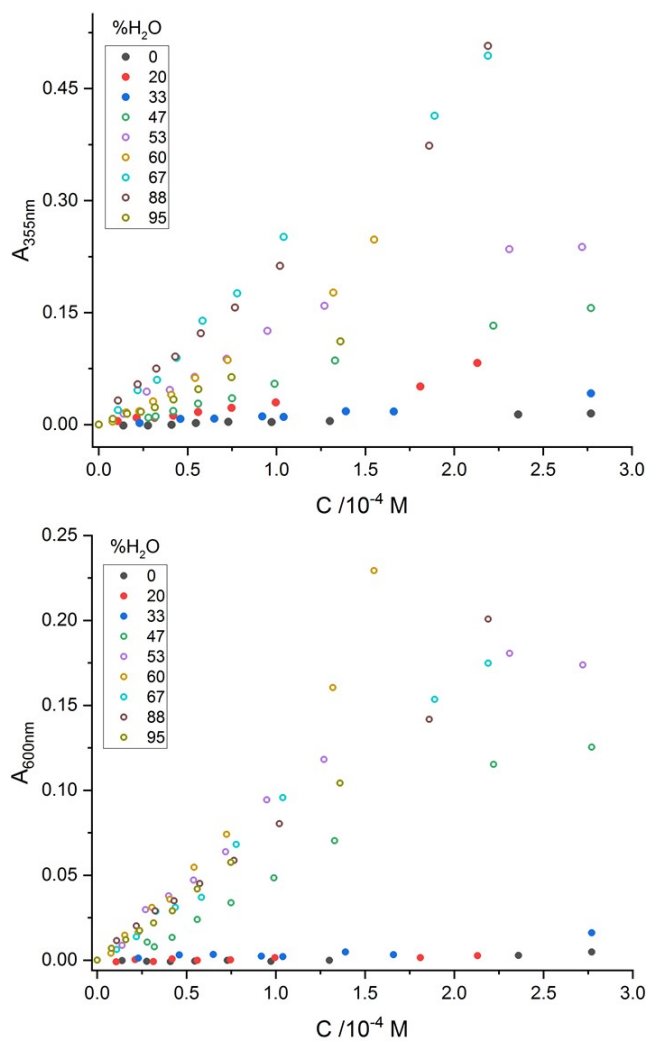


Figure S6. Absorbance vs. concentration of C1 at 355 and 600 nm.

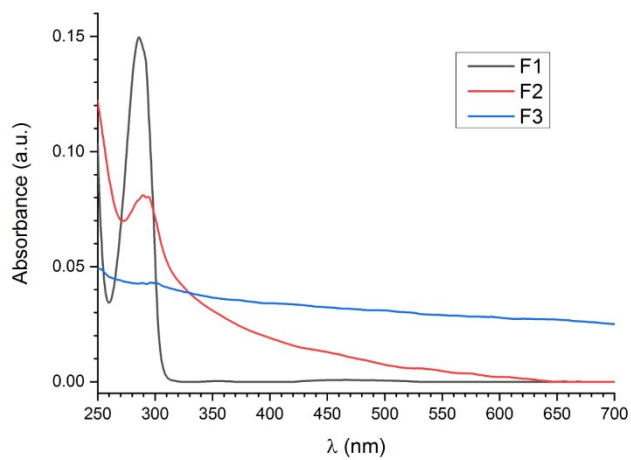


Figure S7. Spectral profiles of F1, F2 and F3.

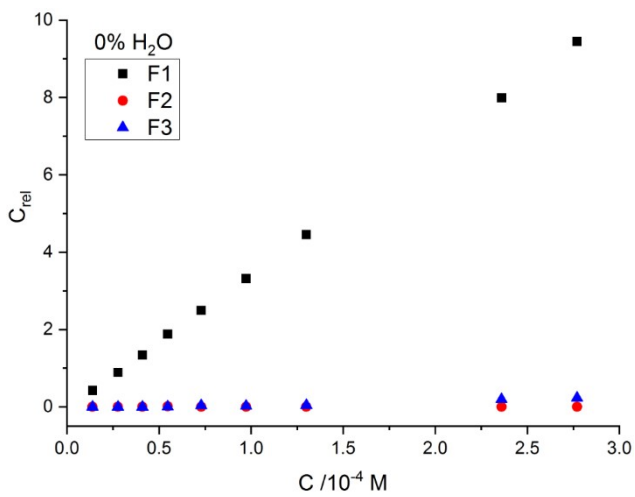
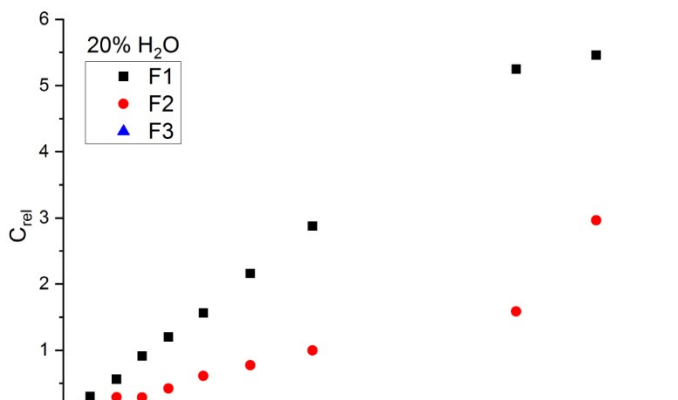


Figure S8. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in pure THF



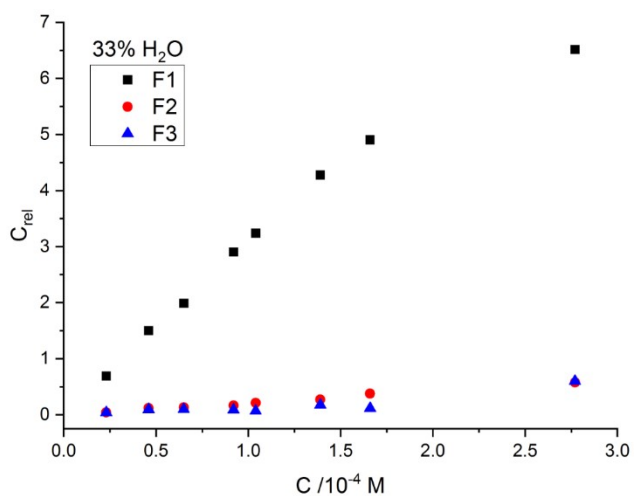


Figure S10. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in THF/H₂O solution at 33% H₂O

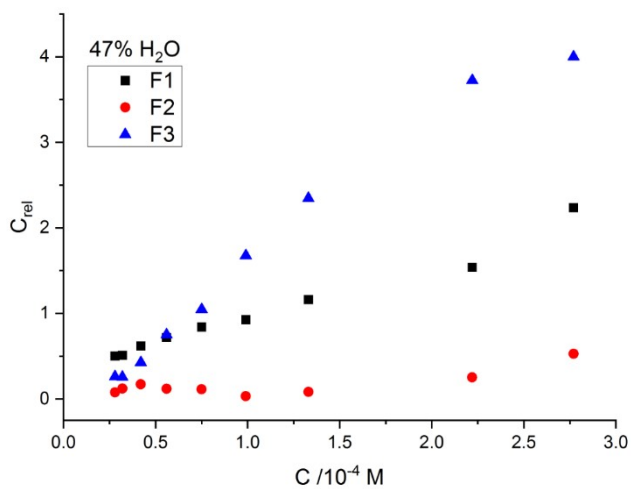
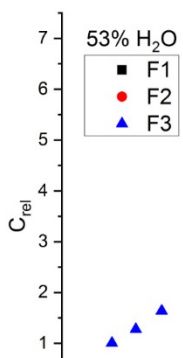


Figure S11. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in THF/H₂O solution at 47% H₂O



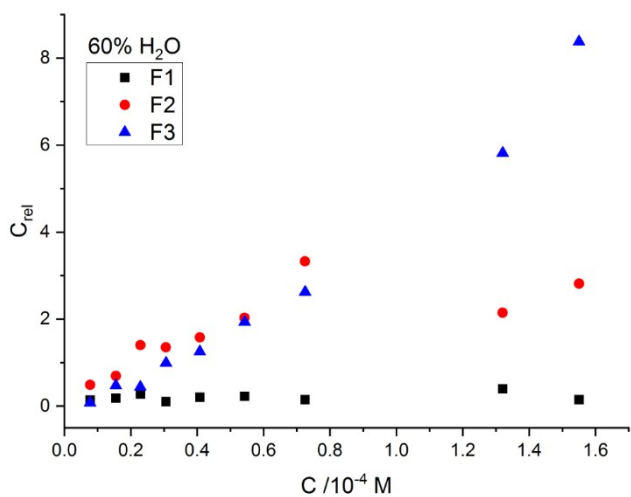


Figure S13. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in THF/H₂O solution at 60% H₂O

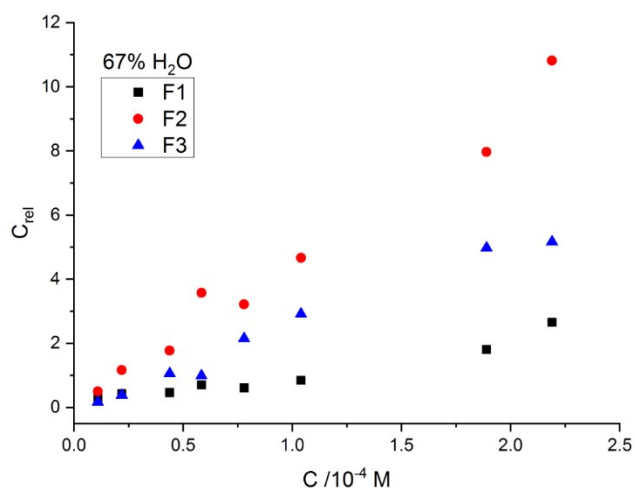
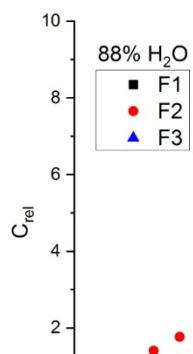


Figure S14. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in THF/H₂O solution at 67% H₂O



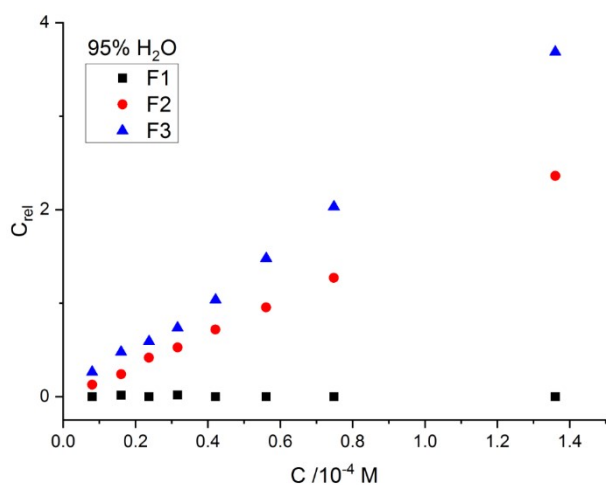


Figure S16. Relative concentrations of F1, F2 and F3 vs. total concentration of C1 in THF/H₂O solution at 95% H₂O

Table S1. DLS measurement of C1 in THF (47%) / H₂O (53%)

Measurement ID	Measurement name	Pdl	Maximum of the distribution in Intensity (nm)	
			Peak 1	Peak 2
1	C153 1	-	818.5	2.864
2	C153 2	-	867.9	2.922
3	C153 3	-	1133	2.894
4	C153 4	-	1100	2.899
5	C153 5	-	936.7	2.909
6	C153 6	-	1151	2.800
Average ±SD (%)		-	1001 ± 145 (94.4)	2.88 ± 0.04 (5.3)



Table S2. DLS measurement of C1 in THF (5%) / H₂O (95%)

Measurement ID	Measurement name	PdI (\pm SD)	Maximum of the distribution in Intensity (nm)
			Peak 1
1	C195 1	0.087	166.0
2	C195 2	0.081	164.6
3	C195 3	0.106	164.4
4	C195 4	0.119	170.2
5	C195 5	0.117	168.3
6	C195 6	0.104	165.2
Average \pm SD (%)		0.10 \pm 0.01	166 \pm 2 (100)

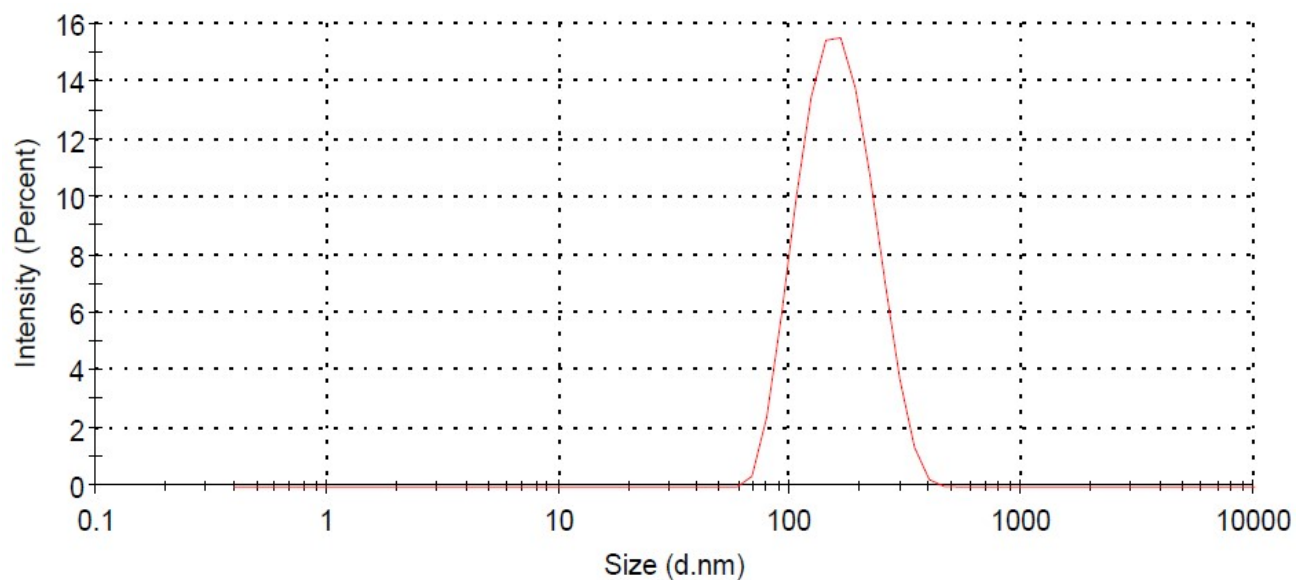


Figure S18. DLS average measurement of C1 in THF (5%) / H₂O (95%)

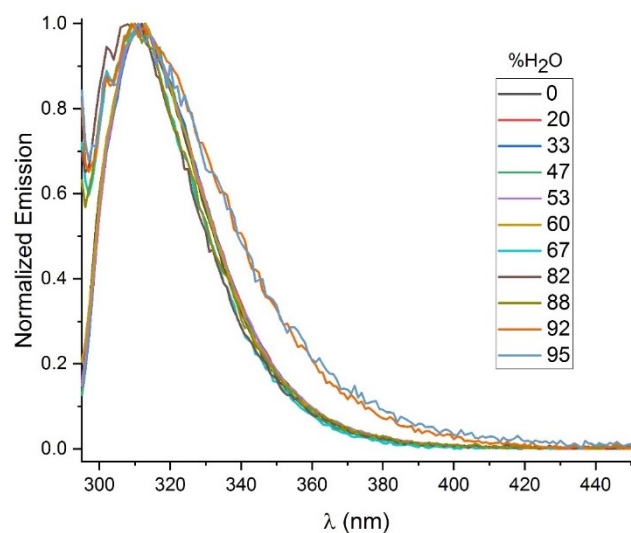


Figure S19. Normalized luminescence spectra of C1 in THF/H₂O mixtures as a function of % H₂O (v:v)

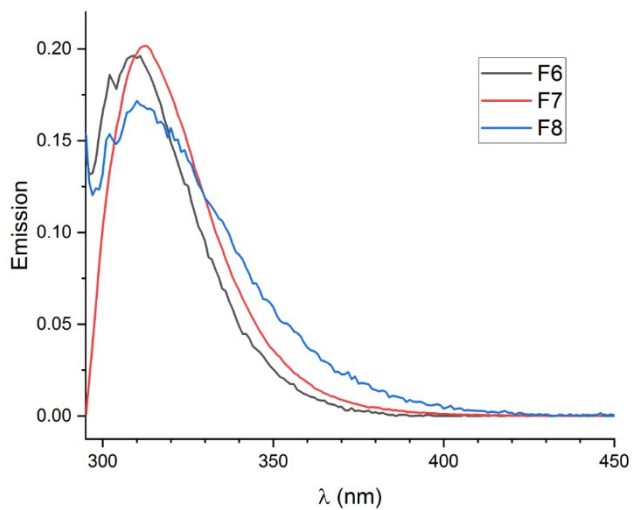
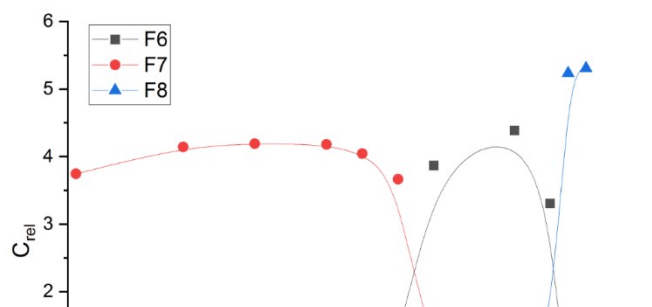


Figure S20. Spectral profiles of F6, F7 and F8



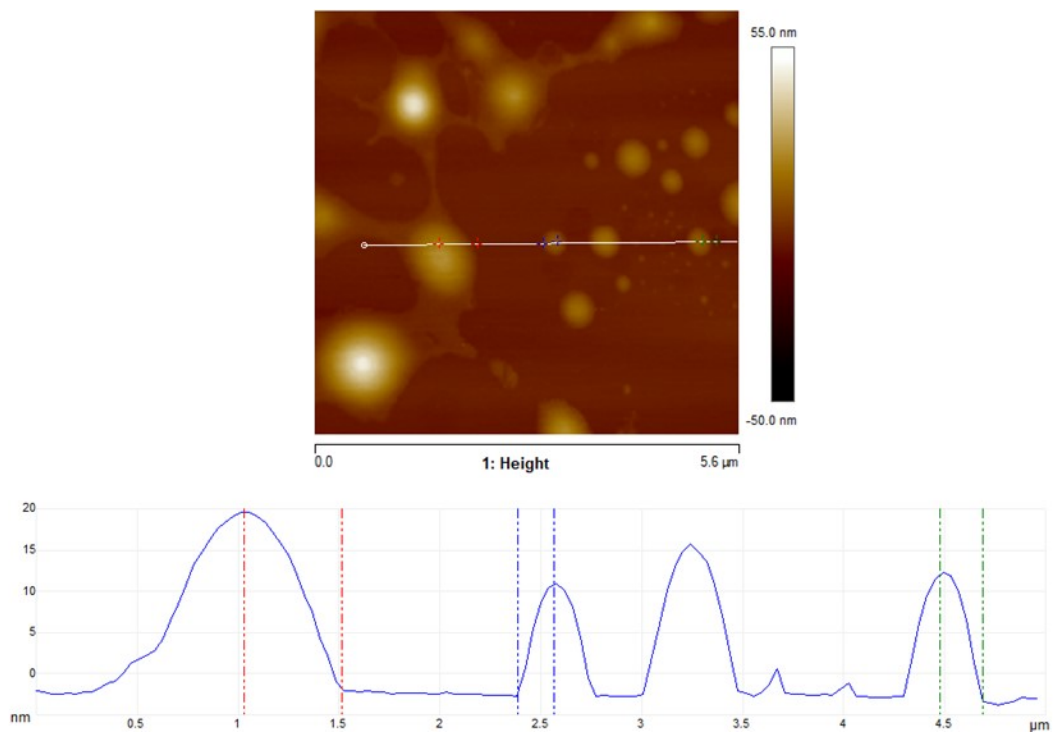


Figure S22. AFM images of C1 in pure THF.

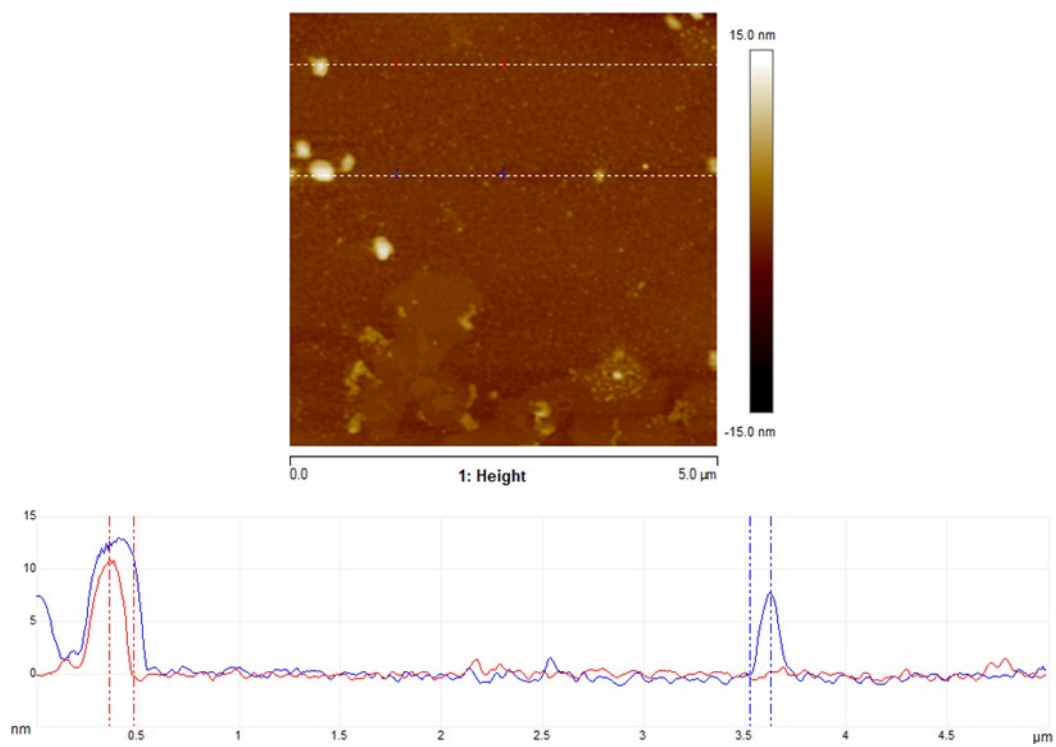


Figure S23. AFM images of C1 in THF (47%) / H₂O (53%).

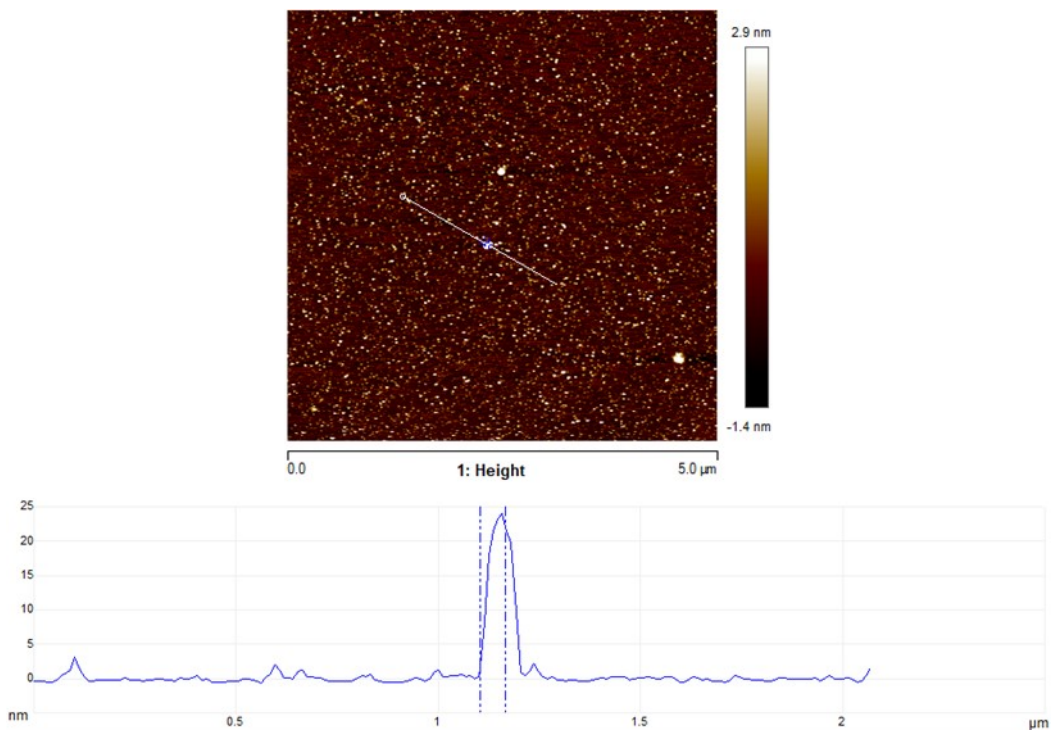
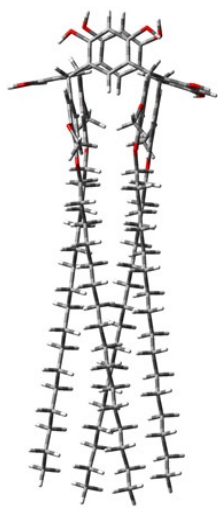
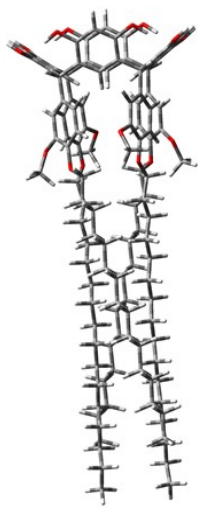


Figure S24. AFM images of C1 in THF (5%) / H₂O (95%).



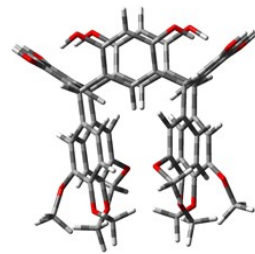
C1-b



C1-c



Cr-b



Cr-c

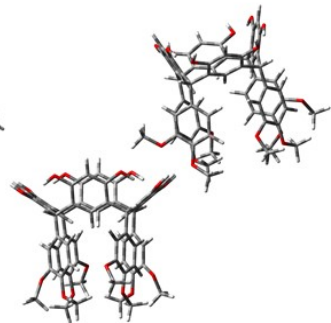
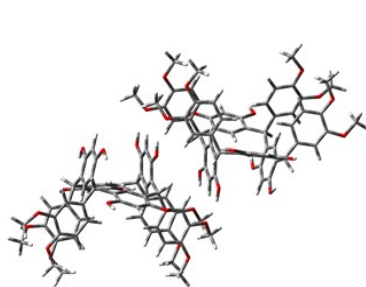
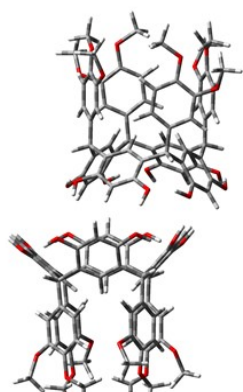
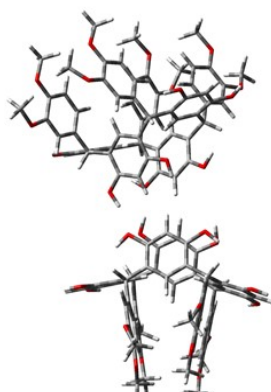


Table S3. Calculated electronic transitions for **C1-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	274.12	4.52	0.023	H-1→LUMO (30%), HOMO→LUMO (36%)	H-1→L+1 (8%), HOMO→L+1 (9%)
2	273.26	4.54	0.246	H-1→LUMO (21%), HOMO→L+1 (59%)	H-3→L+1 (4%)
3	268.05	4.63	0.024	H-2→LUMO (51%), HOMO→LUMO (22%)	H-2→L+2 (3%), H-1→LUMO (4%), H-1→L+1 (6%), HOMO→L+2 (3%)
4	266.07	4.66	0.027	H-3→LUMO (37%)	H-3→L+1 (4%), H-2→LUMO (5%), H-2→L+1 (4%), H-1→LUMO (7%), H-1→L+2 (6%), HOMO→LUMO (8%), HOMO→L+1 (4%), HOMO→L+3

					(7%), HOMO→L+4 (2%)
5	264.62	4.69	0.043	H-1→LUMO (10%), H-1→L+1 (43%)	H-3→LUMO (3%), H-3→L+1 (6%), H-2→L+1 (9%), HOMO→L+1 (8%)
6	263.14	4.71	0.019	H-3→L+1 (24%), H-2→L+1 (28%)	H-4→LUMO (7%), H-3→LUMO (6%), H-1→L+2 (8%), HOMO→L+2 (3%), HOMO→L+3 (5%), HOMO→L+4 (3%)
7	262.98	4.71	0.010	H-2→LUMO (25%), HOMO→LUMO (16%)	H-5→LUMO (3%), H-4→LUMO (6%), H-4→L+1 (5%), H-2→L+2 (4%), H-1→LUMO (7%), H-1→L+1 (3%), H-1→L+2 (4%), HOMO→L+2 (6%), HOMO→L+3 (3%)
8	261.38	4.74	0.054	H-2→L+1 (18%), HOMO→L+3 (14%)	H-5→LUMO (7%), H-5→L+1 (7%), H-4→L+1 (7%), H-3→LUMO (8%), H-1→L+3 (2%), HOMO→LUMO (3%), HOMO→L+4 (7%)
9	259.90	4.77	0.027	H-5→LUMO (18%), H-3→LUMO (10%), H-2→L+1 (14%), H-1→L+1 (19%)	H-4→LUMO (9%), H-1→L+2 (9%), HOMO→LUMO (4%)
10	258.91	4.79	0.053	H-5→L+1 (34%), H-3→L+1 (19%)	H-3→LUMO (7%), H-3→L+4 (3%), H-2→L+1 (4%), H-1→L+1 (6%), H-1→L+2 (3%)
11	257.78	4.81	0.038	H-6→L+1 (10%), HOMO→L+3 (21%)	H-5→LUMO (2%), H-5→L+1 (4%), H-4→L+1 (8%), H-3→L+1 (5%), H-2→L+2 (2%), H-2→L+3 (9%), H-1→L+3 (3%), HOMO→L+1 (4%), HOMO→L+2 (7%)
12	256.11	4.84	0.033	H-4→LUMO (11%), HOMO→L+2 (20%)	H-6→L+1 (8%), H-3→L+1 (9%), H-2→L+1 (3%), H-

					2→L+3 (2%), H-1→L+2 (2%), H-1→L+3 (6%), HOMO→L+1 (4%), HOMO→L+4 (8%), HOMO→L+5 (2%), HOMO→L+7 (2%)
13	255.61	4.85	0.006	H-7→LUMO (19%)	H-7→L+1 (2%), H-5→L+1 (3%), H-4→LUMO (4%), H-4→L+2 (7%), H-3→L+1 (6%), H-3→L+2 (4%), H-3→L+3 (3%), H-2→L+1 (3%), H-1→L+2 (6%), H-1→L+3 (5%), H-1→L+10 (2%), HOMO→L+3 (3%)
14	255.34	4.86	0.022	H-6→L+1 (10%), H-3→L+3 (13%), HOMO→L+2 (10%), HOMO→L+3 (13%)	H-5→L+1 (2%), H-4→LUMO (7%), H-3→L+2 (3%), H-1→L+3 (9%), HOMO→L+4 (5%)
15	254.36	4.87	0.001	H-5→LUMO (35%)	H-7→LUMO (5%), H-4→L+1 (5%), H-4→L+2 (3%), H-3→LUMO (2%), H-2→L+3 (9%), H-1→L+2 (9%), HOMO→L+2 (5%), HOMO→L+3 (2%)
16	253.95	4.88	0.014	H-1→L+2 (17%), H-1→L+4 (12%)	H-7→LUMO (4%), H-5→LUMO (4%), H-4→LUMO (7%), H-4→L+1 (3%), H-3→LUMO (5%), H-3→L+1 (4%), H-3→L+3 (3%), H-2→L+1 (3%), H-2→L+3 (7%), H-1→LUMO (2%), H-1→L+3 (3%), HOMO→L+2 (4%), HOMO→L+7 (2%)
17	253.30	4.89	0.009	H-4→L+1 (29%), HOMO→L+4 (13%)	H-7→LUMO (2%), H-5→L+1 (4%), H-3→L+2 (3%), H-2→L+2 (4%), H-2→L+3 (5%), H-

					2→L+7 (2%), H-1→L+1 (3%), H-1→L+2 (4%), H-1→L+4 (3%), HOMO→L+7 (3%)
18	252.85	4.90	0.030	H-6→L+1 (11%), H-5→L+1 (13%), H-1→L+3 (16%), HOMO→L+4 (10%)	H-7→LUMO (3%), H-6→LUMO (4%), H-4→L+3 (2%), H-3→L+4 (4%), H-1→L+4 (4%), HOMO→L+9 (3%)
19	251.29	4.93	0.007	H-4→LUMO (17%), H-1→L+4 (14%), HOMO→L+6 (14%)	H-2→L+2 (2%), H-2→L+3 (7%), H-2→L+7 (2%), H-1→L+2 (6%), HOMO→L+2 (9%), HOMO→L+5 (3%), HOMO→L+7 (4%)
20	251.02	4.94	0.001	H-1→L+3 (22%), H-1→L+4 (11%)	H-6→LUMO (5%), H-5→L+1 (8%), H-4→L+1 (3%), H-4→L+2 (3%), H-4→L+4 (2%), H-3→L+2 (2%), H-2→L+3 (5%), HOMO→L+4 (7%), HOMO→L+6 (8%), HOMO→L+7 (5%)
21	250.69	4.95	0.018	H-1→L+4 (14%), HOMO→L+5 (14%)	H-7→L+1 (4%), H-6→L+1 (2%), H-5→L+3 (7%), H-4→L+1 (6%), H-3→LUMO (3%), H-3→L+3 (3%), H-3→L+4 (3%), H-3→L+5 (6%), H-2→L+3 (4%), H-1→L+3 (4%), H-1→L+6 (4%), HOMO→L+4 (4%)
22	249.94	4.96	0.007	H-2→L+7 (12%)	H-7→LUMO (3%), H-5→LUMO (5%), H-5→L+2 (4%), H-4→LUMO (6%), H-4→L+1 (4%), H-3→L+3 (3%), H-2→L+3 (5%), H-1→L+2 (6%), H-1→L+7 (3%), HOMO→L+2 (9%),

					HOMO→L+3 (4%), HOMO→L+4 (3%), HOMO→L+6 (3%), HOMO→L+7 (6%)
23	249.24	4.97	0.004	H-2→L+3 (19%), HOMO→L+5 (11%), HOMO→L+7 (15%)	H-6→L+1 (4%), H-5→L+1 (4%), H-4→L+1 (3%), H-3→L+1 (2%), H-3→L+3 (2%), H-3→L+5 (3%), H-1→L+3 (9%), HOMO→L+6 (2%)
24	248.43	4.99	0.018	H-3→L+2 (23%), H-3→L+3 (15%), HOMO→L+5 (19%)	H-6→LUMO (8%), H-6→L+1 (3%), H-5→L+3 (3%), H-2→L+3 (3%)
25	248.23	4.99	0.026	H-2→L+2 (22%), HOMO→L+6 (14%), HOMO→L+7 (13%)	H-6→L+1 (2%), H-3→L+2 (6%), HOMO→L+2 (6%), HOMO→L+3 (6%), HOMO→L+4 (3%), HOMO→L+5 (2%)
26	247.64	5.01	0.001	H-6→LUMO (11%)	H-6→L+1 (7%), H-4→L+1 (2%), H-3→L+2 (9%), H-3→L+3 (5%), H-3→L+4 (3%), H-2→L+1 (3%), H-2→L+4 (9%), H-2→L+7 (2%), H-1→L+7 (3%), HOMO→L+4 (6%), HOMO→L+5 (4%), HOMO→L+7 (3%), HOMO→L+9 (8%)
27	247.02	5.02	0.005	H-7→LUMO (10%), H-2→L+2 (17%)	H-4→L+1 (3%), H-4→L+3 (4%), H-3→LUMO (3%), H-2→LUMO (3%), H-2→L+3 (3%), H-2→L+4 (5%), H-1→L+2 (2%), H-1→L+4 (4%), HOMO→L+6 (8%), HOMO→L+7 (5%), HOMO→L+8 (3%), HOMO→L+9 (3%)
28	246.78	5.02	0.014	H-6→L+1 (10%), H-3→L+4 (13%), H-2→L+4 (23%)	H-7→LUMO (4%), H-6→LUMO (2%), H-4→L+2 (3%), H-

					1→L+5 (4%), H-1→L+6 (7%), HOMO→L+6 (2%), HOMO→L+9 (5%)
29	245.89	5.04	0.013	H-6→LUMO (13%), H-5→L+2 (14%)	H-3→L+2 (9%), H-3→L+3 (2%), H-2→L+4 (2%), H-2→L+7 (4%), H-1→L+5 (5%), H-1→L+7 (8%), HOMO→L+6 (3%), HOMO→L+7 (9%), HOMO→L+9 (4%)
30	245.46	5.05	0.016	H-3→L+4 (10%)	H-7→LUMO (3%), H-7→L+1 (5%), H-5→LUMO (2%), H-5→L+2 (3%), H-5→L+4 (2%), H-4→L+2 (4%), H-4→L+3 (3%), H-3→L+2 (3%), H-3→L+5 (3%), H-3→L+6 (4%), H-1→L+6 (6%), H-1→L+10 (2%), HOMO→L+4 (4%), HOMO→L+5 (7%), HOMO→L+6 (7%), HOMO→L+7 (4%), HOMO→L+9 (4%)
31	244.88	5.06	0.005	H-6→LUMO (11%), HOMO→L+9 (11%)	H-6→L+1 (3%), H-3→L+3 (8%), H-3→L+6 (6%), H-3→L+7 (3%), H-2→L+4 (5%), H-2→L+6 (3%), H-2→L+7 (5%), H-1→L+6 (5%), H-1→L+9 (2%), HOMO→L+6 (4%), HOMO→L+7 (2%), HOMO→L+10 (3%)
32	244.82	5.06	0.007	H-2→L+2 (15%), H-2→L+4 (22%)	H-7→LUMO (4%), H-7→L+1 (2%), H-6→LUMO (3%), H-5→L+3 (7%), H-3→L+2 (3%), H-2→L+3 (4%), H-2→L+7 (3%), H-1→L+6 (4%), H-

					1→L+7 (7%)
33	244.49	5.07	0.010	H-7→L+1 (14%), H-1→L+7 (23%)	H-7→LUMO (9%), H-4→L+4 (2%), H-3→L+4 (4%), H-2→L+7 (2%), H-1→L+4 (4%), H-1→L+6 (4%), H-1→L+8 (4%), HOMO→L+8 (5%)
34	243.66	5.09	0.025	H-5→L+4 (11%)	H-5→L+3 (5%), H-4→L+2 (8%), H-3→L+4 (3%), H-3→L+5 (2%), H-2→L+6 (4%), H-2→L+7 (2%), H-1→L+4 (3%), H-1→L+5 (3%), H-1→L+8 (6%), HOMO→L+5 (2%), HOMO→L+6 (7%), HOMO→L+8 (8%)
35	243.07	5.10	0.001	HOMO→L+8 (11%)	H-7→L+1 (7%), H-5→L+4 (3%), H-4→L+3 (6%), H-3→L+3 (6%), H-3→L+4 (9%), H-3→L+6 (2%), H-3→L+7 (3%), H-2→L+7 (8%), H-2→L+8 (5%), H-1→L+5 (6%), H-1→L+7 (4%), HOMO→L+6 (2%), HOMO→L+7 (3%), HOMO→L+9 (3%)
36	242.71	5.11	0.007	H-1→L+5 (27%)	H-7→LUMO (7%), H-7→L+1 (8%), H-5→L+2 (5%), H-4→L+1 (2%), H-4→L+2 (3%), H-4→L+4 (2%), H-3→L+4 (3%), H-2→L+4 (3%), H-2→L+7 (4%), H-1→L+4 (2%), H-1→L+6 (3%), H-1→L+7 (2%), H-1→L+10 (2%)

37	242.04	5.12	0.013	H-4→L+3 (10%), H-1→L+6 (15%)	H-5→L+2 (3%), H-5→L+6 (3%), H-4→L+2 (2%), H-4→L+4 (3%), H-4→L+5 (2%), H-3→L+4 (3%), H-3→L+6 (9%), H-2→L+6 (5%), H-1→L+7 (2%), HOMO→L+8 (5%), HOMO→L+9 (4%)
38	241.83	5.13	0.011	H-4→L+2 (10%)	H-7→L+1 (6%), H-7→L+2 (6%), H-5→L+2 (8%), H-5→L+3 (9%), H-5→L+4 (3%), H-4→L+3 (7%), H-4→L+5 (3%), H-4→L+6 (3%), H-2→L+7 (3%), H-1→L+5 (3%), H-1→L+6 (7%), H-1→L+7 (3%), HOMO→L+8 (5%)
39	241.46	5.13	0.017	H-7→L+1 (11%), H-3→L+5 (11%)	H-6→LUMO (2%), H-6→L+1 (2%), H-5→L+4 (3%), H-5→L+5 (9%), H-5→L+7 (2%), H-4→L+3 (6%), H-3→L+3 (5%), H-3→L+7 (4%), H-2→L+7 (3%), H-1→L+5 (2%), H-1→L+7 (5%), H-1→L+8 (4%), HOMO→L+9 (2%)
40	241.32	5.14	0.013	H-5→L+3 (10%), H-4→L+3 (10%)	H-7→L+2 (2%), H-7→L+4 (2%), H-6→L+4 (3%), H-5→L+4 (2%), H-4→L+4 (4%), H-3→L+4 (4%), H-3→L+6 (2%), H-2→L+8 (3%), H-1→L+7 (6%), H-1→L+10 (5%), HOMO→L+8 (3%), HOMO→L+9 (7%), HOMO→L+10 (3%)

Table S4. Calculated electronic transitions for **C1-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	296.78	4.18	0.000	HOMO→LUMO (95%)	-
2	287.90	4.31	0.024	H-1→LUMO (55%), HOMO→L+1 (41%)	-
3	287.28	4.32	0.031	H-1→LUMO (39%), HOMO→L+1 (54%)	H-3→LUMO (3%)
4	280.21	4.42	0.014	H-1→L+1 (90%)	H-2→LUMO (8%)
5	278.53	4.45	0.081	H-1→L+3 (16%), HOMO→L+2 (74%)	-
6	278.50	4.45	0.001	H-1→L+2 (32%), HOMO→L+3 (56%)	-
7	274.12	4.52	0.000	H-3→L+1 (15%), H- 2→LUMO (73%)	H-1→L+1 (5%)
8	273.90	4.53	0.002	H-3→LUMO (76%), H-2→L+1 (18%)	-
9	267.00	4.64	0.001	H-1→L+2 (51%), HOMO→L+3 (31%)	H-5→LUMO (4%), H-1→L+5 (6%)
10	266.71	4.65	0.041	H-4→LUMO (33%), H-2→L+1 (38%)	H-5→L+1 (5%), H- 3→LUMO (9%), H- 2→L+2 (2%)
11	266.10	4.66	0.028	H-5→LUMO (32%), H-3→L+1 (38%)	H-4→L+1 (8%), H- 2→LUMO (5%), HOMO→L+3 (4%)
12	265.27	4.67	0.025	H-1→L+3 (70%), HOMO→L+2 (17%)	HOMO→L+5 (7%)
13	262.99	4.71	0.018	H-3→L+2 (43%), H- 2→L+3 (35%)	H-5→LUMO (6%), HOMO→L+4 (3%)
14	262.88	4.72	0.022	H-3→L+3 (21%), H- 2→L+1 (14%), H- 2→L+2 (32%)	H-6→LUMO (4%), H-5→L+1 (4%), H- 4→LUMO (5%), H- 3→LUMO (6%)
15	262.42	4.72	0.008	H-4→LUMO (28%), H-3→L+3 (13%), H- 2→L+1 (15%), H- 2→L+2 (17%)	H-5→L+1 (9%), H- 3→LUMO (2%)
16	262.41	4.72	0.004	H-5→LUMO (28%), H-3→L+1 (39%)	H-6→L+1 (3%), H- 4→L+1 (5%), H- 2→LUMO (7%)
17	258.20	4.80	0.083	HOMO→L+5 (82%)	H-1→L+3 (5%), HOMO→L+2 (4%)

18	258.19	4.80	0.014	H-6→LUMO (38%), H-2→L+1 (10%), H- 1→L+4 (11%)	H-9→L+1 (4%), H- 8→LUMO (2%), H- 5→L+1 (9%), H- 5→L+2 (2%), H- 4→LUMO (5%), H- 4→L+3 (3%)
19	257.50	4.81	0.004	HOMO→L+4 (81%)	H-5→L+3 (3%), H- 4→L+2 (3%), H- 2→L+3 (4%)
20	256.94	4.83	0.050	H-5→L+3 (30%), H- 4→L+2 (33%)	H-5→LUMO (7%), H-3→L+2 (2%), H- 1→L+5 (3%), HOMO→L+4 (8%)
21	256.56	4.83	0.016	H-5→L+2 (35%), H- 4→L+3 (33%)	H-4→LUMO (9%), H-1→L+6 (2%)
22	256.20	4.84	0.002	H-6→L+1 (10%), H- 4→L+1 (12%), H- 2→L+3 (13%), H- 1→L+5 (32%)	H-9→LUMO (6%), H-7→LUMO (3%), H-3→L+2 (2%), H- 1→L+2 (5%)
23	254.41	4.87	0.000	H-4→L+1 (32%), H- 3→L+2 (17%), H- 2→L+3 (17%)	H-7→LUMO (3%), H-6→L+1 (6%), H- 5→LUMO (3%), H- 4→L+2 (2%), H- 1→L+5 (5%), HOMO→L+6 (4%)
24	254.31	4.88	0.000	H-3→L+3 (55%), H- 2→L+2 (40%)	-
25	253.96	4.88	0.000	H-3→L+2 (22%), H- 2→L+3 (22%), H- 1→L+5 (26%), HOMO→L+6 (11%)	H-4→L+1 (6%), HOMO→L+8 (2%)
26	252.80	4.90	0.050	H-5→L+1 (26%), H- 1→L+4 (58%)	H-6→LUMO (2%), H-4→LUMO (5%)
27	251.80	4.92	0.041	H-6→LUMO (31%), H-5→L+1 (32%), H- 1→L+4 (13%)	H-4→LUMO (7%), H-1→L+6 (2%), HOMO→L+7 (3%)
28	251.50	4.93	0.003	H-5→LUMO (10%), H-4→L+1 (24%), HOMO→L+6 (34%)	H-9→LUMO (3%), H-7→LUMO (3%), H-6→L+1 (7%), H- 3→L+2 (3%), H- 1→L+7 (6%)
29	250.85	4.94	0.003	H-6→L+1 (19%), H- 1→L+5 (12%), HOMO→L+6 (15%)	H-9→LUMO (7%), H-7→LUMO (5%), H-5→LUMO (5%), H-4→L+1 (5%), H- 4→L+2 (3%), H- 2→L+4 (2%), H- 1→L+7 (5%)

30	250.42	4.95	0.012	H-1→L+6 (26%), HOMO→L+7 (28%)	H-5→L+1 (7%), H-4→L+3 (2%), H-3→L+3 (3%), H-3→L+4 (3%), H-3→L+6 (3%), H-2→L+5 (2%), H-2→L+7 (6%)
31	248.18	5.00	0.001	H-7→LUMO (69%)	H-9→LUMO (4%), H-6→L+1 (7%), H-3→L+5 (2%), H-2→L+6 (3%), HOMO→L+6 (3%)
32	247.21	5.02	0.036	H-7→LUMO (12%), H-3→L+7 (10%), H-2→L+6 (13%), HOMO→L+6 (13%)	H-6→L+1 (5%), H-3→L+5 (7%), H-2→L+4 (8%), H-2→L+11 (2%), H-1→L+9 (3%), HOMO→L+8 (9%)
33	246.94	5.02	0.004	H-3→L+4 (11%), H-2→L+5 (13%), HOMO→L+7 (14%), HOMO→L+9 (10%)	H-9→L+1 (2%), H-8→LUMO (7%), H-6→LUMO (4%), H-5→L+2 (3%), H-3→L+6 (8%), H-2→L+7 (7%), H-1→L+6 (4%), H-1→L+8 (4%)
34	245.62	5.05	0.007	HOMO→L+8 (40%)	H-6→L+2 (3%), H-5→L+3 (3%), H-2→L+4 (6%), H-2→L+6 (4%), H-1→L+5 (5%), H-1→L+7 (4%), H-1→L+10 (7%), HOMO→L+6 (4%), HOMO→L+11 (6%)
35	245.34	5.05	0.007	HOMO→L+7 (13%), HOMO→L+9 (30%)	H-8→LUMO (3%), H-7→L+1 (2%), H-5→L+2 (9%), H-3→L+4 (8%), H-1→L+6 (8%), H-1→L+11 (7%), HOMO→L+10 (5%)
36	244.96	5.06	0.023	H-8→LUMO (15%), H-7→L+1 (13%), H-5→L+2 (17%), H-4→L+3 (10%)	H-9→L+1 (2%), H-6→LUMO (3%), H-3→L+6 (6%), H-2→L+5 (3%), H-2→L+7 (7%), H-1→L+8 (2%), HOMO→L+7 (5%), HOMO→L+9 (4%)

37	244.72	5.07	0.001	H-5→L+3 (25%), H-4→L+2 (39%)	H-6→L+1 (7%), H-4→L+5 (4%), H-2→L+4 (3%), HOMO→L+8 (8%)
38	244.32	5.07	0.010	H-3→L+5 (41%), H-2→L+4 (18%), HOMO→L+8 (10%)	H-6→L+1 (3%), H-5→L+3 (2%), H-4→L+2 (4%), H-2→L+6 (4%), H-1→L+7 (3%), H-1→L+9 (3%), HOMO→L+11 (3%)
39	244.27	5.08	0.034	H-8→LUMO (11%), H-7→L+1 (14%), H-2→L+5 (23%), HOMO→L+9 (12%)	H-5→L+2 (6%), H-4→L+3 (8%), H-1→L+8 (6%), HOMO→L+7 (5%), HOMO→L+10 (3%)
40	243.77	5.09	0.000	H-5→L+2 (10%), H-4→L+3 (21%), H-2→L+5 (22%)	H-3→L+4 (9%), H-3→L+6 (5%), H-2→L+7 (3%), H-1→L+6 (5%), H-1→L+8 (2%), HOMO→L+7 (7%), HOMO→L+10 (9%)

Table S5. Calculated electronic transitions for **Cr-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	274.12	4.52	0.012	H-1→LUMO (29%), HOMO→LUMO (36%)	H-1→L+1 (9%), HOMO→L+1 (9%)
2	273.07	4.54	0.249	H-1→LUMO (27%), HOMO→L+1 (50%)	H-3→L+1 (3%)
3	268.60	4.62	0.029	H-2→LUMO (49%), HOMO→LUMO (25%)	H-2→L+2 (3%), H-1→L+1 (4%), HOMO→L+1 (5%), HOMO→L+2 (3%)
4	266.25	4.66	0.031	H-3→LUMO (36%), H-2→LUMO (15%)	H-4→LUMO (2%), H-1→LUMO (4%), H-1→L+2 (5%), HOMO→LUMO (7%), HOMO→L+1 (7%), HOMO→L+3 (5%)
5	264.44	4.69	0.019	H-1→LUMO (19%), H-1→L+1 (37%)	H-4→L+1 (2%), H-3→LUMO (5%), H-3→L+1 (4%), H-2→L+1 (3%),

					HOMO→LUMO (4%), HOMO→L+1 (8%)
6	263.12	4.71	0.002	H-2→LUMO (13%), H-2→L+1 (20%), H-1→L+1 (11%), HOMO→LUMO (12%)	H-4→L+1 (5%), H-3→L+1 (5%), H-1→LUMO (2%), HOMO→L+2 (7%), HOMO→L+3 (5%), HOMO→L+4 (2%)
7	262.50	4.72	0.024	H-4→LUMO (14%), H-3→L+1 (15%), H-2→L+1 (15%), H-1→L+2 (14%)	H-5→LUMO (3%), H-4→L+1 (2%), H-3→LUMO (3%), H-2→LUMO (4%), H-2→L+2 (3%), HOMO→L+3 (4%)
8	261.38	4.74	0.047	H-2→L+1 (18%), HOMO→L+3 (18%)	H-5→LUMO (9%), H-5→L+1 (3%), H-4→LUMO (3%), H-4→L+1 (6%), H-3→LUMO (7%), H-1→L+3 (2%), HOMO→LUMO (3%), HOMO→L+2 (4%), HOMO→L+4 (6%)
9	260.26	4.76	0.034	H-5→LUMO (15%), H-3→LUMO (16%), H-2→L+1 (14%), H-1→L+1 (12%), H-1→L+2 (11%)	H-4→LUMO (9%), H-3→L+1 (4%), H-2→LUMO (2%)
10	258.30	4.80	0.039	H-5→L+1 (21%), H-3→L+1 (29%)	H-3→L+4 (3%), H-2→L+1 (7%), H-2→L+3 (2%), H-1→LUMO (3%), H-1→L+1 (9%), HOMO→L+2 (4%)
11	257.78	4.81	0.038	H-6→L+1 (12%), H-4→L+1 (10%), HOMO→L+2 (12%)	H-6→LUMO (3%), H-5→LUMO (3%), H-5→L+1 (4%), H-3→L+1 (3%), H-2→L+2 (5%), H-2→L+3 (5%), H-1→L+3 (3%), HOMO→L+1 (3%), HOMO→L+3 (9%)
12	255.82	4.85	0.021	H-4→LUMO (12%), HOMO→L+2 (14%), HOMO→L+4 (10%)	H-7→LUMO (6%), H-6→L+1 (7%), H-3→L+1 (5%), H-3→L+2 (3%), H-

					1→L+2 (4%), H-1→L+3 (2%), HOMO→L+1 (3%), HOMO→L+3 (3%)
13	255.61	4.85	0.016	H-7→LUMO (12%), H-1→L+2 (13%)	H-7→L+1 (4%), H-6→LUMO (5%), H-5→LUMO (4%), H-5→L+2 (2%), H-4→L+2 (6%), H-3→L+1 (7%), H-3→L+2 (2%), H-2→L+1 (4%), H-2→L+2 (3%), H-1→L+3 (2%), H-1→L+6 (3%), H-1→L+10 (2%)
14	254.88	4.86	0.029	H-3→L+3 (13%), H-1→L+3 (11%), HOMO→L+3 (18%)	H-6→L+1 (8%), H-4→LUMO (6%), H-3→LUMO (2%), H-3→L+1 (3%), HOMO→L+2 (6%), HOMO→L+4 (3%)
15	254.27	4.88	0.003	H-2→L+3 (13%)	H-7→LUMO (8%), H-7→L+1 (3%), H-6→LUMO (3%), H-5→LUMO (9%), H-4→LUMO (3%), H-4→L+1 (5%), H-4→L+2 (4%), H-3→L+3 (4%), H-2→L+2 (6%), H-2→L+7 (2%), HOMO→L+2 (9%), HOMO→L+7 (3%)
16	253.48	4.89	0.008	H-5→LUMO (25%), H-1→L+2 (19%)	H-7→L+2 (4%), H-3→LUMO (7%), H-2→L+1 (2%), H-2→L+2 (5%), H-1→L+3 (6%), H-1→L+4 (4%), HOMO→L+6 (2%), HOMO→L+7 (2%)
17	253.23	4.90	0.019	H-4→LUMO (12%), H-4→L+1 (16%), HOMO→L+4 (15%)	H-6→L+1 (2%), H-3→L+1 (2%), H-3→L+2 (3%), H-3→L+4 (3%), H-1→L+4 (8%), HOMO→L+2 (2%), HOMO→L+5 (7%), HOMO→L+6 (3%)

18	252.77	4.90	0.017	H-5→L+1 (29%), H-4→L+1 (12%), H-1→L+3 (11%)	H-7→LUMO (3%), H-6→LUMO (3%), H-6→L+1 (3%), H-5→LUMO (3%), H-3→L+3 (3%), H-2→L+3 (3%), H-1→L+2 (4%), HOMO→L+5 (4%)
19	252.13	4.92	0.011	HOMO→L+5 (39%)	H-6→L+1 (4%), H-4→LUMO (3%), H-4→L+1 (5%), H-4→L+3 (3%), H-3→L+5 (6%), H-1→L+4 (7%)
20	250.92	4.94	0.005	H-4→LUMO (11%), H-1→L+4 (28%)	H-7→L+1 (4%), H-5→L+3 (3%), H-3→L+4 (2%), H-1→L+2 (3%), H-1→L+3 (4%), H-1→L+6 (5%), HOMO→L+2 (3%), HOMO→L+4 (4%), HOMO→L+5 (6%), HOMO→L+6 (3%), HOMO→L+7 (3%)
21	250.42	4.95	0.007	H-5→L+1 (10%), H-1→L+3 (12%), H-1→L+4 (13%)	H-6→LUMO (3%), H-4→LUMO (2%), H-3→L+3 (3%), H-3→L+4 (2%), H-2→L+3 (9%), HOMO→L+2 (4%), HOMO→L+4 (4%), HOMO→L+6 (6%), HOMO→L+7 (7%)
22	249.78	4.96	0.014	H-2→L+7 (16%), HOMO→L+7 (16%)	H-5→LUMO (2%), H-4→LUMO (4%), H-4→L+1 (4%), H-3→L+3 (4%), H-2→L+3 (6%), H-1→L+3 (3%), H-1→L+7 (4%), HOMO→L+2 (6%), HOMO→L+4 (3%), HOMO→L+6 (5%)
23	249.52	4.97	0.013	H-3→L+2 (10%), H-1→L+3 (19%), HOMO→L+5 (13%)	H-7→L+1 (3%), H-4→L+1 (5%), H-2→L+2 (4%), H-2→L+3 (7%), HOMO→L+2 (4%), HOMO→L+4 (2%),

					HOMO→L+7 (8%)
24	248.56	4.99	0.013	H-2→L+2 (19%), HOMO→L+3 (14%), HOMO→L+4 (10%)	H-7→LUMO (3%), H-3→L+2 (7%), H- 3→L+6 (4%), HOMO→L+2 (2%), HOMO→L+5 (3%), HOMO→L+6 (3%), HOMO→L+7 (7%)
25	248.45	4.99	0.004	H-6→L+1 (13%), H- 3→L+2 (25%)	H-6→LUMO (6%), H-5→L+1 (3%), H- 3→L+3 (9%), H- 2→L+2 (2%), H- 2→L+3 (9%), H- 1→L+3 (3%), HOMO→L+6 (2%), HOMO→L+7 (2%)
26	247.95	5.00	0.002	H-6→LUMO (17%), HOMO→L+9 (13%)	H-6→L+1 (4%), H- 4→L+1 (5%), H- 3→L+3 (6%), H- 3→L+4 (4%), H- 2→L+2 (4%), HOMO→L+6 (7%)
27	246.94	5.02	0.010	H-2→L+3 (12%), H- 2→L+4 (21%)	H-5→L+1 (2%), H- 3→L+2 (6%), H- 2→L+1 (4%), H- 2→L+2 (8%), H- 1→L+7 (4%), HOMO→L+4 (4%), HOMO→L+6 (3%), HOMO→L+7 (7%), HOMO→L+8 (2%)
28	246.82	5.02	0.010	H-2→L+4 (18%), H- 1→L+6 (11%)	H-7→LUMO (7%), H-6→LUMO (3%), H-6→L+1 (8%), H- 4→L+2 (3%), H- 3→L+4 (8%), H- 3→L+6 (3%), H- 1→L+4 (3%), H- 1→L+7 (3%), HOMO→L+6 (5%), HOMO→L+7 (6%)
29	245.98	5.04	0.011	H-6→LUMO (13%), H-5→L+2 (10%), H- 3→L+2 (10%), HOMO→L+6 (10%)	H-5→L+3 (4%), H- 3→L+4 (5%), H- 2→L+2 (2%), H- 2→L+7 (3%), H- 1→L+4 (3%), H- 1→L+6 (6%), H- 1→L+7 (4%),

					HOMO→L+7 (3%)
30	245.63	5.05	0.005		H-7→LUMO (4%), H-5→L+1 (3%), H-5→L+2 (2%), H-4→L+2 (5%), H-3→L+2 (2%), H-3→L+4 (5%), H-2→L+2 (4%), H-2→L+3 (3%), H-2→L+7 (7%), H-1→L+2 (3%), H-1→L+6 (7%), H-1→L+7 (3%), HOMO→L+4 (5%), HOMO→L+6 (4%), HOMO→L+7 (7%), HOMO→L+9 (8%)
31	245.27	5.05	0.017	H-1→L+6 (10%)	H-7→LUMO (8%), H-3→L+6 (6%), H-2→L+2 (6%), H-2→L+6 (2%), H-2→L+7 (5%), H-1→L+5 (4%), H-1→L+8 (9%), H-1→L+10 (7%), HOMO→L+6 (3%), HOMO→L+8 (5%), HOMO→L+9 (5%)
32	244.75	5.07	0.012		H-7→LUMO (5%), H-6→LUMO (6%), H-6→L+1 (3%), H-5→L+4 (2%), H-4→L+1 (4%), H-3→L+5 (2%), H-2→L+3 (6%), H-2→L+4 (8%), H-1→L+5 (4%), H-1→L+6 (7%), H-1→L+7 (8%), H-1→L+8 (2%), HOMO→L+6 (6%), HOMO→L+7 (3%), HOMO→L+8 (3%)
33	244.62	5.07	0.006	H-7→L+1 (10%), H-3→L+3 (12%), H-2→L+4 (17%), H-1→L+7 (14%)	H-5→L+3 (6%), H-3→L+4 (3%), H-1→L+3 (3%), H-1→L+6 (3%), HOMO→L+8 (2%)

34	243.93	5.08	0.015		H-7→LUMO (8%), H-5→L+3 (2%), H-5→L+4 (9%), H-4→L+2 (7%), H-4→L+3 (4%), H-3→L+3 (4%), H-3→L+4 (5%), H-2→L+6 (5%), H-1→L+4 (5%), H-1→L+5 (3%), H-1→L+8 (2%), HOMO→L+4 (3%), HOMO→L+6 (9%), HOMO→L+8 (4%), HOMO→L+9 (4%)
35	243.67	5.09	0.011	H-3→L+5 (10%), H-1→L+5 (40%)	H-5→L+2 (2%), H-4→L+5 (8%), H-3→L+2 (2%), H-3→L+6 (3%), H-2→L+5 (4%), H-2→L+6 (3%), H-1→L+8 (2%), HOMO→L+8 (8%), HOMO→L+9 (2%)
36	242.96	5.10	0.003	H-7→L+1 (13%)	H-4→L+2 (6%), H-4→L+3 (5%), H-3→L+3 (9%), H-3→L+4 (2%), H-3→L+7 (2%), H-2→L+6 (2%), H-2→L+7 (9%), H-2→L+8 (3%), H-1→L+5 (3%), H-1→L+7 (5%), HOMO→L+8 (8%), HOMO→L+9 (3%)
37	242.33	5.12	0.012	H-5→L+2 (15%)	H-7→LUMO (6%), H-7→L+3 (2%), H-4→L+2 (5%), H-4→L+3 (6%), H-4→L+4 (5%), H-3→L+4 (8%), H-2→L+4 (3%), H-2→L+6 (3%), H-1→L+6 (9%), HOMO→L+9 (4%)

38	241.97	5.12	0.026	H-4→L+3 (11%), H-3→L+5 (11%)	H-7→L+1 (5%), H-6→LUMO (2%), H-5→L+5 (3%), H-5→L+6 (4%), H-4→L+2 (3%), H-3→L+3 (4%), H-3→L+6 (5%), H-2→L+5 (8%), H-1→L+8 (3%), HOMO→L+9 (4%)
39	241.73	5.13	0.020	H-1→L+10 (15%), HOMO→L+8 (11%)	H-7→LUMO (3%), H-7→L+2 (7%), H-5→L+3 (7%), H-4→L+6 (6%), H-3→L+7 (2%), H-2→L+8 (3%), H-1→L+6 (5%), H-1→L+7 (4%), HOMO→L+10 (5%)
40	241.35	5.14	0.014	H-2→L+5 (11%), H-1→L+5 (11%)	H-5→L+4 (6%), H-4→L+2 (9%), H-4→L+3 (9%), H-4→L+6 (2%), H-3→L+5 (6%), HOMO→L+5 (2%), HOMO→L+6 (3%), HOMO→L+8 (2%), HOMO→L+9 (7%)

Table S6. Calculated electronic transitions for **Cr-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	297.32	4.17	0.000	HOMO→LUMO (95%)	HOMO→L+3 (2%)
2	288.50	4.30	0.025	H-1→LUMO (56%), HOMO→L+1 (40%)	-
3	287.86	4.31	0.028	H-1→LUMO (38%), HOMO→L+1 (56%)	H-3→LUMO (3%)
4	280.95	4.41	0.012	H-1→L+1 (84%)	H-2→LUMO (7%), HOMO→L+3 (5%)
5	279.61	4.43	0.080	H-1→L+3 (17%), HOMO→L+2 (75%)	-
6	279.58	4.43	0.003	H-1→L+2 (31%), HOMO→L+3 (51%)	H-2→LUMO (6%), H-1→L+1 (3%)
7	275.04	4.51	0.001	H-3→L+1 (15%), H-2→LUMO (70%)	H-1→L+1 (6%), H-1→L+2 (3%)
8	275.00	4.51	0.003	H-3→LUMO (77%),	-

				H-2→L+1 (17%)	
9	267.89	4.63	0.001	H-1→L+2 (55%), HOMO→L+3 (34%)	H-1→L+4 (5%)
10	267.02	4.64	0.031	H-2→L+1 (46%), H- 1→L+3 (21%)	H-4→LUMO (4%), H-3→LUMO (7%), H-3→L+3 (4%), H- 2→L+2 (8%), HOMO→L+2 (3%)
11	266.19	4.66	0.000	H-3→L+1 (63%), H- 3→L+2 (10%), H- 2→L+3 (11%)	H-2→LUMO (7%), H-1→L+1 (2%)
12	265.92	4.66	0.020	H-2→L+1 (17%), H- 1→L+3 (53%), HOMO→L+2 (14%)	H-3→LUMO (6%), HOMO→L+4 (3%)
13	263.51	4.70	0.033	H-3→L+3 (28%), H- 2→L+2 (47%)	H-3→LUMO (3%), H-2→L+1 (4%)
14	263.49	4.71	0.016	H-3→L+1 (13%), H- 3→L+2 (39%), H- 2→L+3 (26%)	H-2→LUMO (6%), HOMO→L+5 (3%)
15	259.56	4.78	0.014	H-6→L+1 (11%), H- 5→LUMO (57%)	H-4→L+1 (4%), H- 4→L+2 (2%), H- 3→L+1 (3%), H- 2→L+3 (3%), H- 1→L+4 (3%)
16	259.25	4.78	0.034	H-4→LUMO (24%), HOMO→L+4 (46%)	H-6→LUMO (3%), H-5→L+1 (8%), H- 2→L+1 (3%)
17	258.24	4.80	0.050	H-6→LUMO (26%), H-5→L+1 (17%), HOMO→L+4 (21%)	H-4→LUMO (5%), H-2→L+2 (3%), H- 1→L+5 (8%)
18	258.11	4.80	0.044	H-6→LUMO (14%), H-4→LUMO (38%), HOMO→L+4 (18%)	H-9→L+1 (4%), H- 2→L+1 (8%), H- 1→L+5 (6%)
19	257.31	4.82	0.016	H-2→L+3 (10%), HOMO→L+5 (82%)	-
20	256.94	4.83	0.000	H-3→L+2 (16%), H- 2→L+3 (26%), H- 1→L+4 (27%)	H-5→LUMO (5%), H-4→L+1 (5%), H- 1→L+2 (4%), HOMO→L+5 (6%), HOMO→L+6 (3%)
21	255.88	4.85	0.002	H-3→L+3 (58%), H- 2→L+2 (33%)	HOMO→L+4 (3%)
22	255.45	4.85	0.003	H-3→L+2 (19%), H- 2→L+3 (19%), H- 1→L+4 (20%), HOMO→L+6 (17%)	H-9→LUMO (2%), H-6→L+1 (2%), H- 4→L+1 (3%), H- 3→L+4 (3%)
23	253.99	4.88	0.000	H-4→L+1 (33%), HOMO→L+6 (26%)	H-9→LUMO (8%), H-6→L+1 (9%), H- 1→L+8 (4%)

24	253.10	4.90	0.003	H-1→L+4 (23%), HOMO→L+6 (22%)	H-6→L+1 (3%), H-5→LUMO (7%), H-5→L+3 (8%), H-4→L+1 (2%), H-4→L+2 (5%), H-3→L+2 (7%), H-1→L+7 (3%), H-1→L+8 (2%), HOMO→L+9 (4%)
25	252.60	4.91	0.015	H-5→L+2 (10%), H-4→LUMO (10%), H-1→L+5 (18%), H-1→L+6 (22%)	H-6→LUMO (2%), H-4→L+3 (9%), H-2→L+8 (3%), HOMO→L+7 (8%), HOMO→L+8 (6%)
26	252.12	4.92	0.084	H-6→LUMO (10%), H-1→L+5 (54%)	H-5→L+1 (5%), H-1→L+6 (8%), HOMO→L+7 (5%), HOMO→L+8 (4%)
27	250.04	4.96	0.004	H-5→L+3 (24%), H-4→L+2 (29%), HOMO→L+6 (10%)	H-6→L+1 (4%), H-6→L+2 (3%), H-5→LUMO (4%), H-4→L+1 (7%), H-1→L+4 (7%)
28	249.89	4.96	0.015	H-5→L+2 (18%), H-4→L+3 (15%), HOMO→L+8 (13%)	H-6→LUMO (3%), H-6→L+3 (3%), H-4→LUMO (3%), H-3→L+5 (4%), H-3→L+6 (3%), H-2→L+4 (5%), H-2→L+8 (3%), H-1→L+6 (8%), H-1→L+10 (3%)
29	248.93	4.98	0.027	H-2→L+6 (15%)	H-7→LUMO (9%), H-6→L+1 (4%), H-5→LUMO (3%), H-3→L+4 (6%), H-3→L+8 (8%), H-2→L+5 (4%), H-2→L+10 (3%), H-1→L+7 (3%), H-1→L+8 (7%), HOMO→L+6 (5%), HOMO→L+9 (5%), HOMO→L+10 (4%)
30	248.80	4.98	0.007	H-5→L+2 (10%), HOMO→L+7 (47%)	H-4→L+3 (6%), H-3→L+6 (8%), H-2→L+8 (4%), H-1→L+6 (7%), H-1→L+10 (4%), HOMO→L+8 (2%)

31	247.07	5.02	0.019	H-7→LUMO (55%), HOMO→L+9 (10%)	H-9→LUMO (3%), H-6→L+1 (7%), H- 5→LUMO (2%), H- 4→L+1 (5%), H- 1→L+8 (2%)
32	246.45	5.03	0.002	H-6→LUMO (27%), H-5→L+1 (43%)	H-8→LUMO (4%), H-7→L+1 (5%), H- 4→LUMO (4%), H- 3→L+5 (4%), H- 2→L+4 (4%)
33	246.05	5.04	0.007	HOMO→L+9 (32%), HOMO→L+10 (12%)	H-7→LUMO (9%), H-6→L+2 (2%), H- 3→L+4 (3%), H- 2→L+5 (9%), H- 1→L+4 (4%), H- 1→L+8 (5%), H- 1→L+11 (6%)
34	246.01	5.04	0.003	H-5→L+1 (13%), H- 3→L+5 (12%), H- 2→L+4 (11%), HOMO→L+8 (30%)	H-3→L+6 (3%), H- 2→L+8 (4%), H- 1→L+10 (3%), HOMO→L+7 (4%), HOMO→L+11 (3%)
35	245.39	5.05	0.002	H-7→LUMO (15%), H-4→L+1 (24%), H- 3→L+4 (18%), H- 2→L+5 (10%)	H-9→LUMO (4%), H-8→L+1 (2%), H- 6→L+1 (2%), H- 5→LUMO (7%), H- 2→L+6 (3%)
36	244.58	5.07	0.005	H-3→L+6 (11%), H- 2→L+4 (40%)	H-5→L+2 (2%), H- 3→L+5 (9%), H- 2→L+8 (5%), H- 1→L+6 (2%), H- 1→L+9 (5%), HOMO→L+8 (7%), HOMO→L+11 (9%)
37	244.50	5.07	0.001	H-6→L+1 (14%), H- 3→L+4 (22%), H- 2→L+5 (11%), HOMO→L+9 (21%)	H-7→LUMO (3%), H-6→L+2 (2%), H- 5→LUMO (5%), H- 4→L+1 (7%), H- 1→L+11 (2%)
38	243.62	5.09	0.001	H-2→L+6 (17%), H- 1→L+7 (21%), HOMO→L+10 (28%)	H-4→L+2 (3%), H- 3→L+4 (3%), H- 3→L+8 (8%), H- 1→L+8 (6%)
39	243.59	5.09	0.022	H-8→LUMO (10%), H-1→L+9 (15%), HOMO→L+11 (28%)	H-9→L+1 (2%), H- 6→L+3 (9%), H- 3→L+6 (4%), H- 1→L+5 (2%), HOMO→L+7 (3%)

40	243.31	5.10	0.047	H-8→LUMO (34%)	H-9→L+1 (8%), H-7→L+1 (2%), H-5→L+1 (6%), H-4→L+3 (2%), H-3→L+5 (2%), H-3→L+6 (5%), H-2→L+4 (7%), H-2→L+8 (3%), H-1→L+9 (3%), HOMO→L+8 (4%), HOMO→L+11 (3%)
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Table S7. Calculated electronic transitions for **D1-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	275.62	4.50	0.020	H-3→LUMO (11%), H-2→L+1 (11%), H-1→L+1 (22%), HOMO→LUMO (24%)	H-1→LUMO (3%), H-1→L+2 (4%), HOMO→L+1 (3%), HOMO→L+3 (5%)
2	275.62	4.50	0.007	H-3→L+1 (11%), H-2→LUMO (11%), H-1→LUMO (23%), HOMO→L+1 (22%)	H-1→L+1 (3%), H-1→L+3 (5%), HOMO→LUMO (3%), HOMO→L+2 (5%)
3	273.97	4.53	0.038	H-3→LUMO (12%), H-2→L+1 (11%), H-1→L+2 (29%), HOMO→L+3 (29%)	H-5→LUMO (3%), H-4→L+1 (4%)
4	273.75	4.53	0.402	H-3→L+1 (12%), H-2→LUMO (12%), H-1→L+3 (28%), HOMO→L+2 (29%)	H-5→L+1 (3%), H-4→LUMO (3%)
5	270.97	4.58	0.020	H-5→L+1 (28%), H-4→LUMO (31%)	H-3→L+2 (4%), H-2→L+3 (4%), H-1→LUMO (5%), H-1→L+3 (5%), HOMO→L+1 (5%), HOMO→L+2 (5%)
6	270.94	4.58	0.006	H-5→LUMO (29%), H-4→L+1 (29%)	H-3→L+3 (4%), H-2→L+2 (4%), H-1→L+1 (5%), H-1→L+2 (5%), HOMO→LUMO (6%), HOMO→L+3 (5%)

7	267.89	4.63	0.057	H-3→L+1 (11%), H-3→L+2 (11%), H-2→LUMO (13%), H-2→L+3 (11%)	H-5→L+2 (7%), H-4→L+3 (6%), H-1→LUMO (9%), H-1→L+3 (3%), HOMO→L+1 (8%), HOMO→L+2 (4%)
8	267.87	4.63	0.058	H-3→LUMO (13%), H-3→L+3 (11%), H-2→L+1 (13%), H-2→L+2 (11%)	H-5→L+3 (7%), H-4→L+2 (6%), H-1→L+1 (7%), H-1→L+2 (3%), HOMO→LUMO (9%), HOMO→L+3 (3%), HOMO→L+4 (2%)
9	265.95	4.66	0.049	H-3→L+2 (14%), H-2→L+3 (14%)	H-11→LUMO (3%), H-10→L+1 (3%), H-5→L+1 (6%), H-5→L+2 (4%), H-4→LUMO (9%), H-4→L+3 (3%), H-3→L+1 (2%), H-2→LUMO (4%), H-1→LUMO (5%), H-1→L+4 (5%), HOMO→L+1 (6%), HOMO→L+5 (5%)
10	265.91	4.66	0.000	H-3→L+3 (14%), H-2→L+2 (15%)	H-11→L+1 (2%), H-10→LUMO (3%), H-5→LUMO (7%), H-5→L+3 (3%), H-4→L+1 (8%), H-4→L+2 (3%), H-3→LUMO (3%), H-2→L+1 (4%), H-1→L+1 (4%), H-1→L+5 (5%), HOMO→LUMO (7%), HOMO→L+4 (5%)
11	263.49	4.71	0.046	-	H-11→LUMO (3%), H-10→L+1 (4%), H-9→L+1 (4%), H-8→LUMO (6%), H-7→L+2 (2%), H-5→L+2 (3%), H-4→L+3 (3%), H-3→L+1 (2%), H-3→L+5 (5%), H-3→L+7 (4%), H-2→LUMO (3%), H-

					2→L+4 (5%), H-2→L+6 (4%), H-1→L+4 (7%), HOMO→L+5 (7%)
12	263.47	4.71	0.021	-	H-11→L+1 (4%), H-10→LUMO (4%), H-9→LUMO (4%), H-8→L+1 (5%), H-7→L+3 (2%), H-5→L+3 (3%), H-4→L+2 (3%), H-3→LUMO (3%), H-3→L+4 (4%), H-3→L+6 (4%), H-2→L+1 (3%), H-2→L+5 (5%), H-2→L+7 (4%), H-1→L+5 (7%), H-1→L+7 (2%), HOMO→L+4 (8%), HOMO→L+6 (2%)
13	262.40	4.72	0.201	H-9→L+1 (10%), H-8→LUMO (14%)	H-11→L+3 (3%), H-10→L+2 (3%), H-7→L+1 (4%), H-6→L+3 (2%), H-3→L+5 (4%), H-2→L+4 (5%), H-1→L+4 (2%), H-1→L+6 (7%), HOMO→L+5 (2%), HOMO→L+7 (8%)
14	262.20	4.73	0.001	H-9→LUMO (10%), H-8→L+1 (12%)	H-11→L+2 (3%), H-10→L+3 (3%), H-7→LUMO (5%), H-6→L+1 (2%), H-3→L+4 (5%), H-2→L+5 (5%), H-1→L+7 (7%), HOMO→L+4 (3%), HOMO→L+6 (7%)
15	261.92	4.73	0.023	H-9→LUMO (18%), H-8→L+1 (12%)	H-11→L+1 (6%), H-10→LUMO (6%), H-9→L+4 (3%), H-8→L+5 (2%), H-7→LUMO (5%), H-6→L+1 (9%), H-4→L+2 (2%), H-3→LUMO (2%), H-1→L+1 (4%), H-1→L+5 (3%)

16	261.86	4.73	0.010	H-9→L+1 (15%), H-8→LUMO (11%), H-6→LUMO (11%)	H-11→LUMO (7%), H-10→L+1 (6%), H-9→L+5 (2%), H-8→L+4 (2%), H-7→L+1 (6%), H-5→L+2 (2%), H-4→L+3 (2%), H-1→LUMO (3%), H-1→L+4 (4%), HOMO→L+5 (2%)
17	259.99	4.77	0.009	H-5→L+3 (13%), H-4→L+2 (17%), H-1→L+1 (17%)	H-5→LUMO (5%), H-3→L+3 (9%), H-2→L+1 (5%), H-2→L+2 (6%), HOMO→LUMO (9%), HOMO→L+4 (3%)
18	259.90	4.77	0.001	H-5→L+2 (14%), H-4→L+3 (17%), H-1→LUMO (18%), HOMO→L+1 (13%)	H-5→L+1 (5%), H-3→L+2 (8%), H-2→LUMO (6%), H-2→L+3 (5%), HOMO→L+5 (2%)
19	259.86	4.77	0.001	H-1→LUMO (14%), HOMO→L+1 (24%)	H-11→LUMO (3%), H-5→L+2 (7%), H-4→LUMO (4%), H-4→L+3 (7%), H-3→L+1 (5%), H-3→L+2 (5%), H-2→LUMO (3%), H-2→L+3 (5%), H-1→L+4 (3%)
20	259.68	4.77	0.000	H-1→L+1 (19%), HOMO→LUMO (24%)	H-11→L+1 (3%), H-5→L+3 (8%), H-4→L+1 (4%), H-4→L+2 (8%), H-3→LUMO (6%), H-3→L+3 (3%), H-2→L+1 (3%), H-2→L+2 (4%)
21	258.79	4.79	0.007	H-1→L+4 (15%), HOMO→L+5 (17%)	H-10→L+1 (2%), H-7→L+2 (4%), H-6→L+3 (4%), H-5→L+5 (7%), H-4→L+4 (7%), H-3→L+5 (5%), H-2→L+4 (6%)
22	258.77	4.79	0.017	H-1→L+5 (16%), HOMO→L+4 (16%)	H-11→L+1 (2%), H-10→LUMO (2%), H-8→L+1 (2%), H-7→L+3 (3%), H-

					6→L+2 (3%), H-5→L+4 (8%), H-4→L+5 (7%), H-3→L+4 (5%), H-2→L+5 (6%)
23	258.15	4.80	0.013	H-1→L+6 (11%), HOMO→L+7 (13%)	H-7→L+1 (3%), H-6→LUMO (3%), H-5→L+2 (4%), H-5→L+7 (5%), H-4→L+3 (3%), H-4→L+6 (5%), H-3→L+7 (5%), H-2→L+6 (5%), H-2→L+9 (2%), H-1→LUMO (3%), H-1→L+9 (5%), HOMO→L+8 (4%)
24	258.14	4.80	0.041	H-1→L+7 (13%), HOMO→L+6 (11%)	H-7→LUMO (3%), H-6→L+1 (3%), H-5→L+6 (5%), H-5→L+9 (2%), H-4→L+2 (3%), H-4→L+7 (6%), H-3→L+6 (4%), H-3→L+9 (2%), H-2→L+7 (5%), H-1→L+8 (4%), HOMO→L+9 (5%)
25	257.16	4.82	0.035	-	H-15→LUMO (4%), H-14→L+1 (4%), H-11→L+4 (3%), H-10→L+5 (2%), H-9→L+7 (2%), H-8→L+6 (2%), H-7→L+2 (6%), H-6→L+3 (6%), H-5→L+5 (5%), H-4→L+4 (5%), H-3→L+7 (2%), H-2→L+6 (2%), H-1→L+6 (2%), HOMO→L+7 (2%), HOMO→L+14 (3%)
26	257.14	4.82	0.039	-	H-15→L+1 (4%), H-14→LUMO (4%), H-11→L+5 (2%), H-10→L+4 (3%), H-8→L+7 (2%), H-7→L+3 (5%), H-6→L+2 (6%), H-

					5→L+4 (4%), H-4→L+5 (6%), H-3→L+6 (3%), H-2→L+7 (2%), H-1→L+7 (3%), H-1→L+14 (2%), HOMO→L+4 (2%), HOMO→L+6 (4%), HOMO→L+10 (2%)
27	256.64	4.83	0.040	H-11→L+3 (11%), H-10→L+2 (11%)	H-13→L+1 (3%), H-13→L+2 (8%), H-12→LUMO (3%), H-12→L+3 (8%), H-5→L+5 (2%), H-3→L+5 (4%), H-3→L+7 (2%), H-2→L+4 (5%)
28	256.62	4.83	0.009	H-11→L+2 (11%), H-10→L+3 (11%)	H-13→LUMO (3%), H-13→L+3 (8%), H-12→L+1 (3%), H-12→L+2 (7%), H-3→L+4 (5%), H-3→L+6 (2%), H-2→L+5 (5%), H-2→L+7 (2%)
29	255.46	4.85	0.025	-	H-11→LUMO (6%), H-10→L+1 (6%), H-9→L+2 (3%), H-8→L+3 (2%), H-7→L+1 (6%), H-6→LUMO (8%), H-6→L+3 (3%), H-4→L+4 (2%), H-3→L+5 (5%), H-2→L+4 (8%), H-1→L+6 (4%), H-1→L+9 (5%), HOMO→L+2 (4%), HOMO→L+8 (5%)
30	255.36	4.86	0.009	-	H-11→L+1 (6%), H-10→LUMO (8%), H-9→L+3 (3%), H-8→L+2 (2%), H-7→LUMO (7%), H-7→L+3 (2%), H-6→L+1 (8%), H-6→L+2 (4%), H-3→L+4 (7%), H-2→L+5 (7%), H-1→L+8 (5%),

					HOMO→L+6 (2%), HOMO→L+9 (4%)
31	254.52	4.87	0.001	H-1→L+2 (32%), HOMO→L+3 (25%)	H-9→L+3 (2%), H- 3→LUMO (5%), H- 3→L+3 (3%), H- 2→L+1 (5%)
32	254.43	4.87	0.008	H-1→L+3 (29%), HOMO→L+2 (21%)	H-11→LUMO (2%), H-10→L+1 (2%), H- 7→L+1 (3%), H- 3→L+1 (7%), H- 3→L+2 (2%), H- 2→LUMO (6%), H- 2→L+6 (2%), HOMO→L+1 (3%)
33	254.34	4.87	0.053	H-3→L+5 (10%)	H-9→L+2 (3%), H- 8→L+3 (3%), H- 7→L+1 (4%), H- 6→LUMO (4%), H- 4→L+4 (4%), H- 2→L+4 (7%), H- 1→L+3 (3%), H- 1→L+6 (2%), H- 1→L+9 (2%), HOMO→L+2 (6%)
34	254.29	4.88	0.002	-	H-9→L+3 (3%), H- 8→L+2 (4%), H- 7→LUMO (6%), H- 6→L+1 (7%), H- 5→L+4 (4%), H- 4→L+5 (3%), H- 3→LUMO (6%), H- 3→L+4 (7%), H- 2→L+1 (3%), H- 2→L+5 (9%), HOMO→L+3 (3%)
35	253.97	4.88	0.000	H-3→L+1 (27%), H- 2→LUMO (26%)	H-11→LUMO (3%), H-10→L+1 (2%), H- 9→L+2 (3%), H- 8→L+3 (3%), H- 2→L+6 (2%), H- 1→LUMO (7%), H- 1→L+3 (3%), HOMO→L+1 (6%)
36	253.88	4.88	0.000	H-3→LUMO (25%), H-2→L+1 (31%)	H-7→LUMO (2%), H-3→L+4 (3%), H- 1→L+1 (7%), H- 1→L+2 (7%), HOMO→LUMO (5%), HOMO→L+3

					(6%)
37	253.76	4.89	0.006	-	H-15→LUMO (6%), H-14→L+1 (7%), H-10→L+2 (2%), H-8→L+3 (3%), H-7→L+2 (9%), H-6→L+3 (7%), H-5→L+5 (3%), H-4→L+4 (3%), H-2→LUMO (2%), H-1→L+3 (2%), H-1→L+10 (2%), HOMO→L+8 (2%)
38	253.75	4.89	0.002	-	H-15→L+1 (4%), H-14→LUMO (4%), H-9→L+3 (4%), H-8→L+2 (8%), H-7→L+3 (8%), H-6→L+2 (5%), H-3→L+6 (4%), H-2→L+7 (3%), H-1→L+8 (3%), HOMO→L+9 (3%)
39	253.65	4.89	0.002	H-10→LUMO (10%)	H-15→L+1 (3%), H-14→LUMO (3%), H-11→L+1 (8%), H-11→L+2 (4%), H-10→L+3 (2%), H-9→L+3 (3%), H-9→L+4 (4%), H-8→L+2 (3%), H-8→L+5 (3%), H-6→L+7 (2%), H-5→L+4 (2%), H-4→L+5 (2%), H-3→L+6 (3%), H-2→L+7 (3%), HOMO→L+3 (7%)
40	253.63	4.89	0.006	HOMO→L+2 (11%)	H-11→LUMO (8%), H-11→L+3 (2%), H-10→L+1 (9%), H-9→L+2 (5%), H-9→L+5 (3%), H-8→L+3 (4%), H-8→L+4 (3%), H-3→L+1 (5%), H-3→L+7 (4%), H-2→L+6 (4%), H-

					1→L+3 (5%)
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Table S8. Calculated electronic transitions for **D1-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	301.32	4.11	0.000	H-1→L+1 (40%), HOMO→LUMO (54%)	-
2	301.24	4.12	0.003	H-1→LUMO (51%), HOMO→L+1 (43%)	-
3	286.96	4.32	0.014	H-1→LUMO (17%), H-1→L+3 (11%), H-1→L+4 (18%), HOMO→L+1 (27%), HOMO→L+5 (21%)	-
4	286.95	4.32	0.020	H-1→L+1 (29%), H-1→L+5 (18%), HOMO→LUMO (17%), HOMO→L+3 (13%), HOMO→L+4 (16%)	H-1→L+2 (2%)
5	285.42	4.34	0.024	H-1→LUMO (28%), H-1→L+3 (10%), H-1→L+4 (11%), HOMO→L+1 (26%), HOMO→L+5 (19%)	HOMO→L+2 (2%)
6	285.25	4.35	0.014	H-1→L+1 (28%), H-1→L+5 (19%), HOMO→LUMO (25%), HOMO→L+3 (11%), HOMO→L+4 (12%)	-
7	282.65	4.39	0.060	H-1→L+3 (16%), H-1→L+4 (11%), HOMO→L+2 (34%)	H-7→LUMO (4%), H-6→L+1 (2%), H-5→LUMO (6%), H-4→L+1 (5%), H-3→L+1 (4%), H-2→LUMO (2%), HOMO→L+5 (5%)
8	282.42	4.39	0.054	H-1→L+2 (29%), HOMO→L+3 (16%), HOMO→L+4 (15%)	H-7→L+1 (3%), H-6→LUMO (2%), H-5→L+1 (5%), H-4→LUMO (5%), H-3→LUMO (5%), H-1→L+5 (7%)

9	279.72	4.43	0.009	H-1→L+7 (33%), HOMO→L+6 (55%)	-
10	279.60	4.43	0.033	H-1→L+6 (54%), HOMO→L+7 (34%)	-
11	278.18	4.46	0.007	H-5→L+1 (19%), H- 4→LUMO (20%), H- 3→LUMO (15%), H- 1→L+2 (14%)	H-7→L+1 (4%), H- 6→LUMO (3%), H- 2→L+1 (5%), HOMO→L+3 (9%), HOMO→L+4 (3%)
12	278.12	4.46	0.012	H-5→LUMO (22%), H-4→L+1 (18%), H- 3→L+1 (12%), HOMO→L+2 (14%)	H-7→LUMO (6%), H-6→L+1 (2%), H- 2→LUMO (7%), H- 1→L+3 (8%), H- 1→L+4 (2%)
13	273.94	4.53	0.005	H-5→LUMO (18%), H-4→L+1 (16%), H- 2→LUMO (18%)	H-7→LUMO (6%), H-6→L+1 (8%), H- 5→L+1 (2%), H- 3→L+1 (8%), H- 3→L+5 (4%), H- 2→L+4 (2%), H- 1→L+3 (2%)
14	273.92	4.53	0.003	H-6→LUMO (10%), H-5→L+1 (16%), H- 4→LUMO (15%), H- 3→LUMO (10%)	H-7→L+1 (5%), H- 4→L+1 (2%), H- 3→L+4 (3%), H- 2→L+1 (9%), H- 2→L+5 (2%), H- 1→L+2 (6%), H- 1→L+5 (4%), HOMO→L+3 (4%)
15	273.66	4.53	0.000	H-1→L+3 (40%), HOMO→L+2 (27%), HOMO→L+5 (20%)	H-2→LUMO (3%), H-1→L+4 (3%)
16	273.57	4.53	0.000	H-1→L+2 (25%), H- 1→L+5 (18%), HOMO→L+3 (35%)	H-7→L+1 (4%), H- 4→LUMO (5%), H- 2→L+1 (2%)
17	272.47	4.55	0.002	H-7→LUMO (27%), H-6→L+1 (27%), H- 2→LUMO (23%)	H-3→L+1 (5%), H- 2→L+4 (2%), HOMO→L+2 (2%)
18	272.30	4.55	0.003	H-7→L+1 (20%), H- 6→LUMO (29%), H- 3→LUMO (10%), H- 2→L+1 (21%)	H-3→L+4 (2%), H- 2→L+5 (3%), H- 1→L+2 (2%)
19	271.79	4.56	0.000	H-1→L+2 (15%), H- 1→L+5 (28%), HOMO→L+4 (44%)	HOMO→L+3 (5%)

20	271.72	4.56	0.000	H-1→L+4 (50%), HOMO→L+2 (14%), HOMO→L+5 (25%)	H-1→L+3 (7%)
21	269.01	4.61	0.018	H-5→L+3 (34%), H- 4→L+2 (30%)	H-7→LUMO (3%), H-6→L+1 (2%), H- 3→L+2 (9%), H- 2→L+3 (2%)
22	268.96	4.61	0.007	H-5→L+2 (35%), H- 4→L+3 (31%)	H-7→L+1 (2%), H- 6→LUMO (3%), H- 3→L+3 (8%), H- 2→L+2 (3%)
23	267.53	4.63	0.020	H-9→LUMO (15%), H-8→L+1 (19%), H- 3→L+4 (15%), H- 2→L+5 (18%)	H-13→LUMO (2%), H-3→L+3 (5%), H- 2→L+1 (8%)
24	267.44	4.64	0.091	H-9→L+1 (16%), H- 8→LUMO (21%), H- 3→L+5 (18%), H- 2→L+4 (16%)	H-8→L+3 (2%), H- 2→L+3 (5%)
25	266.89	4.65	0.015	H-7→L+3 (29%), H- 6→L+2 (31%)	H-5→L+3 (3%), H- 4→L+2 (2%), H- 3→L+2 (3%), H- 1→L+8 (4%), HOMO→L+9 (4%)
26	266.86	4.65	0.015	H-7→L+2 (26%), H- 6→L+3 (33%)	H-9→LUMO (2%), H-5→L+2 (4%), H- 3→L+3 (3%), H- 1→L+9 (3%), HOMO→L+8 (3%)
27	265.24	4.67	0.010	H-9→LUMO (11%)	H-13→LUMO (3%), H-12→L+1 (5%), H- 9→L+3 (2%), H- 8→L+1 (8%), H- 7→L+2 (2%), H- 7→L+5 (6%), H- 6→L+4 (8%), H- 5→L+5 (3%), H- 4→LUMO (3%), H- 4→L+4 (5%), H- 3→L+4 (7%), H- 2→L+1 (5%), H- 2→L+2 (4%), H- 1→L+7 (3%)
28	265.20	4.68	0.011	H-9→L+1 (11%)	H-13→L+1 (3%), H- 12→LUMO (7%), H- 8→LUMO (9%), H- 8→L+3 (2%), H- 7→L+4 (9%), H-

					6→L+5 (5%), H-5→L+4 (4%), H-4→L+5 (5%), H-3→L+2 (5%), H-3→L+5 (5%), H-2→LUMO (3%), H-2→L+4 (3%)
29	264.26	4.69	0.001	H-1→L+6 (29%), HOMO→L+7 (48%)	H-7→LUMO (2%), H-3→L+1 (4%), H-2→LUMO (3%)
30	264.22	4.69	0.001	H-1→L+7 (41%), HOMO→L+6 (25%)	H-11→LUMO (4%), H-10→L+1 (4%), H-3→LUMO (2%), H-1→L+9 (3%), HOMO→L+8 (4%)
31	263.91	4.70	0.005	H-11→L+1 (15%), H-10→LUMO (25%)	H-11→L+2 (7%), H-10→L+3 (7%), H-3→L+1 (5%), H-3→L+5 (2%), H-2→LUMO (5%), H-2→L+6 (4%), H-1→L+8 (6%), HOMO→L+9 (5%)
32	263.79	4.70	0.000	H-11→LUMO (20%), H-10→L+1 (17%), H-1→L+7 (11%)	H-11→L+3 (6%), H-10→L+2 (6%), H-9→LUMO (3%), H-2→L+1 (4%), H-1→L+9 (3%), HOMO→L+6 (8%), HOMO→L+8 (5%)
33	263.39	4.71	0.006	H-3→L+1 (26%), H-2→LUMO (12%)	H-11→L+1 (7%), H-11→L+2 (2%), H-10→LUMO (6%), H-10→L+3 (2%), H-7→LUMO (7%), H-7→L+4 (3%), H-5→LUMO (6%), H-5→L+4 (2%), H-1→L+6 (5%), HOMO→L+7 (7%)
34	263.34	4.71	0.013	H-3→LUMO (14%)	H-11→LUMO (2%), H-10→L+1 (3%), H-7→L+1 (7%), H-7→L+2 (3%), H-6→L+4 (4%), H-5→L+1 (6%), H-4→LUMO (3%), H-4→L+4 (4%), H-3→L+6 (7%), H-2→L+5 (5%), H-

					2→L+7 (6%), H-1→L+9 (6%), HOMO→L+8 (9%)
35	263.16	4.71	0.012	H-1→L+8 (27%), HOMO→L+9 (18%)	H-11→L+1 (4%), H-10→LUMO (7%), H-6→L+2 (4%), H-6→L+5 (2%), H-3→L+7 (3%), H-2→L+6 (6%), HOMO→L+7 (2%)
36	263.14	4.71	0.000	H-11→LUMO (10%), H-3→LUMO (18%), HOMO→L+8 (16%)	H-11→L+3 (2%), H-10→L+1 (5%), H-7→L+1 (5%), H-7→L+5 (2%), H-5→L+1 (3%), H-2→L+1 (9%), H-1→L+7 (2%), H-1→L+9 (9%), HOMO→L+6 (2%)
37	262.40	4.72	0.003	H-2→L+1 (17%), HOMO→L+8 (10%)	H-12→L+1 (3%), H-9→LUMO (3%), H-8→L+1 (3%), H-7→L+1 (3%), H-7→L+5 (5%), H-6→L+4 (6%), H-5→L+1 (2%), H-5→L+5 (4%), H-4→LUMO (5%), H-4→L+4 (8%), H-3→LUMO (8%), H-1→L+9 (7%)
38	262.38	4.73	0.018	H-1→L+8 (11%)	H-12→LUMO (2%), H-8→LUMO (2%), H-7→L+4 (5%), H-6→L+5 (7%), H-5→L+4 (4%), H-4→L+5 (9%), H-3→L+1 (9%), H-3→L+2 (7%), H-3→L+7 (4%), H-2→L+3 (4%), H-2→L+4 (6%), H-2→L+6 (7%), HOMO→L+9 (8%)
39	262.00	4.73	0.020	H-4→LUMO (10%), H-2→L+2 (14%)	H-12→L+1 (5%), H-7→L+1 (6%), H-7→L+5 (5%), H-6→LUMO (6%), H-5→L+1 (6%), H-5→L+5 (4%), H-

					3→L+3 (5%), H-3→L+6 (7%), H-2→L+7 (6%), H-1→L+9 (3%), HOMO→L+8 (4%)
40	261.83	4.74	0.024	H-6→L+1 (10%), H-4→L+1 (16%), H-3→L+1 (12%)	H-9→L+1 (2%), H-8→LUMO (4%), H-7→LUMO (6%), H-5→LUMO (7%), H-3→L+5 (6%), H-2→LUMO (3%), H-2→L+3 (5%), H-2→L+4 (4%), H-2→L+6 (3%), H-1→L+8 (3%), HOMO→L+9 (2%)

Table S9. Calculated electronic transitions for **D2-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	279.17	4.44	0.013	H-3→L+1 (15%), H-2→LUMO (20%), H-1→L+1 (17%), HOMO→LUMO (40%)	-
2	278.80	4.45	0.012	H-3→LUMO (22%), H-2→L+1 (15%), H-1→LUMO (27%), HOMO→L+1 (28%)	-
3	273.49	4.53	0.258	H-5→L+1 (12%), H-4→LUMO (17%), H-1→L+2 (13%), HOMO→L+3 (21%)	H-6→LUMO (2%), H-5→L+5 (2%), H-3→L+2 (4%), H-2→LUMO (2%), H-2→L+3 (4%), H-1→L+1 (6%)
4	273.21	4.54	0.003	H-5→LUMO (18%), H-4→L+1 (14%), H-1→L+3 (16%), HOMO→L+2 (19%)	H-7→LUMO (2%), H-4→L+5 (2%), H-3→L+3 (5%), H-2→L+2 (3%), HOMO→L+1 (5%)
5	271.92	4.56	0.000	H-5→LUMO (10%), H-4→L+1 (11%), H-2→L+1 (19%), H-1→LUMO (11%), HOMO→L+2 (14%)	H-5→L+3 (2%), H-5→L+4 (2%), H-4→L+5 (2%), H-3→LUMO (5%), H-1→L+3 (8%)

6	271.83	4.56	0.010	H-5→L+1 (12%), H-4→LUMO (10%), H-3→L+1 (13%), H-2→LUMO (13%), H-1→L+2 (12%), HOMO→L+3 (12%)	H-5→L+5 (2%), H-4→L+3 (2%), H-4→L+4 (2%), HOMO→LUMO (5%)
7	269.73	4.60	0.004	H-3→LUMO (33%), HOMO→L+1 (30%)	H-6→L+1 (2%), H-2→L+1 (7%), H-1→LUMO (8%), HOMO→L+2 (6%)
8	269.48	4.60	0.032	H-3→L+1 (21%), H-2→LUMO (17%), H-1→L+1 (27%), HOMO→LUMO (14%)	H-5→L+1 (3%), H-1→L+2 (5%)
9	268.75	4.61	0.077	H-7→L+1 (14%), H-6→LUMO (16%)	H-7→L+5 (4%), H-6→L+4 (3%), H-3→L+1 (9%), H-2→LUMO (8%), H-2→L+4 (2%), H-1→L+1 (6%), H-1→L+2 (3%), HOMO→LUMO (9%), HOMO→L+3 (4%)
10	268.71	4.61	0.007	H-7→LUMO (17%), H-6→L+1 (14%), H-2→L+1 (12%), H-1→LUMO (13%)	H-7→L+4 (3%), H-6→L+5 (4%), H-3→LUMO (4%), H-3→L+4 (2%), H-1→L+3 (3%), HOMO→L+1 (3%), HOMO→L+2 (6%)
11	267.24	4.64	0.009	H-3→L+3 (22%), H-2→L+2 (28%)	H-9→L+3 (2%), H-8→L+2 (3%), H-6→L+1 (3%), H-5→LUMO (5%), H-4→L+1 (3%), H-1→LUMO (5%), H-1→L+8 (4%), HOMO→L+9 (3%)
12	267.23	4.64	0.080	H-3→L+2 (20%), H-2→L+3 (28%)	H-9→L+2 (2%), H-8→L+3 (2%), H-7→L+1 (3%), H-6→LUMO (2%), H-5→L+1 (2%), H-4→LUMO (4%), H-1→L+9 (3%), HOMO→LUMO (5%), HOMO→L+8 (5%)

13	264.05	4.70	0.002	H-1→L+5 (18%), HOMO→L+4 (24%)	H-5→L+5 (4%), H-4→L+4 (5%), H-3→L+5 (4%), H-3→L+6 (2%), H-2→L+4 (2%), H-2→L+7 (2%), H-2→L+8 (2%), H-1→L+6 (2%), H-1→L+9 (4%), HOMO→L+8 (3%)
14	264.02	4.70	0.002	H-1→L+4 (22%), HOMO→L+5 (21%)	H-5→L+4 (4%), H-4→L+5 (4%), H-3→L+4 (5%), H-3→L+7 (2%), H-2→L+5 (2%), H-2→L+6 (2%), H-2→L+9 (2%), H-1→L+8 (3%), HOMO→L+6 (3%), HOMO→L+9 (3%)
15	263.72	4.70	0.093	H-1→L+2 (10%)	H-7→L+1 (7%), H-7→L+5 (3%), H-6→LUMO (9%), H-6→L+4 (2%), H-5→L+1 (4%), H-4→LUMO (9%), H-3→L+1 (2%), H-2→LUMO (4%), H-2→L+3 (6%), H-1→L+1 (5%), H-1→L+9 (3%), HOMO→LUMO (3%), HOMO→L+4 (3%), HOMO→L+8 (7%)
16	263.61	4.70	0.035	H-7→LUMO (10%)	H-6→L+1 (8%), H-6→L+5 (2%), H-5→LUMO (7%), H-4→L+1 (3%), H-3→LUMO (3%), H-3→L+3 (9%), H-2→L+1 (3%), H-1→LUMO (3%), H-1→L+8 (8%), HOMO→L+1 (5%), HOMO→L+2 (9%), HOMO→L+9 (4%)
17	263.35	4.71	0.000	H-3→L+3 (11%), H-2→L+2 (18%), H-1→L+3 (27%),	H-2→L+1 (3%), HOMO→L+9 (2%)

				HOMO→L+2 (15%)	
18	263.12	4.71	0.017	H-3→L+2 (30%), H-1→L+2 (16%), HOMO→L+3 (25%)	H-3→L+1 (3%), H-2→L+3 (4%), H-2→L+8 (3%), H-1→L+9 (3%)
19	262.30	4.73	0.000	H-2→L+6 (15%), HOMO→L+6 (18%)	H-5→LUMO (4%), H-4→L+2 (3%), H-3→L+4 (3%), H-3→L+7 (8%), H-1→LUMO (3%), H-1→L+3 (6%), H-1→L+7 (9%), H-1→L+8 (2%), HOMO→L+5 (2%), HOMO→L+9 (2%)
20	262.22	4.73	0.037	H-3→L+6 (13%), HOMO→L+7 (13%)	H-5→L+2 (4%), H-4→LUMO (5%), H-4→L+3 (3%), H-2→LUMO (2%), H-2→L+4 (5%), H-2→L+7 (6%), H-2→L+8 (2%), H-1→L+6 (9%), H-1→L+9 (4%), HOMO→LUMO (3%), HOMO→L+3 (4%), HOMO→L+8 (3%)
21	261.71	4.74	0.019	-	H-7→LUMO (2%), H-5→L+3 (3%), H-5→L+4 (3%), H-4→L+2 (2%), H-4→L+5 (5%), H-3→L+3 (8%), H-3→L+4 (4%), H-3→L+7 (2%), H-2→L+1 (5%), H-2→L+5 (4%), H-2→L+6 (4%), H-1→L+8 (8%), HOMO→L+1 (3%), HOMO→L+2 (3%), HOMO→L+6 (7%), HOMO→L+9 (8%)
22	261.66	4.74	0.051	-	H-6→LUMO (3%), H-5→L+5 (3%), H-4→L+4 (3%), H-3→L+1 (3%), H-

					3→L+5 (5%), H-3→L+6 (7%), H-2→L+3 (8%), H-2→L+4 (3%), H-2→L+7 (4%), H-1→L+1 (5%), H-1→L+2 (3%), H-1→L+6 (8%), H-1→L+9 (6%), HOMO→L+7 (4%), HOMO→L+8 (7%)
23	260.97	4.75	0.055	H-5→L+5 (17%), H-4→L+4 (15%)	H-11→L+1 (3%), H-10→LUMO (3%), H-7→L+5 (5%), H-6→L+4 (4%), H-3→L+5 (5%), H-2→L+4 (8%), H-1→L+5 (2%), HOMO→L+4 (5%), HOMO→L+12 (3%)
24	260.84	4.75	0.026	H-5→L+4 (13%), H-4→L+5 (11%), H-2→L+5 (10%)	H-11→LUMO (2%), H-10→L+1 (3%), H-7→L+4 (5%), H-6→L+5 (5%), H-4→L+1 (3%), H-4→L+2 (3%), H-3→L+4 (8%), H-1→L+4 (3%), HOMO→L+5 (6%)
25	260.77	4.75	0.001	H-5→L+2 (15%), H-4→L+3 (16%)	H-9→L+2 (3%), H-7→L+1 (4%), H-5→L+1 (6%), H-5→L+5 (2%), H-4→LUMO (5%), H-4→L+4 (3%), H-3→L+5 (3%), H-2→LUMO (4%), H-1→L+9 (2%), HOMO→LUMO (4%)
26	260.74	4.75	0.001	H-5→L+3 (15%), H-4→L+2 (14%)	H-8→L+2 (3%), H-6→L+1 (4%), H-5→LUMO (6%), H-5→L+4 (6%), H-4→L+1 (4%), H-4→L+5 (6%), H-3→LUMO (2%), H-1→LUMO (5%)

27	259.66	4.77	0.001	H-3→LUMO (10%), H-2→L+1 (19%), H- 1→LUMO (11%), HOMO→L+1 (14%)	H-5→L+3 (7%), H- 4→L+1 (4%), H- 4→L+2 (7%), H- 2→L+2 (4%), HOMO→L+2 (2%)
28	259.65	4.78	0.004	H-3→L+1 (14%), H- 2→LUMO (12%), H- 1→L+1 (18%)	H-5→L+1 (5%), H- 5→L+2 (7%), H- 4→L+3 (6%), H- 3→L+2 (3%), H- 1→L+2 (3%), HOMO→LUMO (9%)
29	258.13	4.80	0.005	-	H-7→L+4 (2%), H- 3→L+4 (4%), H- 3→L+7 (6%), H- 3→L+8 (2%), H- 3→L+10 (3%), H- 2→L+5 (7%), H- 2→L+9 (2%), H- 2→L+13 (2%), H- 1→L+4 (2%), H- 1→L+7 (7%), H- 1→L+10 (7%), HOMO→L+9 (3%), HOMO→L+11 (8%)
30	258.12	4.80	0.046	HOMO→L+7 (11%), HOMO→L+10 (10%)	H-13→L+2 (2%), H- 3→L+5 (6%), H- 3→L+9 (3%), H- 3→L+13 (2%), H- 2→L+4 (4%), H- 2→L+7 (5%), H- 2→L+8 (3%), H- 2→L+12 (2%), H- 1→L+9 (2%), H- 1→L+11 (7%)
31	257.84	4.81	0.028	-	H-7→L+5 (3%), H- 6→L+4 (3%), H- 5→L+9 (3%), H- 4→LUMO (6%), H- 4→L+8 (4%), H- 3→L+1 (2%), H- 3→L+5 (4%), H- 2→L+4 (6%), H- 1→L+1 (2%), H- 1→L+5 (3%), H- 1→L+6 (2%), H- 1→L+11 (5%), H- 1→L+13 (4%), HOMO→L+4 (2%), HOMO→L+7 (2%),

					HOMO→L+10 (8%), HOMO→L+12 (4%)
32	257.78	4.81	0.027	-	H-7→L+4 (2%), H-6→L+5 (2%), H-5→LUMO (6%), H-5→L+8 (3%), H-4→L+9 (3%), H-3→L+4 (4%), H-2→L+1 (2%), H-2→L+5 (5%), H-1→L+7 (3%), H-1→L+10 (8%), H-1→L+12 (3%), HOMO→L+6 (2%), HOMO→L+11 (8%), HOMO→L+13 (3%)
33	257.22	4.82	0.000	H-5→L+1 (10%)	H-7→L+2 (4%), H-6→L+3 (2%), H-5→L+9 (4%), H-4→LUMO (8%), H-4→L+7 (3%), H-4→L+8 (3%), H-3→L+9 (2%), H-2→LUMO (5%), H-2→L+8 (3%), H-1→L+5 (5%), HOMO→L+4 (4%), HOMO→L+7 (3%), HOMO→L+12 (3%)
34	257.12	4.82	0.006	H-4→L+1 (13%)	H-7→L+3 (3%), H-6→L+2 (4%), H-5→LUMO (9%), H-5→L+7 (4%), H-5→L+8 (4%), H-4→L+9 (4%), H-3→LUMO (6%), H-3→L+4 (2%), H-3→L+8 (2%), H-2→L+9 (3%), H-1→LUMO (2%), H-1→L+4 (3%), HOMO→L+5 (4%)
35	256.46	4.83	0.002	H-5→L+1 (10%), HOMO→L+10 (10%)	H-7→L+2 (3%), H-6→L+3 (3%), H-5→L+5 (3%), H-4→LUMO (4%), H-3→L+1 (2%), H-2→L+12 (3%), H-1→L+5 (2%), H-

					1→L+11 (9%), HOMO→L+8 (2%), HOMO→L+12 (4%)
36	256.33	4.84	0.005	H-4→L+1 (11%)	H-7→L+3 (2%), H-5→LUMO (4%), H-4→L+5 (3%), H-3→L+8 (3%), H-3→L+12 (3%), H-1→L+4 (3%), H-1→L+10 (8%), HOMO→L+5 (5%), HOMO→L+11 (8%)
37	256.23	4.84	0.002	H-4→LUMO (10%)	H-7→L+2 (4%), H-6→L+3 (6%), H-6→L+7 (2%), H-5→L+1 (7%), H-5→L+2 (4%), H-5→L+6 (6%), H-4→L+3 (3%), H-4→L+4 (4%), H-4→L+7 (5%), H-3→L+2 (3%)
38	256.22	4.84	0.001	H-5→LUMO (11%)	H-7→L+3 (6%), H-6→L+2 (4%), H-5→L+3 (3%), H-5→L+4 (3%), H-5→L+7 (5%), H-4→L+1 (9%), H-4→L+2 (5%), H-4→L+6 (5%), H-2→L+2 (3%)
39	256.10	4.84	0.002	-	H-9→L+1 (5%), H-8→LUMO (3%), H-7→L+5 (5%), H-6→L+4 (4%), H-5→L+1 (9%), H-5→L+9 (5%), H-4→LUMO (5%), H-4→L+8 (5%), H-3→L+5 (7%), H-2→L+4 (7%), H-1→L+9 (3%), HOMO→L+8 (4%)
40	256.03	4.84	0.045	-	H-11→LUMO (2%), H-9→LUMO (3%), H-8→L+1 (4%), H-7→L+4 (4%), H-6→L+5 (4%), H-5→L+8 (4%), H-

					4→L+1 (4%), H-4→L+9 (4%), H-3→L+4 (5%), H-3→L+7 (3%), H-2→L+5 (9%), H-1→L+8 (6%), H-1→L+12 (3%), HOMO→L+9 (4%)
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Table S10. Calculated electronic transitions for **D2-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

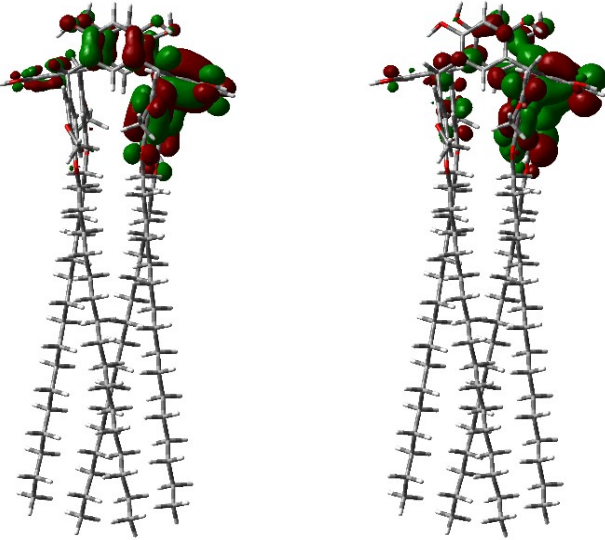
Transition n°	Wavelength (nm)	Energy (eV)	Osc. Strength	Major contribs	Minor contribs
1	298.45	4.15	0.002	HOMO→L+2 (92%)	HOMO→L+8 (3%)
2	298.24	4.16	0.001	H-1→LUMO (91%)	-
3	288.65	4.30	0.030	H-3→LUMO (26%), H-1→L+1 (69%)	-
4	287.97	4.31	0.024	H-3→LUMO (68%), H-1→L+1 (23%)	-
5	287.71	4.31	0.017	H-2→L+2 (93%)	-
6	286.16	4.33	0.022	HOMO→LUMO (38%), HOMO→L+5 (42%)	HOMO→L+3 (5%), HOMO→L+7 (3%), HOMO→L+8 (5%)
7	284.74	4.35	0.015	HOMO→LUMO (55%), HOMO→L+5 (31%)	HOMO→L+6 (3%), HOMO→L+7 (2%), HOMO→L+8 (5%)
8	282.54	4.39	0.049	H-3→L+3 (31%), H-1→L+3 (58%)	-
9	281.29	4.41	0.049	H-2→L+7 (14%), HOMO→L+5 (13%), HOMO→L+7 (40%), HOMO→L+8 (17%)	H-2→L+5 (5%), H-2→L+8 (4%)
10	281.24	4.41	0.051	HOMO→L+7 (33%), HOMO→L+8 (43%)	H-2→L+7 (6%), H-2→L+8 (9%)
11	280.14	4.43	0.030	H-3→L+1 (32%), H-1→L+4 (48%)	H-3→L+3 (4%), H-3→L+4 (6%), H-1→L+3 (3%)
12	279.82	4.43	0.018	H-3→L+1 (61%), H-1→L+4 (22%)	H-6→LUMO (3%), H-3→L+4 (4%), H-1→L+3 (3%)
13	276.47	4.48	0.001	H-2→LUMO (15%), HOMO→L+1 (39%), HOMO→L+3 (34%)	H-2→L+5 (4%)
14	275.81	4.50	0.006	H-2→LUMO (12%), H-2→L+5 (19%),	H-2→L+7 (3%), HOMO→LUMO

				HOMO→L+3 (48%)	(3%), HOMO→L+1 (7%)
15	275.43	4.50	0.009	H-2→L+5 (33%), HOMO→L+1 (37%)	H-5→L+2 (2%), H-4→L+2 (3%), H-2→L+7 (4%), HOMO→L+3 (9%)
16	274.18	4.52	0.003	H-2→LUMO (65%), H-2→L+5 (10%), HOMO→L+1 (11%)	H-5→L+2 (5%), H-4→L+2 (3%)
17	274.00	4.52	0.001	H-6→LUMO (68%), H-6→L+1 (21%)	H-3→L+3 (2%)
18	273.16	4.54	0.004	H-5→L+2 (66%), H-4→L+2 (11%)	H-2→LUMO (2%), H-2→L+5 (9%), H-2→L+7 (2%)
19	271.45	4.57	0.002	H-3→L+3 (25%), H-3→L+6 (14%), H-1→L+3 (16%), H-1→L+6 (29%)	H-1→L+4 (4%)
20	270.79	4.58	0.006	H-3→L+3 (26%), H-3→L+6 (15%), H-1→L+3 (11%), H-1→L+6 (34%)	H-1→L+4 (7%)
21	269.88	4.59	0.002	H-5→L+2 (12%), H-4→L+2 (46%), H-2→L+7 (12%)	H-4→L+5 (7%), H-4→L+7 (4%), H-2→L+8 (3%), HOMO→L+8 (2%)
22	269.23	4.61	0.003	H-4→L+2 (12%), H-2→L+5 (11%), H-2→L+7 (37%), HOMO→L+8 (14%)	H-5→L+2 (2%), H-4→L+5 (3%), H-2→L+8 (3%), HOMO→L+5 (3%), HOMO→L+7 (6%)
23	267.96	4.63	0.000	HOMO→L+6 (85%)	HOMO→L+1 (2%), HOMO→L+4 (3%)
24	267.28	4.64	0.026	H-10→LUMO (23%), H-6→LUMO (13%), H-6→L+1 (50%)	-
25	266.44	4.65	0.000	H-2→L+1 (47%), H-2→L+3 (42%)	HOMO→L+6 (2%)
26	266.21	4.66	0.008	H-2→L+8 (56%)	H-2→L+1 (4%), H-2→L+3 (9%), H-2→L+7 (7%), HOMO→L+7 (6%), HOMO→L+8 (5%), HOMO→L+11 (2%)
27	265.97	4.66	0.001	H-2→L+1 (43%), H-2→L+3 (38%), H-2→L+8 (11%)	H-2→LUMO (2%)

28	265.00	4.68	0.038	H-7→L+2 (27%), H-4→L+5 (34%)	H-8→L+2 (8%), H-4→LUMO (3%), H-4→L+2 (3%), H-4→L+7 (2%)
29	264.86	4.68	0.015	H-3→L+4 (60%), HOMO→L+4 (15%)	H-3→L+9 (4%), H-1→L+4 (8%), H-1→L+9 (4%)
30	264.80	4.68	0.004	H-3→L+4 (11%), HOMO→L+4 (79%)	HOMO→L+6 (3%)
31	263.65	4.70	0.008	H-10→LUMO (49%), H-6→L+1 (16%)	H-11→LUMO (2%), H-10→L+1 (6%), H-10→L+4 (2%), H-6→LUMO (6%), H-3→L+6 (3%)
32	263.31	4.71	0.001	H-1→L+2 (90%)	H-3→L+2 (3%)
33	263.22	4.71	0.002	H-4→LUMO (85%)	H-7→L+2 (2%), H-5→LUMO (4%)
34	262.98	4.71	0.028	H-6→L+3 (22%), H-6→L+4 (54%)	H-10→LUMO (3%), H-3→L+9 (3%)
35	262.71	4.72	0.016	H-5→L+5 (27%), H-5→L+7 (30%)	H-8→L+5 (2%), H-5→L+8 (9%), H-4→L+5 (5%), H-4→L+7 (5%), H-4→L+8 (4%), HOMO→L+11 (6%)
36	262.11	4.73	0.033	H-4→L+7 (27%), H-4→L+8 (27%)	H-9→L+2 (7%), H-5→L+8 (6%), H-4→L+2 (6%), HOMO→L+11 (5%)
37	261.87	4.73	0.019	H-11→LUMO (13%), H-3→L+6 (31%), H-1→L+6 (17%), H-1→L+9 (15%)	H-6→L+4 (5%)
38	261.55	4.74	0.023	H-9→L+2 (25%), H-7→L+2 (18%), H-4→L+5 (15%), H-4→L+8 (11%)	H-2→L+11 (3%)
39	261.14	4.75	0.031	H-11→LUMO (42%), H-3→L+6 (16%)	H-11→L+1 (3%), H-11→L+3 (4%), H-10→LUMO (3%), H-6→L+3 (2%), H-1→L+6 (6%)

40	260.94	4.75	0.023	HOMO→L+11 (43%)	H-8→L+2 (6%), H-8→L+5 (4%), H-7→L+5 (2%), H-5→LUMO (2%), H-5→L+5 (6%), H-4→L+5 (2%), H-4→L+8 (9%), HOMO→L+12 (7%)
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Table S11. NTO analysis of electronic transition 2 of **C1-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
C1-b (2)	4.54 (273.26)	H → L (69.0%) 

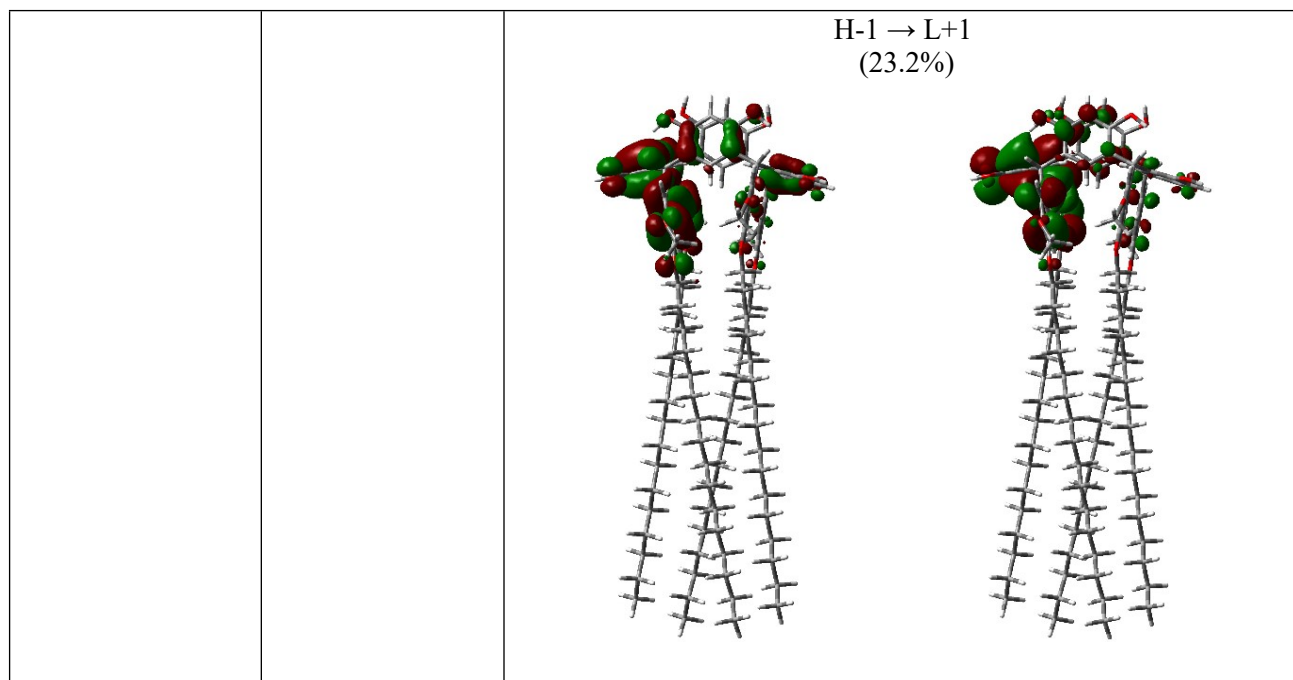
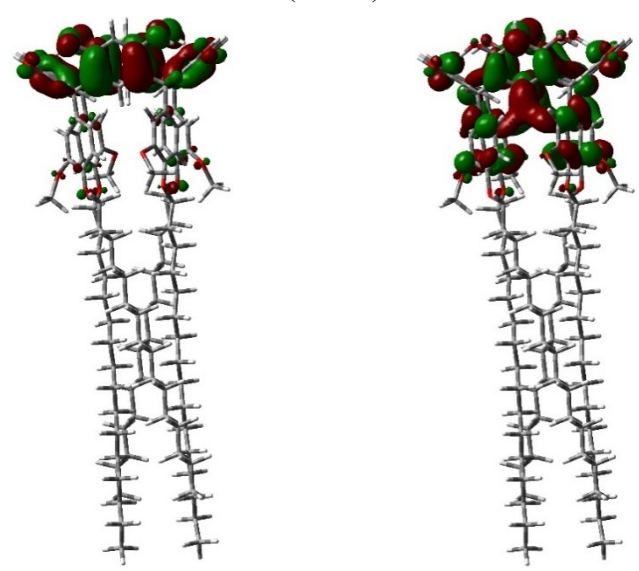
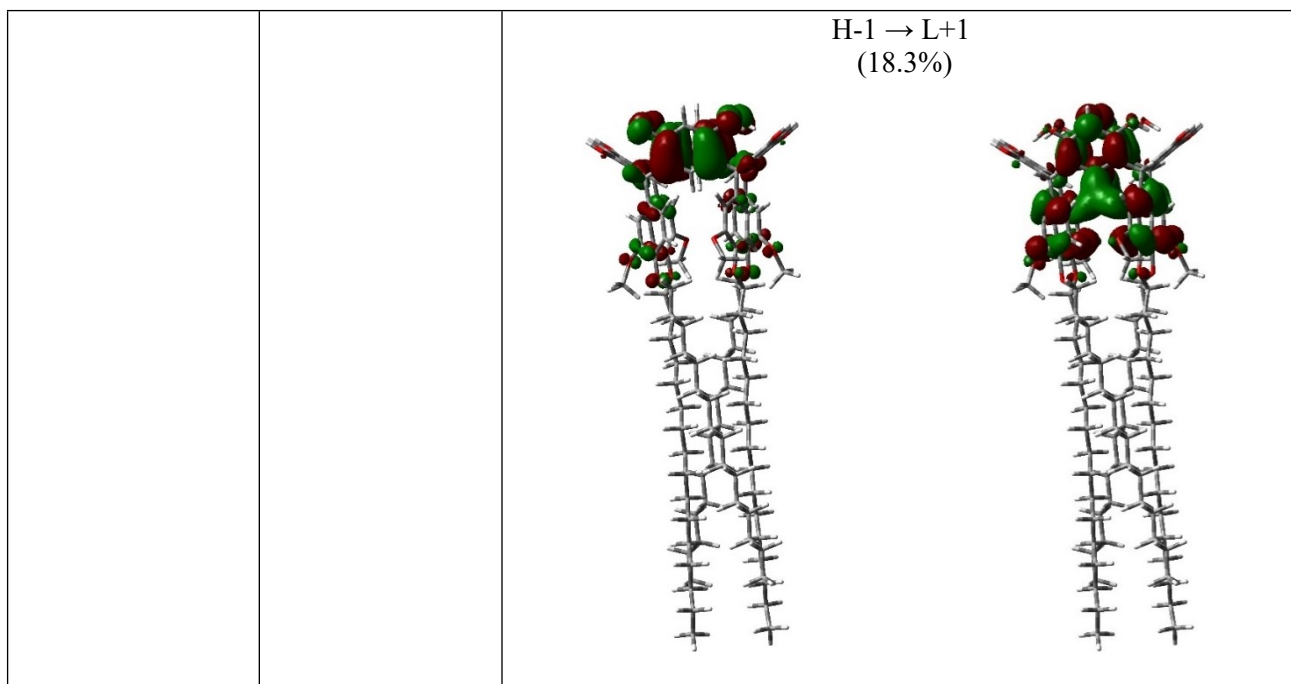
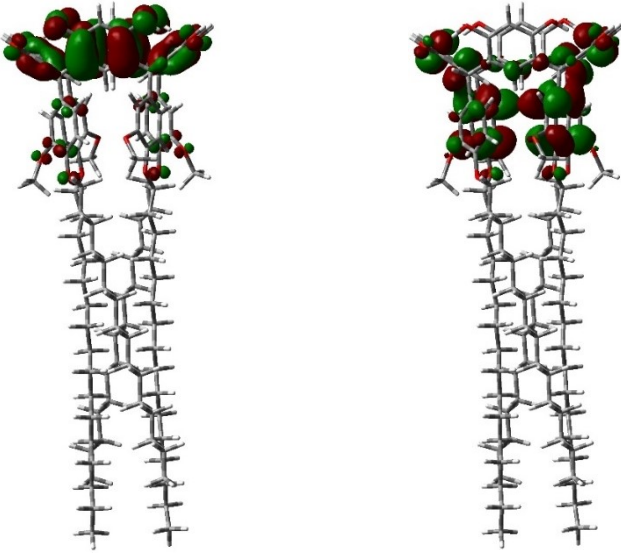
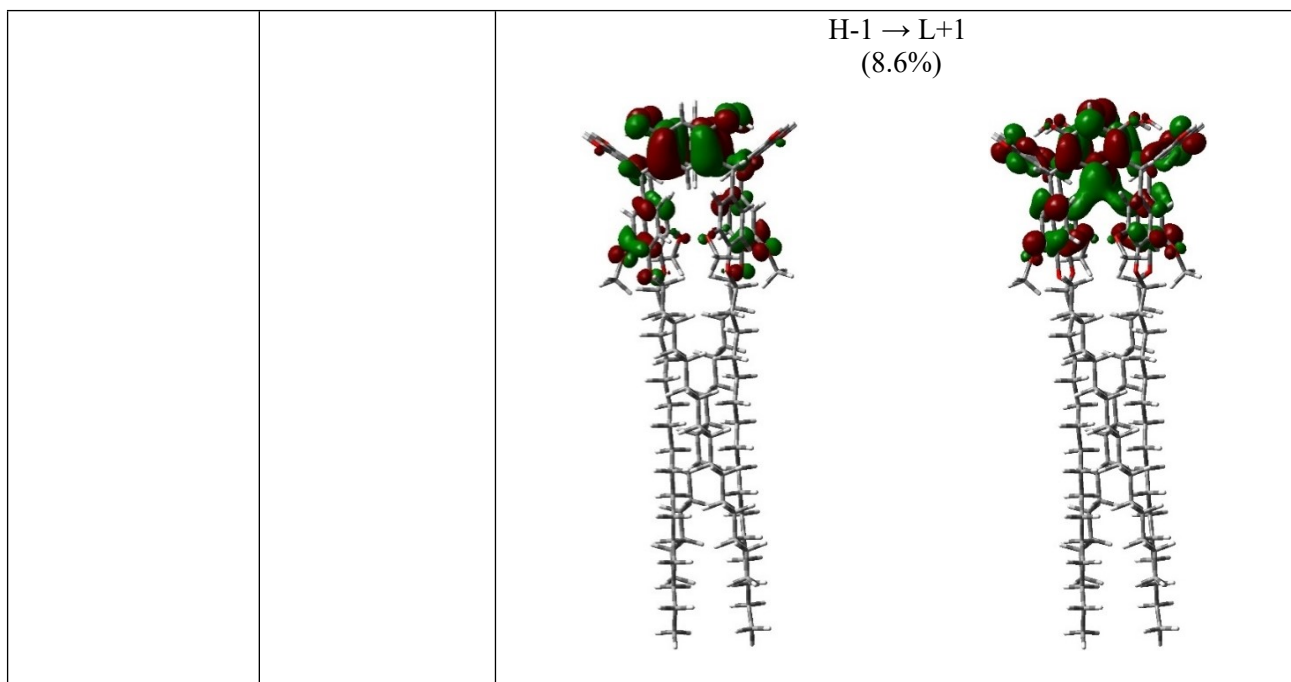


Table S12. NTO analysis of electronic transitions 5, 17 and 20 of **C1-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

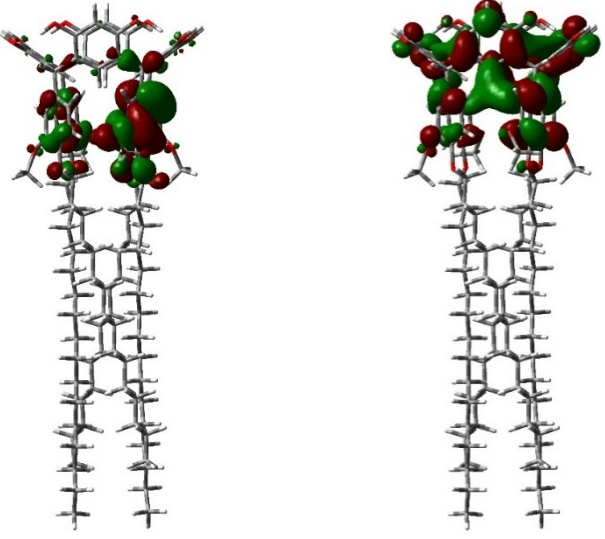
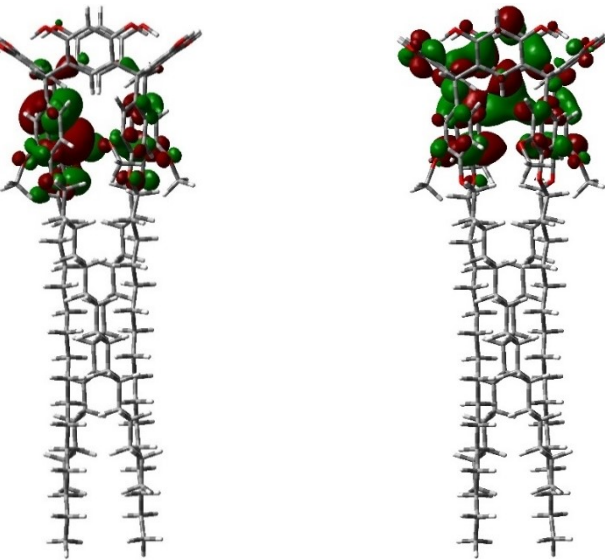
Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
C1-c (5)	4.42 (278.53)	<p>H \rightarrow L (75.3%)</p> 



Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
C1-c (17)	4.80 (258.20)	<p>H → L (86.5%)</p> 



Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
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<p>C1-c (20)</p>	<p>4.83 (256.94)</p>	<p>H → L (38.5%)</p> 
		<p>H-1 → L+1 (38.0%)</p> 

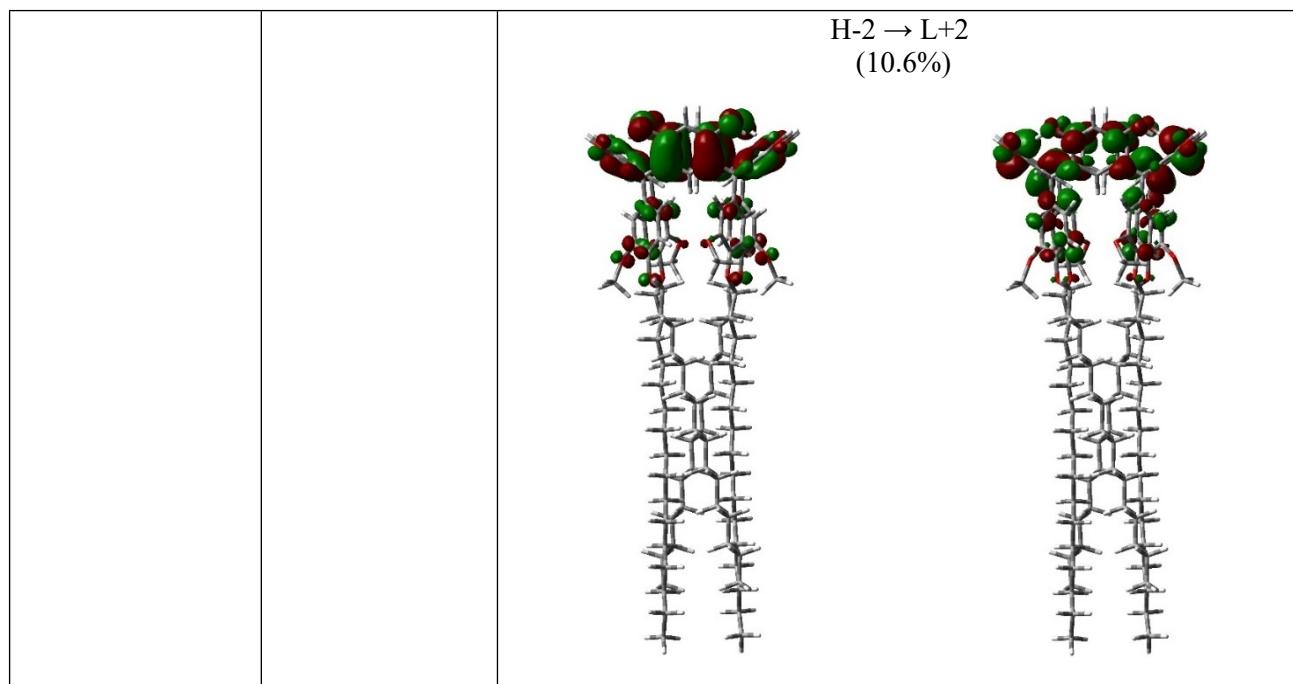


Table S13. NTO analysis of electronic transition 2 of **Cr-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

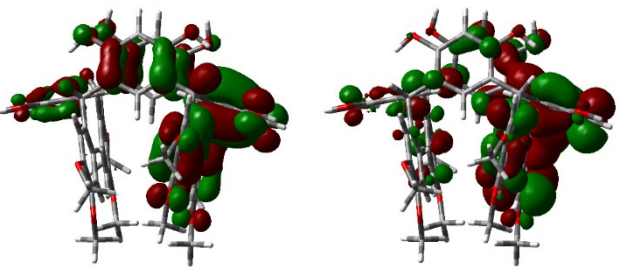
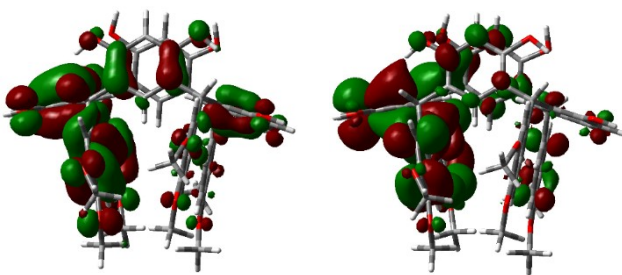
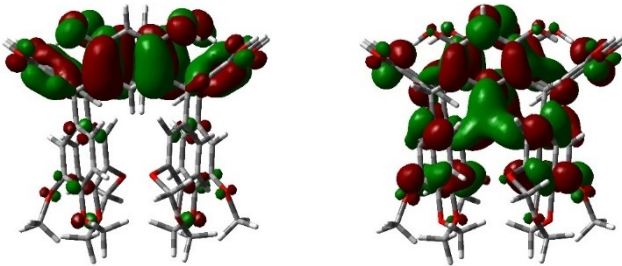
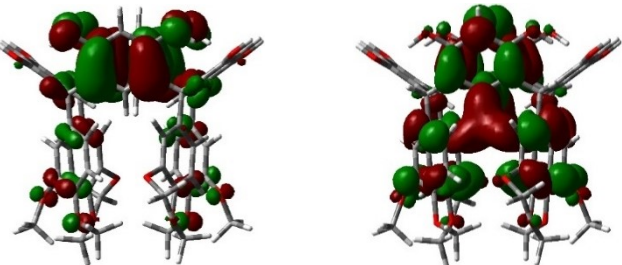
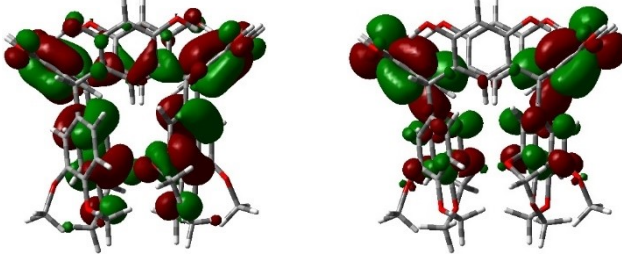
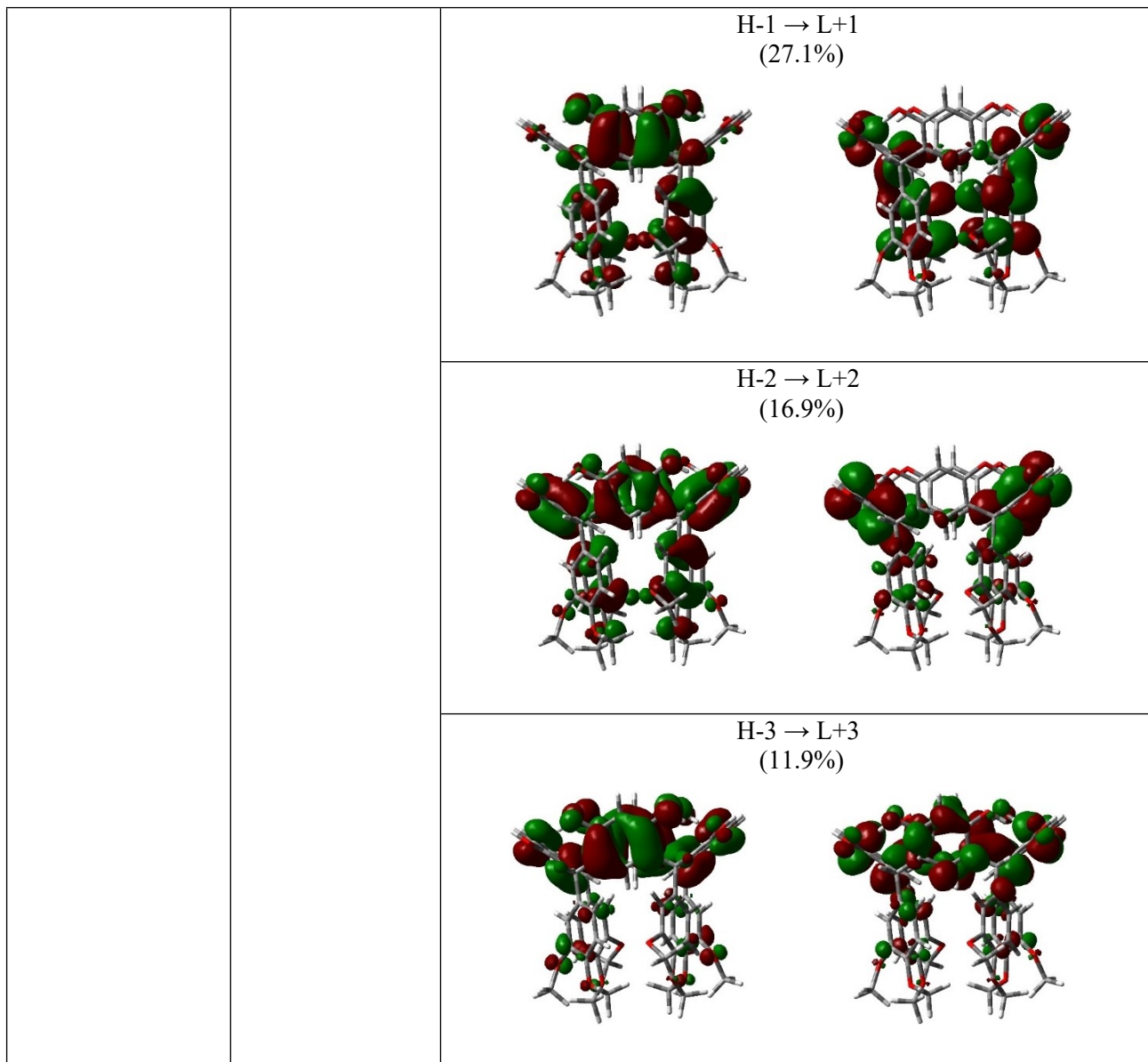
Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
Cr-b (2)	2.54 (273.07)	<p>H \rightarrow L (60.1%)</p> 
		<p>H-1 \rightarrow L+1 (32.3%)</p> 

Table S14. NTO analysis of electronic transitions 5, 17 and 26 of Cr-c at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
Cr-c (5)	4.43 (279.61)	H \rightarrow L (75.7%) 
		H-1 \rightarrow L+1 (18.1%) 
Cr-c (17)	4.80 (258.25)	H \rightarrow L (33.1%) 



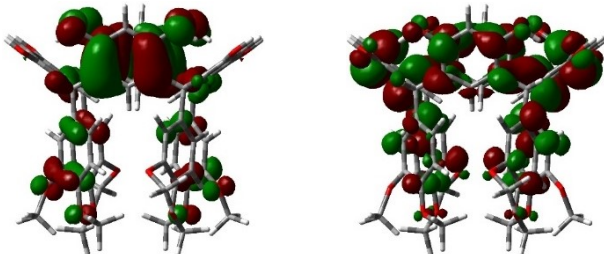
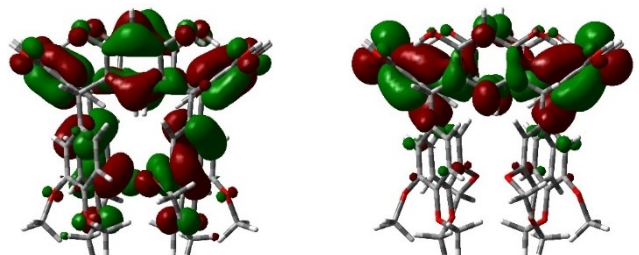
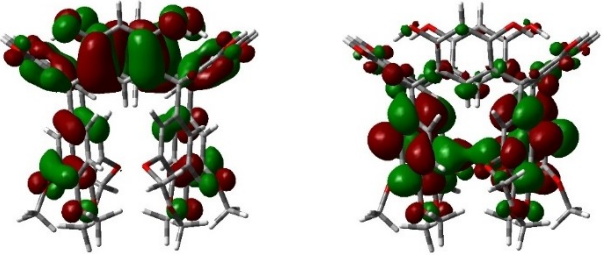
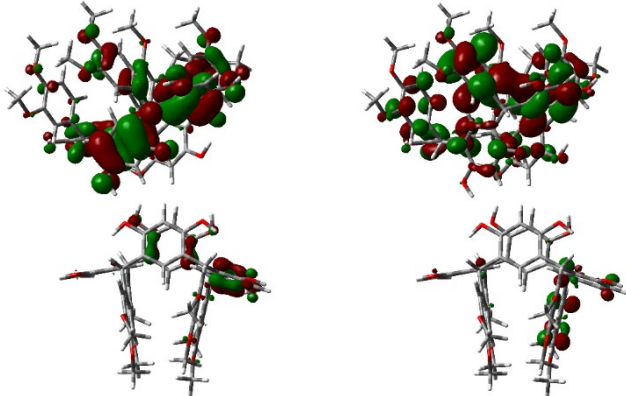
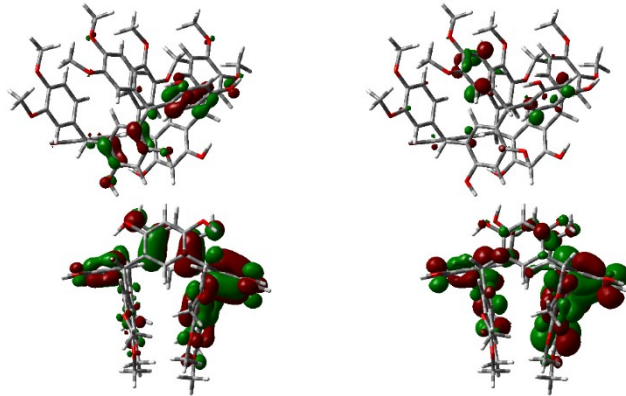
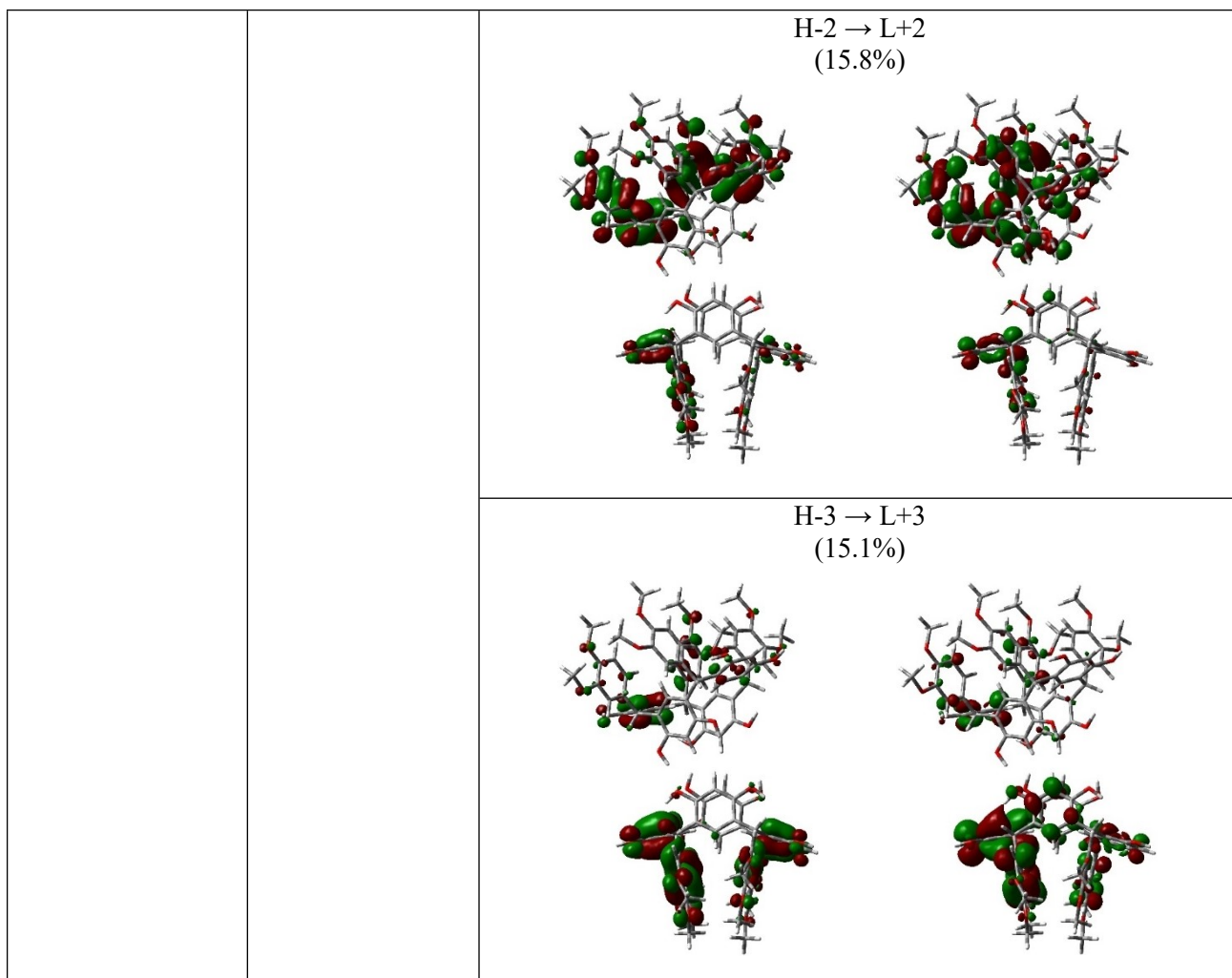
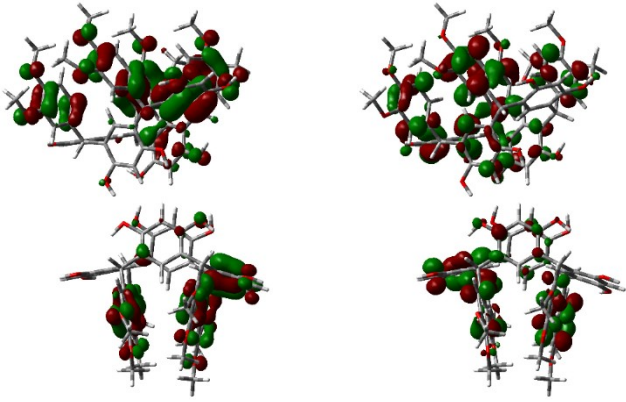
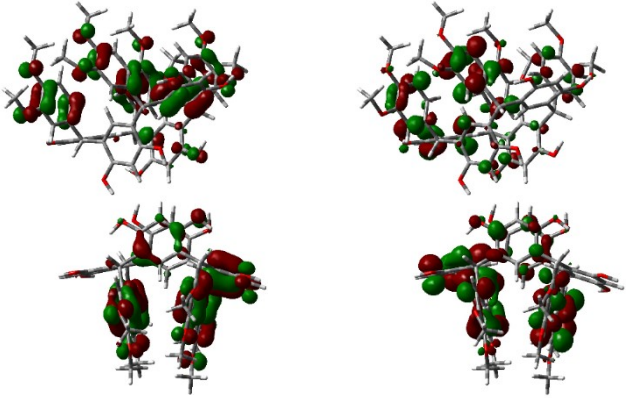
Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
Cr-c (26)	4.92 (252.12)	<p>H \rightarrow L (64.0%)</p> 
		<p>H-1 \rightarrow L+1 (11.1%)</p> 
		<p>H-2 \rightarrow L+2 (10.8%)</p> 

Table S15. NTO analysis of electronic transitions 4 and 13 of **D1-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

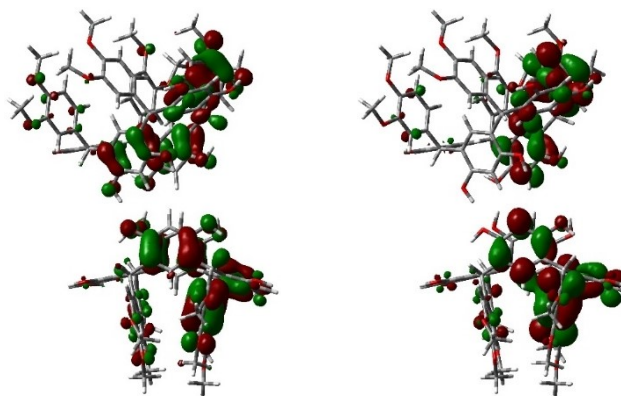
Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D1-b (4)	4.53 (273.75)	<p>H \rightarrow L (31.4%)</p> 
		<p>H-1 \rightarrow L+1 (30.1%)</p> 



Compound	Transition energy	NTO couple
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(State)	(λ) [eV (nm)]	(Contribution)
D1-b (13)	4.73 (262.40)	<p data-bbox="1008 228 1101 256">$H \rightarrow L$</p> <p data-bbox="1008 260 1101 287">(21.1%)</p> 
		<p data-bbox="984 739 1125 766">$H-1 \rightarrow L+1$</p> <p data-bbox="1003 770 1105 798">(19.1%)</p> 

H-2 → L+2
(12.6%)



H-3 → L+3
(10.8%)

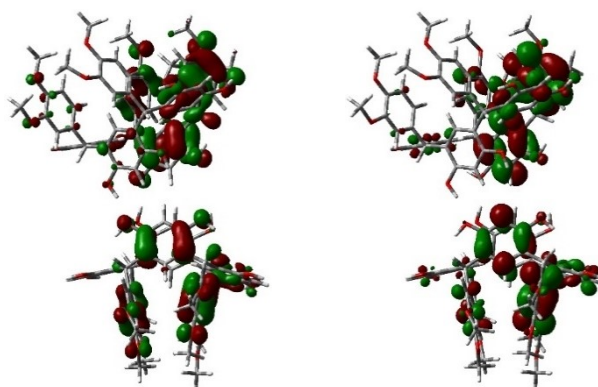
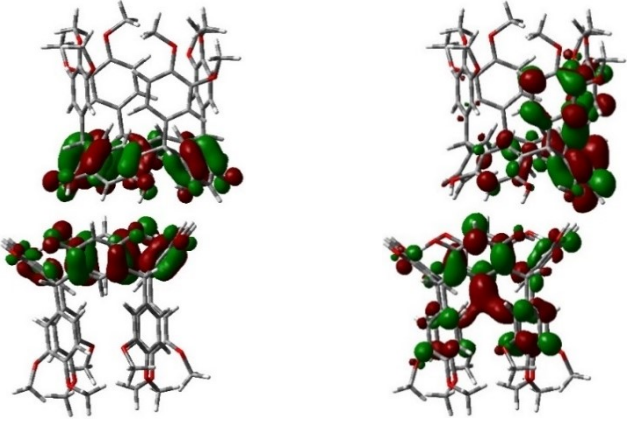
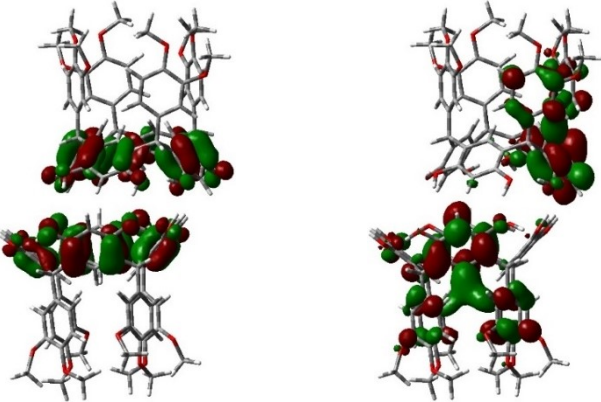
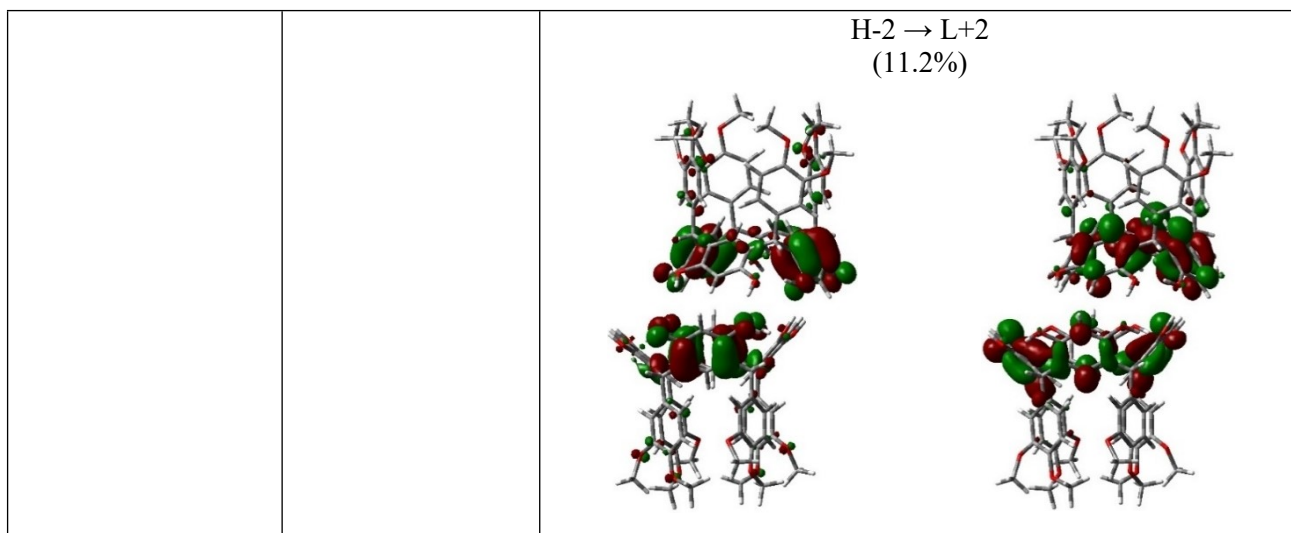


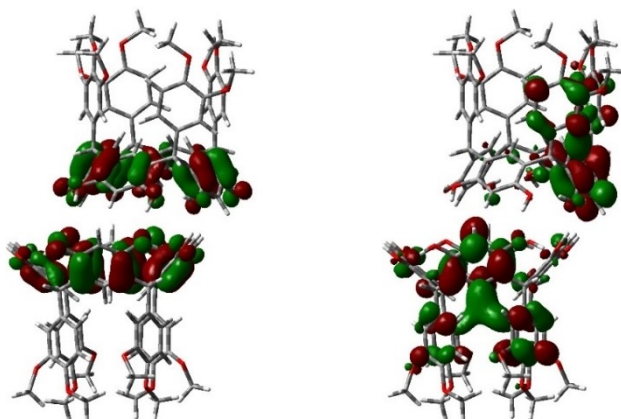
Table S16. NTO analysis of electronic transitions 7, 8 and 24 of **D1-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D2-b (7)	4.39 (282.65)	<p>H \rightarrow L (42.4%)</p> 
		<p>H-1 \rightarrow L+1 (34.7%)</p> 

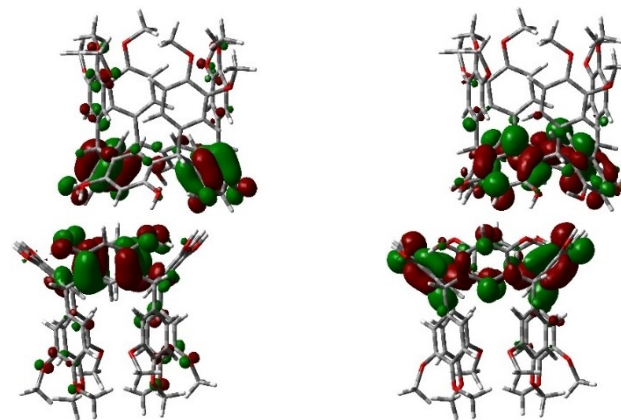


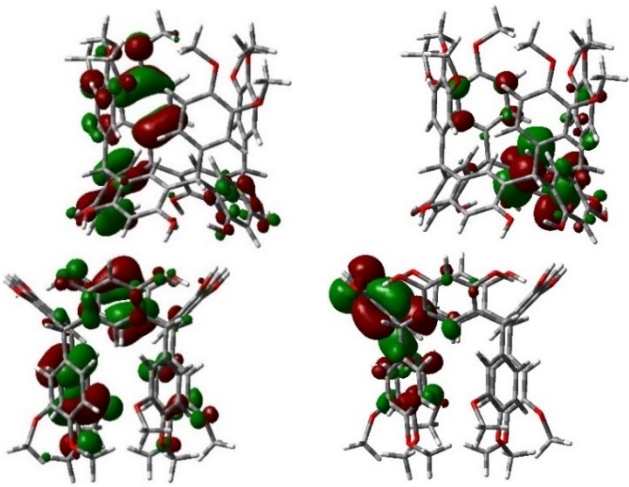
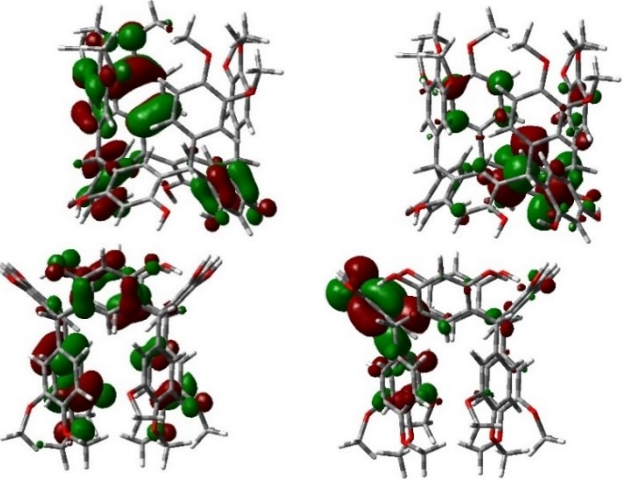
Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D2-b (8)	4.39 (282.42)	<p>H → L (39.6%)</p>

H-1 → L+1
(35.4%)

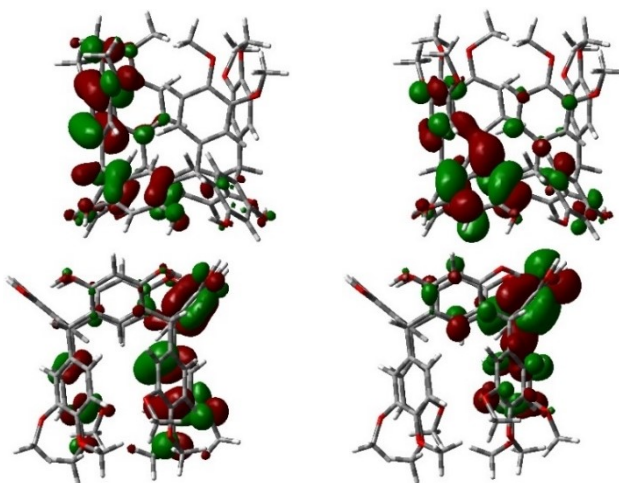


H-2 → L+2
(12.1%)



Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D1-c (24)	4.64 (267.44)	<p data-bbox="998 262 1169 325">H \rightarrow L (33.6%)</p> 
		<p data-bbox="1015 867 1153 930">H-1 \rightarrow L+1 (25.1%)</p> 

H-2 → L+2
(17.9%)



H-3 → L+3
(14.6%)

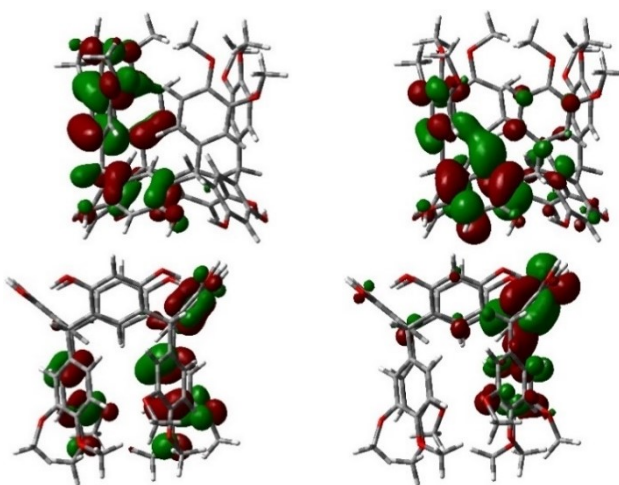
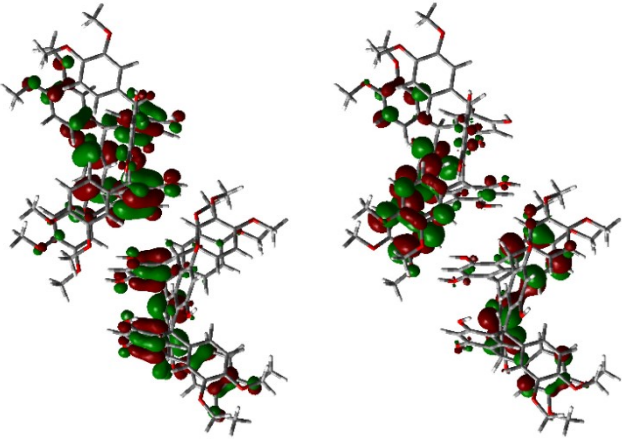
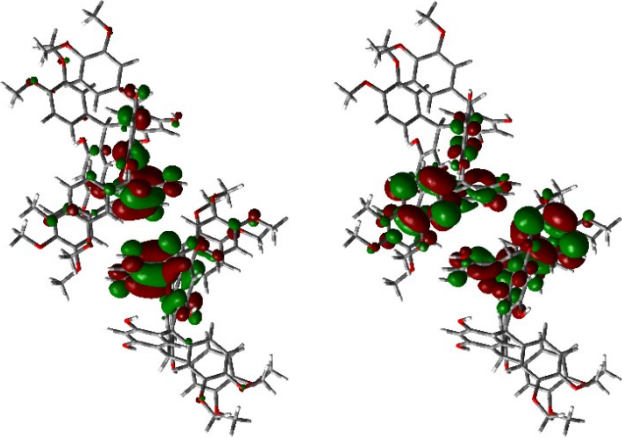
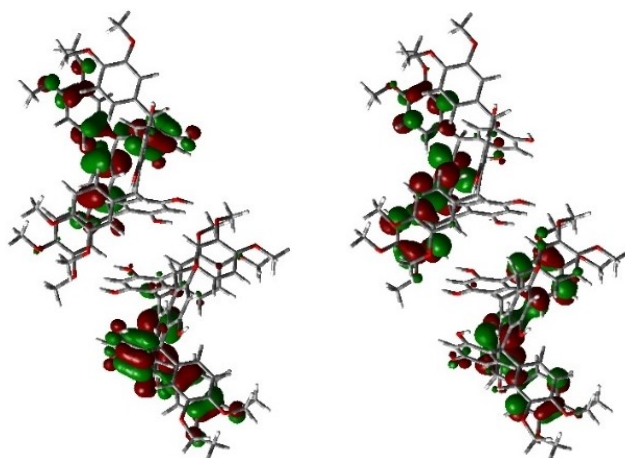


Table S17. NTO analysis of electronic transition 3 of **D2-b** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D2-b (3)	4.53 (273.49)	<p data-bbox="954 394 1052 457">$H \rightarrow L$ (31.6%)</p> 
		<p data-bbox="928 949 1078 1012">$H-1 \rightarrow L+1$ (29.5%)</p> 

H-2 → L+2
(21.8%)



H-3 → L+3
(12.1%)

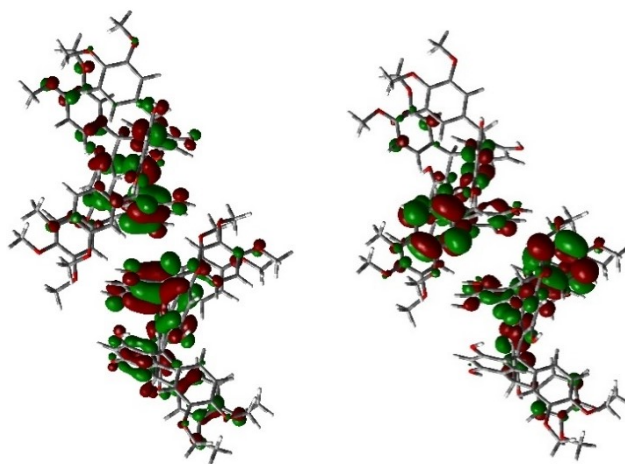
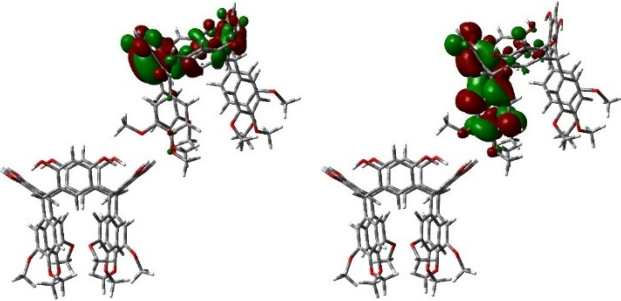
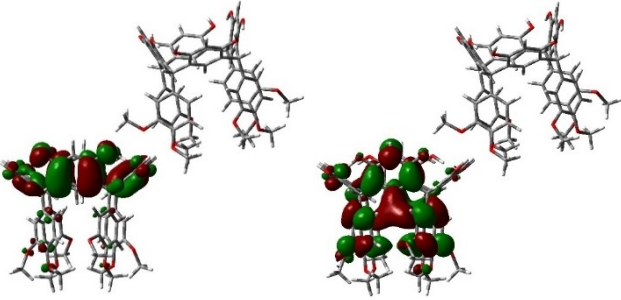
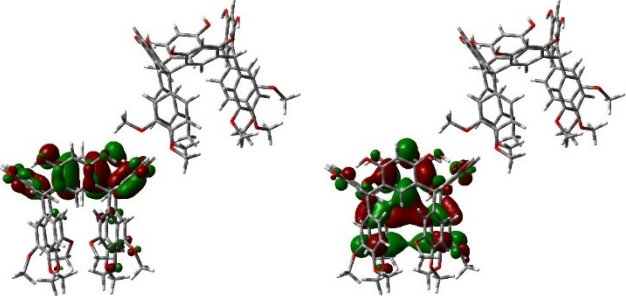


Table S18. NTO analysis of electronic transitions 8, 9 and 10 of **D2-c** at the B3LYP/6-31G(d,p)/PCM(TFH) level of theory

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D2-c (8)	4.39 (282.54)	H \rightarrow L (95.4%) 

Compound (State)	Transition energy (λ) [eV (nm)]	NTO couple (Contribution)
D2-c (9)	4.41 (281.29)	H \rightarrow L (95.2%) 

Compound	Transition energy	NTO couple
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(State)	(λ) [eV (nm)]	(Contribution)
D2-c (10)	4.41 (281.24)	H \rightarrow L (93.9%) 

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