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Supporting Information

Blue-shifted emission and enhanced quantum efficiency via π-bridge elongation in carbazole-carborane dyads

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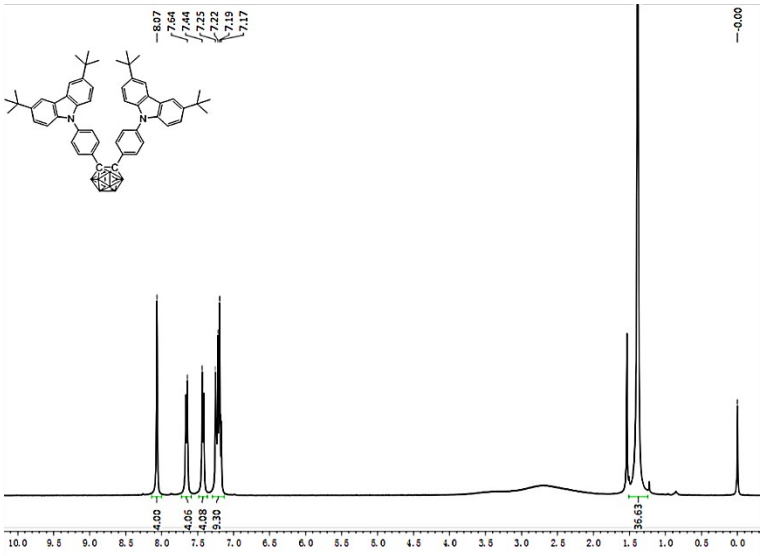
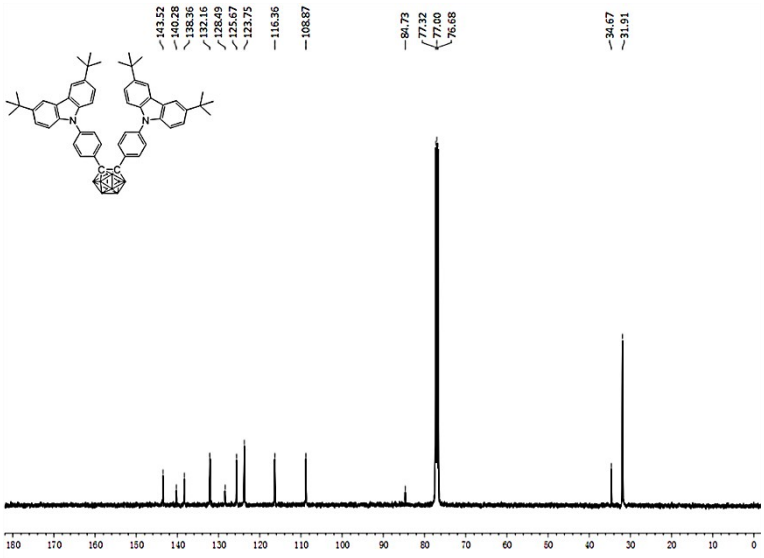


^{1}H NMR spectrum of D-1 ($CDCl_3$)



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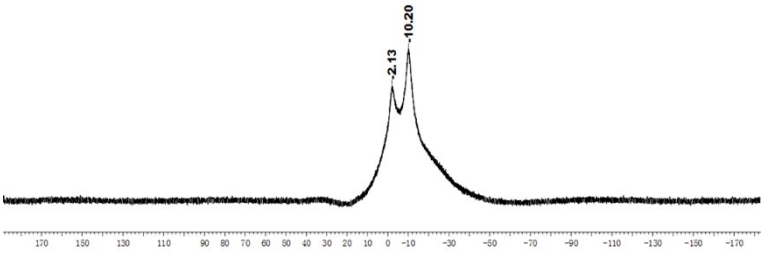

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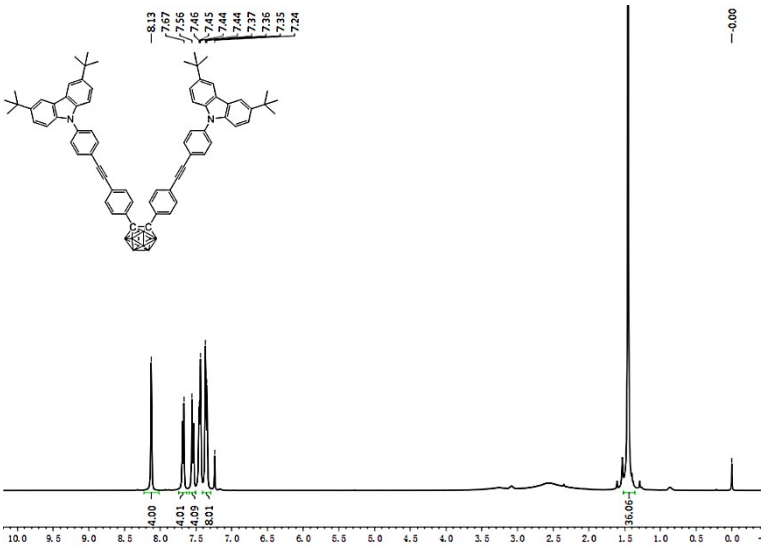

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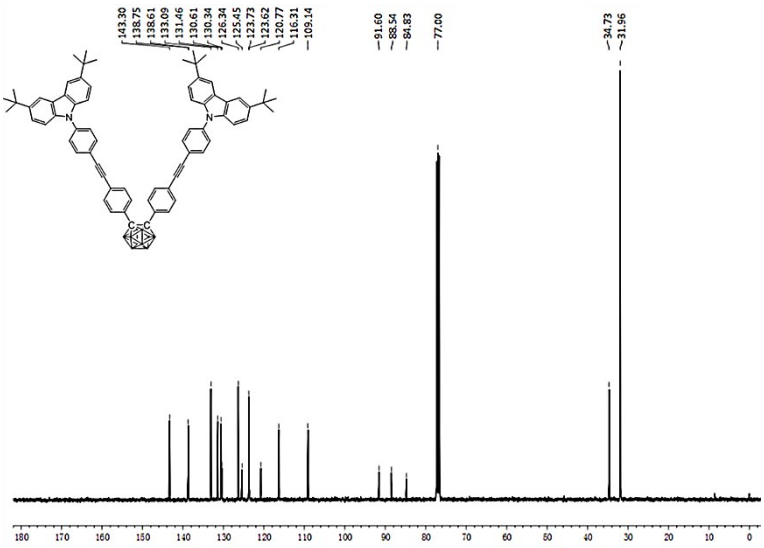

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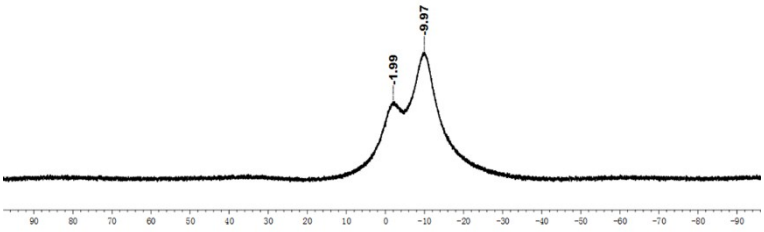

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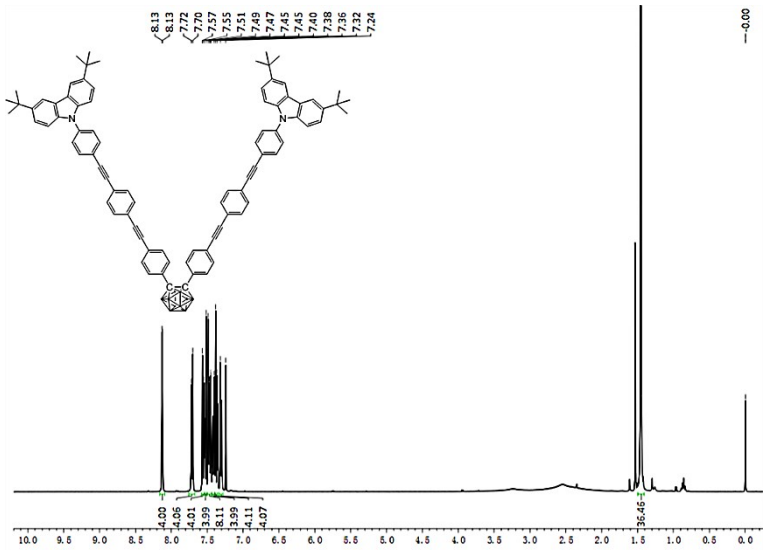

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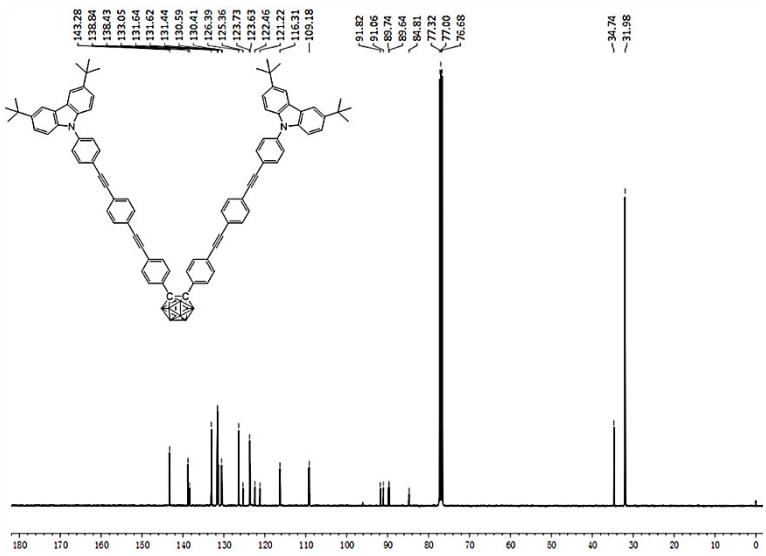

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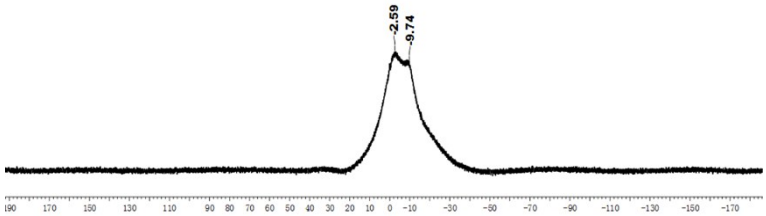

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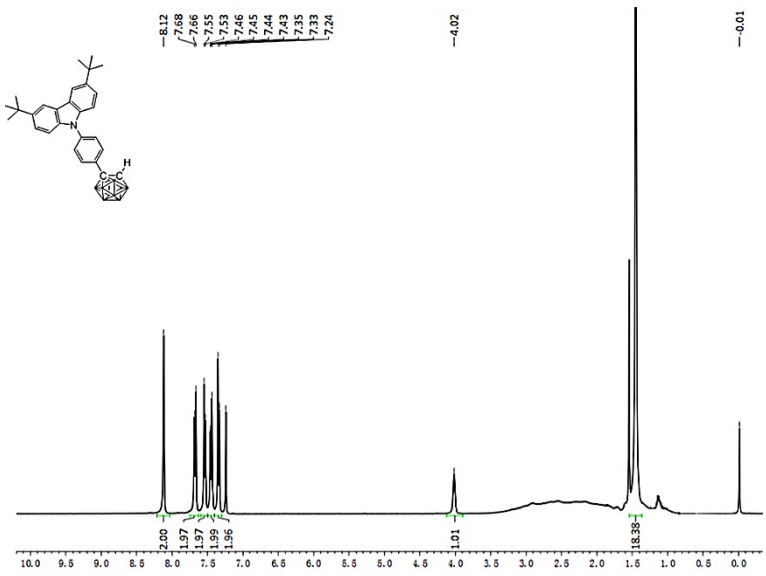

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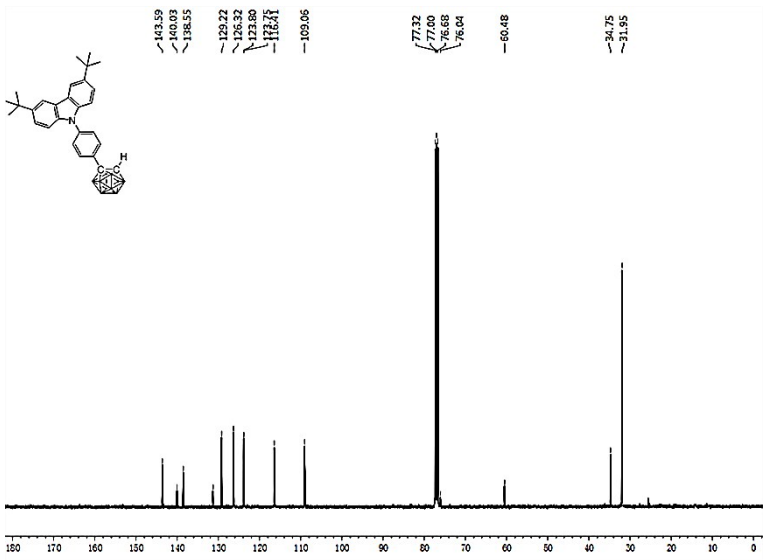

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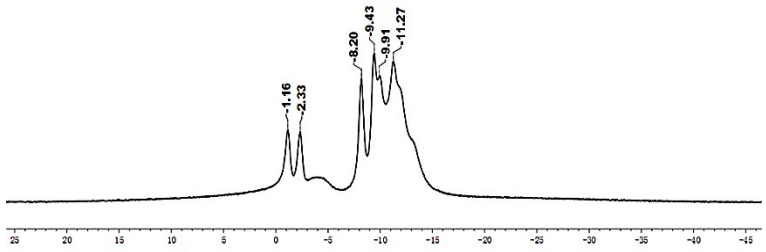

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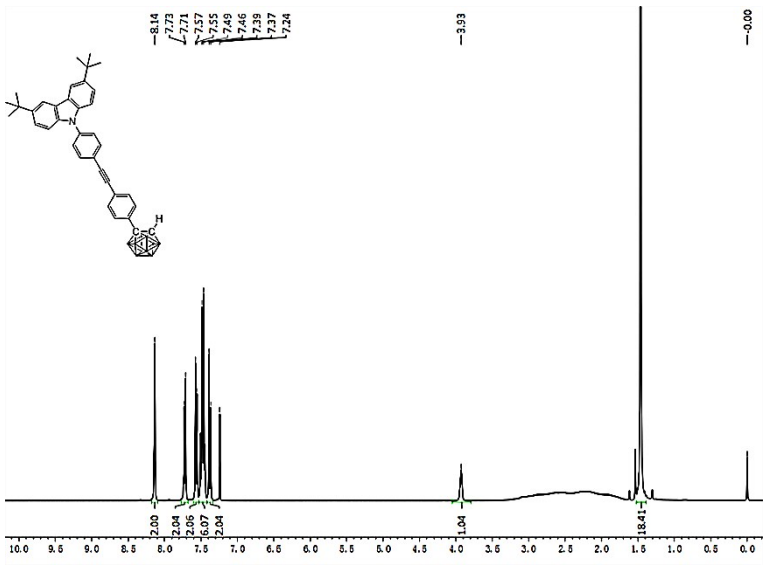

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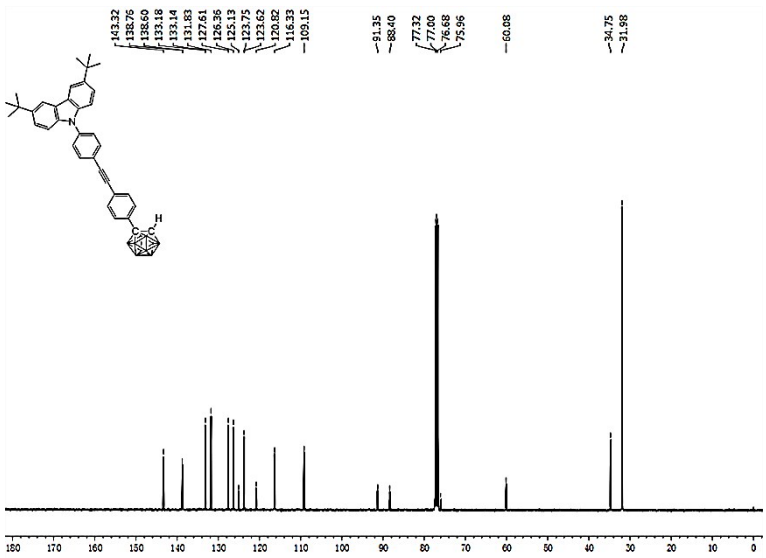

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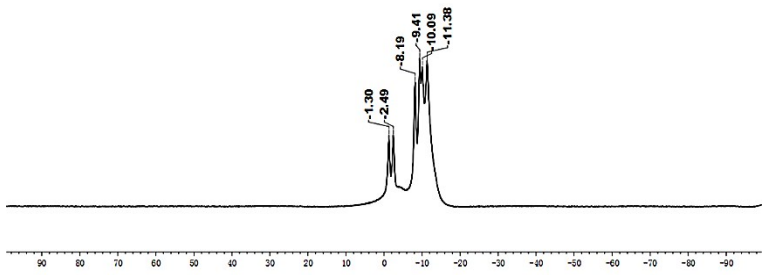

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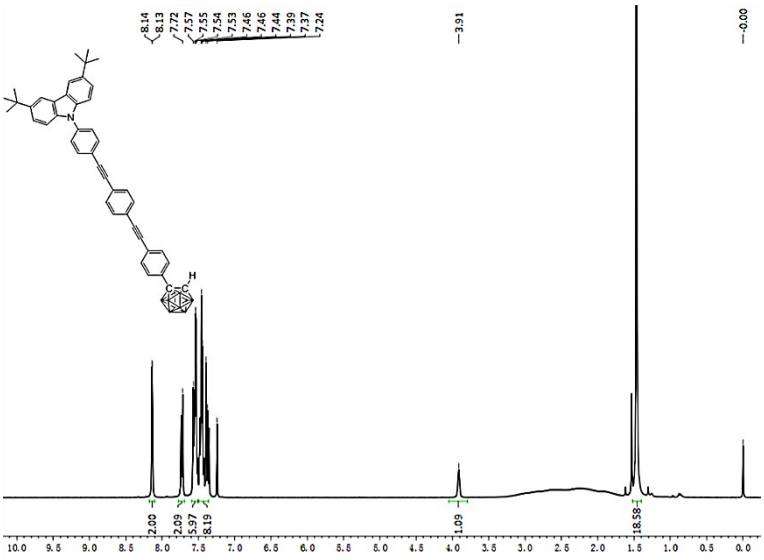

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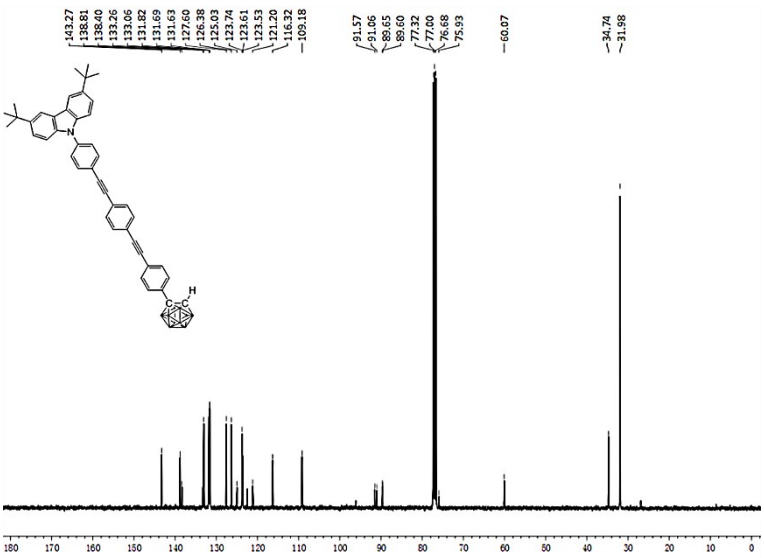

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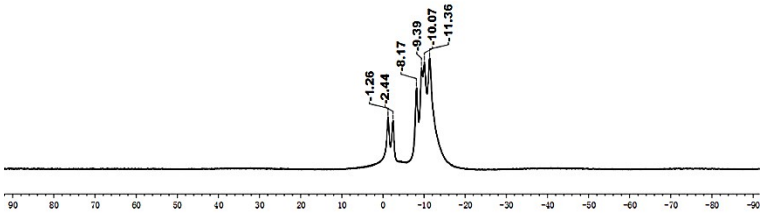


^{11}B {^{1}H} NMR spectrum of M-3 ($CDCl_3$)

1.2 X-ray structural study of D-3

Crystals of **D-3** suitable for the X-ray structural analysis were grown by controlled cooling of a hot hexane/carbon tetrachloride (1:1) solution. A suitable crystal was mounted on a MicroMount (MiTeGen) using Paratone-N oil (Hampton Research) and cooled rapidly to 150 K using an Oxford Cryosystems low-temperature device.[S1] Intensity data were collected on an Agilent SuperNova CCD diffractometer using mirror-monochromated Cu-K_α radiation (λ = 1.54184 Å). N_t (total) reflections were measured by using omega scans and were reduced to N_o unique reflections, with $F_o > 2\sigma(F_o)$ being considered to be observed. The crystal was face-indexed, and a Gaussian grid[S2] absorption correction with beam profile correction was applied. The structure was solved using direct methods and observed reflections were used in least-squares refinement on F^2, with anisotropic thermal parameters refined for non-hydrogen atoms. Hydrogen atoms were constrained in calculated positions and refined with a riding model. Programs used were CrysAlisPro[S3] (control and integration), and SHELXS-97,[S4] SHELXL-2014[S5], Olex2[S6] and Ortep in combination with POV-Ray (structure solution and refinement and molecular graphics). Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC number 1457766. Copies of this information may be obtained, free of charge, from the Director, CCDC, 12 Union Road, Cambridge CB2 1E2, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk). *Crystal data:* $C_{86}H_{82}B_{10}N_2$, M = 1251.63, colourless block, 0.38 × 0.06 × 0.05 mm^3, monoclinic, space group $C2/c$, a = 20.1102(8), b = 26.5248(7), c = 21.3634(5) Å, β = 93.228(3)°, V = 1377.6(6) $Å^3$, Z = 4, D_c = 0.731 g/cm^3, ϑ_{min} = 3.4 º, ϑ_{max} = 72.3 º, 40829 reflections collected, 11080 unique (R_{int} = 0.0460). Final *GooF* = 1.04, R_1 = 0.0634, wR_2 = 0.1817, R indices based on 7088 reflections with $I > 2\sigma(I)$, 448 parameters, 0 restraints, μ = 0.300 mm^{-1}, $(\Delta/\rho)_{min}$ -0.16 e $Å^{-3}$, $(\Delta/\rho)_{max}$ 0.37 e $Å^{-3}$. Disordered lattice solvent molecules could not be modelled and were therefore removed from the refinement using PLATON SQUEEZE.[S7]

2. Determination of photophysical properties

2.1 Absorption spectra of the V-shaped and linear *o-Cb* dyads in different solvents

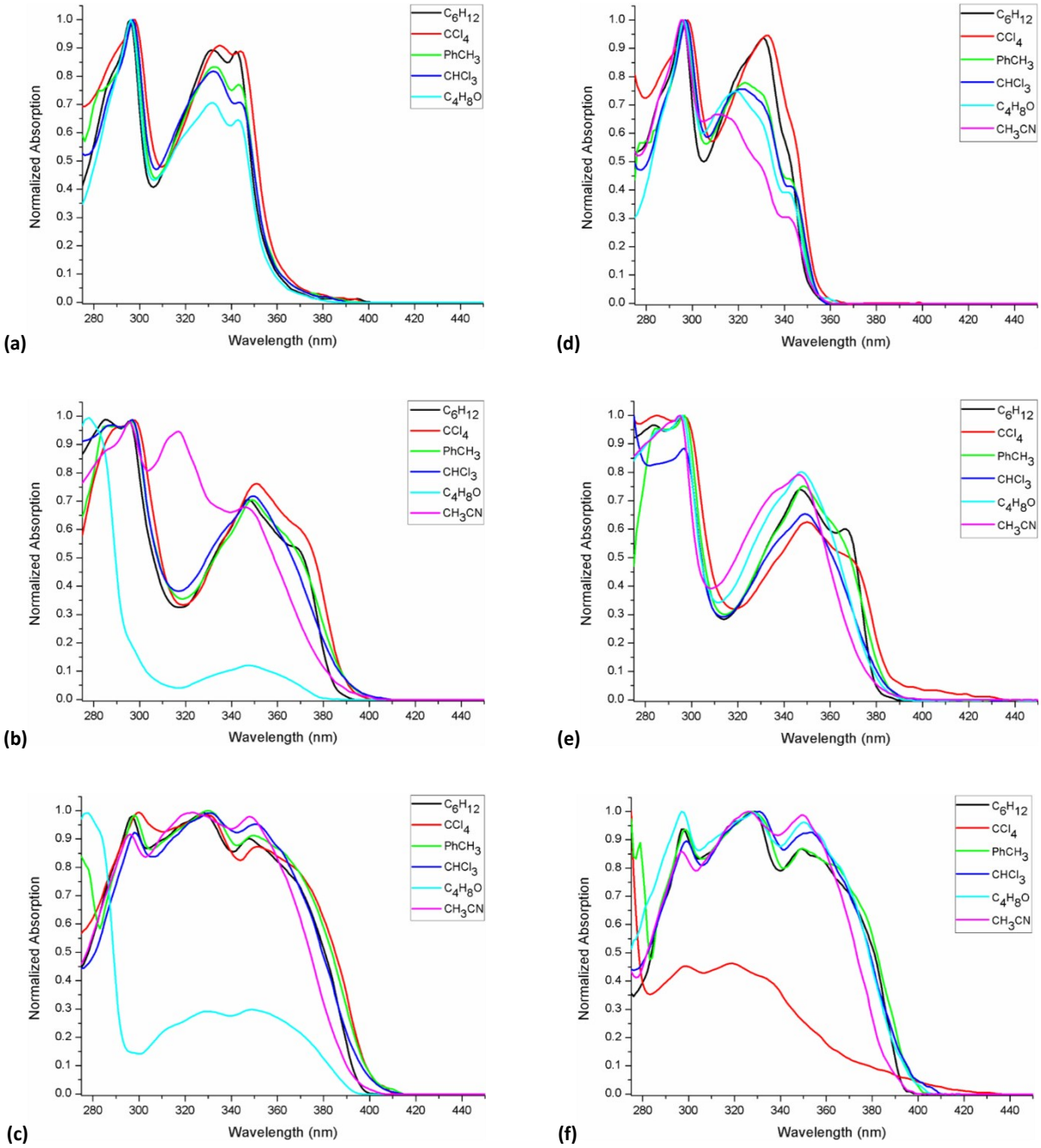


Fig. S2.1 Normalized absorption spectra of the *o-Cb* dyads in different solvents: **D-1** (a)**, D-2** (b), **D-3** (c), **M-1** (d), **M-2** (e) and **M-3** (f) at concentrations of 2 µM. Note that **D-1** is insoluble in CH_3CN. C_6H_{12} = cyclohexane, $PhCH_3$ = toluene, C_4H_8O = tetrahydrofuran (THF).

2.2 PL spectra of the V-shaped and linear *o-Cb* dyads

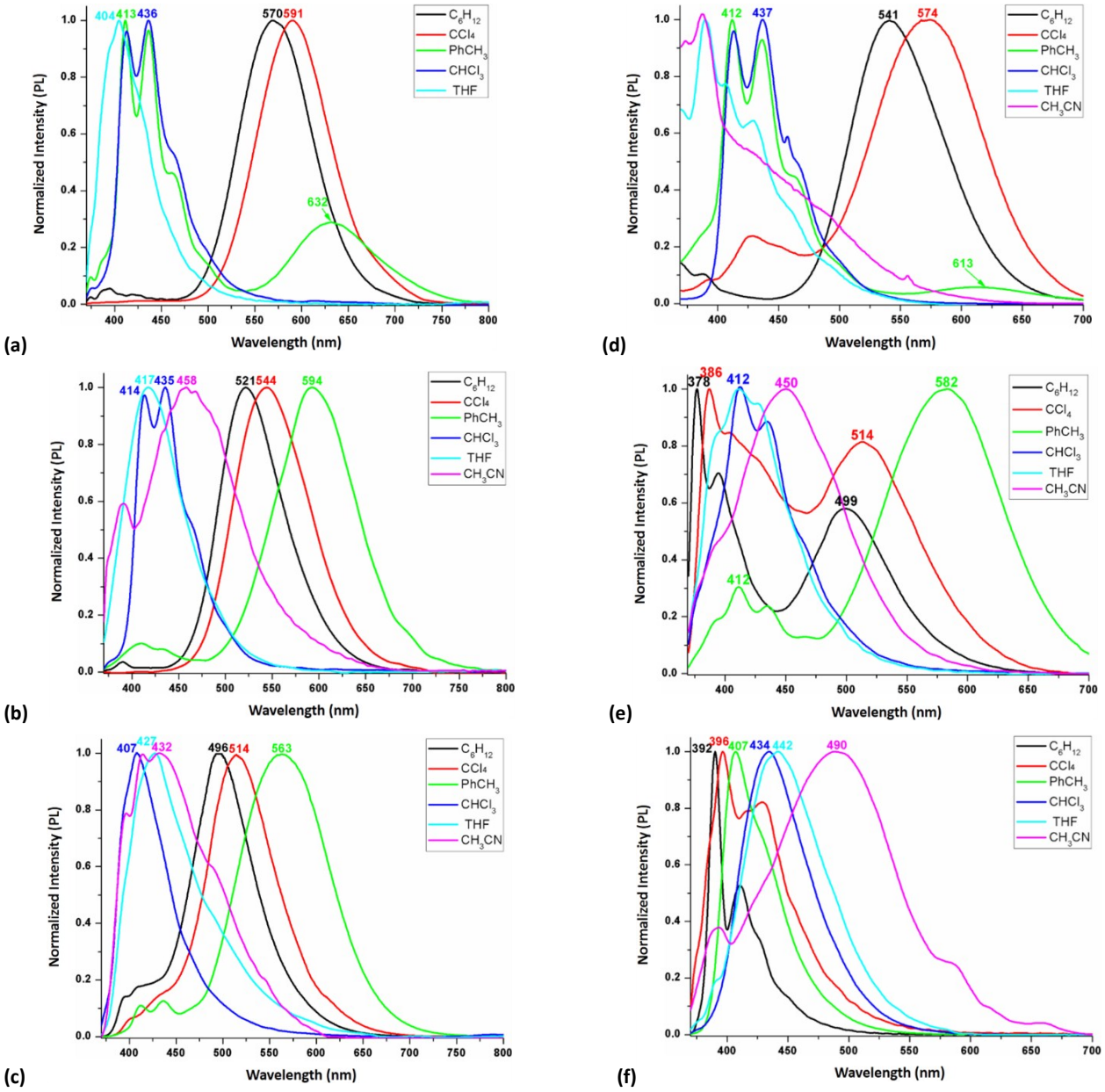


Fig. S2.2 Normalized PL spectra of *o-Cb* dyads in different solvents: **D-1** (a)**, D-2** (b), **D-3** (c), **M-1** (d), **M-2** (e) and **M-3** (f).

Table S1. Summary of quantum efficiency (QE) of *o-Cb* dyads in different solvents.

QE*	C_6H_{12}	CCl_4	Toluene	$CHCl_3$	THF	CH_3CN
D-1	10.2 %	7.1%	5.5%	1%	0.3%	< 0.1%
D-2	16%	35%	18%	1.1%	0.4%	0.4%
D-3	11%	6%	16%	1.8%	0.1%	< 0.1%
M-1	2.3%	0.8%	4.6%	5%	0.4%	0.4%
M-2	13.9%	3.6%	18.6%	0.3%	0.1%	< 0.1%
M-3	86.2%	7.5%	85.3%	8.4%	2.2%	0.3%

*Quinine sulfate solution as standard (Φ = 0.546).

2.3 Comparison of PL of *o-Cb* dyads at different excitation wavelengths

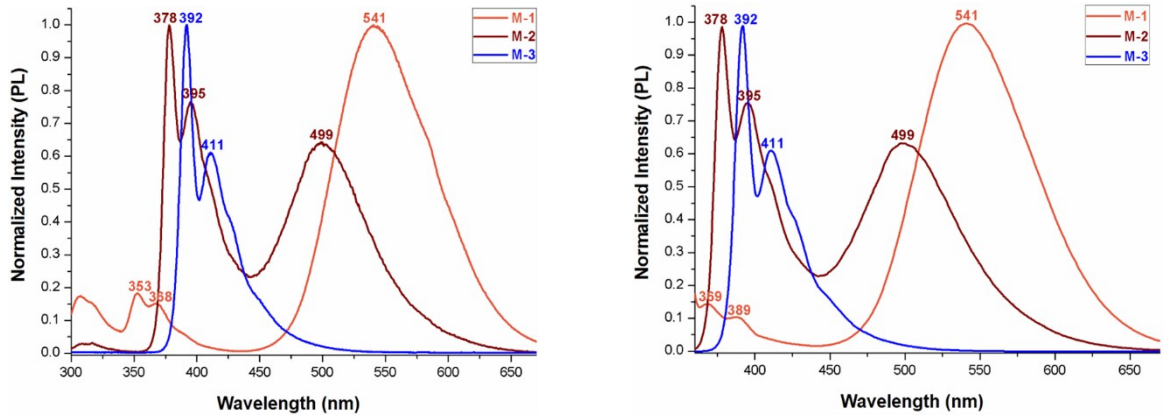


Fig. S2.3 Normalized PL of **M-1**, **M-2** and **M-3** (20 µM) in cyclohexane, excited at 290 nm (left) and 350 nm (right)

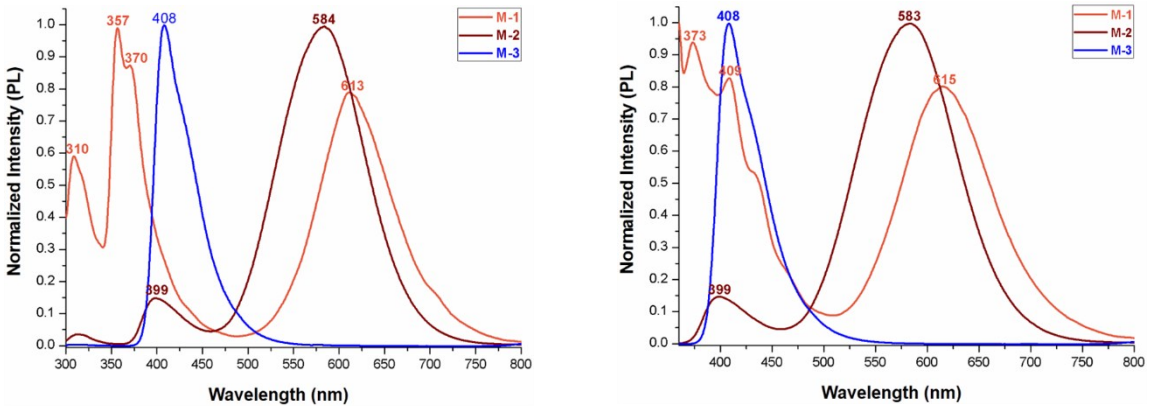


Fig. S2.4 Normalized PL of **M-1**, **M-2** and **M-3** (20 µM) in toluene, excited at 290 nm (left) and 350 nm (right)

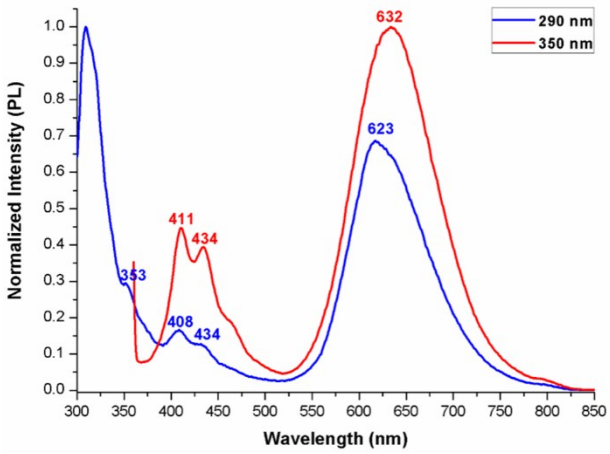


Fig. S2.5 Normalized PL of **D-1** (20 µM) in toluene, excited at 290 nm and 350 nm

2.4 Estimation of the dipole moment of V-shaped *o-Cb* dyads in the excited state

The dipole moments of the V-shaped *o-Cb* dyads were estimated from the Mataga–Lippert equation:

$$V - V_f = \frac{2(\mu_e - \mu_g)^2}{hca^3}\Delta f,\ \Delta f = \left(\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right), \qquad \mu_e - \mu_g = \sqrt[2]{\frac{Shca^3}{2}},\ S = \frac{V_1 - V_2}{\Delta f_1 - \Delta f_2}$$

where μ_e and μ_g are the dipole moments in the excited and ground states, respectively, *c* is the velocity of light, *h* is Planck's constant, S is the slope of the plots and *a* is the radius of the Onsager cavity around the fluorophore. The solvent dielectric constant (ε) and refraction index (n) are included in the term, Δf. The Onsager radii were obtained from the optimized excited state structures obtained from TD-DFT calculations at the 6-31g (d, p) level of theory, and were taken as half of the distance between the N atom and the carborane cluster. The value of μ_g was obtained by DFT calculations of the ground states.

Table S2. Dipole moments (μ_e) of D-1, D-2 and D-3 in the excited state obtained from Mataga-Lippert plots.

Compound	Radius/Å (*a*)	*S* / cm^{-1}	μ_e-μ_g / D	μ_g / D	μ_e / D
D-1	**3.21**	**282194.32**	**30**	**5**	**35**
D-2	**6.55**	**—[#]**	**87**	**5**	**92**
D-3	**9.98[*]**	**—[#]**	**164**	**5**	**169**

*** optimized at the 6-31g level of theory. [#] using the same *S* value as D-1.**

3. Theoretical calculations

3.1 TD-DFT calculations at the ground state

Table S3. Summary of electronic transitions of all *o-Cb* dyads from the ground state to the lowest five excited states

	λ_{calc}	f	Assignment (>5%)		λ_{calc}	f	Assignment (>5%)
	290.78	0.1728	H-1 → L (44.4%); H-1 → L+1 (6.4%); H → L (13.8%); H → L+1 (35.4%)		281.87	0.4365	H → L (93.6%); H → L+1 (6.4%)
	284.32	0.5342	H-1 → L (17.8%); H-1 → L+1 (21.5%); H-1 → L+2 (10.8%); H → L (39.5%); H → L+1 (10.4%)		275.61	0.0001	H-1 → L+4 (8.8%); H → L (7.2%); H → L+1 (84.0%);
D-1	281.82	0.0200	H-1 → L+3 (11.0%); H → L+2 (27.5%); H → L+3 (42.1%); H → L+4 (6.6%)	**M-1**	257.69	0.0029	H-4 → L (7.4%); H-3 → L+2 (5.5%); H → L+2 (87.1%);
	280.83	0.0176	H-1 → L (5.4%); H-1 → L+2 (58.2%); H-1 → L+3 (7.5%); H → L (6.5%); H → L +3 (14.2%)		248.45	0.1675	H-1 → L+1 (82.0%); H → L+4 (12.5%);
	262.02	0.0065	H → L (14.8%); H → L+1 (17.9%); H → L+3 (5.9%); H → L+4 (28.8%); H → L+5 (26.8%)		240.34	0.0002	H-1 → L (89.4%)
	319.41	0.8205	H-5 → L (7.9%); H-4 → L+1 (6.1%); H-1 → L (42.1%); H → L+1 (38.6%)		314.73	1.3248	H-2 → L (8.9%); H → L (82.5%); H → L+3 (8.6%)
D-2	311.11	1.6579	H-1 → L+1 (40.8%); H → L (45.4%)	**M-2**	278.29	0.0276	H-1→ L+6 (9.4%); H → L+1 (86.0%)
	278.45	0.0155	H-1 → L+2 (35.5%); H-1 → L+4 (8.5%); H → L+3 (44.1%)		262.96	0.5767	H-2 → L (88.3%); H → L+3 (7.3%)
	278.38	0.0461	H-1 → L+3 (44.0%); H → L+2 (35.6%); H → L+4 (8.6)		256.67	0.0034	H-4 → L (11.8%); H → L+4 (76.8%)
	266.57	0.2601	H-5 → L (50.1%); H-4 → L+1 (37.1%); H → L+1 (6.2%)		254.72	0.0004	H-1 → L (88.9%); H-1 → L+3 (11.1%)
	339.32	1.5156	H-5 → L (14.9%); H-4 → L+1 (11.9%); H-1 → L (25.4%); H-1 → L+1 (9.7%); H → L (8.1%); H → L+1 (20.8%)		333.97	2.6162	H-2 → L (25.5%); H → L (62.6%); H → L+1 (9.4%)
	329.94	3.5488	H-5 → L (6.2%); H-4 → L (5.0%); H-4 → L+1 (7.6%); H-1 → L (21.8%); H-1 → L+1 (9.1%); H → L (10.9%);	**M-3**	288.24	0.2665	H-2→ L (62.5%); H → L (10.7%); H → L+1 (18.7%)
D-3			H → L+1 (26.3%)				
	290.58	0.0953	H-5 → L (28.4%); H-5 → L+1 (6.0%); H-4 → L (5.4%); H-4 → L+1 (20.2%); H-1 → L (5.3%); H-1 → L+2 (7.7%); H-1 → L+3 (5.6%); H → L+1 (5.4%); H → L+3 (5.8%)		278.85	0.0368	H-2→ L+2 (11.0%); H-1 → L+8 (9.2%); H → L+2 (79.8%)
	286.28	0.4114	H-5 → L (20.7%); H-5 → L+1 (12.3%); H-4 → L (17.6%); H-4 → L+1 (25.0%); H → L+2 (5.3%); H → L+3 (6.1%)		256.89	0.0001	H-1 → L (78.1%); H-1 → L+1 (17.9%)
	278.84	0.0324	H-5 → L+5 (11.4%); H-3 → L+15 (9.2%); H-1 → L+5 (79.4%)		256.79	0.0035	H-6 → L (7.2%); H-6 → L+1 (7.3%); H-3 → L+4 (5.1%); H → L+4 (77.7%);

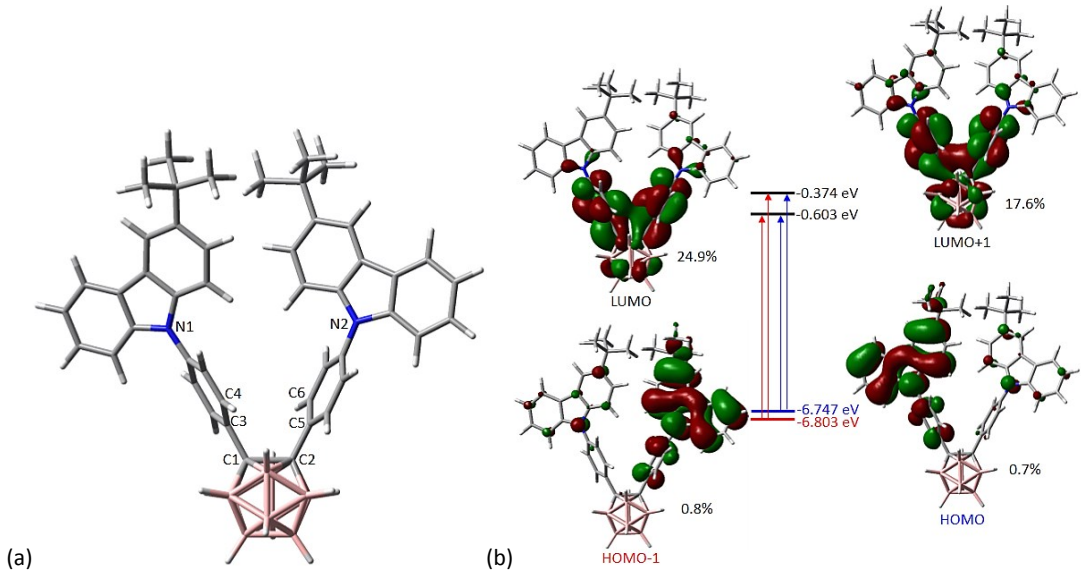


Fig. S3.1 (a) Optimized ground state structure of **D-1**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.683, C1–N1 5.724, C2–N2 5.712, C2–C1–C3–C4 76.26, C1–C2–C5–C6 67.71. The calculated dipole moment is 5.1135 Debye. (b) Calculated electron excitation of **D-1** from the ground state to the lowest excited state. The assignment of the transition is H-1 → L (44.4%), H-1 → L+1 (6.4%), H → L (13.8%) and H → L+1 (35.4%).

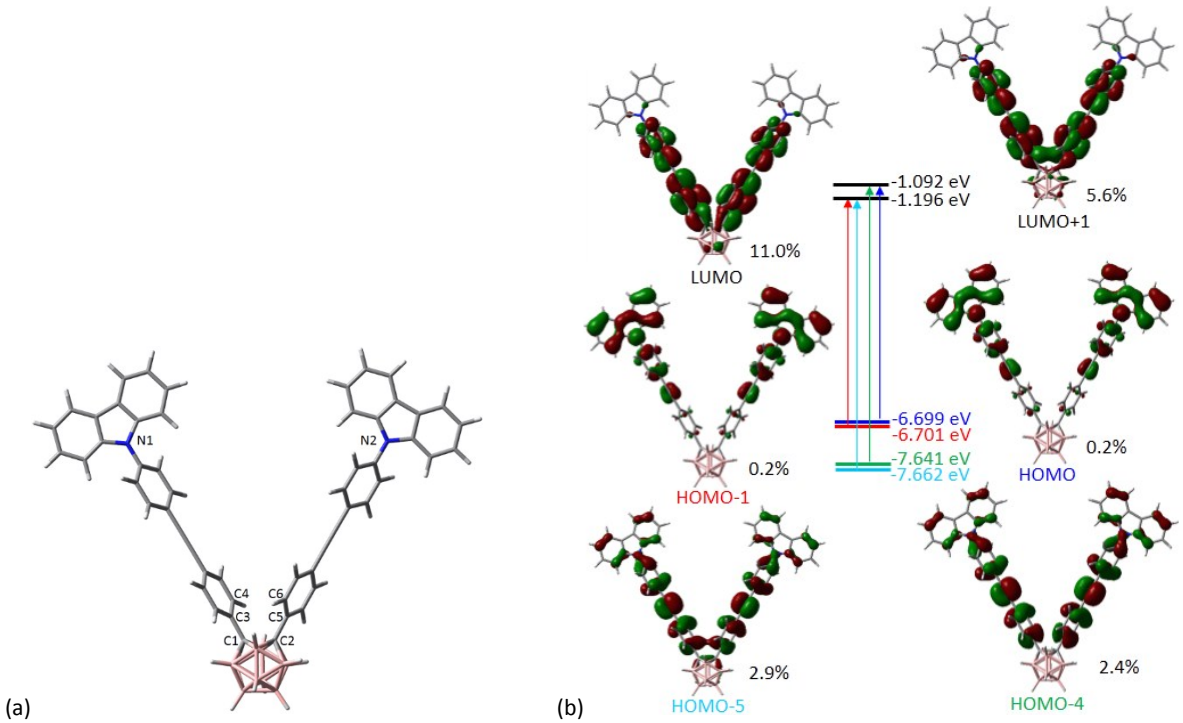


Fig. S3.2 (a) Optimized ground state structure of **D-2**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.683, C1–N1 12.597, C2–N2 12.597, C2–C1–C3–C4 71.34, C1–C2–C5–C6 70.89. The calculated dipole moment is 4.9817 Debye; (b) Calculated electron excitation of **D-2** from its ground state to the lowest excited state. The assignment of the transition is H-5 → L (7.9%), H-4 → L+1 (6.1%), H-1 → L (42.1%) and H → L+1 (38.6%).

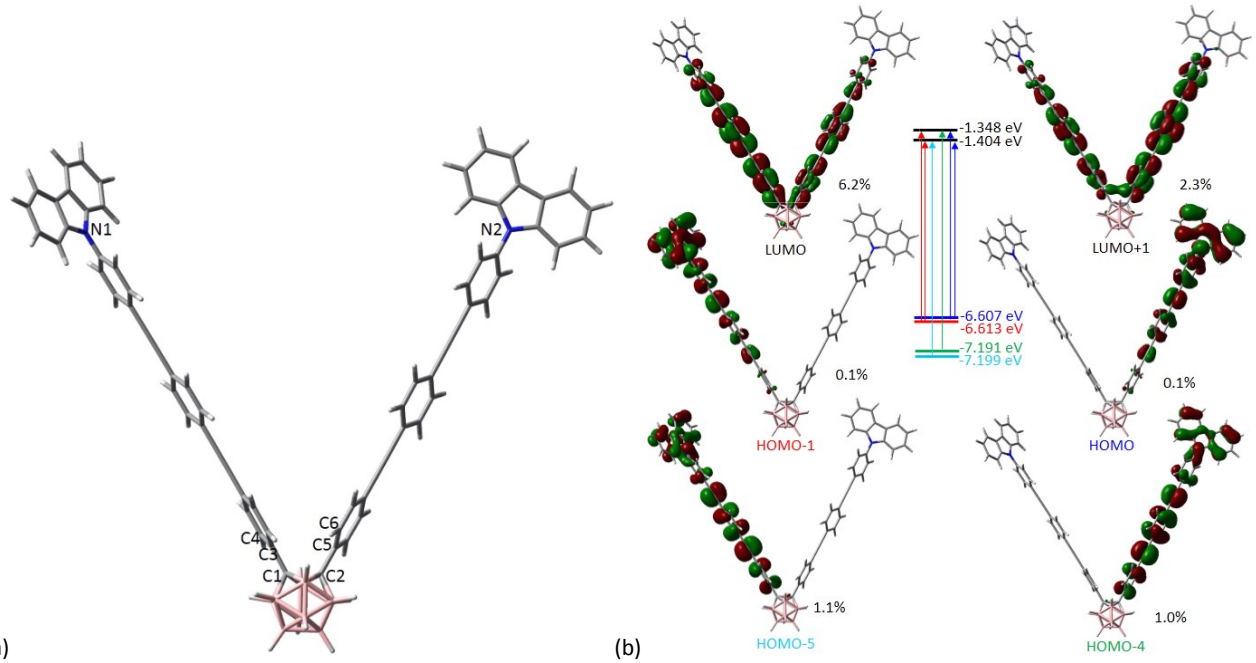


Fig. S3.3 (a) Optimized ground state structure of **D-3**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.690, C1–N1 19.458, C2–N2 19.474, C2–C1–C3–C4 94.67, C1–C2–C5–C6 74.60. The calculated dipole moment is 5.1990 Debye; (b) Calculated electron excitation of **D-3** from the ground state to the lowest excited state. The assignment of the transition is H-5 → L (14.9%), H-4 → L+1 (11.9%), H-1 → L (25.4%), H-1 → L+1 (9.7%), H → L (8.1%) and H → L+1 (20.8%).

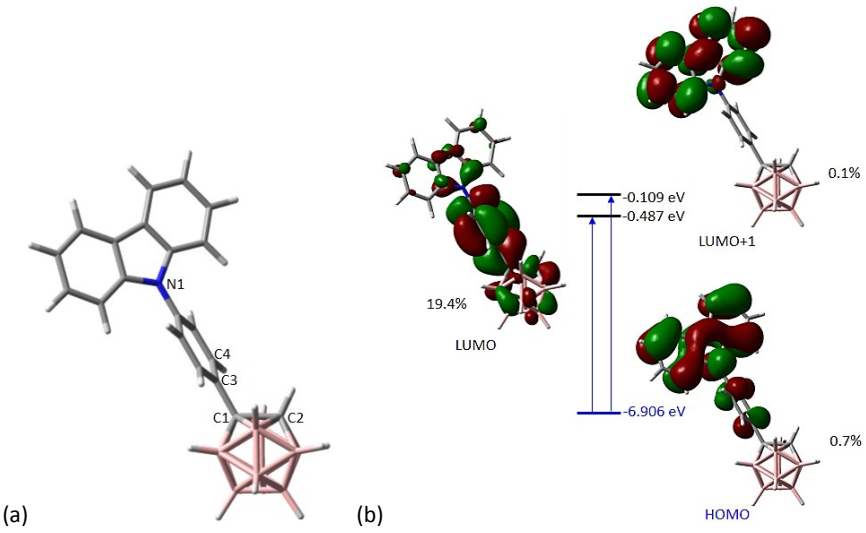
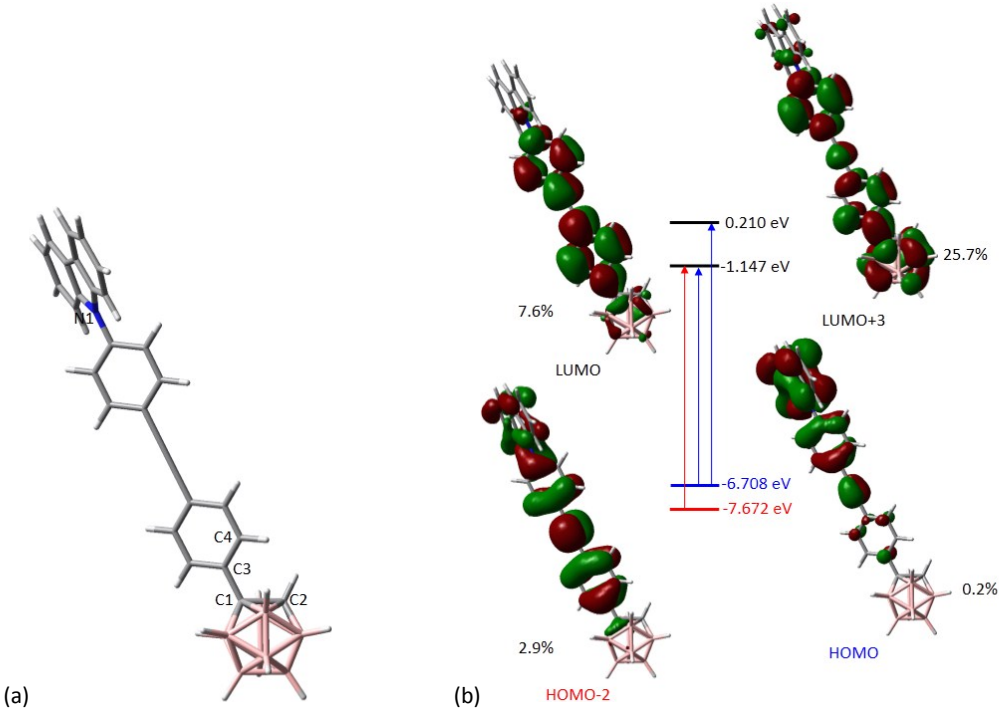
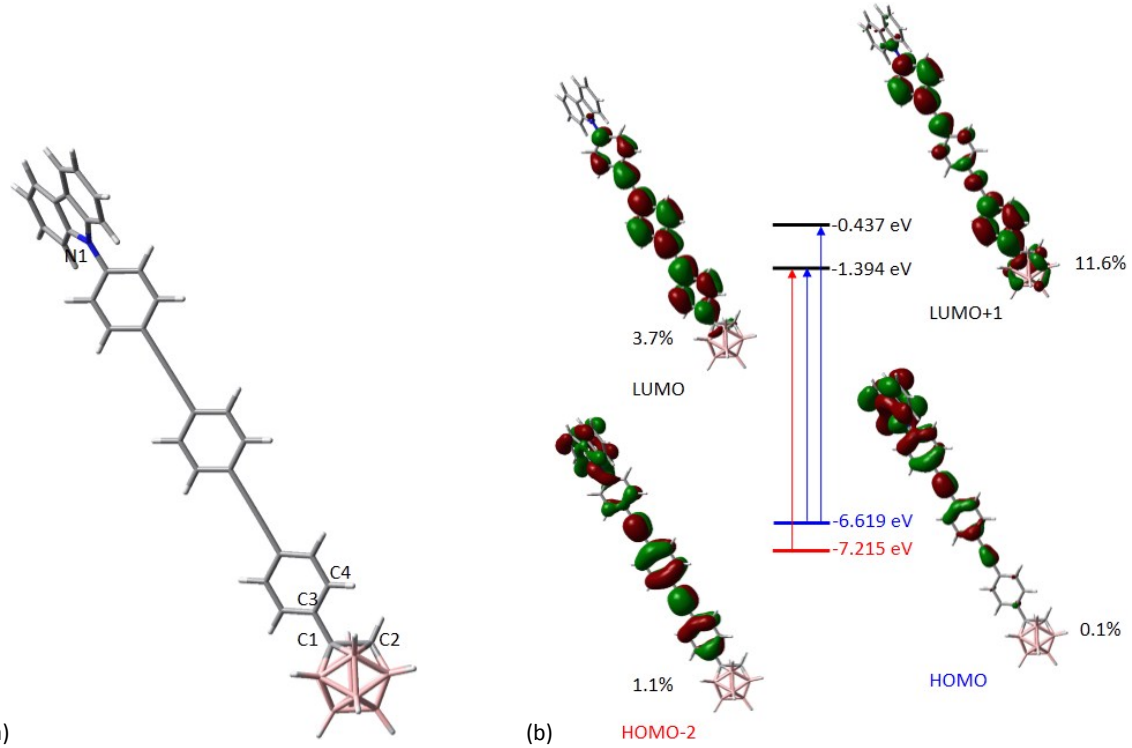


Fig. S3.4 (a) Optimized ground state structure of **M-1**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.643, C1–N1 5.724, C2–C1–C3–C4 81.96. The calculated dipole moment is 4.4254 Debye; (b) Calculated electron excitation of **M-1** from the ground state to the lowest excited state. The assignment of the transition is H → L (93.6%) and H → L+1 (6.4%).



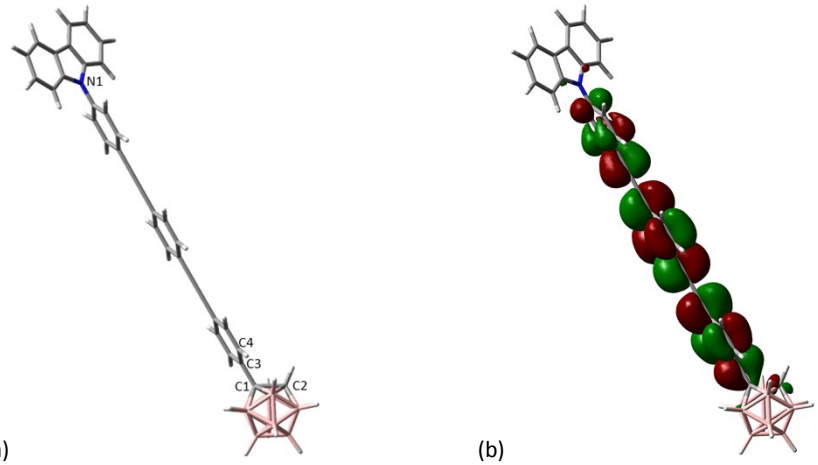
(a) (b)

Fig. S3.5 (a) Optimized ground state structure of **M-2**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.627, C1–N1 12.596, C2–C1–C3–C4 29.80. The calculated dipole moment is 4.6412 Debye; (b) Calculated electron excitation of **M-2** from the ground state to the lowest excited state. The assignment of the transition is H-2 → L (8.9%), H → L (82.5%) and H → L+3 (8.6%).



(a) (b)

Fig. S3.6 (a) Optimized ground state structure of **M-3**. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.627, C1–N1 19.467, C2–C1–C3–C4 27.70. The calculated dipole moment is 4.7159 Debye; (b) Calculated electron excitation of **M-3** from the ground state to the lowest excited state. The assignment of the transition is H-2 → L (25.5%), H → L (62.6%) and H → L+1 (9.4%).



(a) (b)

Fig. S3.7 (a) Optimized structure of **M-3** at its anion state. Selected bond lengths (Å) and dihedral angles (°): C1–C2 1.682, C1–N1 19.500, C2–C1–C3–C4 82.89; (b) The highest semi-occupied molecular orbital (HSOMO) of M-3 anion.

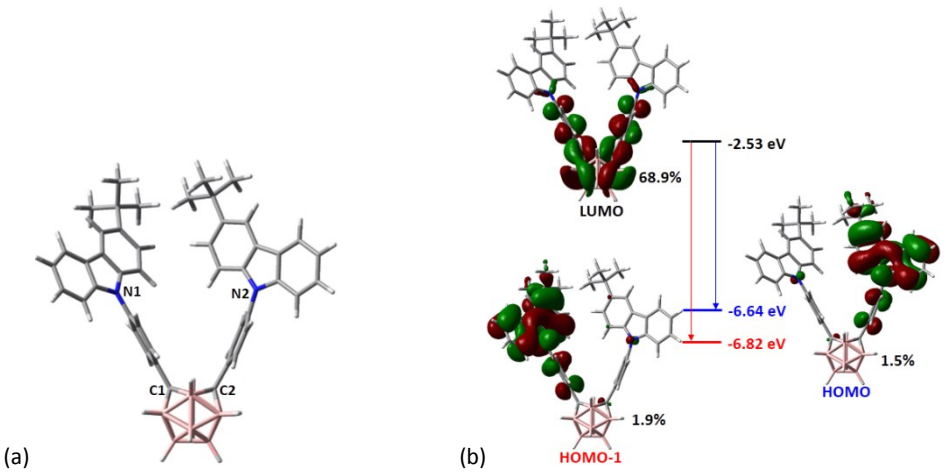
3.2 TD-DFT calculations at the excited state

Table S4. Electronic transitions of selected *o-Cb* dyads at the LE or CT excited state.

Compound	Basis set	Emission type	λ_{calc} (nm)	f	Assignment (> 5%)
D-1	**6-31g(d, P)**	**CT**	444.83	0.2116	H-1 → L (5.4%); H → L (91.3%)
D-2	**6-31g(d, P)**	**CT**	425.11	0.9057	H-4 → L (26.3%); H → L (70.4%)
D-3	**6-31g**	**CT**	431.31#	1.0805	H-6 → L (7.5%); H-2 → L (44.7%); H → L (42.0%)
M-2	**6-31g(d, P)**	**LE**	358.18	1.6526	H → L (91.2%)
M-2	**6-31g(d, P)**	**CT***	406.36*	1.2281*	H-2 → L (22.1%); H → L (73.4%)
M-3	**6-31g(d, P)**	**LE**	387.23	2.8522	H-1 → L (9.4%); H → L (86.3%)

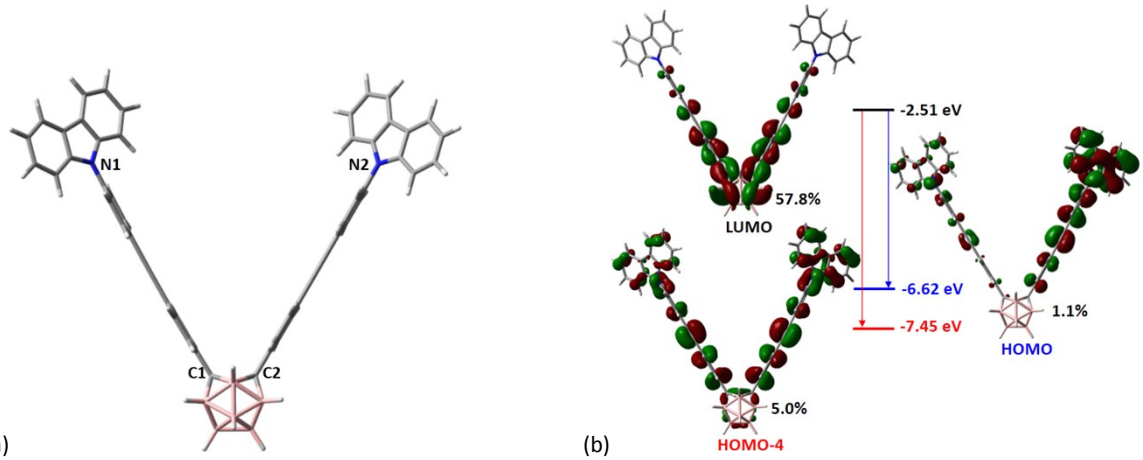
The calculated excitation energy has been underestimated due to a lower-level basic set, 6-31G.

* The data were obtained from an estimated structure by merging the geometry of the **M-2** anion with that of the **M-2** cation.



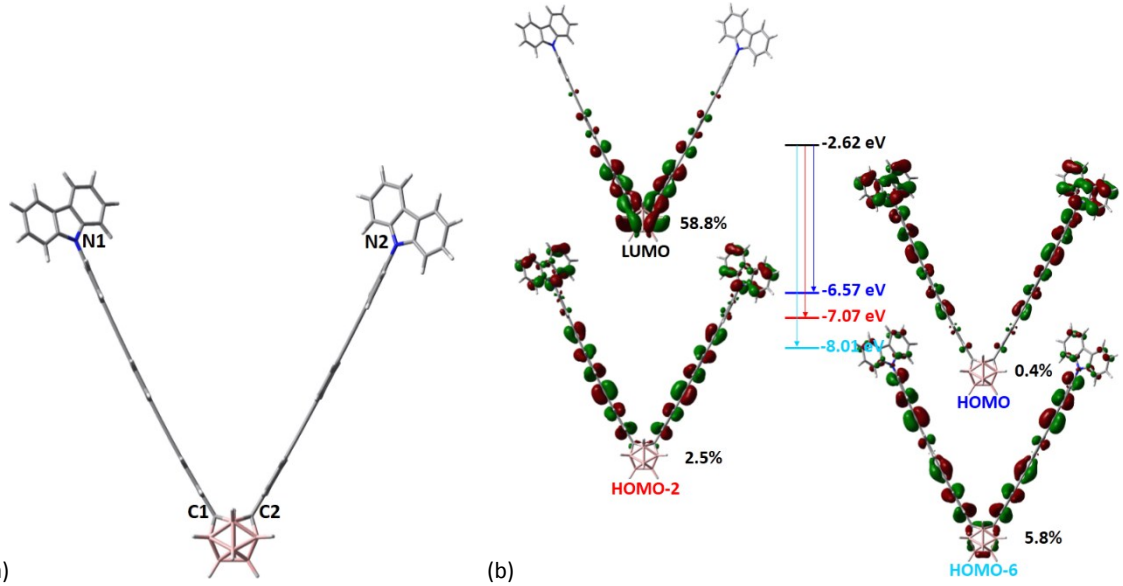
(a) (b)

Fig. S3.7 (a) Optimized structure of the lowest singlet excited state of **D-1**. Selected bond lengths (Å): C1–C2 2.291, C1–N1 5.695, C2–N1 7.131; (b) Calculated electron transition of **D-1** at the lowest singlet excited state. The assignment of the transition is H-1 → L (5.4%) and H → L (91.3%).



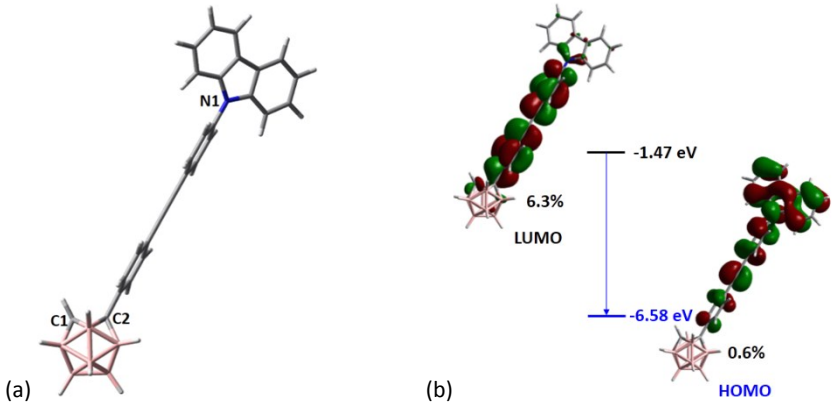
(a) (b)

Fig. S3.8 (a) Optimized structure of the lowest singlet excited state of **D-2**. Selected bond lengths (Å): C1–C2 2.245, C1–N1 12.499, C2–N1 13.722; (b) Calculated electron transition of **D-2** at the lowest singlet excited state. The assignment of the transition is H-4 → L (26.3%) and H → L (70.4%).



(a) (b)

Fig. S3.9 (a) Optimized structure of the lowest singlet excited state of **D-3**. Selected bond lengths (Å): C1–C2 2.271, C1–N1 19.408, C2–N1 20.528; (b) Calculated electron transition of **D-3** at the lowest singlet excited state. The assignment of the transition is H-6 → L (7.5%), H-2 → L (44.7%) and H → L (42.0%).



(a) (b)

Fig. S3.10 (a) Optimized structure of the local excited state of **M-2**. Selected bond lengths (Å): C1–C2 1.667, C2–N1 12.566; (b) Calculated electron transition of **M-2** at the local excited state. The assignment of the transition is H → L (91.2%).

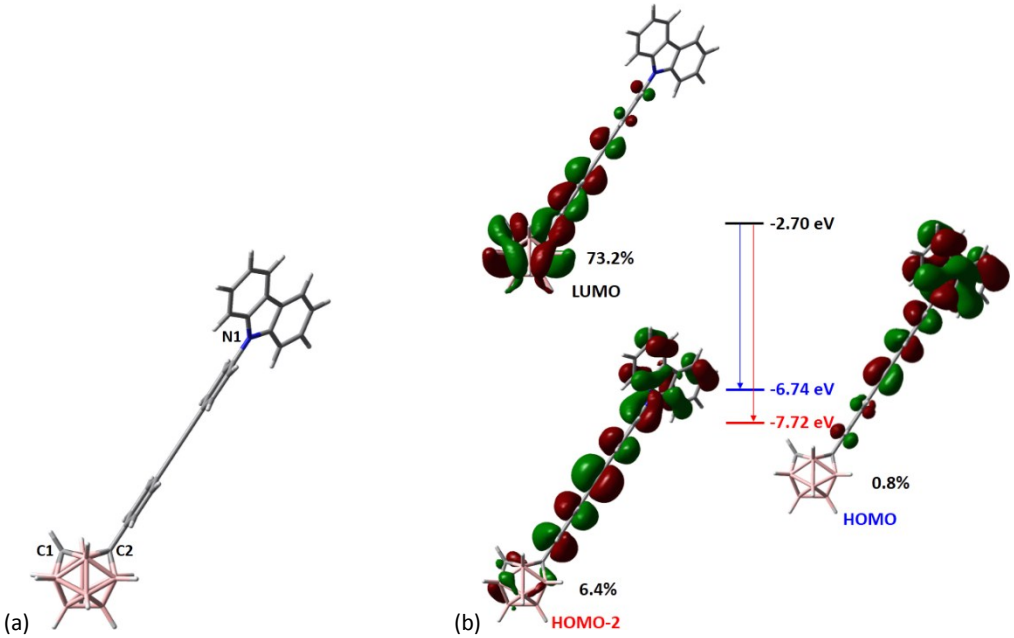


Fig. S3.11 (a) Estimated charge-transfer excited-state structure of **M-2**. Selected bond lengths (Å): C1–C2 2.321, C2–N1 12.566; (b) Calculated charge-transfer excited-state electronic transition of **M-2**. The assignment of the transition is H-2 → L (22.1%) and H → L (73.4%).

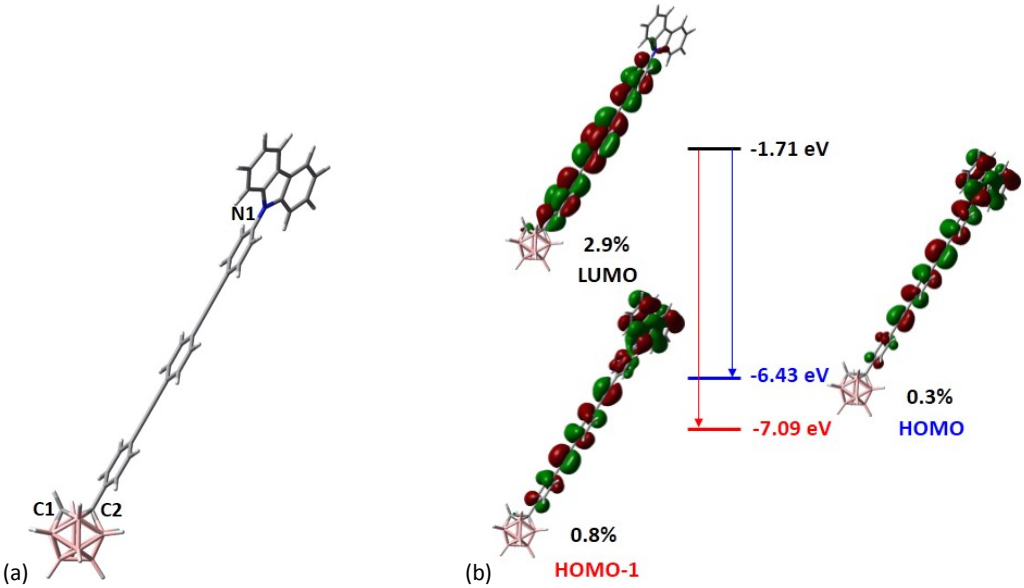


Fig. S3.12 (a) Optimized local excited-state structure of **M-3**. Selected bond lengths (Å): C1–C2 1.654, C2–N1 19.416; (b) Calculated local excited state electronic transition of **M-3**. The assignment of the transition is H-1 → L (9.4%) and H → L (86.3%).

3.3 Cartesian coordinates of *o-Cb* dyads in the ground state

D-1	X	Y	Z	**D-2**	X	Y	Z
N	3.419328	-1.213981	-0.051635	C	2.962311	3.342529	-0.041244
N	-3.678686	-1.224357	-0.23982	C	3.039305	4.225388	1.044399
B	-0.33497	4.200178	1.444361	C	2.359877	5.433391	1.015566
H	-0.482446	3.421535	2.314823	H	2.43212	6.104217	1.864145
B	1.170918	5.05063	1.101487	C	1.593416	5.79912	-0.09632
H	2.105236	4.817444	1.786671	C	1.515243	4.917168	-1.177986
B	1.344895	5.132649	-0.65559	H	0.928878	5.171565	-2.051698
H	2.402114	4.969326	-1.15779	C	2.186846	3.703772	-1.150812
B	-0.052429	4.335488	-1.381349	H	2.120542	3.026702	-1.995065
H	0.036451	3.651608	-2.334768	C	0.886023	7.12895	-0.098964
B	-0.286186	5.952313	1.54634	C	-0.792191	7.13855	0.027112
H	-0.380652	6.475658	2.603538	B	0.149622	7.595783	1.379764
B	0.756209	6.541912	0.236089	H	0.238335	6.865932	2.29896
H	1.431809	7.507337	0.347543	B	-1.31476	8.478562	0.948323
B	0.00306	6.088551	-1.307683	H	-2.274823	8.315966	1.618198
H	0.130413	6.709337	-2.307131	B	-1.435646	8.472516	-0.81368
B	-1.507049	5.232315	-0.950293	H	-2.484595	8.328164	-1.337557
H	-2.451016	5.125018	-1.653134	B	-0.050641	7.585946	-1.455099
B	-1.67822	5.149078	0.804411	H	-0.146409	6.850097	-2.368802
H	-2.745301	5.010144	1.292042	B	0.161193	9.352106	1.387556
B	-1.005709	6.601995	0.05771	H	0.244887	9.928508	2.417764
H	-1.624506	7.610789	0.047328	B	-0.821603	9.904884	0.017989
C	0.630075	3.782443	0.094375	H	-1.466111	10.896692	0.057084
C	-1.042763	3.84058	-0.077891	B	-0.043804	9.342257	-1.476186
C	1.310307	2.438423	0.05804	H	-0.121381	9.911496	-2.510867
C	2.023238	2.05444	-1.082046	B	1.422832	8.456522	-1.03048
H	2.063566	2.713857	-1.941818	H	2.380932	8.278826	-1.6993
C	2.685886	0.835915	-1.134006	B	1.543887	8.46265	0.731448
H	3.218897	0.539674	-2.031078	H	2.591343	8.311889	1.256429
C	2.673665	-0.018459	-0.028778	B	0.944937	9.895101	-0.110814
C	1.950963	0.349218	1.108539	H	1.599889	10.879704	-0.157657
H	1.951545	-0.301514	1.976381	H	3.636528	3.955717	1.908284
C	1.273884	1.561258	1.145633	C	4.788759	-1.150187	-0.98162
H	0.737497	1.829882	2.04686	C	5.938508	-0.434133	1.021294
C	4.776265	-1.301004	-0.388369	C	5.502164	-2.339069	-0.96592
C	5.647656	-0.310448	-0.844347	H	4.070233	-0.954853	-1.770137
H	5.317864	0.710512	-0.997007	C	6.639979	-1.629896	1.047795
C	6.968006	-0.673132	-1.078706	H	6.099231	0.311077	1.792616
H	7.663578	0.07932	-1.435913	C	6.427987	-2.586761	0.051437
C	7.421344	-1.981354	-0.861428	H	5.36073	-3.080348	-1.745578
H	8.458542	-2.228501	-1.060152	H	7.345987	-1.840267	1.844574

C	6.555976	-2.95426	-0.383179	C	8.527099	-3.934636	0.192371
H	6.906781	-3.964404	-0.194226	C	6.583228	-5.076463	-0.026301
C	5.225582	-2.613423	-0.137233	C	9.505711	-2.943282	0.27512
C	4.097344	-3.350413	0.39442	C	8.859333	-5.305692	0.169262
C	3.947804	-4.657984	0.845212	C	5.240994	-5.446962	-0.117682
H	4.805466	-5.325551	0.828341	C	7.61552	-6.036209	0.032438
C	2.717817	-5.104011	1.331274	C	10.828757	-3.354812	0.360246
C	1.633839	-4.20675	1.308909	H	9.244784	-1.890751	0.262363
H	0.65575	-4.533389	1.647259	C	10.197822	-5.692516	0.256368
C	1.754333	-2.89077	0.866485	C	4.953578	-6.803937	-0.174574
H	0.890192	-2.234747	0.869428	H	4.45101	-4.704054	-0.132785
C	3.005862	-2.459155	0.433807	C	7.299093	-7.394754	-0.027251
C	-1.774174	2.528158	-0.162072	C	11.176084	-4.713907	0.356185
C	-1.627514	1.673872	-1.257594	H	11.610685	-2.605312	0.427803
H	-1.005233	1.958542	-2.096101	H	10.466412	-6.744535	0.240037
C	-2.276399	0.448777	-1.290611	C	5.968411	-7.77141	-0.135714
H	-2.170797	-0.206604	-2.148608	H	3.91817	-7.120975	-0.246357
C	-3.076535	0.048091	-0.219726	H	8.084978	-8.142812	0.017702
C	-3.246295	0.902171	0.870736	H	12.220302	-4.998963	0.425199
H	-3.858495	0.585092	1.708577	H	5.706762	-8.822935	-0.183712
C	-2.600852	2.13094	0.893187	N	7.14325	-3.802595	0.072429
H	-2.725169	2.779443	1.753343	C	5.000463	-0.18067	0.009641
C	-3.008078	-2.416951	-0.514865	C	3.66877	2.100011	-0.021143
C	-1.656755	-2.642386	-0.760562	C	4.275345	1.051421	-0.009537
H	-0.939584	-1.828355	-0.786573	C	-1.515829	5.817572	0.036589
C	-1.245798	-3.95357	-0.972779	C	-2.281946	5.447807	-1.074164
H	-0.190873	-4.124522	-1.15545	C	-1.455441	4.949323	1.13042
C	-2.139042	-5.0406	-0.94876	C	-2.978282	4.249142	-1.090208
C	-3.485443	-4.78612	-0.682586	H	-2.341023	6.10837	-1.931786
H	-4.200516	-5.603944	-0.643643	C	-2.144232	3.745461	1.116283
C	-3.926056	-3.484166	-0.456166	H	-0.870472	5.207665	2.003878
C	-5.21595	-2.907433	-0.126874	C	-2.919519	3.380319	0.007861
C	-6.490882	-3.44533	0.053958	H	-3.575285	3.976469	-1.953306
H	-6.653304	-4.514696	-0.042183	H	-2.09243	3.079515	1.970325
C	-7.544898	-2.593084	0.351082	C	-3.644481	2.148334	0.002859
H	-8.541289	-2.996518	0.495207	C	-4.266051	1.108489	0.006648
C	-7.336429	-1.210557	0.458132	C	-5.006724	-0.114485	0.005547
H	-8.176942	-0.56084	0.679659	C	-5.947712	-0.371507	-1.002429
C	-6.078156	-0.649146	0.282857	C	-4.806063	-1.072167	1.010524
H	-5.927398	0.422741	0.351138	C	-6.661797	-1.560095	-1.012965
C	-5.021277	-1.515259	0.001988	H	-6.100563	0.3649	-1.783731
C	-1.679735	-6.479963	-1.201378	C	-5.532083	-2.253418	1.010814
C	-2.064264	-7.357803	0.00159	H	-4.085597	-0.873798	1.796512
H	-3.149206	-7.412338	0.129342	C	-6.45961	-2.505718	-0.003907

H	-1.692362	-8.378472	-0.137285	H	-7.369602	-1.773861	-1.807242
H	-1.640599	-6.957585	0.927446	H	-5.398456	-2.985494	1.800458
C	-0.163685	-6.567961	-1.406167	C	-8.569544	-3.839149	-0.130343
H	0.153407	-6.023448	-2.301315	C	-6.634684	-4.992152	0.109184
H	0.386936	-6.159748	-0.551086	C	-9.540914	-2.842115	-0.229683
H	0.129943	-7.615263	-1.530867	C	-8.911892	-5.207247	-0.087851
C	-2.370102	-7.023191	-2.463416	C	-5.295469	-5.37147	0.208989
H	-3.458905	-7.015312	-2.357597	C	-7.673926	-5.944913	0.062605
H	-2.111776	-6.417163	-3.336891	C	-10.866737	-3.245408	-0.311779
H	-2.056563	-8.055338	-2.654157	H	-9.272534	-1.791368	-0.231582
C	2.613252	-6.524107	1.900494	C	-10.252889	-5.585735	-0.172316
C	2.99491	-7.552231	0.823166	C	-5.018437	-6.729517	0.28736
H	2.939738	-8.565875	1.23426	H	-4.499829	-4.634507	0.214168
H	2.31664	-7.491514	-0.033146	C	-7.367977	-7.304719	0.143856
H	4.013651	-7.394399	0.457815	C	-11.223883	-4.60171	-0.288723
C	1.202795	-6.84771	2.40007	H	-11.643028	-2.491341	-0.39202
H	0.469673	-6.805736	1.589178	H	-10.529085	-6.635448	-0.141268
H	1.184086	-7.86172	2.810725	C	-6.040464	-7.689774	0.261228
H	0.886467	-6.159688	3.190391	H	-3.985618	-7.053193	0.366352
C	3.58136	-6.655485	3.089481	H	-8.159497	-8.04736	0.108934
H	4.617644	-6.483251	2.785265	H	-12.269982	-4.880214	-0.355986
H	3.334948	-5.930206	3.87089	H	-5.787023	-8.742379	0.326323
H	3.518152	-7.661008	3.519022	N	-7.184941	-3.715678	-0.009469

D-3	X	Y	Z	**M-1**	X	Y	Z
C	-0.558817	0.03592	-0.149943	C	1.077255	-0.009116	0.034446
C	-0.430655	-0.193282	1.226725	C	0.36766	-0.830951	-0.843282
C	0.791159	-0.016169	1.857032	C	-1.019866	-0.834855	-0.824896
H	0.87089	-0.19992	2.922382	H	-1.554224	-1.488167	-1.505044
C	1.9189	0.387625	1.134282	C	-1.729861	-0.004821	0.048534
C	1.793976	0.600291	-0.241301	C	-1.010517	0.80245	0.933836
H	2.653601	0.894958	-0.829519	H	-1.530208	1.420641	1.654919
C	0.572	0.43122	-0.876114	C	0.378214	0.799879	0.931286
H	0.4846	0.60271	-1.943174	H	0.929342	1.408233	1.640709
C	3.232314	0.567404	1.848594	C	-3.237983	-0.039731	0.059423
C	3.784988	2.139104	2.130229	C	-4.085605	1.130481	-0.723497
B	3.150817	1.221575	3.429746	B	-4.009989	-0.40721	-1.435905
H	2.085455	1.502508	3.846801	H	-3.329635	-0.534082	-2.390101
B	4.590569	2.223244	3.628505	B	-5.499627	0.542766	-1.442033
H	4.479924	3.234555	4.230792	H	-5.833624	1.018444	-2.47059
B	5.485136	2.179248	2.104196	B	-5.545741	1.500846	0.043001
H	5.982769	3.160108	1.67102	H	-5.910781	2.624019	0.019264
B	4.590118	1.148488	0.986409	B	-4.086049	1.145854	0.972988
H	4.493219	1.385522	-0.16104	H	-3.480018	1.994692	1.519123

B	4.544005	0.581089	4.28797	B	-5.530241	-1.172265	-0.997565
H	4.476336	0.395048	5.454765	H	-6.004522	-1.984343	-1.715649
B	6.002663	1.16833	3.463292	B	-6.489167	0.00868	-0.075626
H	7.004248	1.411302	4.045211	H	-7.670453	0.045551	-0.135519
B	6.000215	0.509611	1.814194	B	-5.607801	0.387603	1.421999
H	6.981333	0.277574	1.194701	H	-6.136473	0.697732	2.434194
B	4.551066	-0.492362	1.627708	B	-4.110475	-0.561683	1.426644
H	4.393454	-1.379393	0.862865	H	-3.475224	-0.897862	2.364893
B	3.658445	-0.445332	3.150259	B	-4.065791	-1.521389	-0.063198
H	2.902442	-1.310833	3.425881	H	-3.405339	-2.50038	-0.111145
B	5.425681	-0.480231	3.169121	B	-5.602968	-1.267738	0.776937
H	6.002117	-1.445917	3.538271	H	-6.136334	-2.163518	1.337024
H	-1.298253	-0.506409	1.796756	H	0.909419	-1.453895	-1.547166
C	-4.344655	0.069369	-3.302943	C	3.294591	1.134324	-0.038295
C	-5.22152	-1.055046	-1.346715	C	3.308126	-1.130767	0.052018
C	-5.569167	-0.072501	-3.933758	C	2.928778	2.477674	-0.130242
H	-3.521124	0.561888	-3.808263	C	4.646766	0.732684	-0.047323
C	-6.445588	-1.198473	-1.978339	C	2.959095	-2.477551	0.158471
H	-5.075576	-1.434442	-0.341289	C	4.655389	-0.715055	0.013521
C	-6.636125	-0.708083	-3.279505	C	3.948863	3.416724	-0.203937
H	-5.715494	0.30749	-4.938851	H	1.887677	2.779977	-0.154293
H	-7.269132	-1.69075	-1.472895	C	5.653314	1.697015	-0.122337
C	-7.900584	-0.852374	-3.92914	C	3.990814	-3.405828	0.195989
C	-8.973473	-0.972563	-4.479841	H	1.922863	-2.790544	0.222658
C	-10.237712	-1.111709	-5.132264	C	5.673908	-1.668896	0.053048
C	-11.296641	-1.781234	-4.501192	C	5.298535	3.036205	-0.195189
C	-10.437784	-0.579307	-6.414664	H	3.69247	4.468849	-0.274368
C	-12.525623	-1.906811	-5.131098	H	6.697501	1.399265	-0.129655
H	-11.149074	-2.187933	-3.506712	C	5.335347	-3.011488	0.138231
C	-11.660064	-0.72127	-7.053554	H	3.74793	-4.460328	0.277313
H	-9.619251	-0.068038	-6.909397	H	6.71463	-1.360556	0.023855
C	-12.712145	-1.381704	-6.41277	H	6.069107	3.79721	-0.254212
H	-13.354854	-2.398565	-4.633072	H	6.115296	-3.764607	0.169509
H	-11.807747	-0.335453	-8.056951	N	2.485985	-0.002405	0.020849
C	-14.665749	-2.711322	-7.221232	H	-3.478967	1.89292	-1.196711
C	-14.680642	-0.489791	-7.664211				
C	-14.322032	-4.005953	-6.828872				
C	-15.853161	-2.444941	-7.935029				
C	-14.395477	0.875218	-7.72556				
C	-15.863542	-1.024247	-8.216922				
C	-15.207515	-5.027606	-7.145				
H	-13.393116	-4.209752	-6.307937				
C	-16.726818	-3.490253	-8.239522				
C	-15.309134	1.69218	-8.377732				

H	-13.499676	1.285628	-7.272947
C	-16.765926	-0.180823	-8.86721
C	-16.40123	-4.77731	-7.837588
H	-14.965118	-6.044055	-6.85197
H	-17.643816	-3.295516	-8.787506
C	-16.480585	1.174139	-8.949398
H	-15.111446	2.757341	-8.441508
H	-17.679295	-0.582037	-9.295955
H	-17.069618	-5.60051	-8.06562
H	-17.170754	1.842684	-9.452598
N	-13.958958	-1.519121	-7.059197
C	-4.155335	-0.418958	-2.001068
C	-1.8206	-0.130813	-0.800673
C	-2.89211	-0.266101	-1.350101
C	2.977574	3.305785	1.627223
C	3.177466	3.81335	0.339505
C	2.057903	3.943605	2.464983
C	2.458626	4.910458	-0.108988
H	3.912863	3.361623	-0.315258
C	1.338243	5.043973	2.02283
H	1.912708	3.588778	3.478357
C	1.525006	5.539385	0.725674
H	2.621744	5.298575	-1.108262
H	0.629375	5.532022	2.682387
C	0.798842	6.677718	0.25695
C	0.206961	7.647247	-0.164746
C	-0.469304	8.79289	-0.686563
C	-0.31774	9.140971	-2.037715
C	-1.280741	9.586887	0.138218
C	-0.957716	10.256164	-2.550588
H	0.308975	8.526174	-2.674458
C	-1.920193	10.703352	-0.374796
H	-1.398511	9.318727	1.182424
C	-1.765952	11.053644	-1.724985
H	-0.838849	10.525826	-3.594244
H	-2.544842	11.319236	0.262821
C	-2.417151	12.209383	-2.25542
C	-2.96172	13.191364	-2.711074
C	-3.598637	14.351109	-3.251671
C	-3.436063	14.686509	-4.603893
C	-4.393334	15.172317	-2.437906
C	-4.058195	15.807868	-5.131407
H	-2.828578	14.04982	-5.237764
C	-5.000121	16.304576	-2.959582

H	-4.515143	14.921319	-1.389878
C	-4.839132	16.62573	-4.310097
H	-3.957254	16.054087	-6.183461
H	-5.59202	16.95705	-2.32599
C	-4.831677	18.771404	-5.58865
C	-6.80523	18.118289	-4.689264
C	-3.490603	18.88867	-5.956859
C	-5.779253	19.763417	-5.918423
C	-7.831923	17.415321	-4.056785
C	-7.041848	19.345061	-5.344292
C	-3.12221	20.010465	-6.687552
H	-2.760101	18.138967	-5.673403
C	-5.382588	20.881475	-6.654328
C	-9.099054	17.981975	-4.069961
H	-7.65049	16.457729	-3.581379
C	-8.325599	19.893298	-5.342613
C	-4.055162	20.996496	-7.040065
H	-2.085819	20.126265	-6.987914
H	-6.104049	21.650478	-6.913996
C	-9.347798	19.210513	-4.699653
H	-9.915482	17.458153	-3.583362
H	-8.518237	20.838254	-5.841584
H	-3.732105	21.858529	-7.613649
H	-10.350335	19.624243	-4.687319
N	-5.461796	17.774763	-4.842701

M-2	X	Y	Z	**M-3**	X	Y	Z
C	2.48363	-0.015826	0.105074	C	6.001831	-0.084249	-0.032793
C	3.19567	0.858412	-0.72678	C	6.753921	-1.062156	0.631291
C	4.582212	0.856905	-0.724755	C	8.140319	-1.015562	0.612952
H	5.104913	1.565326	-1.359212	H	8.69363	-1.804974	1.111264
C	5.29484	-0.021137	0.096829	C	8.81151	0.011982	-0.056035
C	4.586742	-0.886189	0.93394	C	8.062921	0.980348	-0.728885
H	5.121619	-1.564932	1.587004	H	8.565659	1.774973	-1.265871
C	3.199447	-0.883766	0.940334	C	6.677142	0.933846	-0.719671
H	2.657416	-1.558676	1.593461	H	6.104644	1.69061	-1.244299
C	6.801314	-0.034748	0.096445	C	10.315903	0.080149	-0.079195
C	7.557857	0.377347	-1.283781	C	11.131671	-0.576437	1.166391
B	7.575924	1.498118	-0.00013	B	11.144422	-1.408292	-0.320621
H	6.879804	2.446879	-0.076672	H	10.480245	-2.377733	-0.42303
B	8.994714	1.222384	-1.017979	B	12.587834	-1.291084	0.693725
H	9.286574	2.070925	-1.786625	H	12.933383	-2.266902	1.263176
B	8.995896	-0.474646	-1.531102	B	12.548115	0.26313	1.547053
H	9.286077	-0.752574	-2.642012	H	12.865622	0.316622	2.683661

B	7.568898	-1.265625	-0.839148	B	11.072261	1.121028	1.070448
H	6.859572	-2.001955	-1.427569	H	10.358429	1.691684	1.816335
B	9.151007	1.26953	0.747184	B	12.683943	-0.968492	-1.045787
H	9.673575	2.178663	1.294945	H	13.217696	-1.724654	-1.782972
B	10.034901	0.048619	-0.198134	B	13.559134	0.06698	0.10793
H	11.210683	0.086677	-0.32662	H	14.739058	0.049417	0.195909
B	9.146538	-1.489392	-0.090363	B	12.616561	1.55745	0.343551
H	9.66514	-2.55224	-0.131495	H	13.099689	2.608817	0.591066
B	7.720236	-1.210748	0.919862	B	11.167907	1.436308	-0.665353
H	7.160092	-2.034968	1.552354	H	10.56095	2.351243	-1.098622
B	7.717831	0.481763	1.43945	B	11.204486	-0.112556	-1.522347
H	7.113076	0.8038	2.402441	H	10.577891	-0.252498	-2.514795
B	9.243723	-0.409159	1.320654	B	12.701983	0.794929	-1.261718
H	9.840659	-0.709978	2.297287	H	13.255807	1.312958	-2.170335
H	6.909293	0.615802	-2.116796	H	10.522155	-1.007769	1.949762
H	2.651544	1.542167	-1.368793	H	6.242476	-1.862391	1.154455
C	-2.311877	-0.872537	0.902465	C	1.227642	0.78434	-0.806657
C	-2.283337	0.859872	-0.783724	C	1.217813	-1.036244	0.788889
C	-3.698317	-0.863118	0.889483	C	-0.156764	0.794072	-0.804449
H	-1.775988	-1.538757	1.569778	H	1.78085	1.483787	-1.42387
C	-3.669416	0.856507	-0.811676	C	-0.167045	-1.025774	0.791695
H	-1.724895	1.523425	-1.434987	H	1.762651	-1.743491	1.40466
C	-4.384064	-0.002127	0.028307	C	-0.872507	-0.110044	-0.004211
H	-4.263156	-1.50931	1.553494	H	-0.701968	1.501337	-1.419753
H	-4.211251	1.504814	-1.492598	H	-0.720134	-1.724654	1.40956
C	-6.609623	-1.124988	-0.125089	C	-2.301124	-0.094273	-0.000116
C	-6.609446	1.129314	0.098172	C	-3.51274	-0.073926	0.00106
C	-6.250577	-2.462888	-0.293973	C	-4.941872	-0.048554	0.002885
C	-7.959699	-0.715443	-0.116042	C	-5.638409	0.869791	-0.796466
C	-6.252229	2.465875	0.281301	C	-5.668542	-0.941238	0.804562
C	-7.959617	0.725933	0.028908	C	-7.024774	0.888868	-0.801966
C	-7.275661	-3.389748	-0.426685	H	-5.07954	1.555788	-1.423634
H	-5.210737	-2.768015	-0.332706	C	-7.05468	-0.910413	0.814362
C	-8.971468	-1.667998	-0.251687	H	-5.132999	-1.647267	1.429833
C	-7.277943	3.397599	0.366351	C	-7.739703	0.001744	0.007255
H	-5.213722	2.766112	0.366329	H	-7.567048	1.578388	-1.44086
C	-8.972008	1.683181	0.117932	H	-7.619704	-1.580082	1.454612
C	-8.623503	-3.002516	-0.400791	C	-9.94642	1.159889	0.179369
H	-7.025231	-4.437351	-0.558983	C	-9.984765	-1.078326	-0.165176
H	-10.014001	-1.364308	-0.246252	C	-9.565424	2.479739	0.425663
C	-8.624946	3.016358	0.280468	C	-11.303715	0.779528	0.116845
H	-7.028915	4.444264	0.508394	C	-9.648487	-2.4102	-0.411931
H	-10.014663	1.384323	0.066329	C	-11.328234	-0.651667	-0.105426
H	-9.397748	-3.754555	-0.507187	C	-10.575259	3.419587	0.582201

H	-9.399839	3.77199	0.351424	H	-8.520817	2.760115	0.503711
N	-5.794518	0.000294	0.005454	C	-12.299701	1.744632	0.278333
C	-1.586488	-0.008086	0.069572	C	-10.689462	-3.314564	-0.572032
C	1.054363	-0.016055	0.100674	H	-8.613887	-2.726113	-0.487493
C	-0.15696	-0.012437	0.088	C	-12.356358	-1.581935	-0.26987
				C	-11.929377	3.062138	0.504538
				H	-10.307909	4.453691	0.774384
				H	-13.347597	1.463652	0.232345
				C	-12.030789	-2.911124	-0.496705
				H	-10.45713	-4.356964	-0.764834
				H	-13.394074	-1.26517	-0.22595
				H	-12.691255	3.823651	0.631003
				H	-12.817644	-3.646359	-0.625601
				N	-9.150711	0.026556	0.008449
				C	1.932626	-0.130444	-0.009381
				C	4.573228	-0.120209	-0.017585
				C	3.361723	-0.132078	-0.010968

M-3 anion	X	Y	Z
C	-5.976214	-0.06106	0.066279
C	-6.733161	-0.922001	-0.775559
C	-8.110652	-0.893982	-0.781196
H	-8.641837	-1.58447	-1.426698
C	-8.831054	-0.002871	0.039385
C	-8.089133	0.830088	0.90279
H	-8.609906	1.499649	1.580029
C	-6.712859	0.806748	0.919797
H	-6.167358	1.457999	1.59453
C	-10.320329	0.038472	0.046941
C	-11.139276	0.920324	-1.12824
B	-11.188065	-0.767364	-1.201674
H	-10.594907	-1.30955	-2.062268
B	-12.610184	0.228535	-1.559119
H	-12.951647	0.3026	-2.689154
B	-12.531233	1.666599	-0.541087
H	-12.817655	2.729804	-0.973399
B	-11.056143	1.551118	0.434609
H	-10.356117	2.48046	0.621509
B	-12.753088	-1.191156	-0.506353
H	-13.31859	-2.165723	-0.873133
B	-13.587853	0.324011	-0.088225
H	-14.766575	0.433035	-0.14905
B	-12.615386	1.155118	1.151142
H	-13.083337	1.860045	1.98065

B	-11.20322	0.145277	1.498525
H	-10.583565	0.129013	2.504872
B	-11.287715	-1.298944	0.47993
H	-10.71732	-2.285786	0.793026
B	-12.770029	-0.614308	1.171138
H	-13.354946	-1.184943	2.029735
H	-10.486952	1.393918	-1.851313
H	-6.203439	-1.616842	-1.418723
C	-1.211183	0.782877	0.924176
C	-1.209796	-0.916197	-0.819698
C	0.160215	0.788839	0.916928
H	-1.757174	1.434458	1.599417
C	0.161683	-0.905733	-0.826024
H	-1.754507	-1.574571	-1.489379
C	0.899726	-0.053451	0.041205
H	0.706032	1.446222	1.587348
H	0.708618	-1.556803	-1.501675
C	2.303348	-0.042548	0.032826
C	3.527438	-0.030885	0.02559
C	4.938145	-0.018036	0.017257
C	5.667943	0.79401	0.915383
C	5.671645	-0.81691	-0.889609
C	7.05207	0.796153	0.913769
H	5.122095	1.409068	1.622622
C	7.055495	-0.79481	-0.903948
H	5.128481	-1.441591	-1.590463
C	7.758053	0.006708	0.000952
H	7.604152	1.404388	1.62476
H	7.609994	-1.393435	-1.621173
C	9.982009	1.142373	-0.142721
C	10.000505	-1.093527	0.121339
C	9.606018	2.475525	-0.323359
C	11.340363	0.753252	-0.101598
C	9.6464	-2.432015	0.306842
C	11.352236	-0.683937	0.06589
C	10.618587	3.415872	-0.444993
H	8.559635	2.756864	-0.371311
C	12.339153	1.721847	-0.227218
C	10.67419	-3.356838	0.418767
H	8.60494	-2.729096	0.36588
C	12.366774	-1.637325	0.181555
C	11.973358	3.049203	-0.394454
H	10.355271	4.459497	-0.586472
H	13.38667	1.435461	-0.19761

C	12.022656	-2.969867	0.353545
H	10.428185	-4.404146	0.564078
H	13.409495	-1.335243	0.14098
H	12.737935	3.812756	-0.492947
H	12.799534	-3.721839	0.444736
N	9.179302	0.018177	-0.00669
C	-1.95464	-0.070391	0.055222
C	-4.579724	-0.072544	0.063693
C	-3.349242	-0.074285	0.059944

3.4 Cartesian coordinates of *o-Cb* dyads in the excited state

D-1	X	Y	Z	**D-2**	X	Y	Z
N	0.067402	-6.377372	3.198924	C	-0.860576	-0.053722	-0.258948
B	0.728161	0.207829	3.390902	C	-0.890592	0.0915	1.152146
H	-0.13536	-0.101956	4.144541	C	0.274919	0.246688	1.86113
B	2.474271	0.039744	3.896973	H	0.244683	0.353203	2.939466
H	2.777633	-0.388803	4.961469	C	1.532744	0.264106	1.206503
B	3.232862	-0.417649	2.337097	C	1.557816	0.087823	-0.200226
H	4.12316	-1.193154	2.207479	H	2.515018	0.070688	-0.708769
B	1.788954	-0.423483	1.216713	C	0.395217	-0.064002	-0.91725
H	1.753488	-1.235027	0.351278	H	0.423646	-0.194219	-1.993711
B	1.779181	1.647403	3.687198	C	2.756388	0.450814	1.961716
H	1.681138	2.351195	4.636426	C	3.62289	2.497202	2.283416
B	3.344208	1.249351	2.929931	B	2.745229	1.471471	3.361694
H	4.383389	1.676258	3.310219	H	1.695179	1.850322	3.759864
B	2.992544	0.921591	1.21181	B	4.255552	2.381275	3.784713
H	3.792129	1.087072	0.351986	H	4.211165	3.359492	4.452941
B	1.299468	1.296787	0.877457	B	5.228193	2.199178	2.286962
H	0.928023	1.637176	-0.196589	H	5.922018	3.040094	1.820117
B	0.538108	1.748475	2.433608	B	4.125562	1.211926	1.237009
H	-0.417015	2.44235	2.555733	H	4.099093	1.409619	0.06838
B	2.196324	2.265426	2.067789	B	4.000251	0.768031	4.44703
H	2.426763	3.407938	1.847748	H	3.85537	0.646881	5.61726
C	1.807941	-1.013897	2.845206	B	5.565963	1.181314	3.704064
C	0.312643	0.303963	1.715507	H	6.558776	1.350189	4.329819
C	0.780326	-7.572598	3.181445	B	5.548405	0.479195	2.066617
C	2.161798	-7.759222	3.223266	H	6.535189	0.150259	1.498337
H	2.841919	-6.916817	3.273091	B	4.090423	-0.490461	1.867558
C	2.622463	-9.072821	3.213185	H	4.030307	-1.41532	1.127649
H	3.690002	-9.259751	3.240128	B	3.115282	-0.305399	3.364985
C	1.734707	-10.151854	3.179734	H	2.32018	-1.092798	3.758413
H	2.125691	-11.163256	3.175492	B	4.884581	-0.419912	3.455626
C	0.349814	-9.950682	3.164864	H	5.391547	-1.393533	3.903719

H	-0.328579	-10.797564	3.158159	H	-1.848878	0.080368	1.66032
C	-0.132446	-8.652209	3.16678	C	-4.412938	-0.456135	-3.658575
C	-1.468241	-8.062984	3.177526	C	-5.562358	-0.37168	-1.515058
C	-2.746688	-8.580305	3.149689	C	-5.62784	-0.532615	-4.3053
H	-2.894124	-9.65575	3.12553	H	-3.488559	-0.477714	-4.224889
C	-3.862034	-7.713122	3.137355	C	-6.776631	-0.450928	-2.161646
C	-3.640683	-6.324767	3.111376	H	-5.521179	-0.287927	-0.434755
H	-4.484008	-5.645646	3.059044	C	-6.824689	-0.529082	-3.565539
C	-2.365351	-5.774759	3.126717	H	-5.671954	-0.635735	-5.384022
H	-2.213179	-4.702759	3.073394	H	-7.703723	-0.412877	-1.600088
C	-1.283191	-6.658436	3.190492	C	-8.416791	0.126101	-5.364785
C	-5.267198	-8.308701	3.105598	C	-9.139963	-1.405528	-3.847343
C	-5.479805	-8.99741	1.74497	C	-7.702612	1.107334	-6.053455
H	-6.483782	-9.431383	1.699735	C	-9.736677	-0.215534	-5.72248
H	-5.376952	-8.279041	0.926772	C	-9.23231	-2.349294	-2.823636
H	-4.755598	-9.801935	1.586004	C	-10.197732	-1.19374	-4.754714
C	-6.345647	-7.237173	3.294868	C	-8.324009	1.705896	-7.142742
H	-6.361007	-6.506452	2.47892	H	-6.70889	1.409736	-5.744613
H	-7.328988	-7.716199	3.331375	C	-10.339454	0.398722	-6.817594
H	-6.201677	-6.697046	4.237071	C	-10.429548	-3.043574	-2.698838
C	-5.422061	-9.344049	4.234245	H	-8.400044	-2.551516	-2.159681
H	-5.258324	-8.883227	5.212781	C	-11.387541	-1.903191	-4.611365
H	-6.434947	-9.757571	4.215119	C	-9.62288	1.352426	-7.530447
H	-4.724734	-10.179079	4.129171	H	-7.790884	2.470609	-7.697539
C	-0.97545	-0.238	1.28604	H	-11.355642	0.142355	-7.100503
C	-1.106779	-0.978143	0.096462	C	-11.500647	-2.820325	-3.573738
C	-2.13221	-0.042738	2.066742	H	-10.530888	-3.781023	-1.909749
C	-2.326524	-1.511248	-0.287326	H	-12.206966	-1.747	-5.305946
H	-0.231944	-1.143172	-0.522219	H	-10.077075	1.839411	-8.386334
C	-3.358744	-0.549556	1.67552	H	-12.421145	-3.379291	-3.44599
H	-2.059764	0.544363	2.976258	N	-8.055101	-0.601107	-4.222401
C	-3.465461	-1.297047	0.495825	C	-4.351251	-0.369936	-2.247626
H	-2.404399	-2.108765	-1.190126	C	-2.057808	-0.180346	-0.976666
H	-4.249827	-0.345348	2.260846	C	-3.120126	-0.2757	-1.579851
C	-5.280357	-1.642843	-1.182768	C	2.993258	3.680589	1.716603
C	-5.647315	-2.454317	0.894179	C	3.386065	4.168412	0.449975
C	-4.758921	-0.995623	-2.305163	C	1.987944	4.382253	2.418587
C	-6.574643	-2.205536	-1.191421	C	2.798475	5.289626	-0.094068
C	-5.553476	-2.861301	2.224871	H	4.17206	3.653061	-0.090818
C	-6.81484	-2.715809	0.143633	C	1.394954	5.502835	1.877783
C	-5.547422	-0.959641	-3.44765	H	1.688767	4.033347	3.400513
H	-3.783029	-0.525	-2.281948	C	1.782246	5.976255	0.605669
C	-7.347113	-2.155987	-2.351248	H	3.112155	5.658441	-1.064716
C	-6.664549	-3.473237	2.801242	H	0.624297	6.035255	2.424818

H	-4.652777	-2.685677	2.8038	C	1.166056	7.11943	0.047029
C	-7.906899	-3.32908	0.746362	C	0.62957	8.103519	-0.431427
C	-6.82405	-1.538802	-3.479466	C	0.007513	9.247145	-0.990218
H	-5.165317	-0.464576	-4.334405	C	0.395613	9.727239	-2.256011
H	-8.34392	-2.586526	-2.367054	C	-1.011205	9.924741	-0.292
C	-7.860519	-3.699442	2.093659	C	-0.208426	10.845436	-2.802208
H	-6.596795	-3.763555	3.844716	H	1.189849	9.218241	-2.790864
H	-8.808348	-3.499702	0.163328	C	-1.62249	11.036382	-0.84218
H	-7.409999	-1.493315	-4.391035	H	-1.323803	9.552725	0.677448
N	-4.719423	-1.805976	0.084987	C	-1.225386	11.507033	-2.100917
C	-9.119983	-4.275575	2.749993	H	0.115205	11.234233	-3.762061
C	-9.577449	-5.535521	1.997029	H	-2.42971	11.537929	-0.318762
H	-10.482437	-5.94434	2.458939	C	-2.100974	13.84021	-1.990994
H	-9.806969	-5.319197	0.950028	C	-2.368319	12.731011	-3.95105
H	-8.801456	-6.306352	2.018833	C	-1.726547	14.235364	-0.70587
C	-8.89638	-4.642081	4.220051	C	-2.783328	14.712335	-2.864196
H	-8.119435	-5.40406	4.333764	C	-2.408312	11.769443	-4.961447
H	-8.614389	-3.767252	4.814047	C	-2.955642	14.003026	-4.116673
H	-9.822702	-5.044835	4.640257	C	-2.083614	15.51435	-0.299492
C	-10.238161	-3.21959	2.688034	H	-1.165032	13.576654	-0.053039
H	-9.935944	-2.305964	3.208404	C	-3.130106	15.992418	-2.432661
H	-10.48201	-2.954482	1.655487	C	-3.021141	12.121223	-6.157057
H	-11.148019	-3.603024	3.162276	H	-1.989563	10.780057	-4.816646
C	1.484232	-2.41637	3.042915	C	-3.565733	14.331818	-5.326827
C	0.610018	-2.835191	4.070945	C	-2.784244	16.384549	-1.146705
C	1.979651	-3.399399	2.152183	H	-1.806349	15.846984	0.695382
C	0.169542	-4.140268	4.143385	H	-3.656343	16.671374	-3.096761
H	0.268325	-2.109595	4.799431	C	-3.589248	13.389219	-6.345429
C	1.555625	-4.708924	2.222762	H	-3.065187	11.393332	-6.960655
H	2.674181	-3.098219	1.37596	H	-4.02056	15.308143	-5.464142
C	0.616471	-5.077248	3.199398	H	-3.048639	17.375839	-0.795012
H	-0.507566	-4.457197	4.930805	H	-4.058805	13.6292	-7.293201
H	1.890425	-5.441283	1.49451	N	-1.849901	12.637531	-2.65681

D-3	X	Y	Z	**M-3** (LE)	X	Y	Z
C	-17.908804	-0.863575	-9.646065	C	-5.964141	-0.010674	0.037502
C	-16.669233	-0.89095	-9.042959	C	-6.699829	-0.904952	-0.773996
H	-16.539399	-1.391085	-8.091381	C	-8.081316	-0.88154	-0.779455
C	-15.545574	-0.272041	-9.648388	H	-8.614352	-1.594792	-1.395953
C	-15.727278	0.353483	-10.909105	C	-8.792312	0.036355	0.009136
H	-14.872733	0.810082	-11.393056	C	-8.065762	0.907429	0.837851
C	-16.964118	0.382601	-11.51731	H	-8.592812	1.599711	1.484674
H	-17.092178	0.864186	-12.479571	C	-6.685405	0.891222	0.85438

C	-14.24816	-0.281142	-9.000323	H	-6.138661	1.570796	1.498749
C	-13.657715	1.36037	-7.546864	C	-10.294348	0.059197	0.028933
B	-14.143909	-0.289154	-7.262885	C	-11.123764	0.87068	-1.149657
H	-15.132408	-0.481458	-6.642694	B	-11.153865	-0.823909	-1.171725
B	-12.724234	0.544315	-6.460376	H	-10.553378	-1.37848	-2.019142
H	-12.780095	0.904816	-5.334943	B	-12.593379	0.135973	-1.535932
B	-12.040572	1.514275	-7.827652	H	-12.948769	0.170608	-2.662222
H	-11.584796	2.60139	-7.727244	B	-12.526203	1.613088	-0.568388
B	-13.177269	1.081924	-9.197391	H	-12.835582	2.652339	-1.03827
H	-13.460266	1.897494	-10.006511	B	-11.042627	1.568083	0.392562
B	-12.596219	-1.164783	-6.903221	H	-10.348725	2.51065	0.531586
H	-12.484068	-1.968178	-6.042379	B	-12.69341	-1.248103	-0.431576
B	-11.278933	-0.02762	-7.341708	H	-13.241015	-2.246962	-0.752932
H	-10.222457	-0.020528	-6.809323	B	-13.548215	0.264848	-0.051686
B	-11.512293	0.373375	-9.075674	H	-14.728025	0.349045	-0.098385
H	-10.617242	0.679208	-9.785881	B	-12.579449	1.159483	1.143012
B	-12.814498	-0.632197	-9.732049	H	-13.046737	1.883116	1.954638
H	-12.860819	-0.942727	-10.872782	B	-11.138839	0.192699	1.50083
B	-13.495729	-1.60286	-8.364605	H	-10.490061	0.222468	2.488248
H	-14.05413	-2.639516	-8.479594	B	-11.207085	-1.290292	0.532021
B	-11.738564	-1.30229	-8.473184	H	-10.598086	-2.245845	0.86837
H	-11.004646	-2.191732	-8.737177	B	-12.691603	-0.612975	1.227234
H	-18.760643	-1.337003	-9.172333	H	-13.246115	-1.166385	2.114713
C	-14.567161	2.445151	-7.231661	H	-10.498591	1.334599	-1.902692
C	-14.557538	3.648006	-7.983849	H	-6.164356	-1.618781	-1.390182
C	-15.487865	2.33754	-6.158021	C	-1.20577	0.870665	0.871994
C	-15.432538	4.674812	-7.697347	C	-1.207054	-0.937359	-0.786626
H	-13.843475	3.752869	-8.791205	C	0.16129	0.873272	0.871466
C	-16.365203	3.360536	-5.867568	H	-1.75858	1.557497	1.503762
H	-15.490259	1.434853	-5.559949	C	0.160059	-0.938424	-0.789685
C	-16.366855	4.551513	-6.637979	H	-1.76069	-1.625386	-1.416367
H	-15.41662	5.588404	-8.279758	C	0.89549	-0.031419	0.039079
H	-17.065467	3.267166	-5.045941	H	0.71351	1.561569	1.502194
C	-18.089862	-0.214355	-10.893986	H	0.711366	-1.626585	-1.421365
C	-19.359213	-0.152806	-11.498147	C	2.280983	-0.027974	0.034788
C	-20.465013	-0.078637	-12.02083	C	3.516998	-0.02299	0.029912
C	-21.737841	0.023024	-12.617723	C	4.905948	-0.01639	0.023344
C	-22.878647	-0.529065	-11.986897	C	5.640115	0.892149	0.841349
C	-21.902136	0.689126	-13.856263	C	5.64104	-0.917244	-0.802272
C	-24.128173	-0.413311	-12.565607	C	7.013889	0.900014	0.829675
H	-22.75725	-1.040759	-11.039827	H	5.092999	1.566652	1.490733
C	-23.152278	0.803197	-14.433079	C	7.01485	-0.909873	-0.805835
H	-21.031572	1.110759	-14.343934	H	5.094319	-1.597897	-1.445533
C	-24.290882	0.258216	-13.797988	C	7.725416	-0.000795	0.00777

H	-24.998885	-0.834444	-12.077751	H	7.566025	1.567671	1.482776
H	-23.274156	1.314869	-15.380112	H	7.566948	-1.571528	-1.465053
C	-25.574283	0.394986	-14.385913	C	9.934519	1.145744	-0.060948
C	-26.674365	0.529658	-14.893304	C	9.948421	-1.121063	0.048302
C	-27.954747	0.702248	-15.488608	C	9.567558	2.48547	-0.194415
C	-29.111879	0.191357	-14.86939	C	11.287167	0.744931	-0.050873
C	-28.087817	1.395793	-16.707312	C	9.598521	-2.464732	0.187786
C	-30.361515	0.378072	-15.443442	C	11.29607	-0.7048	0.018772
H	-29.01839	-0.334078	-13.926554	C	10.588763	3.424647	-0.268971
C	-29.335441	1.570098	-17.288611	H	8.527864	2.785069	-0.255786
H	-27.200378	1.780106	-17.195651	C	12.293098	1.704692	-0.13084
C	-30.482751	1.067862	-16.658086	C	10.631218	-3.392232	0.24807
H	-31.254808	0.01601	-14.948023	H	8.56333	-2.775982	0.264795
H	-29.433011	2.07414	-18.242988	C	12.313843	-1.653092	0.084512
C	-17.279812	5.583487	-6.351188	C	11.936739	3.044808	-0.229711
C	-18.088697	6.466873	-6.093569	H	10.333125	4.474192	-0.369637
C	-19.032073	7.468788	-5.7886	H	13.337494	1.408263	-0.126264
C	-19.0755	8.676135	-6.526304	C	11.974035	-2.997118	0.188886
C	-19.962136	7.281075	-4.737714	H	10.389072	-4.444523	0.353298
C	-20.010177	9.650731	-6.229392	H	13.354657	-1.344923	0.065031
H	-18.363337	8.825002	-7.328865	H	12.708278	3.804523	-0.292512
C	-20.893767	8.256382	-4.442126	H	12.755	-3.748012	0.240656
H	-19.932509	6.359358	-4.169355	N	9.121161	0.007562	-0.000748
C	-20.938856	9.459709	-5.182718	C	-1.93807	-0.032968	0.042778
H	-20.039156	10.572257	-6.798098	C	-4.56005	-0.023515	0.040544
H	-21.605741	8.109051	-3.639094	C	-3.331811	-0.029921	0.041975
C	-21.911431	10.441364	-4.863454				
C	-22.771978	11.244426	-4.547125				
C	-23.799177	12.137497	-4.134049				
C	-24.06993	13.3248	-4.84024				
C	-24.575509	11.832215	-2.998351				
C	-25.082125	14.178421	-4.423305				
H	-23.470539	13.574183	-5.707497				
C	-25.594713	12.678886	-2.588556				
H	-24.377787	10.915301	-2.456284				
C	-25.855719	13.859896	-3.297797				
H	-25.269758	15.107141	-4.949295				
H	-26.211984	12.423832	-1.735157				
C	-27.887153	15.265501	-3.715909				
C	-27.11517	15.169118	-1.570025				
C	-28.113972	15.070357	-5.07971				
C	-28.74923	16.064771	-2.928602				
C	-26.371019	14.939553	-0.411184				
C	-28.256746	16.005282	-1.563665				

C	-29.207287	15.716946	-5.650902
H	-27.474161	14.430201	-5.6744
C	-29.83898	16.703883	-3.523623
C	-26.809486	15.539848	0.766594
H	-25.477171	14.328278	-0.42429
C	-28.677715	16.595892	-0.370602
C	-30.05968	16.531142	-4.88677
H	-29.40554	15.583026	-6.70794
H	-30.505164	17.319351	-2.929176
C	-27.953641	16.354686	0.792923
H	-26.25146	15.37661	1.68121
H	-29.552183	17.23693	-0.354591
H	-30.899554	17.02084	-5.364443
H	-28.267916	16.803635	1.727374
C	-32.72931	0.267015	-17.4303
C	-32.252055	2.47769	-17.734185
C	-32.676201	-1.100017	-17.151684
C	-33.859334	0.854492	-18.046732
C	-31.672703	3.747886	-17.724536
C	-33.556548	2.262137	-18.238006
C	-33.792419	-1.868022	-17.474549
H	-31.796717	-1.554666	-16.712979
C	-34.967126	0.06427	-18.360794
C	-32.412871	4.798856	-18.260241
H	-30.688834	3.917352	-17.304808
C	-34.279657	3.331433	-18.770423
C	-34.930039	-1.295537	-18.067102
H	-33.778135	-2.93182	-17.26809
H	-35.838624	0.503924	-18.833082
C	-33.70017	4.596501	-18.784776
H	-31.986135	5.795071	-18.267011
H	-35.279481	3.17785	-19.161174
H	-35.781205	-1.9221	-18.304643
H	-34.246833	5.436321	-19.196387
N	-26.893141	14.720926	-2.883946
N	-31.751884	1.259511	-17.24247

M-2(LE)	X	Y	Z	**M-2***(CT)	X	Y	Z
C	2.345529	-0.082476	0.167601	C	2.205706	0.068828	0.383903
C	3.07007	1.065168	-0.26806	C	2.916246	1.18358	-0.104924
C	4.445747	1.066075	-0.2834	C	4.295668	1.189996	-0.122798
H	4.967704	1.961666	-0.60167	H	4.831277	2.057443	-0.494378
C	5.18548	-0.064108	0.123057	C	5.04057	0.083564	0.34576
C	4.475857	-1.190206	0.586095	C	4.320162	-1.029546	0.836407

H	5.015798	-2.056788	0.94828	H	4.874762	-1.885458	1.207141
C	3.099222	-1.209864	0.604766	C	2.940757	-1.036445	0.85789
H	2.570897	-2.086252	0.964191	H	2.404167	-1.897917	1.243923
C	6.679985	-0.021854	0.131326	C	6.48522	0.089881	0.324574
C	7.547577	-0.667466	-1.137123	C	7.757437	-0.65409	-1.468999
B	7.443787	1.016781	-1.012701	B	7.38219	0.898196	-0.953944
H	6.763295	1.585476	-1.789255	H	6.769061	1.608839	-1.684237
B	8.946693	0.211124	-1.486627	B	9.05714	0.318813	-1.475669
H	9.275557	0.29768	-2.618561	H	9.530559	0.631272	-2.52009
B	9.012862	-1.342377	-0.647499	B	9.074038	-1.317882	-0.788288
H	9.387671	-2.313932	-1.206663	H	9.560941	-2.273972	-1.299388
B	7.554197	-1.489894	0.3431	B	7.403343	-1.376839	0.001469
H	6.962921	-2.505776	0.418143	H	6.803396	-2.403752	0.004394
B	8.965489	1.499934	-0.27028	B	8.909431	1.463145	-0.137792
H	9.426333	2.563055	-0.513187	H	9.372243	2.552032	-0.253473
B	9.945209	0.032165	-0.037615	B	9.921294	0.000298	0.036222
H	11.126688	0.042122	-0.112875	H	11.109502	0.028486	0.075998
B	9.077569	-1.030748	1.096151	B	8.934292	-1.164092	0.96564
H	9.619859	-1.784601	1.83047	H	9.415083	-2.000682	1.660303
B	7.578917	-0.215885	1.568031	B	7.467533	-0.372119	1.530681
H	6.957762	-0.382401	2.55998	H	6.935916	-0.703366	2.541482
B	7.509739	1.341096	0.725525	B	7.451623	1.289551	0.834385
H	6.849515	2.220539	1.15945	H	6.906722	2.23432	1.308143
B	9.058941	0.7294	1.328163	B	8.971394	0.564778	1.401403
H	9.59445	1.251129	2.2465	H	9.493993	0.981755	2.385415
H	6.938025	-1.113561	-1.913186	H	7.298024	-1.036827	-2.370614
H	2.519055	1.94517	-0.581338	H	2.360476	2.044654	-0.463714
C	-2.406261	-1.231324	0.674214	C	-2.56387	-1.058561	0.927079
C	-2.409958	1.057302	-0.223905	C	-2.584522	1.159364	-0.029086
C	-3.774454	-1.226661	0.686521	C	-3.950127	-1.05919	0.955792
H	-1.857294	-2.094337	1.034165	H	-2.009682	-1.913762	1.298159
C	-3.777908	1.063515	-0.198256	C	-3.97102	1.150381	-0.020688
H	-1.864384	1.916319	-0.598328	H	-2.046432	2.018414	-0.414624
C	-4.49166	-0.078764	0.254044	C	-4.661152	0.043028	0.476837
H	-4.324157	-2.076067	1.079452	H	-4.494771	-1.90799	1.35811
H	-4.33165	1.91767	-0.574826	H	-4.532055	1.995309	-0.408416
C	-6.713791	-1.102792	-0.182733	C	-6.891902	-1.037118	0.151024
C	-6.694116	0.962256	0.749563	C	-6.891976	1.105954	0.857639
C	-6.35773	-2.299063	-0.808043	C	-6.529859	-2.305836	-0.306411
C	-8.063135	-0.730363	0.00644	C	-8.245046	-0.658743	0.29466
C	-6.313579	2.156809	1.363856	C	-6.52933	2.377976	1.305401
C	-8.05056	0.599663	0.595073	C	-8.2451	0.716854	0.746031
C	-7.389356	-3.149244	-1.190517	C	-7.552231	-3.197888	-0.596645
H	-5.321216	-2.54642	-1.004147	H	-5.487888	-2.576904	-0.436476

C	-9.076424	-1.593173	-0.389265	C	-9.253917	-1.577043	-0.003472
C	-7.329072	3.015024	1.77084	C	-7.551662	3.26231	1.618531
H	-5.270608	2.396925	1.533011	H	-5.486801	2.657599	1.410399
C	-9.047205	1.470322	1.014992	C	-9.253949	1.62754	1.066859
C	-8.730443	-2.809377	-0.977609	C	-8.902125	-2.844352	-0.443758
H	-7.147426	-4.089196	-1.674561	H	-7.299492	-4.191315	-0.953684
H	-10.118634	-1.322457	-0.252463	H	-10.298009	-1.298219	0.105636
C	-8.677561	2.684811	1.592446	C	-8.901929	2.898063	1.497567
H	-7.06792	3.953835	2.247107	H	-7.298398	4.25815	1.968428
H	-10.094492	1.207037	0.905147	H	-10.298064	1.340312	0.982663
H	-9.51077	-3.494838	-1.289932	H	-9.674571	-3.569199	-0.678268
H	-9.444467	3.376552	1.92361	H	-9.674243	3.617181	1.749497
N	-5.885125	-0.073479	0.273085	N	-6.079759	0.037526	0.494922
C	-1.664532	-0.089892	0.214944	C	-1.85339	0.052864	0.439044
C	0.955603	-0.092222	0.181853	C	0.785435	0.062066	0.402826
C	-0.282957	-0.093335	0.197018	C	-0.430729	0.057678	0.419601

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