nature photonics

SUPPLEMENTARY INFORMATION

https://doi.org/10.1038/s41566-019-0476-5

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Narrowband deep-blue organic light-emitting diode featuring an organoboron-based emitter

Yasuhiro Kondo[1], Kazuki Yoshiura[2], Sayuri Kitera[2], Hiroki Nishi[2], Susumu Oda[2], Hajime Gotoh[2], Yasuyuki Sasada[1], Motoki Yanai[1] and Takuji Hatakeyama[2]*

[1]JNC Petrochemical Corporation, Ichihara, Japan. [2]Department of Chemistry, School of Science and Technology, Kwansei Gakuin University, Sanda, Japan. *e-mail: hatake@kwansei.ac.jp

General Procedure. All the reactions dealing with air- or moisture-sensitive compounds were carried out in a dry reaction vessel (small scale, a Schlenk flask; large scale, a three-neched round bottomed flask) under a positive pressure of nitrogen. Air- and moisture-sensitive liquids and solutions were transferred *via* a syringe or a Teflon cannula. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel containing a fluorescent indicator (Merck, #1.05715.0009). TLC plates were visualized by exposure to ultraviolet light (254 nm or 365 nm) and/or by immersion in a basic staining solution of $KMnO_4$ followed by heating on a hot plate. Organic solutions were concentrated by rotary evaporation at *ca.* 10–50 mmHg. Flash column chromatography was performed on Merck silica gel 60 (spherical, neutral, 140–325 mesh) as described by Still et al.[1] Gel permeation chromatography was performed on a JAIGEL-1H and 2H (20 mm i.d.) with an LC-9130 (Japan Analytical Industry Co., Ltd.). Proton nuclear magnetic resonance (^{1}H NMR), carbon nuclear magnetic resonance (^{13}C NMR) and boron nuclear magnetic resonance (^{11}B NMR) spectra were recorded on JEOL ECX400 (400 MHz) NMR spectrometers or JEOL ECX500 (500 MHz) NMR spectrometers. Proton chemical shift values are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the tetramethylsilane (δ 0), $(CDCl_2)_2$ (δ 6.00) or $CDCl_3$ (δ 7.26). ^{13}C NMR spectra were recorded at 101 MHz or 126 MHz: carbon chemical shift values are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane, and are referenced to the carbon resonance of tetramethylsilane (δ 0), $(CDCl_2)_2$ (δ 73.8), or $CDCl_3$ (δ 77.0). ^{11}B NMR spectra were recorded at 128 MHz or 160 MHz: boron chemical shift values are reported in parts per million (ppm, δ scale) and are referenced to the external standard boron signal of $BF_3 \cdot Et_2O$ (δ 0). Data are presented as: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, sept = septet, m = multiplet and/or multiplet resonances, br = broad), coupling constant in hertz (Hz), signal area integration in natural numbers, and assignment (*italic*). IR spectra were recorded on an ATR-FTIR spectrometer (FT/IR-4200, JASCO). Characteristic IR absorptions are reported in cm^{-1}. Melting points were recorded on a Fisher-Johns 12-144-1Q melting point apparatus (according to the limitations of the apparatus, the compounds which did not melt up to 300 °C are presented as ">300 °C" after confirming that is not decomposed using NMR). Glass-transition temperatures were measured by Perkin Elmer Diamond DSC. High-resolution mass spectra (HRMS) were obtained by the electron impact (EI) method with a JEOL JMS-T100GCv instrument, by the atmospheric pressure chemical ionization (APCI) method with a BRUKER DALTONICS micrOTOF instrument, and by the direct analysis in real time (DART) method with IonSense SVP100 and JEOL JMS-T100LP instruments. Low-resolution mass spectra (LRMS) were obtained by the electron impact (EI) method with a Shimadzu GCMS-QP2010 Ultra instrument. Thermogravity and differential thermal analysis

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(1) Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923–2925.

was performed using a Rigaku TG8120 under flowing N_2 with 10 K min^{-1} lamp rate. Purity of isolated compounds was determined by ^1H NMR analyses, GC analysis on a Shimadzu GC-2025 instrument equipped with an FID detector and a capillary column (ZB-1MS, Phenomenex, 10 m × 0.10 mm i.d., 0.10 μm film thickness), or HPLC analysis on a JASCO UV-2070 Plus instrument equipped with a reversed-phase C18 column (InertSustain™ C18, GL Siences Inc., 4.6 mm × 250 mm i.d.). Sublimation was conducted by an ULVAC VPC–050/051 instrument (10^1–10^{-3} Pa).

Materials. Materials were purchased from Wako Pure Chemical Industries, Ltd. (Wako), Tokyo Chemical Industry Co., Ltd. (TCI), Aldrich Inc. (Aldrich), and other commercial suppliers, and were used after appropriate purification, unless otherwise noted.

Solvent. Anhydrous solvents were purchased from above-described suppliers and/or dried over Molecular Sieves 4A and degassed before use. Water content of the solvent was determined with a Karl Fischer Moisture Titrator (AQ-2200, Hiranuma Sangyo Co., Ltd.) to be less than 20 ppm.

Computational method. The calculations were performed using the Gaussian 09 package[2] based on the density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods with the B3LYP hybrid functional[3]. All structures were optimized using DFT (S_0 states) or TD-DFT (S_1 and T_1 state) method with a 6-31G(d) basis set[4]. Franck-Condon analyses of emission spectra were performed according to the literature[5] using the Gaussian 16 package[6]. All calculations were performed in the gas phase.

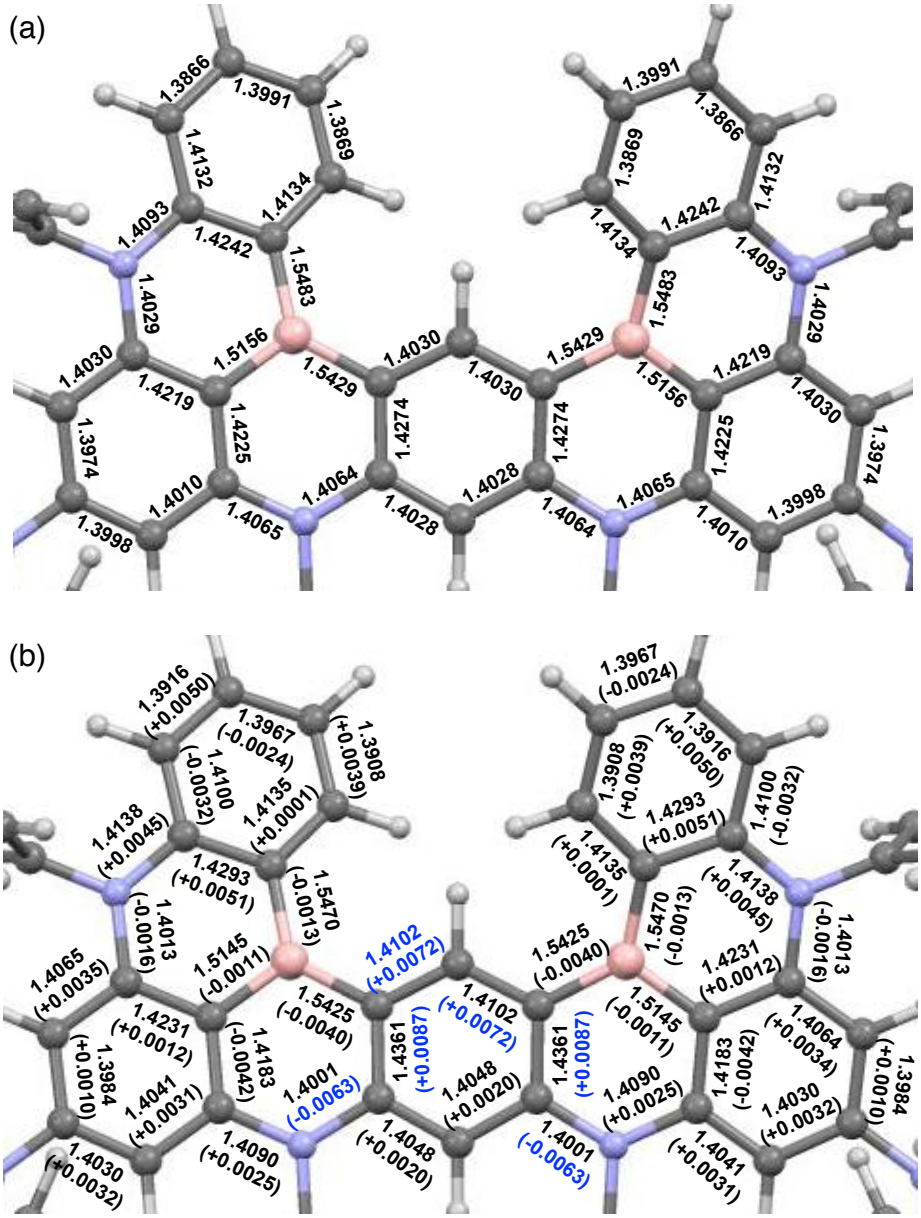
(2) Frisch, M. J. et al. Gaussian 09, Revision C.01. (Gaussian, 2010).

(3) (a) Becke, A. D. *J. Chem. Phys.* **98**, 5648–5652 (1993). (b) Stephens, P. J., Devlin, F. J., Chabalowski, C. F. & Frisch, M. J. *J. Phys. Chem.* **98**, 11623–11627 (1994).

(4) (a) Ditchfield, R., Hehre, W. J. & Pople, J. *J. Chem. Phys.* **54**, 724–728 (1971). (b) Frisch, M. J., Pople, J. A. & Binkley, J. S. *J. Chem. Phys.* **80**, 3265–3269 (1984).

(5) Santoto, F., Lami, A., Improta, R. & Borone, V. *J. Chem. Phys.* **128**, 224311 (2008).

(6) Frisch, M. J. et al. Gaussian 16, Revision B.01. (Gaussian, 2018).



bond-length change (Å)	
0.0087	0.0031
0.0087	0.0031
0.0072	0.0025
0.0072	0.0025
0.0063	0.0024
0.0063	0.0024
0.0051	0.0020
0.0051	0.0020
0.0050	0.0016
0.0050	0.0016
0.0045	0.0013
0.0045	0.0013
0.0042	0.0012
0.0042	0.0012
0.0039	0.0011
0.0039	0.0011
0.0035	0.0010
0.0034	0.0010
0.0032	0.0004
0.0032	0.0004
0.0032	0.0001
0.0032	0.0001
average change (Å)	
0.0032	

Figure S1. Bond lengths of the optimized structures of **ν-DABNA** in the (a) S_0 and (b) S_1 states. Changes between the S_0 and S_1 states are shown in parenthesis.

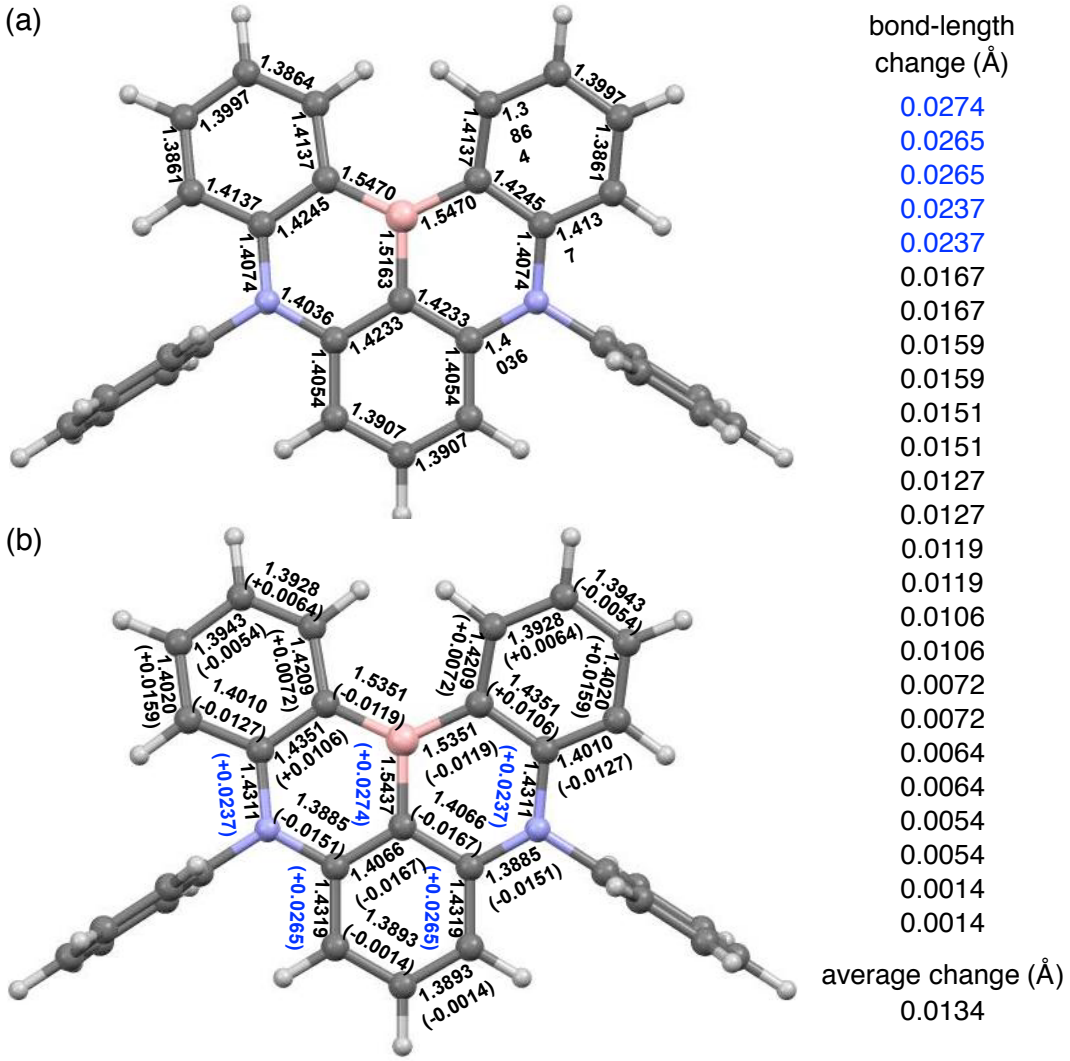


Figure S2. Bond lengths of the optimized structures of **DABNA-1** in the (a) S_0 and (b) S_1 states. Changes between the S_0 and S_1 states are shown in parenthesis.

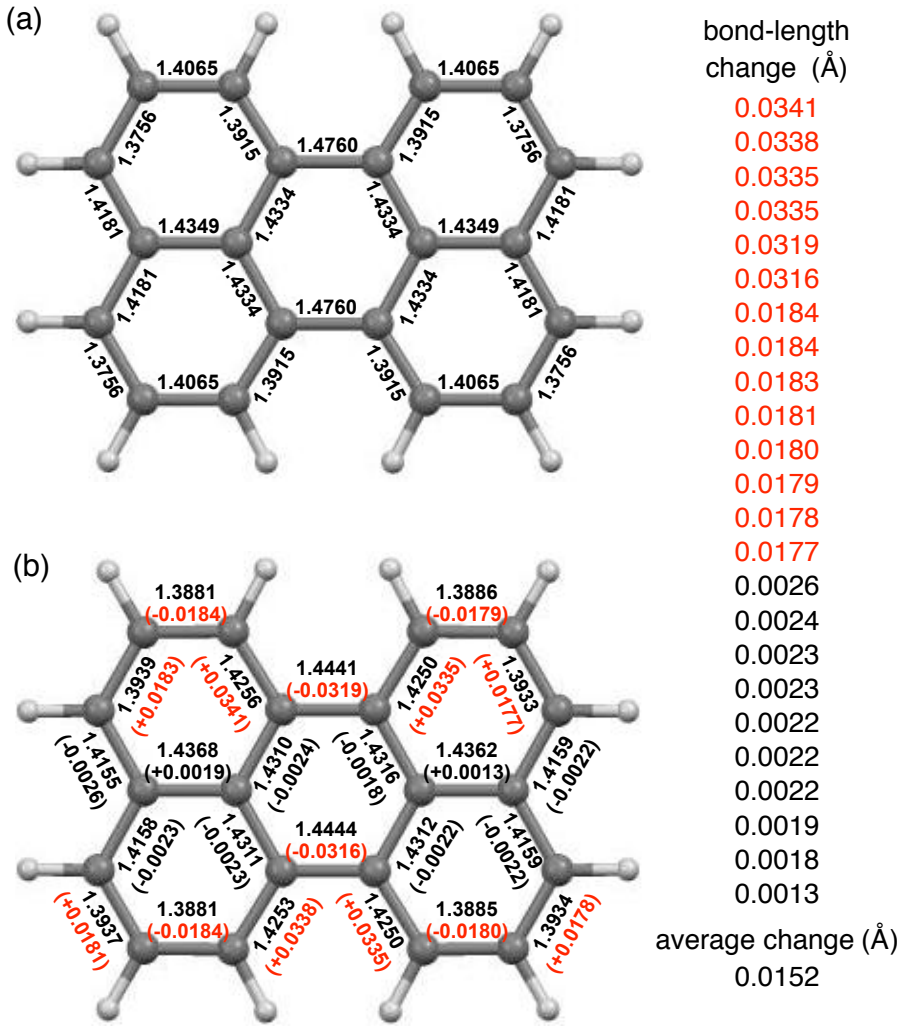


Figure S3. Bond lengths of the optimized structures of perylene in the (a) S_0 and (b) S_1 states. Changes between the S_0 and S_1 states are shown in parenthesis.

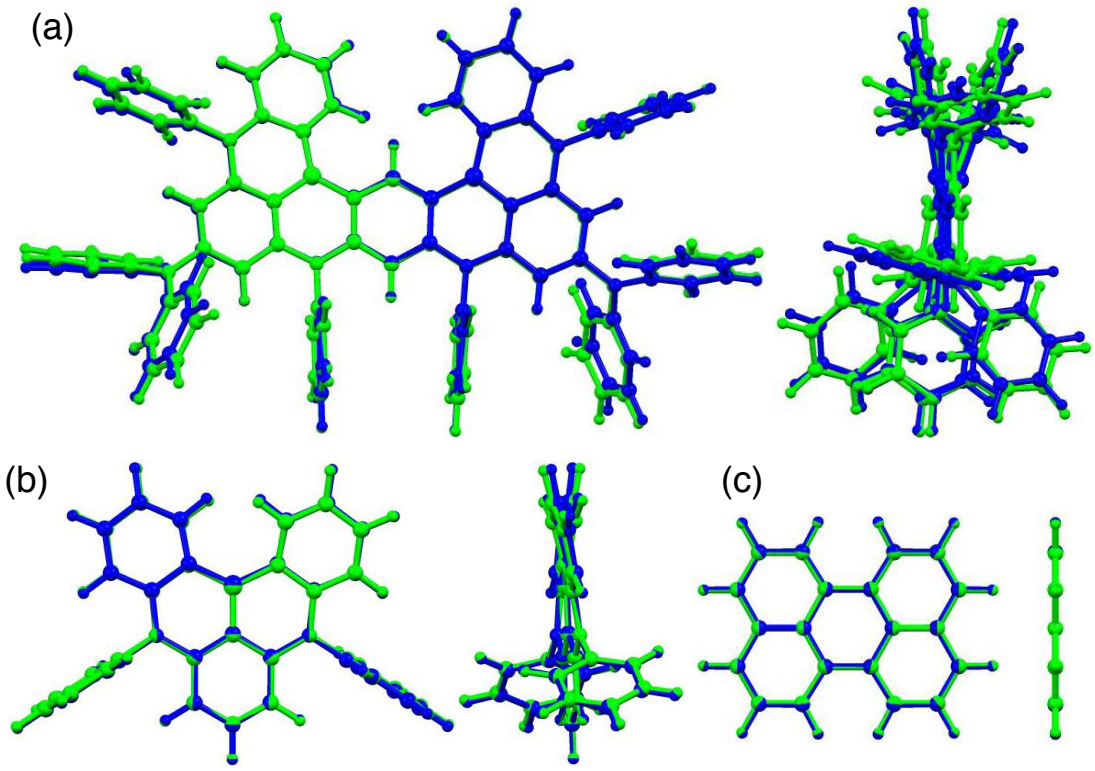


Figure S4. Comparison of the optimized structures of (a) **ν-DABNA**, (b) **DABNA-1**, and (c) perylene in the S_0 (green) and S_1 (blue) states.

Table S1. Summary of electronic energy (E) for **ν-DABNA, DABNA-1** and perylene at the S_0 and S_1 structures at the B3LYP/6-31G(d) level.

compound	$E_{(S0@S0)}$[a] (A.U.)	$E_{(S0@S1)}$[a] (A.U.)	$E_{(S1@S0)}$[b] (A.U.)	$E_{(S1@S1)}$[b] (A.U.)
ν-DABNA	-3383.171976	-3383.170821	-3383.065359	-3383.066542
DABNA-1	-1290.260356	-1290.255484	-1290.145214	-1290.149026
perylene	-769.4061188	-769.400552	-769.2995204	-769.3054566

[a] Electronic energy of S_0 at the optimized S_0 or S_1 structure, respectively. [c] Electronic energy of S_1 at the optimized S_0 or S_1 structure, respectively.

Table S2. Correlation between FWHM, $\Delta E(E_{(S1@S0)} - E_{(S1@S1)})$, and average change in bond length for **ν-DABNA, DABNA-1,** and perylene at the B3LYP/6-31G(d) level.

compound	FWHM[a] (nm/meV)	FWHM[b] (nm/meV)	ΔE[c] (meV)	average change in bond length (Å)
ν-DABNA	18/109	14/79	32	0.0032
DABNA-1	28/162	21/127	104	0.0134
perylene	–	42/247	162	0.0152

[a] Full width at half maximum (nm, meV) of EL spectra. [b] Full width at half maximum (nm, meV) of PL spectra in toluene (0.02 mM) at 298 K. [c] $\Delta E = E_{(S1@S0)} - E_{(S1@S1)}$ in Table S1.

Table S3. Summary of TD-DFT calculation for **ν-DABNA**, **DABNA-1** and perylene at the S_0, S_1, and T_1 structures at the B3LYP/6-31G(d) level with related spectroscopic data.

compound	optimized structure	transition	wavelength (nm)	energy (eV)	oscillator strength	coefficient of HOMO–LUMO	experimental λ_{ab} (nm)	experimental λ_{em} (nm)
ν-DABNA	S_0	S_0–S_1	427.65	2.8992	0.6876	0.69323	457[a]	—
		S_0–T_1	481.76	2.5735	0.0000	0.67124	—	—
	S_1	S_1–S_0	436.94	2.8376	0.7145	0.69416	—	468[a]
	T_1	T_1–S_0	496.43	2.4975	0.0000	0.67390	—	471[b]
DABNA-1	S_0	S_0–S_1	395.71	3.1332	0.2047	0.69746	439[a]	—
	S_1	S_1–S_0	428.00	2.8969	0.1389	0.70010	—	450[a]
perylene	S_0	S_0–S_1	427.43	2.9007	0.3613	0.70450	439[a]	—
	S_1	S_1–S_0	479.13	2.5877	0.3587	0.70782	—	448[a]

[a] Absorption and emission maxima in toluene at 298 K (0.02 mM solution). [b] Emission maxima at 77 K in 2-methyltetrahydrofuran (saturated solution).

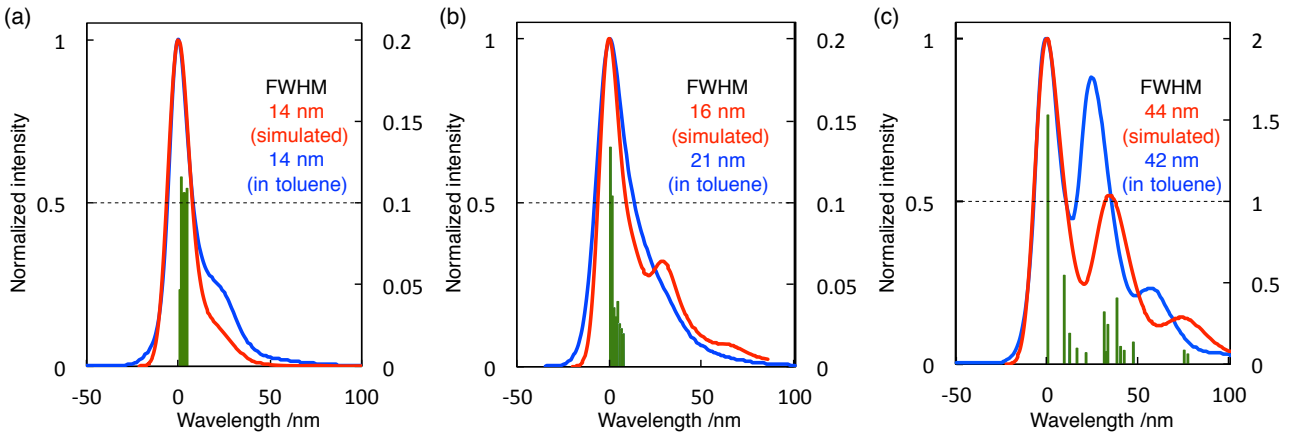


Figure S4. Comparison between emission spectra simulated by Franck-Condon analysis on the S_1–S_0 transition (red) and emission spectra (blue) in toluene (0.02 mM solution) of (a) **ν-DABNA**, (b) **DABNA-1** and (c) perylene at the (TD)B3LYP/6-31G(d) level. Band broadening simulated by mean of Gaussian functions with half-widths at half-maximum of 300.0 cm^{-1}.

Table S5. Summary of Franck-Condon analysis on the S_1–S_0 transition of **ν-DABNA**, **DABNA-1** and perylene at the (TD)B3LYP/6-31G(d) level.

compound	transition ($S_1 \rightarrow S_0$)	frequency (cm^{-1})	relative frequency (cm^{-1})	line density	dipole strength (a.u.)
ν-DABNA	$0 \rightarrow 0$	22173.534	0	28.98	0.04699
	$0 \rightarrow 3^1 1^1$	22154.354	-19.1795	71.13	0.1157
	$0 \rightarrow 3^1 1^2$	22146.844	-26.6897	65.27	0.1063
	$0 \rightarrow 7^1 3^1 1^1$	22136.073	-37.4607	66.87	0.1092
DABNA-1	$0 \rightarrow 0$	23520.167	0	104.5	0.1338
	$0 \rightarrow 1^1$	23497.092	-23.0750	80.85	0.1040
	$0 \rightarrow 1^2$	23474.017	-46.1500	37.59	0.04852
	$0 \rightarrow 7^1$	23442.490	-77.6767	27.63	0.03586
	$0 \rightarrow 7^1 1^1$	23419.415	-100.7518	23.24	0.03030
	$0 \rightarrow 10^1$	23393.101	-127.0661	30.32	0.03968
	$0 \rightarrow 10^1 1^1$	23370.026	-150.1411	19.84	0.02608
	$0 \rightarrow 13^1$	23312.129	-208.0375	17.40	0.02310
	$0 \rightarrow 13^1 1^1$	23289.054	-231.1125	14.99	0.01998
perylene	$0 \rightarrow 0$	21358.819	0	812.4	1.530
	$0 \rightarrow 9^1$	21001.024	-357.7948	270.9	0.5457
	$0 \rightarrow 19^1$	20802.811	-556.0082	90.50	0.1894
	$0 \rightarrow 9^2$	20643.229	-715.5896	45.33	0.09784
	$0 \rightarrow 19^1 9^1$	20445.016	-913.8030	31.33	0.07028
	$0 \rightarrow 60^1$	20020.945	-1337.8741	131.6	0.3209
	$0 \rightarrow 63^1$	19959.000	-1399.8191	31.12	0.07685
	$0 \rightarrow 65^1$	19949.533	-1409.2859	98.46	0.2436
	$0 \rightarrow 73^1$	19739.020	-1619.7990	157.3	0.4061
	$0 \rightarrow 60^1 9^1$	19663.150	-1695.6690	41.38	0.1085
	$0 \rightarrow 65^1 9^1$	19591.738	-1767.0807	31.73	0.08442
	$0 \rightarrow 73^1 9^1$	19381.225	-1977.5938	48.83	0.1356
	$0 \rightarrow 73^1 60^1$	18401.146	-2957.6731	25.06	0.08566
	$0 \rightarrow 73^1 65^1$	18329.734	-3029.0849	18.03	0.06260

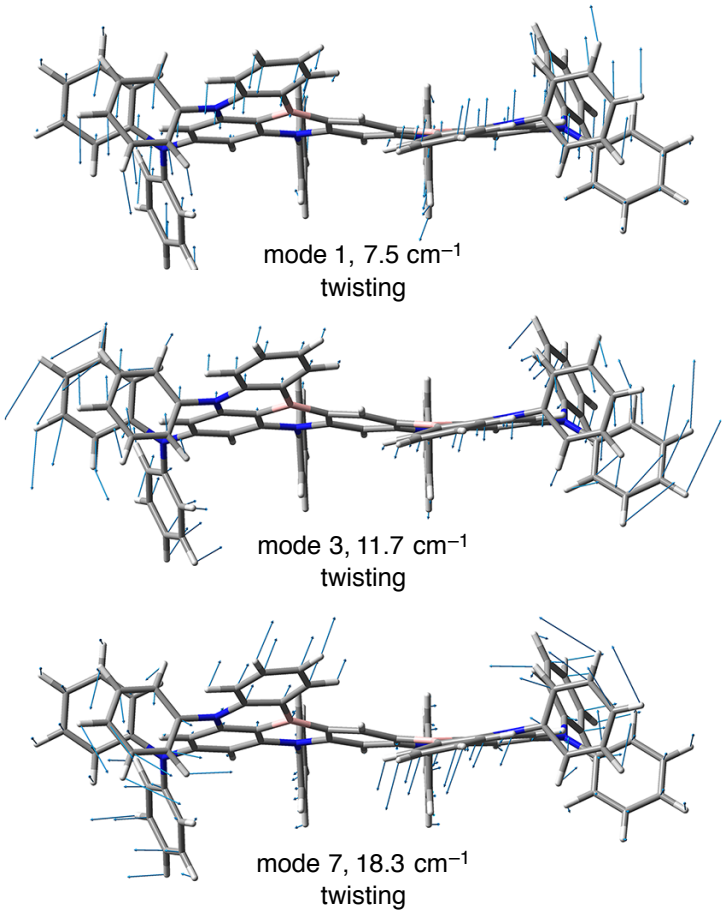


Figure S6. Vibrational modes in the S_0 state involved in the Franck-Condon spectral progression of **ν-DABNA** at the (TD)B3LYP/6-31G(d) level.

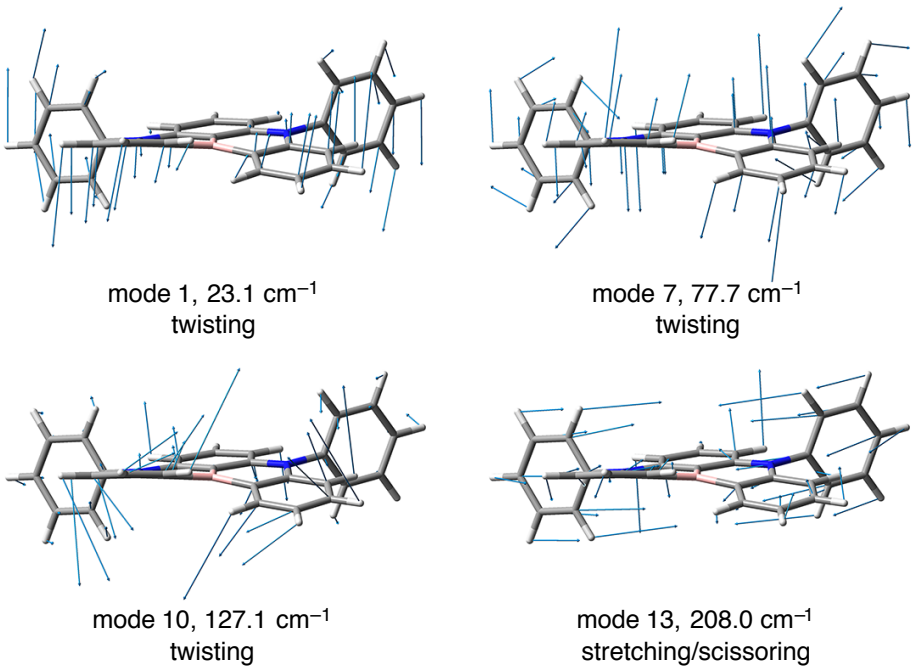


Figure S7. Vibrational modes in the S_0 state involved in the Franck-Condon spectral progression of **DABNA-1** at the (TD)B3LYP/6-31G(d) level.

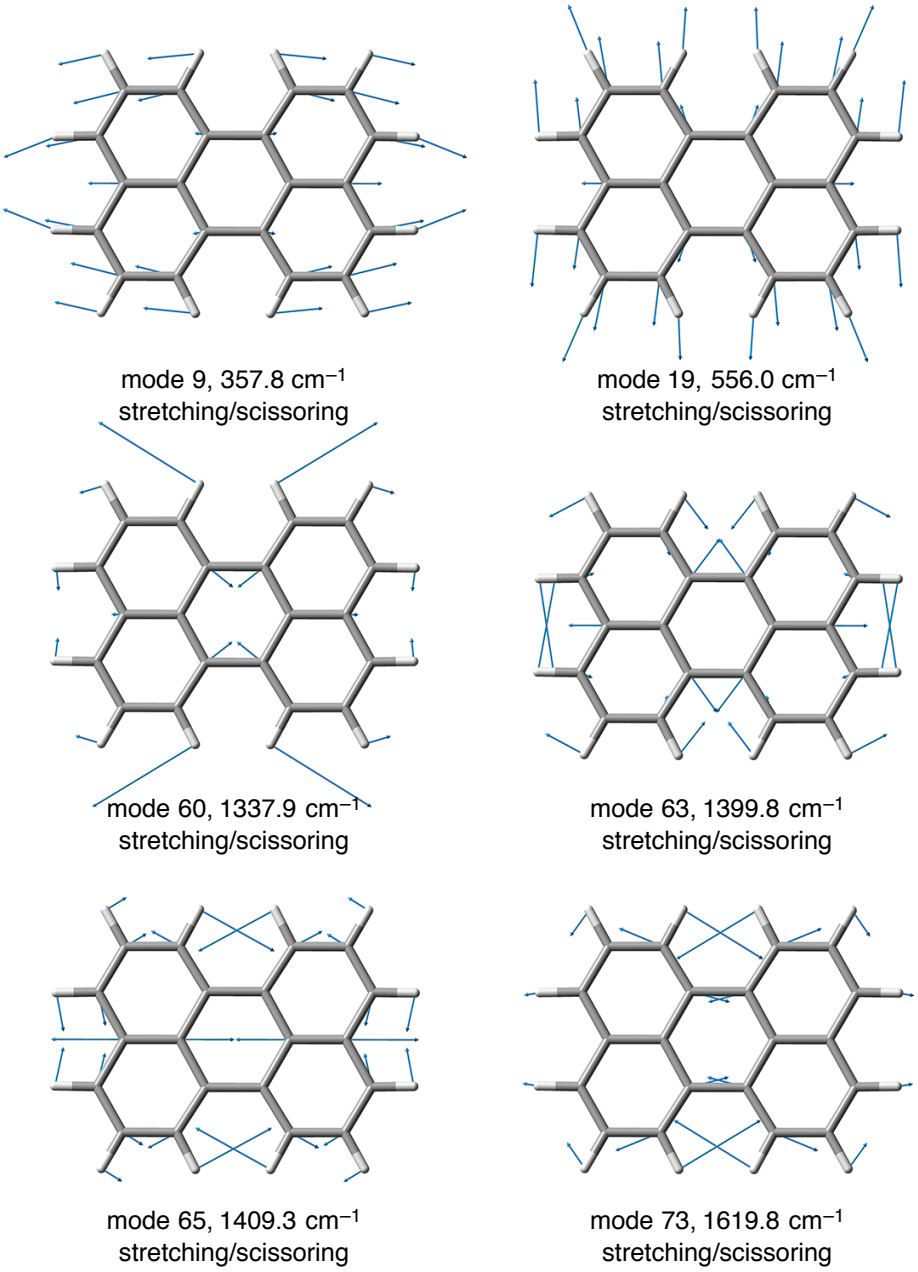
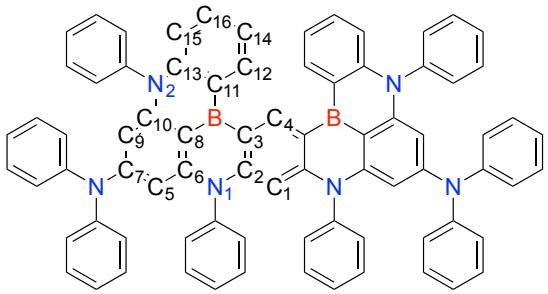
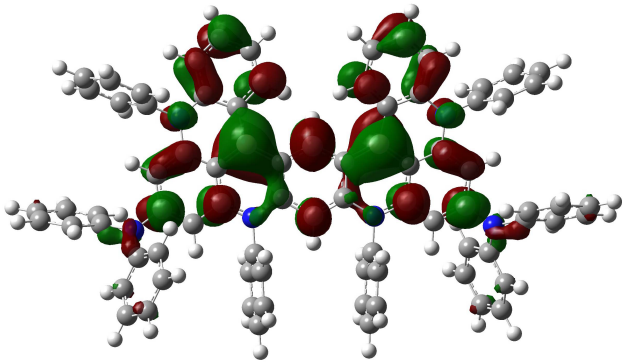
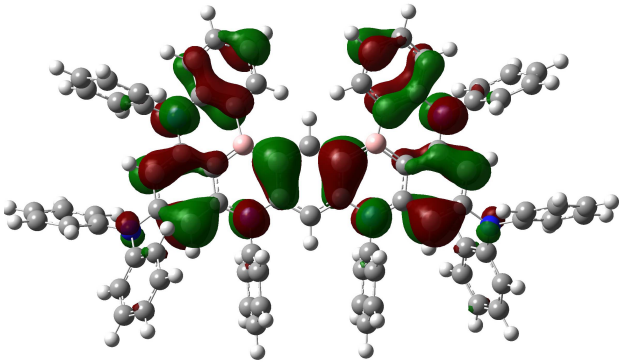


Figure S8. Vibrational modes in the S_0 state involved in the Franck-Condon spectral progression of perylene at the (TD)B3LYP/6-31G(d) level.







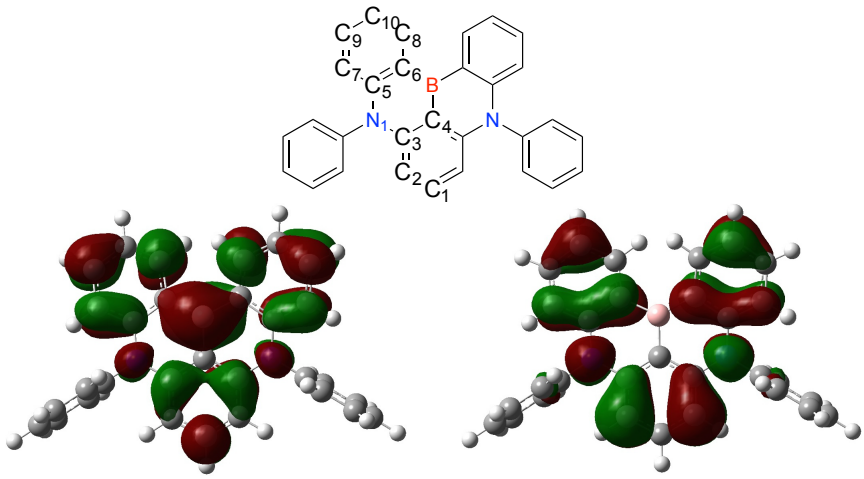
LUMO (–1.17 eV)

	coefficient (LUMO)	
	2PX	3PX
B	**-0.19131**	**-0.20039**
N_1	-0.04520	-0.05970
C_1	**0.11390**	**0.13997**
C_2	-0.04243	-0.05275
C_3	-0.04712	-0.03667
C_4	**0.21689**	**0.21921**
C_5	0.00181	0.01095
C_6	**0.13840**	**0.12867**
C_7	**-0.15357**	**-0.14994**
C_8	-0.04243	-0.05275
C_9	0.06162	**0.08109**
C_{10}	**0.09847**	**0.09529**
N_2	**-0.09240**	**-0.10327**
C_{11}	-0.02114	-0.01884
C_{12}	**0.10271**	**0.09870**
C_{13}	0.06774	0.05720
C_{14}	-0.02728	-0.01925
C_{15}	0.07169	**0.08827**
C_{16}	**-0.10639**	**-0.11814**

HOMO (–4.57 eV)

	coefficient (HOMO)	
	2PX	3PX
B	0.00996	0.01506
N_1	**-0.16100**	**-0.13532**
C_1	0.00000	0.00000
C_2	**0.08784**	0.06167
C_3	**0.17335**	**0.13874**
C_4	0.00000	0.00000
C_5	**0.18009**	**0.15406**
C_6	0.03017	0.02221
C_7	0.03609	0.02249
C_8	-0.04765	-0.04012
C_9	**-0.12300**	**-0.10778**
C_{10}	-0.07362	-0.05264
N_2	**0.18107**	**0.15431**
C_{11}	**-0.08904**	**-0.08260**
C_{12}	0.00746	-0.00195
C_{13}	-0.06239	-0.04372
C_{14}	**0.09175**	**0.07749**
C_{15}	-0.07028	-0.06004
C_{16}	0.03207	0.02425

Figure S9. The highest occupied and lowest-unoccupied Kohn–Sham orbitals of **ν-DABNA** along with coefficients of 2PX/3PX basis functions, major component of π-orbital, in the S_0 states calculated at the B3LYP/6-31G(d) level (isovalue = 0.02). X-Axis is vertical direction to the sheet (π-plane). Orbital energies are shown in parentheses.

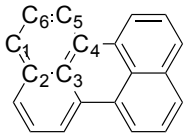


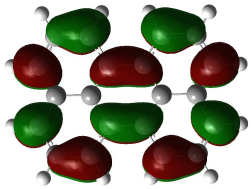
LUMO (–1.08 eV) HOMO (–4.74 eV)

	coefficient (LUMO)	
	2PX	3PX
B	**0.27439**	**0.29108**
N_1	**0.13704**	**0.15426**
C_1	**0.17884**	**0.19608**
C_2	-0.04061	-0.05852
C_3	**-0.15234**	**-0.14262**
C_4	0.00135	0.00707
C_5	-0.09846	-0.08160
C_6	0.05667	0.05642
C_7	**-0.12274**	**-0.15530**
C_8	**-0.17347**	**-0.18131**
C_9	**0.17542**	**0.20061**
C_{10}	0.03625	0.02600

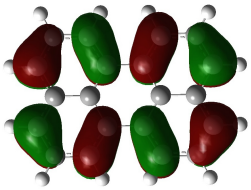
	coefficient (HOMO)	
	2PX	3PX
B	0.00000	0.00000
N_1	**0.25903**	**0.22001**
C_1	0.00000	0.00000
C_2	**-0.24552**	**-0.20966**
C_3	-0.09910	-0.06817
C_4	0.00000	0.00000
C_5	-0.08920	-0.06209
C_6	**-0.13064**	**-0.10958**
C_7	-0.11113	-0.09560
C_8	0.02213	0.01290
C_9	0.04257	0.03096
C_{10}	**0.14106**	**0.11790**

Figure S10. The highest occupied and lowest-unoccupied Kohn–Sham orbitals of **DABNA-1** along with coefficients of 2PX/3PX basis functions, major component of π-orbital, in the S_0 states calculated at the B3LYP/6-31G(d) level (isovalue = 0.02). X-Axis is vertical direction to the sheet (π-plane). Orbital energies are shown in parentheses.





LUMO (–1.89 eV)



HOMO (–4.95 eV)

	coefficient (LUMO)	
	2PX	3PX
C_1	**0.19502**	**0.20348**
C_2	0.00000	0.00000
C_3	0.00000	0.00000
C_4	**0.15516**	**0.15367**
C_5	**-0.17947**	**-0.19244**
C_6	-0.07654	-0.07726

	coefficient (HOMO)	
	2PX	3PX
C_1	**0.19320**	**0.15480**
C_2	0.00000	0.00000
C_3	0.00000	0.00000
C_4	**-0.15188**	**-0.11202**
C_5	**-0.17699**	**-0.14572**
C_6	0.07832	0.06547

Figure S11. The highest occupied and lowest-unoccupied Kohn–Sham orbitals of perylene along with coefficients of 2PX/3PX basis functions, major component of π-orbital, in the S_0 states calculated at the B3LYP/6-31G(d) level (isovalue = 0.02). X-Axis is vertical direction to the sheet (π-plane). Orbital energies are shown in parentheses.

Measurement of absorption and emission characteristics. UV–visible absorption and PL spectra were measured using the UV-2600 (Shimadzu) and FluoroMax-4P (HORIBA) at 77 and 298 K. Furthermore, the absolute PL quantum yields were measured using C11347 and C9920-02G spectrometers (Hamamatsu Photonics), whereas PL decays were measured using a C11367 spectrometer (298 K, Hamamatsu Photonics) and then fitted using a single exponential function to determine the lifetimes of prompt and delayed fluorescence. The thin films of **DOBNA-OAr** 1 wt% doped with **ν-DABNA** were prepared on quartz substrates using a co-deposition technique; the quartz substrates were cleaned in a detergent solution at 60 °C for 5 min and then in distilled water at room temperature (298 K) for 10 min using ultrasonication. After pre-drying using a jet spin washer, the substrates were finally dried for 5 min in an oven at 423 K. The evaporation rates of **DOBNA-OAr** and **ν-DABNA** were 0.4 nm s^{-1} and 0.04 nm s^{-1}, respectively. The thickness of the deposited film was 60 nm.

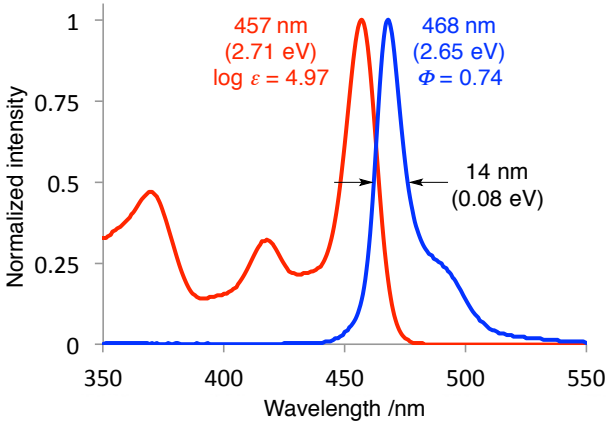


Figure S12. Normalized absorption (red) and fluorescence (blue) spectra of **ν-DABNA** in toluene (0.02 mM solution, excited at 340 nm) at 298 K with absorption/emission maxima (nm, eV), absorption coefficient at an absorption maximum (ε), absolute fluorescence quantum yield (Φ), and full width at half maximum (nm, eV).

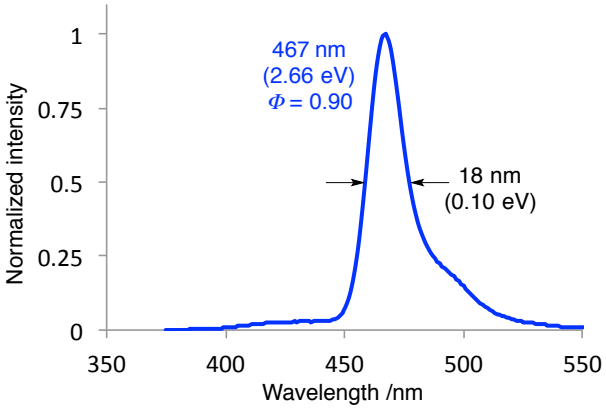


Figure S13. Normalized PL spectra of **ν-DABNA** in **DOBNA-OAr** (1 wt% doped film, excited at 365 nm) at 298 K with emission maxima (nm, eV), absolute fluorescence quantum yield (Φ), and full width at half maximum (nm, eV).

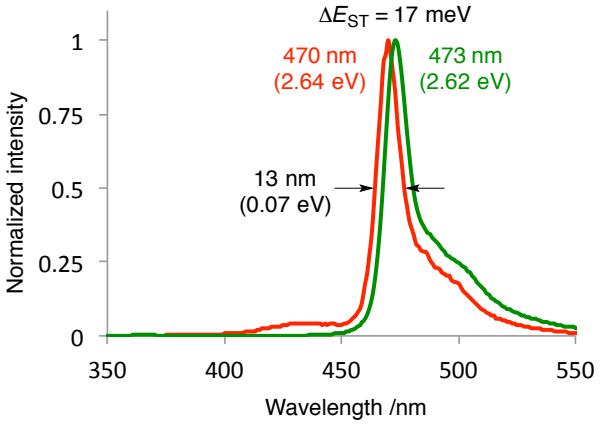


Figure S14. Normalized PL spectra with/without delay time of 100–200 μs (green/red) of **ν-DABNA** in **DOBNA-OAr** (1 wt% doped film) at 77 K (excited at 365 nm) with emission maxima (nm, eV) and full width at half maximum (nm, eV).

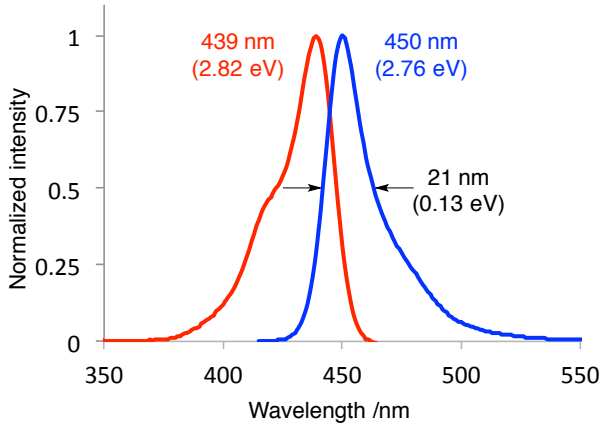


Figure S15. Normalized absorption (red) and fluorescence (blue) spectra of **DABNA-1** in toluene (0.02 mM solution, excited at 405 nm) at 298 K with absorption/emission maxima (nm, eV) and full width at half maximum (nm, eV)

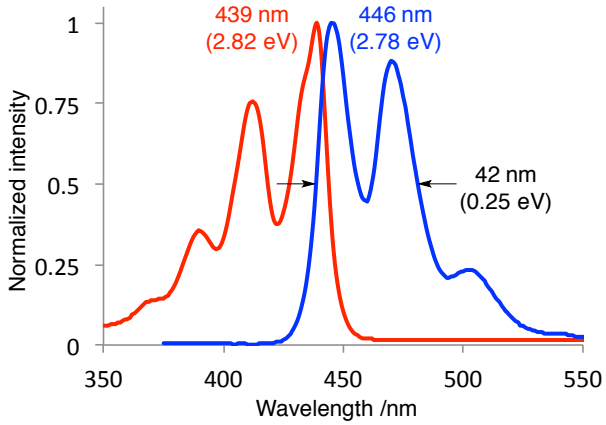


Figure S16. Normalized absorption (red) and fluorescence (blue) spectra of perylene in toluene (0.02 mM solution, excited at 365 nm) at 298 K with absorption/emission maxima (nm, eV) and full width at half maximum (nm, eV).

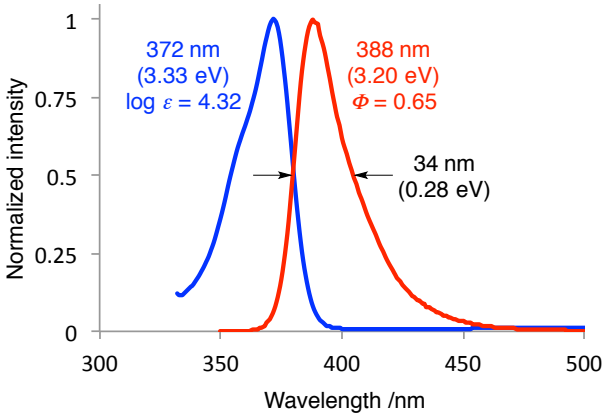


Figure S17. Normalized absorption (red) and fluorescence (blue) spectra of **DOBNA-OAr** in toluene (0.02 mM solution, excited at 340 nm) at 298 K with absorption/emission maxima (nm, eV) and full width at half maximum (nm, eV)

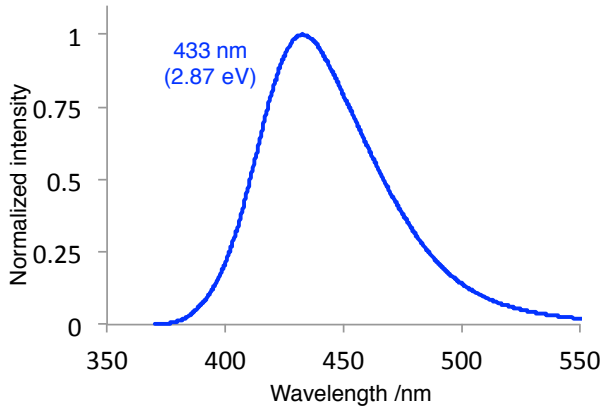


Figure S18. Normalized PL spectra of **DOBNA-OAr** (vacuum deposited film, excited at 360 nm) at 298 K with emission maxima (nm, eV).

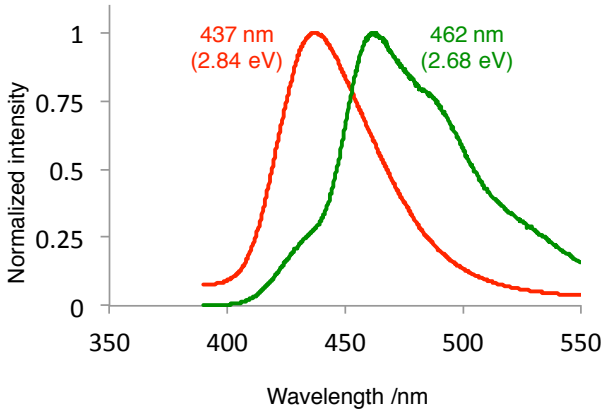


Figure S19. Normalized PL spectra with/without delay time of 100 μs (green/red) of **DOBNA-OAr** (vacuum deposited film, excited at 360 nm) at 77 K (excited at 360 nm) with emission maxima (nm, eV).

Estimation of the rate constants. Rate constants for **ν-DABNA** in **DOBNA-OAr** (1 wt% doped film) at 298 K shown in **Figure 3b** were determined from the measurements of quantum yields and lifetimes of the fluorescence and TADF components according to equations 1–14[7].

$\Phi = 0.902$

$\Phi_F = 0.817$

$\Phi_{TADF} = 0.085$

$\tau_F = 4.07$ ns

$\tau_{TADF} = 4.05$ μs

$k_F = 2.00 \times 10^7$ s^{-1}	$k_F = \Phi_F/\tau_F$	(1)
$k_{IC} = 2.17 \times 10^7$ s^{-1}	$\Phi = k_F/(k_F + k_{IC})$	(2)
$k_{ISC} = 2.32 \times 10^7$ s^{-1}	$\Phi_F = k_F/(k_F + k_{IC} + k_{ISC})$	(3)
$\Phi_{IC} = 0.089$	$\Phi_{IC} = k_{IC}/(k_F + k_{IC} + k_{ISC})$	(4)
$\Phi_{ISC} = 0.094$	$\Phi_{ISC} = 1 - \Phi_F - \Phi_{IC} = k_{ISC}/(k_F + k_{IC} + k_{ISC})$	(5)
$k_{TADF} = 2.23 \times 10^5$ s^{-1}	$k_{TADF} = \Phi_{TADF}/\Phi_{ISC}\tau_{TADF}$	(6)
$k_{RISC} = 2.01 \times 10^5$ s^{-1}	$k_{RISC} = k_F k_{TADF}\Phi_{TADF}/k_{ISC}\Phi_F$	(7)

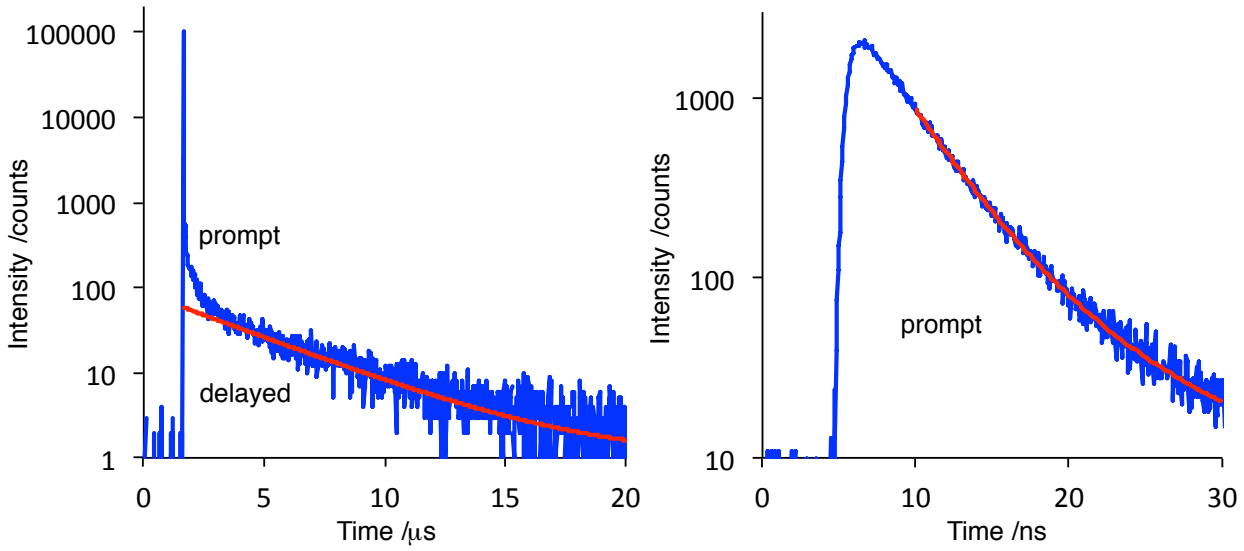


Figure S20. Transient decay spectra of **ν-DABNA** in **DOBNA-OAr** (1 wt% doped film) at 298 K (excited at 365 nm). The red curves represent the single and double exponential fitting data.

(7) Masui, K., Nakanotani, H. & Adachi, C. *Org. Electron.* **14**, 2721–2726 (2013).

Estimation of the activation energy. The activation energy (ΔE_a^{TADF}) for the reverse intersystem crossing (RISC) was calculated from Arrhenius plots of k_{RISC} vs. 1/T according to the literature.[8]

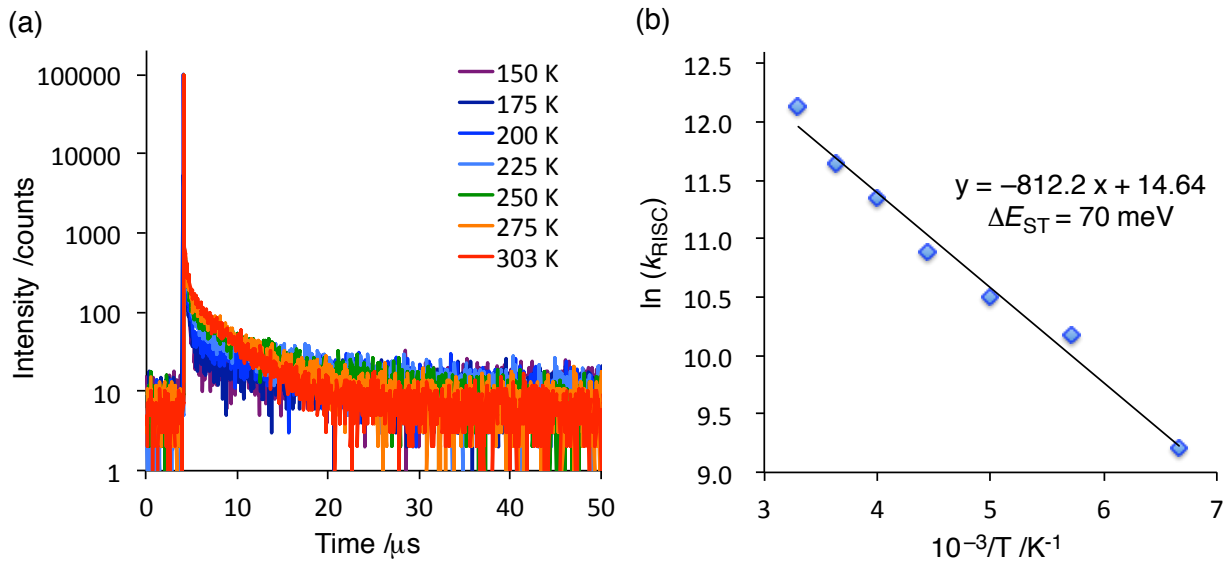


Figure S21. (a) Transient decay spectra of ν-**DABNA** in **DOBNA-OAr** (1 wt% doped film) at different temperatures (from 150 to 303 K, excited at 365 nm). (b) Arrhenius plot of the RISC rate constant (k_{RISC}).

(8) Uoyama, H., Goushi, K., Shizu, K., Nomura, H. & Adachi, C. *Nature* **492**, 234–238 (2012).

Measurement of ionization potential and optical band gap. Ionization potentials (I_p) of the thin films were measured using photoelectron yield spectroscopy with a PYS-201 system (Sumitomo Heavy Industries) at room temperature (298 K). The UV–visible absorption spectra of the thin films were measured using a UV-2600 spectrophotometer (Shimadzu). Furthermore, the optical band gaps (E_g) were estimated based on the absorption edge wavelength. The electron affinities (E_a) were calculated using the I_p and E_g values. Thin films of **ν-DABNA** and **DOBNA-OAr** were vacuum-deposited on the cleaned glass substrates at a rate of 0.2 nm s^{-1}. The ITO-coated glass substrates were cleaned in a detergent solution for 5 min and then in distilled water for 10 min using ultrasonication. After pre-drying the substrates using a jet spin washer, they were finally dried for 5 min in an oven at 423 K. The thickness of the deposited films was 60–80 nm. The pressure of the vacuum system was 5.0×10^{-3} Pa, and the film thickness was controlled using a calibrated quartz crystal microbalance during the deposition. The spectra are described in the Supporting Information.

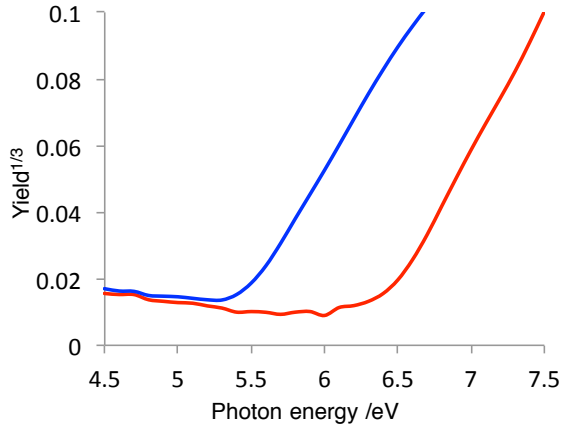


Figure S22. Photoelectron yield spectra of the vacuum-deposited thin films of **ν-DABNA** (blue) and **DOBNA-OAr** (red) after light illumination from a D_2 lamp *in vacuo*.

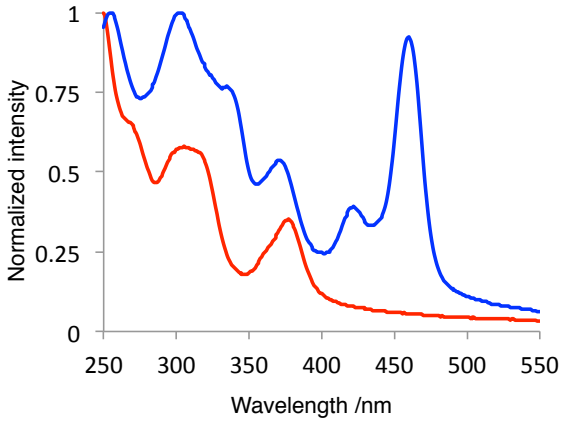


Figure S23. Normalized absorption spectra of the vacuum-deposited thin films of **ν-DABNA** (blue) and **DOBNA-OAr** (red).

Device fabrication and measurement of EL characteristics. OLEDs were fabricated on glass substrates coated with a patterned transparent ITO conductive layer. The substrates were cleaned in a detergent solution at 60 °C for 5 min and then in distilled water at room temperature (298 K) for 10 min in an ultrasonic bath. Subsequently, they were pre-dried using a jet spin washer, and then dried for 5 min in an oven at 423 K, before being finally treated with UV/ozone plasma. The pressure during the vacuum evaporation was 5.0×10^{-4} Pa, and the film thickness was controlled using a calibrated quartz crystal microbalance during deposition. After the deposition of all layers, the OLED test modules were encapsulated with a capping glass in an evaporation chamber filled with nitrogen. The OLED characteristics of all fabricated devices were evaluated at room temperature (298 K) in an air atmosphere using a voltage–current–luminance measuring system, comprising a source meter (Keithley 2400) and spectral radiance meter (Topcon SR-3AR). The EQE was calculated using the EL spectrum, assuming the light-emitting surface to be a perfect diffusion surface: adding up all radiance elements from every angle and inputting them into the formula for obtaining EQE. OLEDs were fabricated three times to check reproducibility. The second-best dataset was shown in **Figure 4** in the manuscript. The other two datasets were shown in Figure S25.

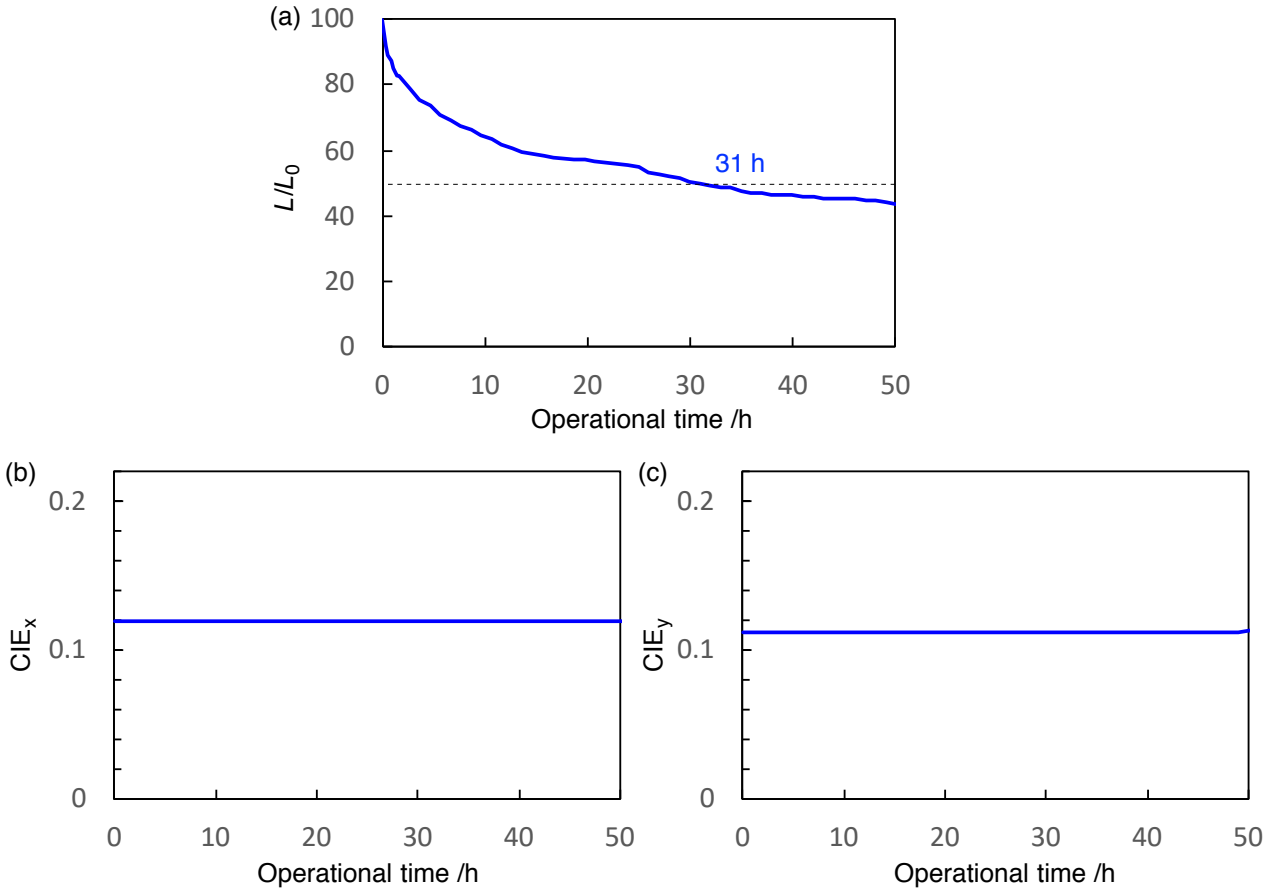


Figure S24. The emission luminance (a) and colour (b, c) changes with operational time of the OLED reported in **Figure 4** (L_0: initial luminance = 100 cd m^{-2}).

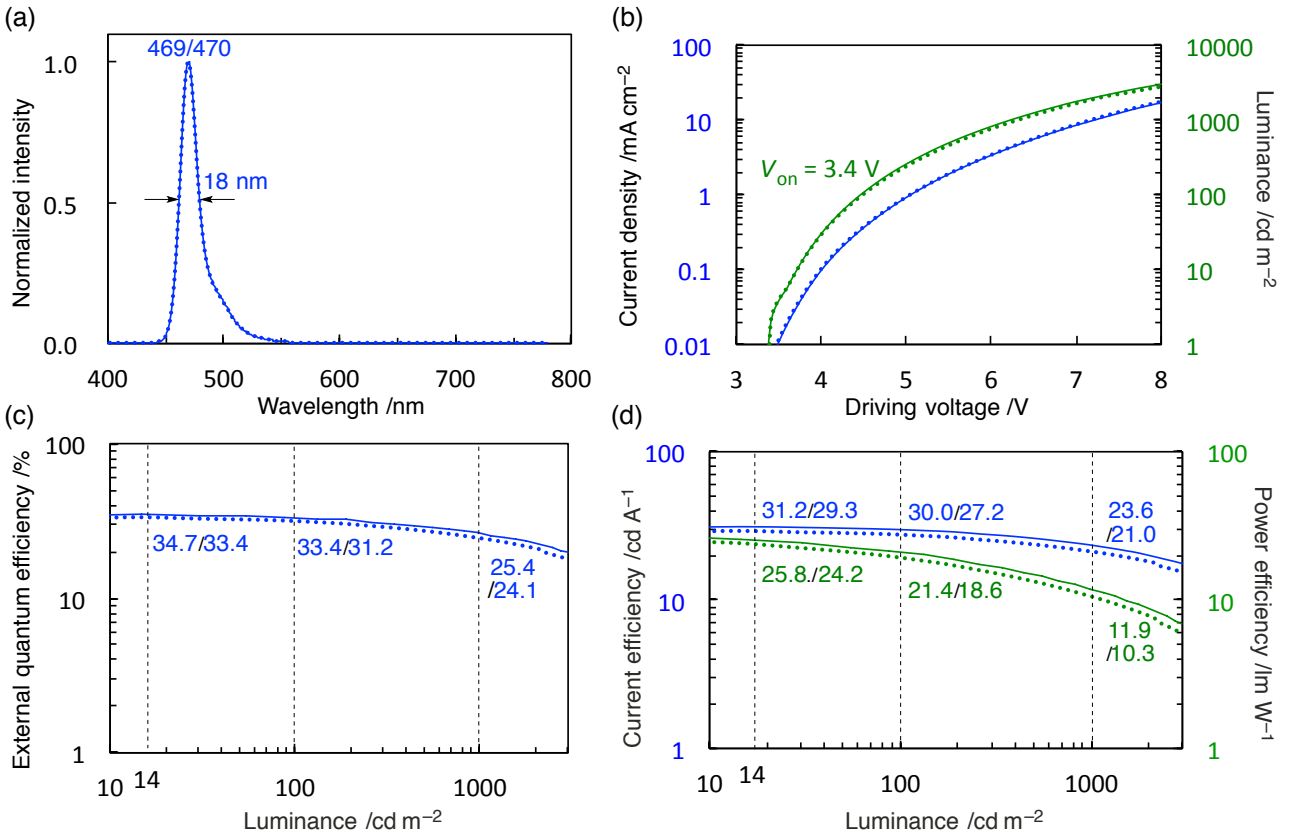


Figure S25. OLED Performance. (a) Normalized EL spectra. (b) Current density and luminance versus driving voltage characteristics. (c) External quantum efficiency versus luminance characteristics. (d) Current and power efficiency versus luminance characteristics.

Thermogravimetric-differential thermal analysis (TG-DTA). TG-DTA profiles of **ν-DABNA** were measured from room temperature to 500 °C with heating rate of 10 °C/min on a Thermo plus EVO II (Rigaku).

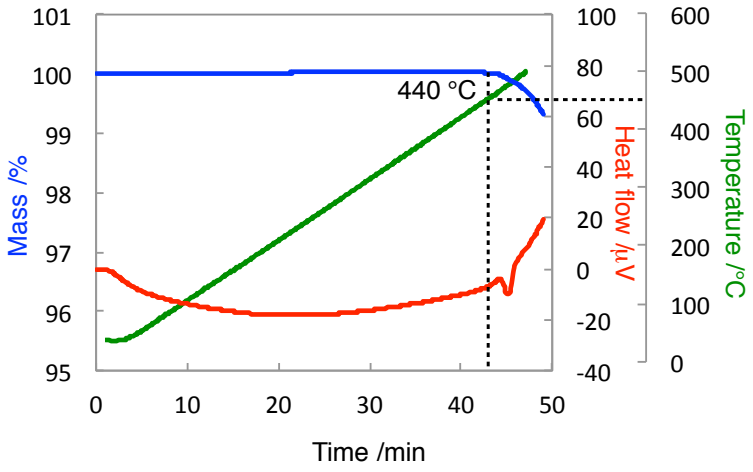
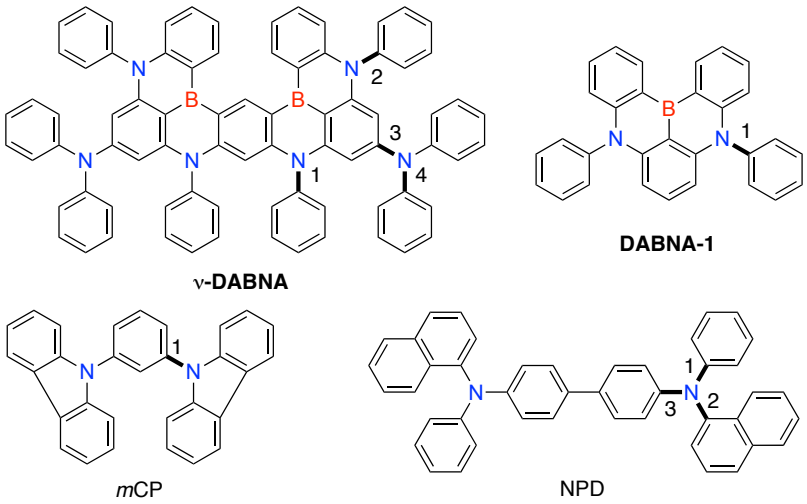


Figure S26. Thermogravimetric-differential thermal analysis profiles (blue/red) of **ν-DABNA**.

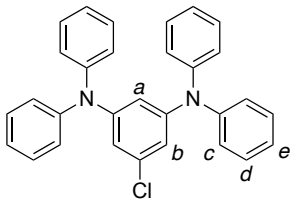


molecule	enthalpy[a] *H* (hartree)	bond number	enthalpy[a] of fragments *H* (hartree)		BDE[b], *ΔH* (hartree)	BDE[b], *ΔH* (kcal mol^{-1})
ν-DABNA	–3381.98898	1	–3150.40712	–231.46834	0.11352	76.3
		2	–3150.40768	–231.46834	0.11296	76.0
		3	–2864.05559	–517.81828	0.11512	77.4
		4	–3150.40359	–231.46834	0.11705	78.7
DABNA-1	–1289.80445	1	–1058.22343	–231.46834	0.11268	75.8
*m*CP	–1264.35396	1	–747.57458	–516.65061	0.12877	86.6
NPD	–1804.81819	1	–1573.2412	–231.46834	0.10865	73.1
		2	–1419.6440	–385.06249	0.11172	75.1
		3	–1133.2914	–671.41610	0.11072	74.5

[a] Sum of electronic and thermal enthalpies. [b] Bond dissociation enthalpy.

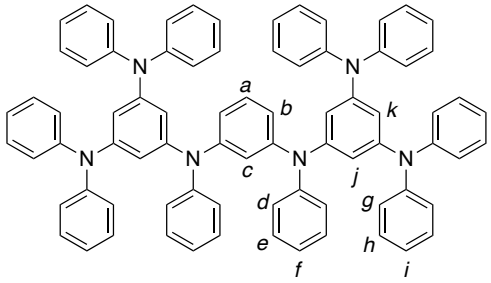
Figure S27. Bond dissociation enthalpies (*ΔH*) of **ν-DABNA**, **DABNA-1**, *m*CP, and NPD at the B3LYP/6-31G(d) level.

Synthesis of 5-chloro-N^1,N^1,N^3,N^3-tetraphenylbenzene-1,3-diamine



Diphenylamine (10.1 g, 60 mmol), sodium *tert*-butoxide (8.60 g, 90 mmol), SPhos (0.493 g, 1.2 mmol), tris(dibenzylideneacetone)palladium(0) (0.549 g, 0.60 mmol) and 1,3-dibromo-5-chlorobenzene (8.11 g, 30 mmol) were dissolved in toluene (300 mL) under a nitrogen atmosphere. After stirring at 80 ºC for 15 h, the reaction mixture was filtered with a pad of Florisil® (eluent: toluene). After the solvent was removed *in vacuo*, the crude product was washed with hexane by using a sonicator to obtain the title compound (5.66 g, 43% yield, >99% pure on NMR analysis) as a white solid. IR (neat): cm^{-1} 3064, 3032, 1576, 1568, 1489, 1437, 1310, 1288, 1244, 1174, 1098, 895, 750, 689, 652, 613; mp: 129.3–130.1 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.57 (d, J = 2.0 Hz, 2H, *b*), 6.66 (t, J = 2.0 Hz, 1H, *a*), 7.01 (t, J = 7.2 Hz, 4H, *e*), 7.06 (d, J = 7.6 Hz, 8H, *c*), 7.22 (dd, J = 7.2, 7.6 Hz, 8H, *d*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 115.7 (1C), 116.5 (2C), 123.4 (4C), 124.6 (8C), 129.2 (8C), 135.1 (1C), 146.9 (4C), 149.3 (2C); HRMS (DART) *m*/*z* $[M+H]^+$ calcd for $C_{30}H_{23}ClN_2$ 447.1628; observed 447.1611.

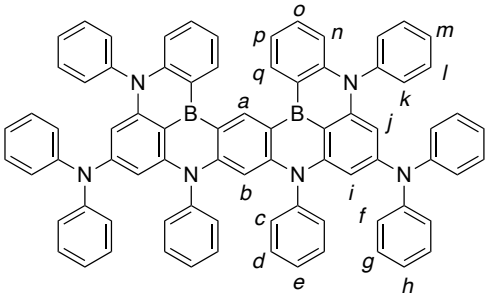
Synthesis of N^1,$N^{1'}$-(1,3-phenylene)bis(N^1,N^3,N^3,N^5,N^5-pentaphenylbenzene-1,3,5-triamine)



5-Chloro-N^1,N^1,N^3,N^3-tetraphenylbenzene-1,3-diamine (4.80 g, 11 mmol), sodium *tert*-butoxide (1.47 g, 15 mmol), tri-*tert*-butylphosphine (60.7 mg, 0.30 mmol), tris(dibenzylideneacetone) palladium(0) (0.140 g, 0.15 mmol) and N^1,N^3-diphenylbenzene-1,3-diamine (1.34 g, 5.1 mmol) were dissolved in toluene (200 mL) under a nitrogen atmosphere. After stirring at 110 ºC for 8 h, the reaction mixture was filtered with a pad of Florisil® (eluent: toluene). After the solvent was removed *in vacuo*, the crude product was washed with methanol and hexane by using a sonicator to obtain the title compound (4.80 g, 87% yield, >99% pure on NMR analysis) as a white solid. IR (neat): cm^{-1} 3065, 3032, 1489, 1456, 1290, 1169, 1040, 893, 843, 770, 750, 692, 644; mp: 257.8–258.5 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.38 (d, J = 2.0 Hz, 4H, *j*), 6.42 (t, J = 2.0 Hz, 2H, *k*), 6.58 (dd, J = 2.0, 8.0 Hz, 2H, *b*), 6.70 (t, J = 2.0 Hz, 1H, *c*), 6.83–6.90 (m, 14H, *d*, *f*, *i*), 6.94–7.01 (m, 17H, *a*, *g*), 7.08–7.15 (m, 20H, *e*, *h*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 114.4 (2C), 114.7 (4C), 118.3 (2C), 119.3 (1C),

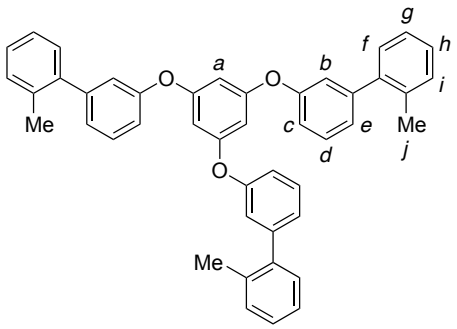
122.2 (2C), 122.6 (8C), 123.3 (4C), 123.9 (16C), 128.8 (4C), 129.0 (16C), 129.3 (1C), 147.1 (2C), 147.2 (8C), 147.9 (2C), 148.6 (2C), 148.9 (4C); HRMS (DART) *m*/*z* $[M+H]^+$ calcd for $C_{78}H_{60}N_6$ 1081.4958; observed 1081.4959.

Synthesis of *N*⁷,*N*⁷,*N*¹³,*N*¹³,5,9,11,15-octaphenyl-5,9,11,15-tetrahydro-5,9,11,15-tetraaza-19b, 20b-diboradinaphtho[3,2,1-*de*:1',2',3'-*jk*]pentacene-7,13-diamine (ν-DABNA)



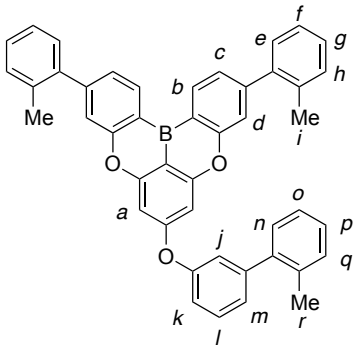
Boron tribromide (1.13 mL, 12 mmol) was added to a solution of *N*¹,*N*¹'-(1,3-phenylene)bis (*N*¹,*N*³,*N*³,*N*⁵,*N*⁵-pentaphenylbenzene-1,3,5-triamine) (3.24 g, 3.0 mmol) in *o*-dichlorobenzene (40 mL) at room temperature under a nitrogen atmosphere. After stirring at 180 ºC for 20 h, the reaction mixture was allowed to cool to room temperature. After addition of *N*,*N*-diisopropylethylamine (7.70 mL, 45 mmol) at 0 ºC, the solvent was removed *in vacuo*. The crude product was washed with hexane, acetonitrile, and toluene by using a sonicator to obtain the title compound (2.40 g, 73% yield, 85% pure on HPLC analysis) as a yellow solid. The residue was dissolved in toluene and then filtered with a pad of Florisil® (eluent: toluene). After the solvent was removed *in vacuo*, the crude product was purified by recrystallization from *o*-dichlorobenzene. The crude product was purified by sublimation (440 ºC, 1.0×10^{-4} Pa) to obtain the title compound (1.17 g, 36% yield, >99% pure on NMR analysis) as a yellow solid. IR (neat): cm^{-1} 3061, 3034, 2918, 2361, 2313, 1562, 1489, 1323, 1261, 1159, 1024, 1003, 820, 750, 694, 648; mp: >300 ºC; ^{1}H NMR (500 MHz, $(CDCl_2)_2$) δ 5.72 (s, 2H, *i*), 5.74 (s, 2H, *j*), 5.86 (s, 1H, *b*), 6.83 (d, *J* = 8.5 Hz, 2H, *n*), 6.88–6.93 (m, 12H, *f*, *h*), 7.05 (d, *J* = 7.5 Hz, 4H, *c*), 7.12 (dd, *J* = 7.0, 9.0 Hz, 8H, *g*) 7.12–7.19 (m, 6H, *d*, *e*) 7.32 (d, *J* = 8.0 Hz, 4H, *k*), 7.38 (dd, *J* = 6.8, 8.0 Hz, 2H, *p*), 7.41–7.45 (m, 4H, *m, o*), 7.47 (dd, *J* = 7.5, 8.0 Hz 4H, *l*), 9.30 (d, *J* = 8.0 Hz, 2H, *q*), 10.5 (s, 1H, *a*); ^{13}C NMR (126 MHz, $(CDCl_2)_2$) δ 99.5 (2C), 103.4 (1C), 116.8 (2C), 120.0 (2C), 123.1 (4C), 125.3 (8C), 127.1 (2C), 127.4 (2C), 127.6 (2C), 128.5 (8C), 129.6 (4C), 129.8 (4C), 130.2 (4C + 2C), 130.3 (4C), 135.0 (2C), 142.1 (2C), 142.5 (2C), 143.3 (1C), 146.8 (4C), 147.9 (2C + 2C), 148.0 (2C), 150.1 (2C), 151.1 (2C). The NMR signal of the carbon α to the boron was not observed.; ^{11}B NMR (160 MHz, $(CDCl_2)_2$) δ 36.7; HRMS (LDI) *m*/*z* $[M]^+$ calcd for $C_{78}H_{54}B_2N_6$ 1096.4613; observed 1096.4616.

Synthesis of 1,3,5-tris((2'-methyl-[1,1'-biphenyl]-3-yl)oxy)benzene



A solution of 2'-methyl-[1,1'-biphenyl]-3-ol in *N*-methylpyrrolidone (NMP, 16.5 mL, 1.00 M, 17 mmol) was added to mixture of 1,3,5-trifluorobenzene (0.540 mL, 5.2 mmol) and cesium carbonate (5.38 g, 17 mmol), at room temperature under a nitrogen atmosphere. After stirring at 90 ºC for 18 h and 160 ºC for 26 h, the reaction mixture was filtered with a pad of Florisil® (eluent: ethyl acetate), and then concentrated *in vacuo*. The crude product was purified by silica gel column chromatography (eluent: hexane/toluene = 10/1) to obtain the title compound (2.88 g, 88% yield, 97% pure on NMR analysis) as a colorless oil. IR (neat): cm^{-1} 3059, 2953, 1597, 1578, 1566, 1497, 1474, 1456, 1418, 1379, 1296, 1271, 1260, 1200, 1184, 1159, 1034, 1009, 995, 943, 895, 872, 837, 789, 754, 725, 700, 623; ^{1}H NMR （400 MHz, $CDCl_3$） δ 2.21 (s, 9H, *j*), 6.43 (s, 3H, *a*), 6.99–7.02 (m, 6H, *b*, *e*), 7.06 (d, *J* = 7.9 Hz, 3H, *c*), 7.16–7.25 (m, 12H, *f*, *g*, *h*, *i*), 7.33 (dd, *J* = 7.9, 8.2 Hz, 3H, *d*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.4 (3C), 103.3 (3C), 117.8 (3C), 120.3 (3C), 124.8 (3C), 125.8 (3C), 127.5 (3C), 129.5 (3C), 129.6 (3C), 130.3 (3C), 135.2 (3C), 141.0 (3C), 143.8 (3C), 155.9 (3C), 160.0 (3C); HRMS (DART) *m/z* $[M]^+$ calcd for $C_{45}H_{36}O_3$ 625.2743, observed 625.2751.

Synthesis of 7-((2'-methyl-[1,1'-biphenyl]-3-yl)oxy)-3,11-di-*o*-tolyl-5,9-dioxa-13b-boranaphtho [3,2,1-*de*]anthracene (DOBNA-OAr)



Boron triiodide (3.89 g, 9.9 mmol) was added to a solution of 1,3,5-tris((2'-methyl-[1,1'-biphenyl] -3-yl)oxy)benzene (1.55 g, 2.48 mmol) in *o*-dichlorobenzene (30 mL) at room temperature under a nitrogen atmosphere. After stirring at 180 ºC for 3 h, the reaction mixture was allowed to cool to room temperature and hydrogen iodide was removed *in vacuo*. After phosphorus buffer solution (pH 7, 100 mL) was added to the reaction mixture, the aqueous layer was separated and extracted with

dichloromethane (300 mL, three times). The combined organic layers were concentrated *in vacuo*. Acetic acid (3.0 mL, 52.4 mmol) was added to crude product in toluene (100 mL) at room temperature under atmosphere. After stirring at 90 ºC for 26 h, saturated sodium carbonate (100 mL) was added to the reaction mixture, and then the aqueous layer was extracted with toluene (500 mL, three times). The solvent of the combined organic layer was removed *in vacuo*. The crude product was purified by silica gel column chromatography (eluent: hexane/toluene = 5/1) to obtain the title compound (1.42 g, 91% yield, 98% pure on NMR analysis) as a white solid. IR (neat): cm^{-1} 3057, 3016, 2951, 2922, 1630, 1612, 1599, 1580, 1543, 1499, 1476, 1431, 1406, 1385, 1344, 1308, 1298, 1287, 1271, 1260, 1242, 1188, 1157, 1123, 1099, 1070, 1026, 1007, 1001, 935, 908, 881, 868, 816, 800, 789, 758, 729, 702, 677, 665; mp: 186.0–189.2 ºC; ^{1}H NMR（500 MHz, $CDCl_3$）δ 2.33 (s, 3H, *r*), 2.38 (s, 6H, *i*), 6.88 (s, 2H, *a*), 7.16–7.18 (m, 2H, *j*, *k*), 7.20 (td, *J* = 1.2, 7.5 Hz, 1H, *m*), 7.23–7.36 (m, 12H, *b*, *e*, *f*, *h*, *n*, *o*, *q*), 7.37 (dd, *J* = 1.7, 8.0 Hz, 2H, *c*), 7.46–7.49 (m, 3H, *d*, *l*), 8.72 (d, *J* = 8.0 Hz, 2H, *b*); ^{13}C NMR (126 MHz, $CDCl_3$) δ 20.5 (3C), 98.5 (2C), 118.7 (2C), 118.8 (1C), 121.3 (1C) 124.3 (2C), 125.6 (1C), 125.8 (1C), 125.9 (2C), 127.6 (1C), 127.8 (2C), 129.7 (2C + 2C), 130.4 (1C), 130.5 (2C), 134.1 (2C), 135.3 (1C), 135.3 (2C), 140.9 (3C), 144.1 (1C), 147.3 (2C), 155.3 (1C), 158.8 (2C), 160.4 (2C), 163.9 (1C). The NMR signal of the carbon α to the boron was not observed.; ^{11}B NMR (128 MHz, $CDCl_3$) δ 38.7; HRMS (DART) *m/z* $[M]^+$ calcd for $C_{45}H_{33}BO_3$ 633.2609, observed 633.2640.

^{1}H, ^{13}C and ^{11}B NMR spectra for isolated compounds

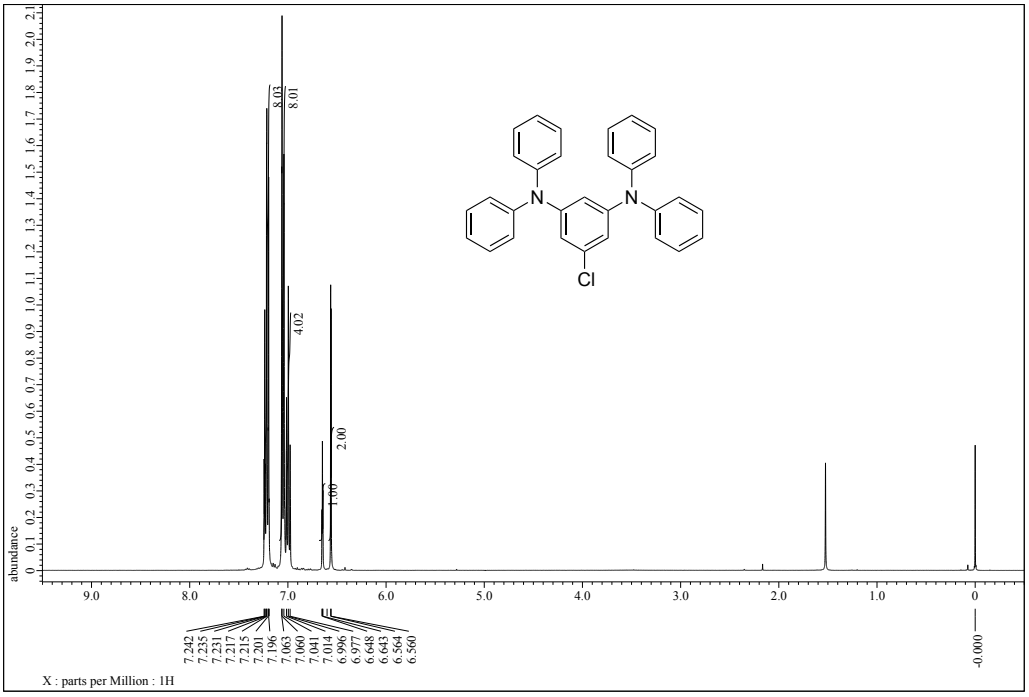


Figure S28. ^{1}H NMR spectrum of 5-chloro-N^1,N^1,N^3,N^3-tetraphenylbenzene-1,3-diamine in $CDCl_3$ at 25 ºC.

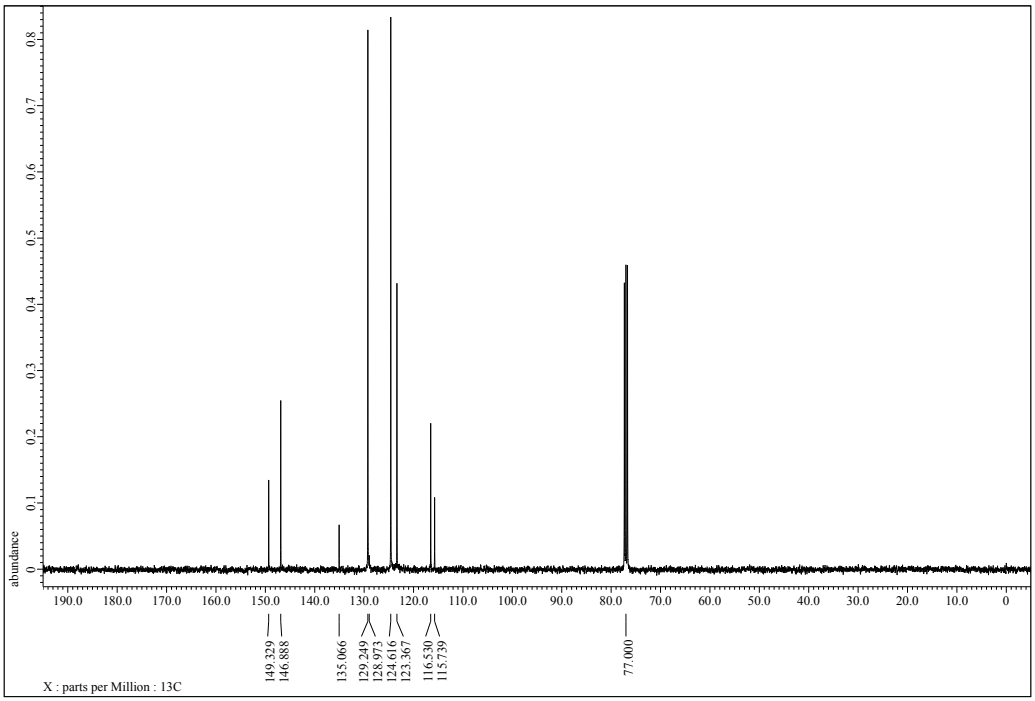


Figure S29. ^{13}C NMR spectrum of 5-chloro-N^1,N^1,N^3,N^3-tetraphenylbenzene-1,3-diamine in $CDCl_3$ at 25 ºC.

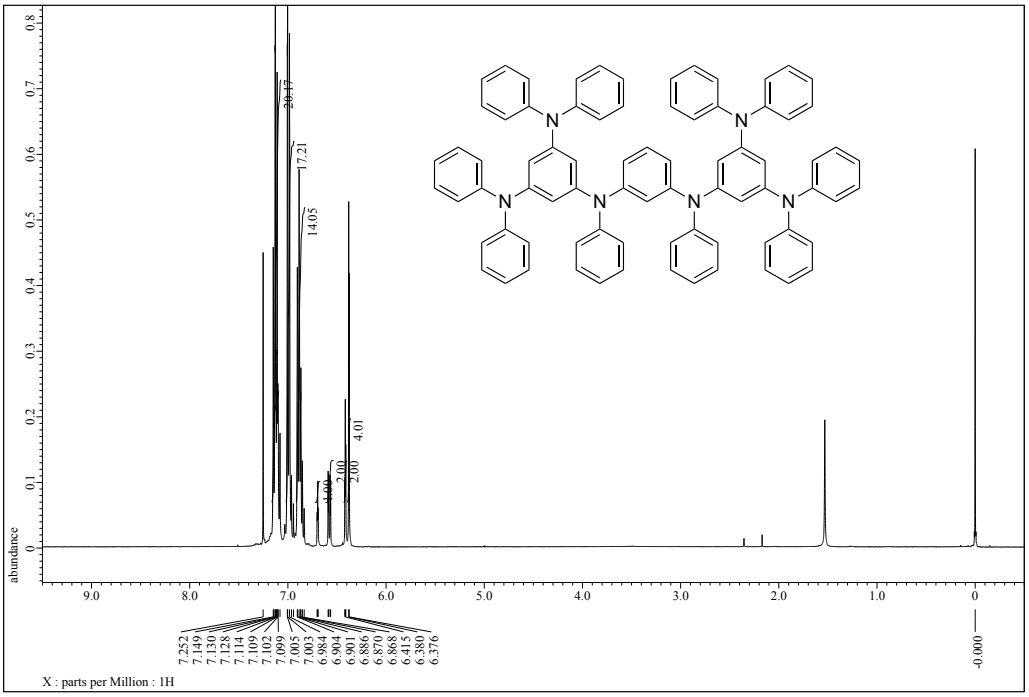


Figure S30. ^{1}H NMR spectrum of N^{1},$N^{1'}$-(1,3-phenylene)-bis(N^{1},N^{3},N^{3},N^{5},N^{5}-pentaphenylbenzene -1,3,5-triamine) in $CDCl_3$ at 25 ºC.

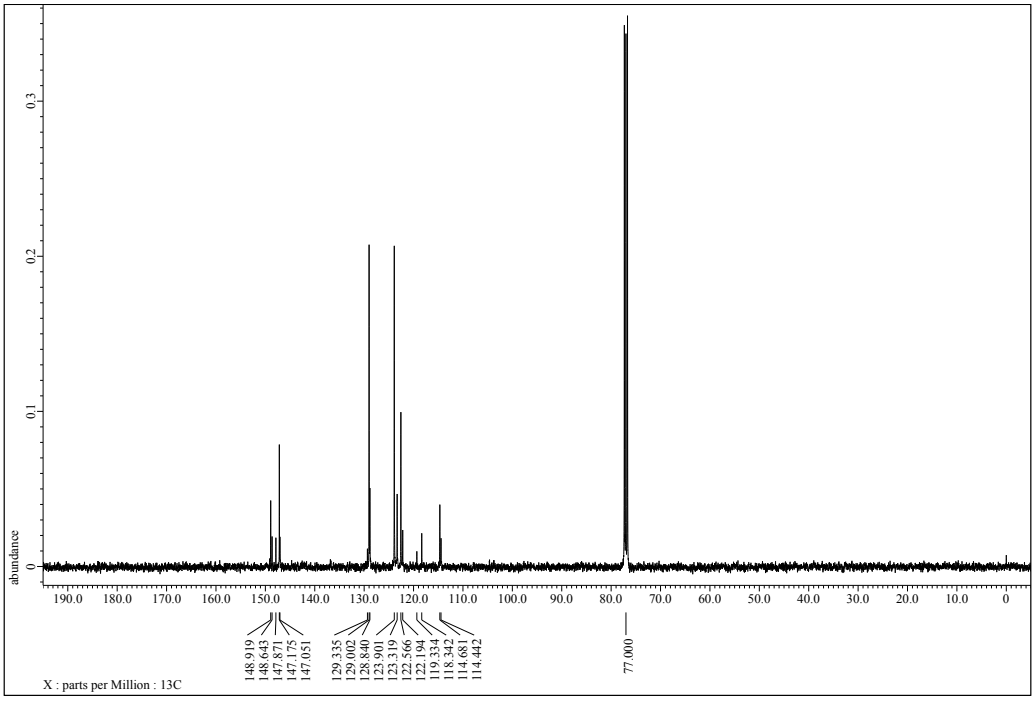


Figure S31. ^{13}C NMR spectrum of N^{1},$N^{1'}$-(1,3-phenylene)-bis(N^{1},N^{3},N^{3},N^{5},N^{5}-pentaphenylbenzene -1,3,5-triamine) in $CDCl_3$ at 25 ºC.

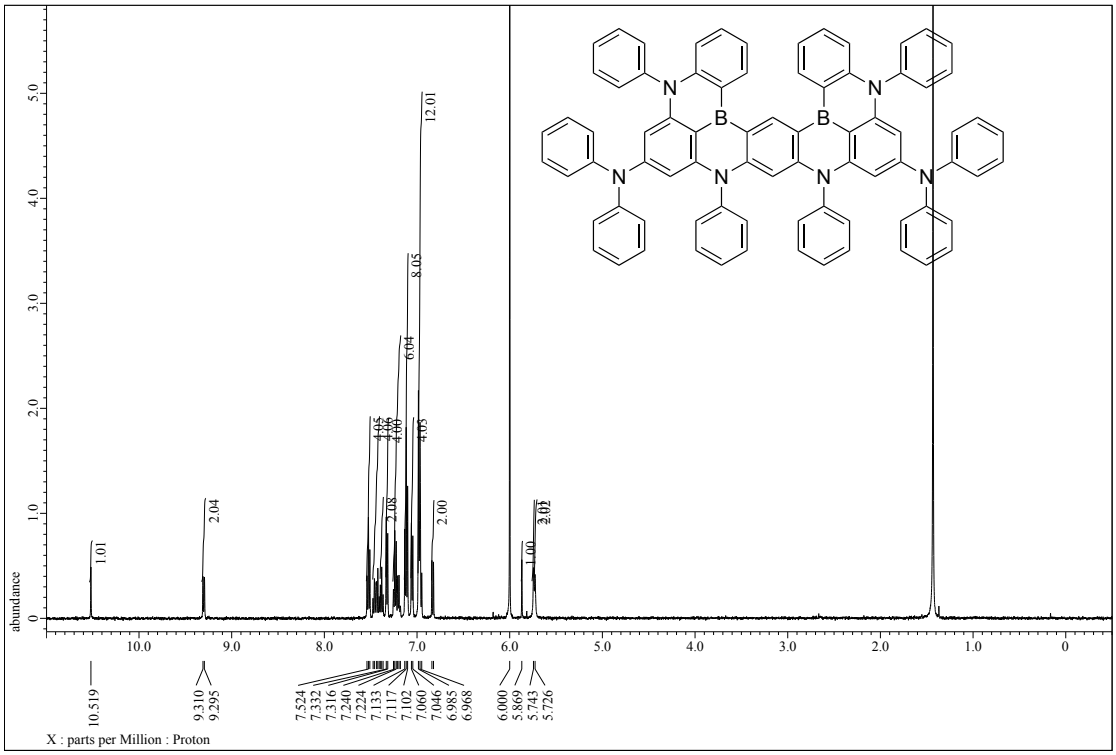


Figure S32. ^{1}H NMR spectrum of **ν-DABNA** in $(CDCl_2)_2$ at 130 ºC.

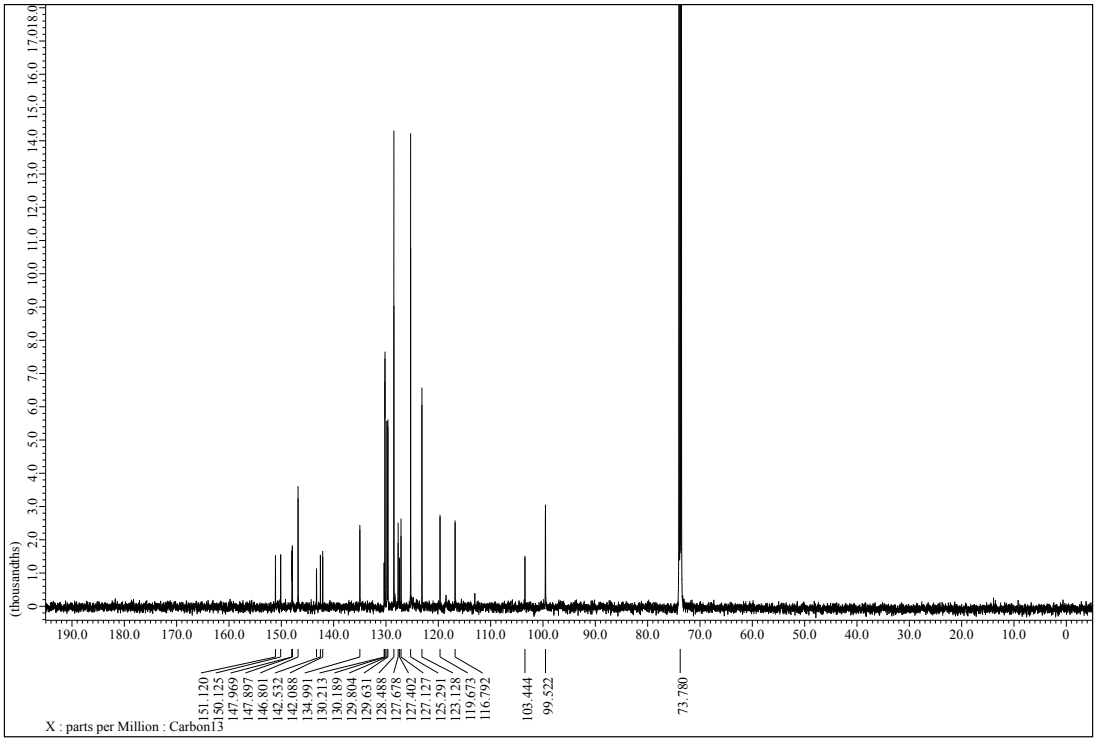


Figure S33. ^{13}C NMR spectrum of **ν-DABNA** in $(CDCl_2)_2$ at 130 ºC.

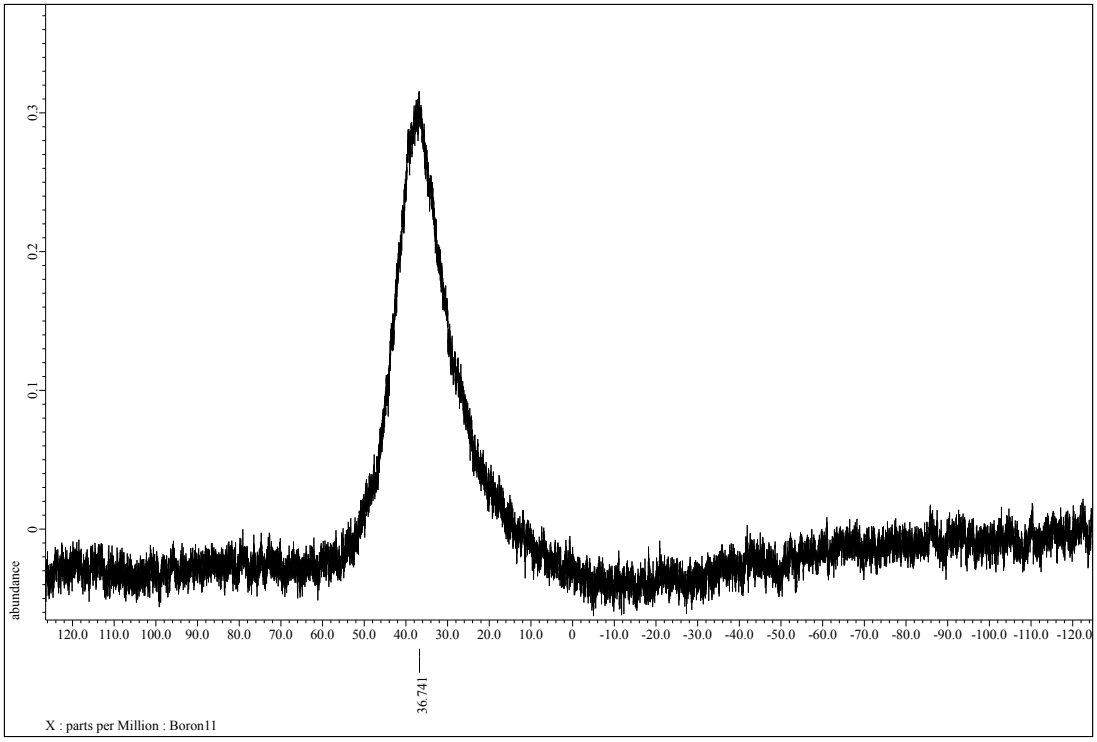


Figure S34. ^{11}B NMR spectrum of **ν-DABNA** in $(CDCl_2)_2$ at 130 ºC.

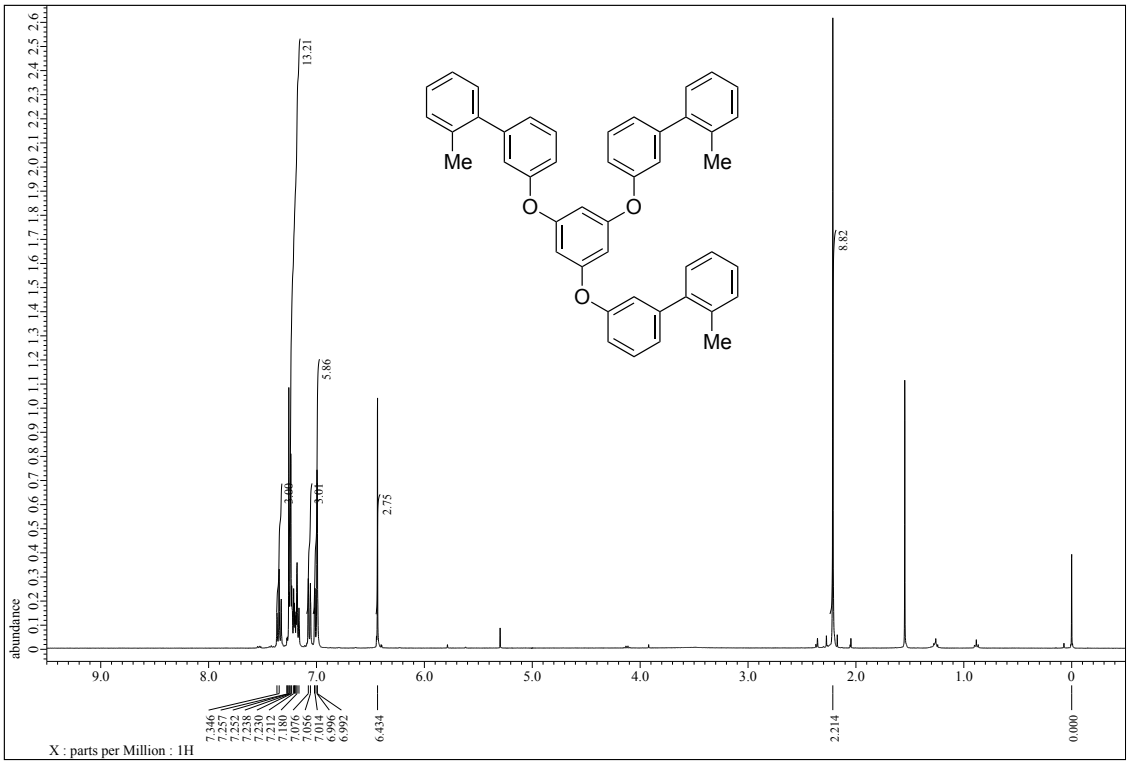


Figure S35. ^{1}H NMR spectrum of 1,3,5-tris((2'-methyl-[1,1'-biphenyl]-3-yl)oxy)benzene in $CDCl_3$ at 25 ºC.

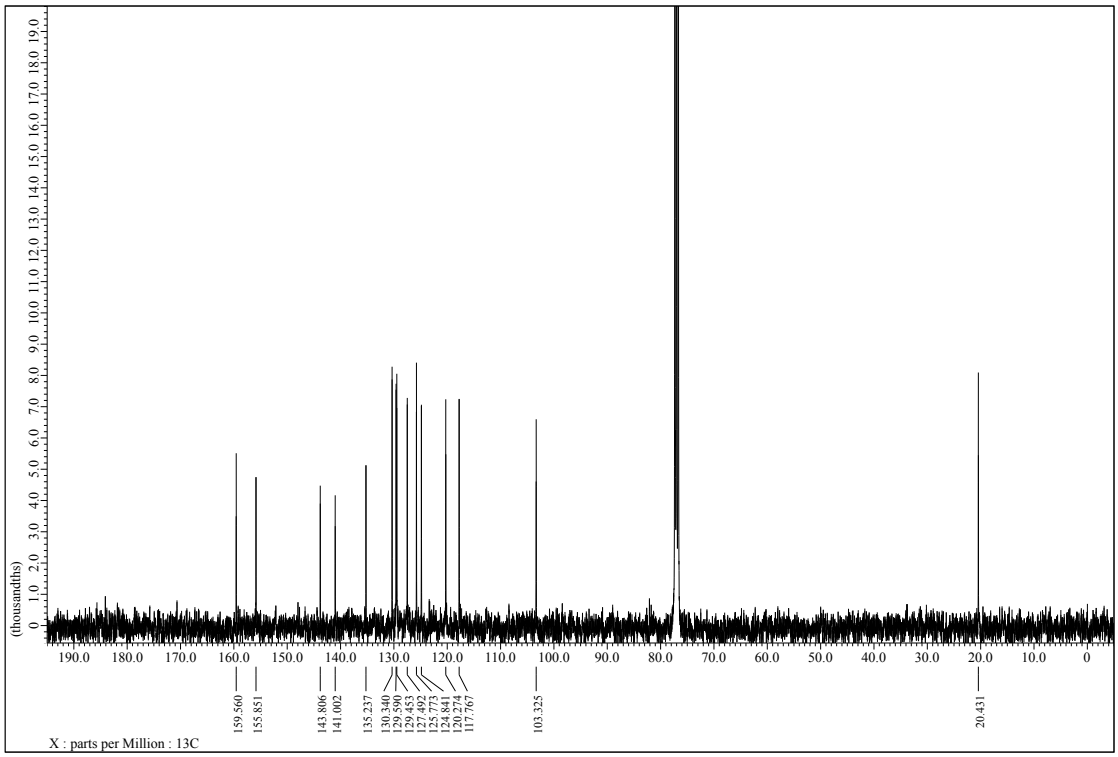


Figure S36. ^{13}C NMR spectrum of 1,3,5-tris((2'-methyl-[1,1'-biphenyl]-3-yl)oxy)benzene in $CDCl_3$ at 25 ºC.

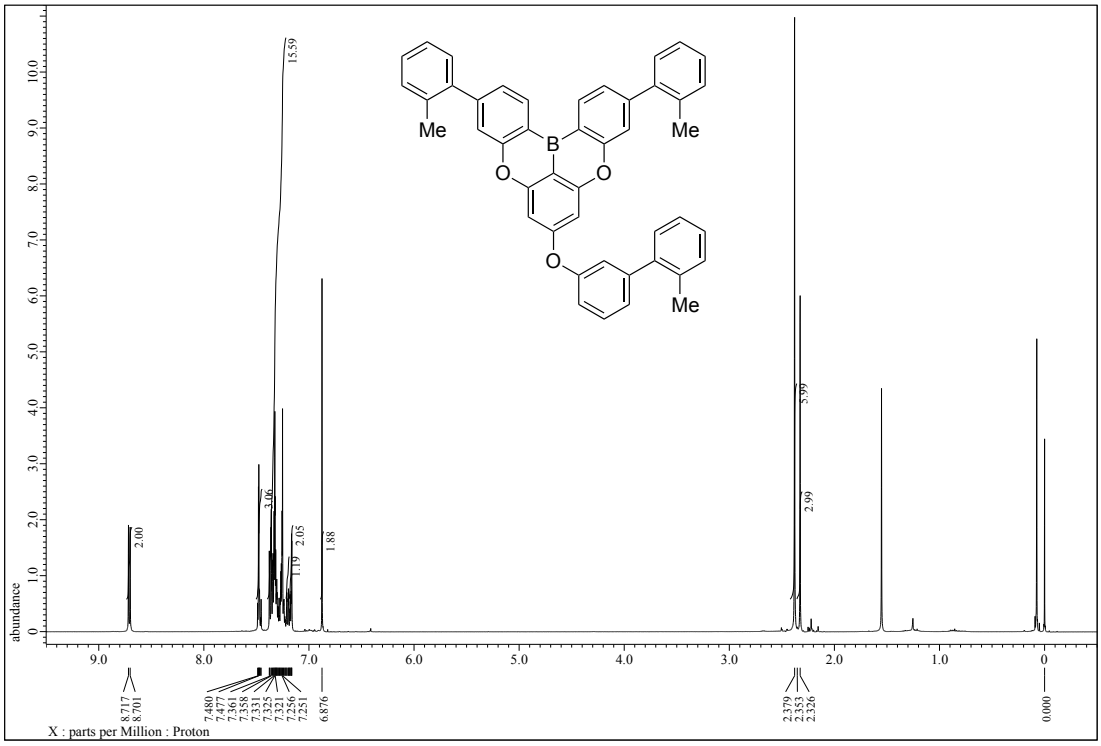


Figure S37. ^{1}H NMR spectrum of **DOBNA-OAr** in $CDCl_3$ at 25 ºC.

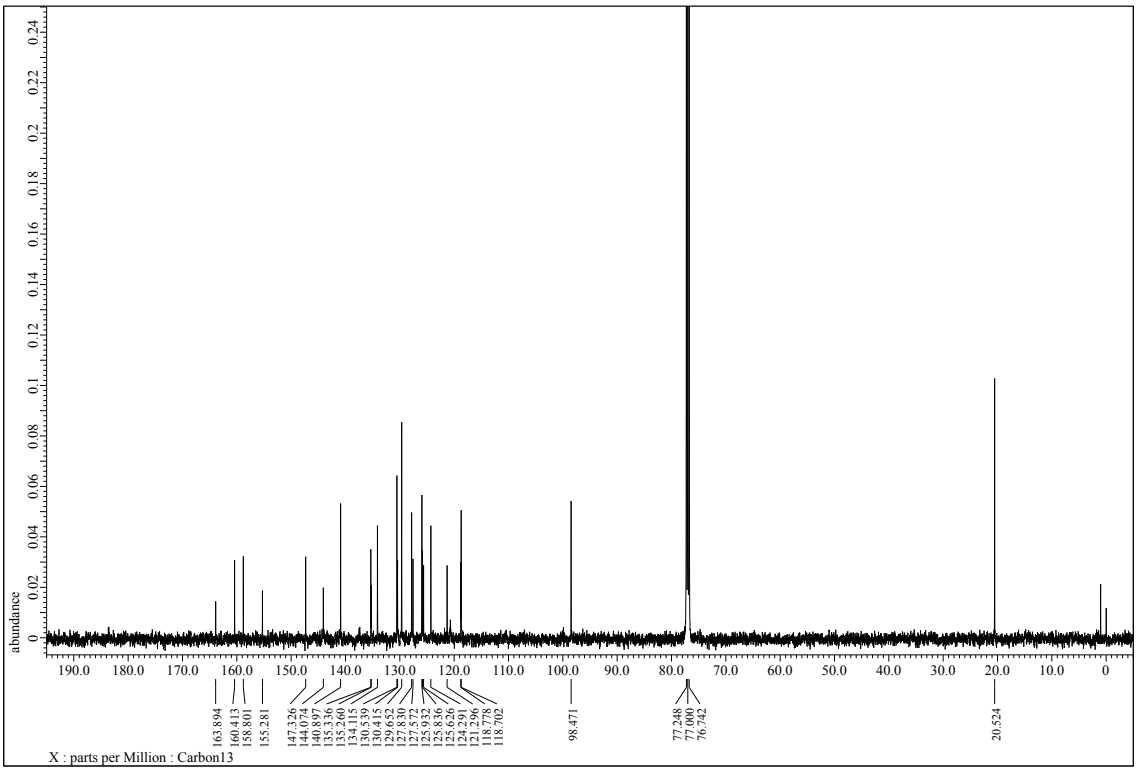


Figure S38. ^{1}H NMR spectrum of **DOBNA-OAr** in $CDCl_3$ at 25 ºC.

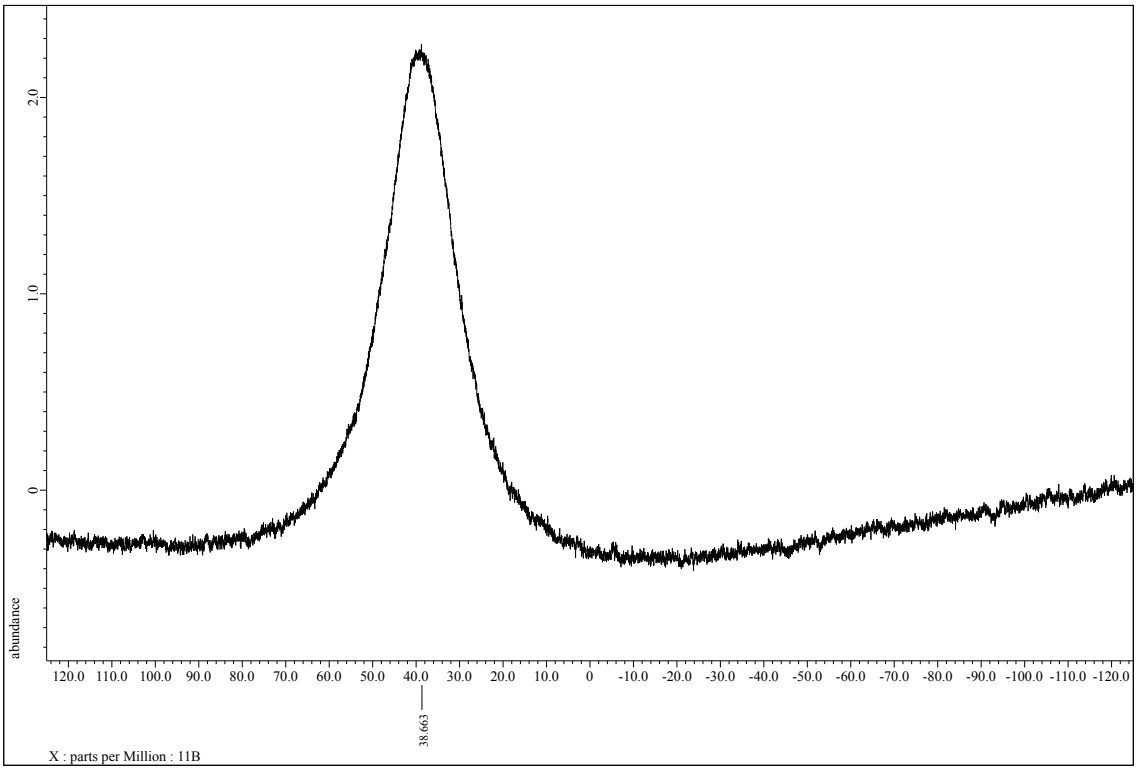


Figure S39. ^{11}B NMR spectrum of **DOBNA-OAr** in $CDCl_3$ at 25 ºC.

Cartesian coordinates

ν-DABNA (S_0, C_2 symmetry)

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H(B3LYP) = -3381.988983 hartree

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ν-DABNA (S_1, C_1 symmetry)

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H	2.08596800	-2.41796000	2.78535600
C	-1.34810400	-2.18314200	4.57413600
H	-2.19200100	-2.23814800	2.58162400
C	-0.17356800	-2.20006500	5.32919500
H	1.98100900	-2.29870400	5.27354400
H	-2.31376600	-2.12221800	5.06816000
H	-0.22359900	-2.15098800	6.41344600
C	0.04616100	2.33425400	2.54551600
C	1.28703100	2.24942100	3.18183200
C	-1.13101000	2.35117000	3.29723100
C	1.34769500	2.18338400	4.57433200
H	2.19184100	2.23833000	2.58190400
C	-1.06523100	2.28375300	4.68960500
H	-2.08615400	2.41826000	2.78513000
C	0.17306700	2.20039100	5.32925100
H	2.31328900	2.12246000	5.06847100
H	-1.98151300	2.29904800	5.27330300
H	0.22295500	2.15135800	6.41350700
N	-0.38296500	5.29440600	-2.80332300
N	0.38317400	-5.29427400	-2.80321600
C	0.27284800	-6.62594100	-3.34651200
C	1.39187300	-7.46175500	-3.39137600
C	-0.95961300	-7.07399600	-3.82781500
C	1.27459900	-8.74852000	-3.91840000
H	2.34239900	-7.09778100	-3.01340400
C	-1.07164600	-8.36112100	-4.35565400
H	-1.81785300	-6.41010500	-3.78654400
C	0.04420300	-9.19937600	-4.40136800
H	2.14462900	-9.39842100	-3.94995200
H	-2.03091000	-8.70795100	-4.72983000
H	-0.04481200	-10.20184200	-4.81080600
C	-0.27250700	6.62603600	-3.34665000
C	-1.39148400	7.46190500	-3.39171000
C	0.96005600	7.07401800	-3.82777000
C	-1.27406000	8.74864500	-3.91876100
H	-2.34208900	7.09798900	-3.01387900
C	1.07224400	8.36112900	-4.35562000

H	1.81824900	6.41007500	-3.78633300
C	-0.04356500	9.19942100	-4.40155900
H	-2.14404300	9.39859600	-3.95049500
H	2.03158700	8.70791600	-4.72965300
H	0.04554900	10.20186200	-4.81101300
C	-1.40767800	-7.23529400	2.57181300
C	-2.64970700	-6.64149200	2.28667100
C	-1.20510800	-7.80744900	3.84012500
C	-3.65710100	-6.61967400	3.24873400
H	-2.81753900	-6.20483700	1.30755000
C	-2.22497500	-7.79423000	4.78871600
H	-0.24612600	-8.25792700	4.07470400
C	-3.45610600	-7.19858200	4.50383200
H	-4.61186700	-6.15929100	3.00734400
H	-2.04858900	-8.24099900	5.76392900
H	-4.24651900	-7.18579400	5.24892800
C	0.45641600	-8.38425600	1.43895300
C	-0.07824900	-9.68136400	1.51246100
C	1.83187400	-8.22994400	1.19693500
C	0.74853900	-10.79287700	1.36111000
H	-1.14145300	-9.81106600	1.68732200
C	2.64680400	-9.34740600	1.03106200
H	2.25271600	-7.23110300	1.14270000
C	2.11438400	-10.63616100	1.11606800
H	0.31612000	-11.78839500	1.42148400
H	3.70928500	-9.20767200	0.84818200
H	2.75443300	-11.50515500	0.99247900
C	-0.45674800	8.38422000	1.43926500
C	0.07743400	9.68151200	1.51326800
C	-1.83215200	8.22950900	1.19716300
C	-0.74976100	10.79277300	1.36232900
H	1.14058600	9.81155700	1.68819100
C	-2.64747700	9.34674100	1.03167300
H	-2.25263200	7.23054900	1.14253900
C	-2.11554400	10.63566000	1.11719300
H	-0.31771300	11.78843800	1.42307900
H	-3.70990100	9.20668500	0.84870600
H	-2.75591700	11.50446200	0.99391700
C	1.40791600	7.23557400	2.57152600
C	1.20551500	7.80749100	3.83996600
C	2.64997200	6.64196300	2.28606200
C	2.22557600	7.79429200	4.78834500
H	0.24651900	8.25781100	4.07480600
C	3.65755000	6.62012600	3.24793200
H	2.81765500	6.20544800	1.30685300
C	3.45672300	7.19883600	4.50314400
H	2.04932100	8.24090600	5.76366700
H	4.61233000	6.15989300	3.00630400
H	4.24728500	7.18606400	5.24808700
C	0.72182400	-4.24408000	-3.68710700
C	0.77875000	-2.89370100	-3.22224000
C	1.01545100	-4.55394300	-5.03093100
C	1.41330400	-3.55558600	-5.91490500
H	0.94850700	-5.57413300	-5.38585200
H	1.63760600	-3.81724100	-6.94576700
C	-0.72163600	4.24421000	-3.68717700
C	-1.01515100	4.55400900	-5.03104100
C	-0.77861700	2.89383700	-3.22225900
C	-1.41298600	3.55562100	-5.91499300
H	-0.94812100	5.57417600	-5.38601200
H	-1.63720200	3.81721200	-6.94588000
C	0.01876700	6.26568900	-0.61460600
H	0.05429200	7.26086400	-1.03471400
C	0.15745600	4.82875800	1.34124800
H	0.27008800	4.73973900	2.41268900
C	0.18656700	6.10743500	0.76462700
C	1.53874900	-2.23653900	-5.47302900
H	1.87404200	-1.45678000	-6.15186600
C	1.22517100	-1.92856500	-4.15349200
H	1.35138000	-0.90594000	-3.81768900
C	-1.53848400	2.23659000	-5.47307200
H	-1.87376400	1.45683100	-6.15190800

C	-1.22500000	1.92866600	-4.15350100
H	-1.35123500	0.90606000	-3.81765000

ν-DABNA (T_1, C_1 symmetry)

E(B3LYP) = -3383.07877886 hartree

B	0.38831300	-2.60486400	-1.75267700
B	-0.38821900	2.60498800	-1.75266300
N	0.00947700	-2.41406500	1.10511800
N	-0.00929200	2.41423800	1.10511600
N	-0.39654600	5.29994500	-2.79917700
N	0.39659900	-5.29985000	-2.79912600
N	-0.39854500	-7.24620200	1.59847700
N	0.39861400	7.24641400	1.59835700
C	-0.00382400	3.69880300	0.52573300
C	-0.04929100	1.22226800	0.37340900
C	-0.15302400	1.24684100	-1.06028800
C	-0.20227500	3.82174500	-0.87483600
C	0.00009700	0.00007800	1.06286300
C	0.00005600	0.00008300	-1.70057800
C	0.15319000	-1.24668200	-1.06030500
C	0.04948200	-1.22209700	0.37338100
C	0.00398000	-3.69863300	0.52575200
C	0.20240300	-3.82159500	-0.87483400
H	0.00009000	0.00005500	2.14056400
H	-0.00002800	0.00009800	-2.78000800
C	0.20136400	-5.13629700	-1.42019300
C	-0.17354000	-4.82692000	1.34067000
C	-0.20130200	5.13642400	-1.42024000
C	-0.02002000	-6.26471300	-0.61095700
H	-0.05171300	-7.26086700	-1.02955600
C	-0.19756500	-6.10621400	0.76803700
H	-0.29815000	-4.73623100	2.41090400
C	-0.07760600	-2.33130800	2.54354300
C	1.09113600	-2.35177500	3.30799000
C	-1.32536600	-2.24196400	3.16537600
C	1.00990600	-2.28270400	4.69944300
H	2.05170100	-2.42272500	2.80670400
C	-1.40133400	-2.17445800	4.55702400
H	-2.22332600	-2.22878300	2.55531700
C	-0.23527300	-2.19453500	5.32499600
H	1.91947100	-2.30055300	5.29341900
H	-2.37219600	-2.11007600	5.04025900
H	-0.29716600	-2.14439000	6.40857100
C	0.07778300	2.33151200	2.54356300
C	1.32553600	2.24214700	3.16539700
C	-1.09096100	2.35199300	3.30798900
C	1.40148300	2.17465000	4.55706100
H	2.22350300	2.22894900	2.55534300
C	-1.00975300	2.28291900	4.69944300
H	-2.05153200	2.42294400	2.80669700
C	0.23541200	2.19478200	5.32502200
H	2.37233100	2.11026600	5.04030600
H	-1.91934100	2.30078300	5.29339000
H	0.29728100	2.14466100	6.40859500
C	0.29028500	-6.63335400	-3.34035500
C	1.40922700	-7.46954700	-3.37316800
C	-0.93843800	-7.08118600	-3.83089100
C	1.29544900	-8.75751700	-3.89805700
H	2.35658500	-7.10563200	-2.98732000
C	-1.04676500	-8.36954500	-4.35639800
H	-1.79661100	-6.41674500	-3.79840700
C	0.06890100	-9.20858900	-4.39042900
H	2.16515700	-9.40813800	-3.92025400
H	-2.00305500	-8.71674700	-4.73762900
H	-0.01736800	-10.21205200	-4.79790800
C	-0.29022000	6.63342800	-3.34043500
C	-1.40916300	7.46961500	-3.37331600
C	0.93853400	7.08124800	-3.83091200
C	-1.29535400	8.75757000	-3.89823300
H	-2.35654200	7.10570700	-2.98751200

C	1.04689200	8.36960200	-4.35643400
H	1.79669900	6.41679900	-3.79836100
C	-0.06878000	9.20862700	-4.39056300
H	-2.16505000	9.40820000	-3.92050600
H	2.00320500	8.71681200	-4.73762000
H	0.01749400	10.21207100	-4.79806200
C	-1.46839100	-7.25143400	2.53009800
C	-2.70691500	-6.67790300	2.19400600
C	-1.30810000	-7.81471100	3.80814900
C	-3.75234600	-6.66841700	3.11494100
H	-2.84187800	-6.24540800	1.20790100
C	-2.36536600	-7.81455000	4.71532100
H	-0.35249300	-8.24935700	4.08312700
C	-3.59335100	-7.23988400	4.37932400
H	-4.70337000	-6.22296000	2.83379000
H	-2.22080300	-8.25509400	5.69862500
H	-4.41310200	-7.23694700	5.09214300
C	0.46507500	-8.36583900	1.47622200
C	-0.03760500	-9.67576800	1.55635500
C	1.84138600	-8.18116300	1.26070700
C	0.81983100	-10.76767100	1.43788200
H	-1.10055600	-9.83062000	1.71079800
C	2.68740300	-9.27994300	1.12694200
H	2.23886700	-7.17306400	1.20153400
C	2.18634300	-10.58047800	1.21884900
H	0.41092500	-11.77285000	1.50300400
H	3.74961900	-9.11539900	0.96388100
H	2.85029300	-11.43466900	1.12073000
C	-0.46511300	8.36596200	1.47623800
C	0.03744300	9.67592300	1.55674000
C	-1.84138700	8.18121800	1.26053700
C	-0.82007600	10.76777600	1.43842600
H	1.10036100	9.83083900	1.71136000
C	-2.68747300	9.27996200	1.12689000
H	-2.23878100	7.17311100	1.20109600
C	-2.18654400	10.58051800	1.21916900
H	-0.41127400	11.77298800	1.50383300
H	-3.74965600	9.11536700	0.96365900
H	-2.85056200	11.43467000	1.12116600
C	1.46831500	7.25157400	2.53014800
C	1.30783700	7.81468900	3.80823500
C	2.70690500	6.67812900	2.19413600
C	2.36500500	7.81451000	4.71551900
H	0.35217800	8.24927500	4.08314000
C	3.75222100	6.66857000	3.11520400
H	2.84199000	6.24572800	1.20800500
C	3.59304300	7.23991200	4.37961700
H	2.22031100	8.25496600	5.69885800
H	4.70330100	6.22318000	2.83413500
H	4.41271200	7.23695500	5.09253500
C	0.73926700	-4.25083300	-3.68097900
C	0.78610000	-2.89842500	-3.21768800
C	1.04724800	-4.56349700	-5.02158200
C	1.44830500	-3.56725700	-5.90431000
H	0.98819500	-5.58534900	-5.37312700
H	1.68403600	-3.82993500	-6.93218800
C	-0.73922300	4.25091600	-3.68099200
C	-1.04718500	4.56352000	-5.02161800
C	-0.78602300	2.89851300	-3.21766200
C	-1.44822400	3.56723800	-5.90430200
H	-0.98811800	5.58535400	-5.37321100
H	-1.68394400	3.82985000	-6.93218900
C	0.02006200	6.26485300	-0.61102000
H	0.05171800	7.26100700	-1.02961300
C	0.17366300	4.82709900	1.34064500
H	0.29828900	4.73642300	2.41087800
C	0.19763000	6.10637000	0.76798000
C	1.56362600	-2.24559600	-5.46315800
H	1.90281800	-1.46666800	-6.14102600
C	1.23708000	-1.93453200	-4.14893900
H	1.35569500	-0.91034700	-3.81557800
C	-1.56350900	2.24557800	-5.46310900

H	-1.90268500	1.46664100	-6.14096400
C	-1.23697100	1.93456800	-4.14888000

DABNA-1 (S_0, C_2 symmetry)

E(B3LYP) = -1290.26035584 hartree

H(B3LYP) = -1289.804450 hartree

B	0.00000000	0.00000000	-1.31267100
N	0.00000000	2.44026800	0.22910000
N	0.00000000	-2.44026800	0.22910000
C	-0.00372900	-1.22410000	0.92985900
C	0.00000000	0.00000000	0.20363000
C	0.00372900	1.22410000	0.92985900
C	0.01990900	1.21881500	2.33511800
C	0.00000000	0.00000000	3.00457100
C	-0.01990900	-1.21881500	2.33511800
H	0.03258200	2.14069400	2.90083800
H	0.00000000	0.00000000	4.09191000
H	-0.03258200	-2.14069400	2.90083800
C	0.19059500	-2.54070300	-1.16173200
C	0.33750500	-3.81997700	-1.74512000
C	0.25055200	-1.37428700	-1.97722900
C	0.60595100	-3.94903300	-3.09886400
H	0.26019200	-4.71129600	-1.13580800
C	0.57053200	-1.56373900	-3.34116600
C	0.75022600	-2.81607800	-3.90809000
H	0.72421700	-4.94373600	-3.52164600
H	0.99862400	-2.91673100	-4.96093200
C	-0.19059500	2.54070300	-1.16173200
C	-0.25055200	1.37428700	-1.97722900
C	-0.33750500	3.81997700	-1.74512000
C	-0.57053200	1.56373900	-3.34116600
C	-0.60595100	3.94903300	-3.09886400
H	-0.26019200	4.71129600	-1.13580800
C	-0.75022600	2.81607800	-3.90809000
H	-1.35553300	0.91039400	-3.81547000
H	-0.72421700	4.94373600	-3.52164600
H	-0.99862400	2.91673100	-4.96093200
C	-0.12486100	-3.65588100	0.99374300
C	-1.39114600	-4.19509400	1.23312600
C	1.01439800	-4.29082600	1.49700400
C	-1.51725600	-5.37037500	1.97552700
H	-2.26605900	-3.68930000	0.83580500
C	0.88432000	-5.46538200	2.23935600
H	1.99170700	-3.85920400	1.30254400
C	-0.38085800	-6.00649500	2.47933000
H	-2.50329200	-5.78788200	2.15976200
H	1.77118900	-5.95713700	2.62949000
H	-0.48051900	-6.92116600	3.05727900
C	0.12486100	3.65588100	0.99374300
C	1.39114600	4.19509400	1.23312600
C	-1.01439800	4.29082600	1.49700400
C	1.51725600	5.37037500	1.97552700
H	2.26605900	3.68930000	0.83580500
C	-0.88432000	5.46538200	2.23935600
H	-1.99170700	3.85920400	1.30254400
C	0.38085800	6.00649500	2.47933000
H	2.50329200	5.78788200	2.15976200
H	-1.77118900	5.95713700	2.62949000
H	0.48051900	6.92116600	3.05727900
H	0.70589100	-0.68739800	-3.96507900
H	-0.70589100	0.68739800	-3.96507900

DABNA-1 (S_1, C_1 symmetry)

E(B3LYP) = -1290.14902727 hartree

B	-0.00190900	0.00021000	-1.36525500
N	0.00105800	2.41951200	0.22912800
N	-0.00318200	-2.41920100	0.22896700

C	-0.01102100	-1.20537900	0.90315200
C	-0.00106800	0.00015900	0.17848000
C	0.00966200	1.20564900	0.90321300
C	0.02525800	1.20587900	2.33506400
C	0.00047800	0.00008100	3.02477900
C	-0.02505000	-1.20568100	2.33502500
H	0.04846900	2.13666700	2.88528900
H	0.00106700	0.00005300	4.11024500
H	-0.04766900	-2.13649400	2.88522800
C	0.15185100	-2.55065500	-1.18766000
C	0.19799300	-1.37729700	-2.01268200
C	-0.15551300	2.55106600	-1.18732500
C	-0.20252800	1.37775600	-2.01237400
C	-0.26930700	3.83800000	-1.72910700
C	-0.46359300	1.61772700	-3.38829800
C	-0.47626400	4.01555100	-3.10428200
H	-0.20705900	4.71201700	-1.09400700
C	-0.59240400	2.89572900	-3.92677300
H	-0.55838100	5.01977700	-3.50944400
H	-0.78355200	3.01612600	-4.99075900
C	-0.09886300	-3.63300400	1.00425600
C	-1.35492100	-4.18358600	1.26864400
C	1.05902600	-4.25231500	1.48257300
C	-1.45224900	-5.35203900	2.02673000
H	-2.24246600	-3.69338800	0.88018400
C	0.95585900	-5.41990100	2.24060600

perylene (S_0, D_{2h} symmetry)

E(B3LYP) = -769.40611859 hartree

C	0.00000000	2.42264400	2.88607800
C	0.00000000	2.42729100	1.47962800
C	0.00000000	1.24985100	0.73800400
C	0.00000000	0.00000000	1.43974400
C	0.00000000	0.00000000	2.87468500
C	0.00000000	1.23260100	3.57591400
H	0.00000000	2.15767500	4.66285700
H	0.00000000	3.36861000	3.42085800
H	2.02736400	-3.81566300	1.25739800
C	-0.29869700	-5.97021300	2.51357300
H	-2.42969900	-5.77757800	2.23595900
H	1.85573000	-5.89857200	2.61665300
H	-0.37674100	-6.87909400	3.10368700
C	0.09748200	3.63323100	1.00445500
C	1.35377100	4.18394100	1.26747800
C	-1.05993400	4.25229100	1.48423900
C	1.45181800	5.35228700	2.02563700
H	2.24093300	3.69392700	0.87791200
C	-0.95604700	5.41976900	2.24234200
H	-2.02847400	3.81553100	1.26014300
C	0.29874900	5.97022000	2.51392400
H	2.42945200	5.77792800	2.23379600
H	-1.85554500	5.89824900	2.61952100
H	0.37735200	6.87901600	3.10409300
H	-0.59563900	0.76590600	-4.04451400
C	0.45755800	-1.61719100	-3.38890200
H	0.58887500	-0.76533400	-4.04523000
C	0.58578300	-2.89516700	-3.92758600
H	0.77580600	-3.01550200	-4.99178800
C	0.47050100	-4.01503900	-3.10503800
H	0.55214600	-5.01925000	-3.51035200
C	0.26501000	-3.83756000	-1.72963500
H	0.20339200	-4.71161500	-1.09450900

C	0.00000000	1.24985100	-0.73800400
C	0.00000000	-1.24985100	0.73800400
C	0.00000000	-1.24985100	-0.73800400
C	0.00000000	0.00000000	-1.43974400
C	0.00000000	-2.42729100	-1.47962800
C	0.00000000	-2.42729100	1.47962800
C	0.00000000	-2.42264400	2.88607800
C	0.00000000	-1.23260100	3.57591400
H	0.00000000	-1.21767500	4.66285700
H	0.00000000	-3.36861000	3.42085800

H	0.00000000	-3.38813400	0.97734700
H	0.00000000	3.38813400	0.97734700
H	0.00000000	3.36861000	3.42085800
H	0.00000000	1.21767500	4.66285700
C	0.00000000	2.42729100	-1.47962800
C	0.00000000	2.42264400	-2.88607800
C	0.00000000	1.23260100	-3.57591400
C	0.00000000	0.00000000	-2.87468500
C	0.00000000	-2.42264400	-2.88607800
C	0.00000000	-1.23260100	-3.57591400
H	0.00000000	3.38813400	-0.97734700
H	0.00000000	3.36861000	-3.42085800
H	0.00000000	1.21767500	-4.66285700
H	0.00000000	-1.21767500	-4.66285700
H	0.00000000	-3.36861000	-3.42085800
H	0.00000000	-3.38813400	-0.97734700

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perylene (S_1, C_1 symmetry)

E(B3LYP) = -769.30547356 hartree

C	0.00005100	2.44096900	2.86387100
C	0.00002600	2.45603700	1.47536500
C	0.00028200	1.24633600	0.72215700
C	-0.00004000	0.00005900	1.42657000
C	0.00002900	-0.00011200	2.86276100
C	0.00013800	1.23313500	3.55841600
C	0.00016200	1.24577300	-0.72196400
C	-0.00006200	-1.24583200	0.72229700
C	-0.00011000	-1.24590900	-0.72209200
C	-0.00004600	-0.00001800	-1.42614400
C	-0.00001800	-2.45591900	-1.47537600
C	-0.00007800	-2.45559100	1.47529900
C	-0.00028300	-2.44085000	2.86374000
C	0.00003300	-1.23315100	3.55870200
H	0.00027300	-1.22278500	4.64552100
H	-0.00067000	-3.38010100	3.41044700
H	0.00005800	-3.41182500	0.96685900
H	-0.00023300	3.41214800	0.96670000
H	0.00002900	3.38009400	3.41077700
H	0.00024900	1.22293600	4.64530900
C	-0.00006600	2.45596800	-1.47544900
C	-0.00008600	2.44142800	-2.86342200
C	-0.00006300	1.23297200	-3.55816700
C	0.00014800	-0.00001400	-2.86295300
C	0.00005800	-2.44111600	-2.86343800
C	-0.00000200	-1.23314200	-3.55860400
H	-0.00005200	3.41186100	-0.96636000
H	-0.00016600	3.38017600	-3.41087800
H	-0.00005100	1.22361500	-4.64507600
H	-0.00000800	-1.22342300	-4.64543900
H	0.00010400	-3.38009100	-3.41059900
H	-0.00017700	-3.41179200	-0.96626300

ν-DABNA_radical_1 (S_0, C_1 symmetry)

E(B3LYP) = -3151.491157 hartree

H(B3LYP) = -3150.407120 hartree

B	2.807377	1.542183	0.248795
B	-2.417176	1.546314	-0.436121
N	2.517317	-1.366283	-0.090880
N	-2.241656	-1.328481	-0.179216
N	-5.087709	2.630070	-0.276787
N	5.575204	2.422780	0.285357
N	7.250309	-2.119010	-0.273357
N	-7.053542	-1.769869	0.362461
C	-3.513366	-0.740577	-0.101184
C	-1.042628	-0.592324	-0.186100
C	-1.057548	0.835043	-0.247056
C	-3.635580	0.672526	-0.231007
C	0.183059	-1.266957	-0.139328

C	0.182410	1.493306	-0.083210
C	1.422875	0.868258	0.052626
C	1.409651	-0.569893	-0.055204
C	3.756455	-0.806821	-0.054998
C	3.985888	0.598225	0.105346
H	0.244325	-2.346755	-0.166528
H	0.152591	2.574255	-0.062207
C	5.317615	1.056975	0.130463
C	4.841890	-1.704407	-0.164011
C	-4.938302	1.240500	-0.155150
C	6.396714	0.151867	-0.025240
H	7.418589	0.504753	-0.037549
C	6.157316	-1.221486	-0.156448
H	4.631236	-2.763619	-0.253095
C	-2.158098	-2.768115	-0.176207
C	-2.057628	-3.464115	1.031256
C	-2.179441	-3.462848	-1.387866
C	-1.978837	-4.857275	1.024182
H	-2.041219	-2.909618	1.964611
C	-2.099334	-4.856149	-1.390551
H	-2.256420	-2.906447	-2.317187
C	-1.999613	-5.554425	-0.185561
H	-1.901111	-5.396816	1.963879
H	-2.113899	-5.394717	-2.334044
H	-1.937529	-6.639143	-0.189045
C	6.944570	2.873228	0.213968
C	7.731368	2.909456	1.368116
C	7.478710	3.269185	-1.014659
C	9.055486	3.343201	1.290540
H	7.300852	2.597282	2.314794
C	8.802994	3.703714	-1.087235
H	6.852747	3.235141	-1.901351
C	9.592192	3.741304	0.064226
H	9.667252	3.367735	2.187894
H	9.217177	4.011220	-2.043386
H	10.623460	4.078123	0.005917
C	-6.401418	3.187615	-0.071227
C	-7.300415	3.282658	-1.137176
C	-6.772017	3.631584	1.200440
C	-8.570255	3.822358	-0.928548
H	-6.998321	2.931549	-2.119253
C	-8.042383	4.172607	1.404711
H	-6.061960	3.549883	2.017942
C	-8.942502	4.268236	0.341517
H	-9.268491	3.892407	-1.757912
H	-8.328094	4.517564	2.394609
H	-9.931901	4.687468	0.502279
C	7.181948	-3.215613	-1.176013
C	6.618053	-3.055722	-2.452083
C	7.682032	-4.474474	-0.805602
C	6.548033	-4.135973	-3.329670
H	6.235842	-2.084403	-2.749056
C	7.624665	-5.543402	-1.697493
H	8.111985	-4.608239	0.181832
C	7.054058	-5.384365	-2.962174
H	6.105855	-3.994264	-4.312350
H	8.015668	-6.510938	-1.393413
H	7.003627	-6.222303	-3.651602
C	8.417407	-1.926372	0.517903
C	9.694094	-2.049982	-0.052075
C	8.307356	-1.615906	1.882829
C	10.833470	-1.874487	0.731523
H	9.785119	-2.285659	-1.107724
C	9.451936	-1.425525	2.654491
H	7.322467	-1.529001	2.330831
C	10.721263	-1.557213	2.086749
H	11.814468	-1.974429	0.274216
H	9.348758	-1.189080	3.710456
H	11.611452	-1.416167	2.693253
C	-8.258792	-1.489670	-0.338081
C	-9.499088	-1.563869	0.315943
C	-8.227008	-1.141425	-1.698343

C	-10.677995	-1.302454	-0.380073
H	-9.531230	-1.827277	1.368362
C	-9.409615	-0.864969	-2.381209
H	-7.272196	-1.090777	-2.211656
C	-10.642489	-0.947438	-1.730061
H	-11.629066	-1.364405	0.142614
H	-9.366093	-0.598928	-3.434340
H	-11.563119	-0.738960	-2.267839
C	-7.000205	-2.872049	1.259388
C	-7.585316	-4.100910	0.914775
C	-6.368643	-2.745120	2.507226
C	-7.545675	-5.172806	1.804558
H	-8.069118	-4.207895	-0.050882
C	-6.318501	-3.827871	3.382810
H	-5.921564	-1.795321	2.782587
C	-6.909677	-5.046302	3.041273
H	-8.003736	-6.116875	1.520918
H	-5.826997	-3.711322	4.345371
H	-6.875300	-5.885819	3.729905
C	4.567657	3.375118	0.538951
C	3.189112	3.003670	0.575925
C	4.946411	4.717552	0.775156
C	3.993963	5.672637	1.088540
H	5.987794	5.008669	0.727688
H	4.311741	6.695923	1.272504
C	-4.044555	3.499169	-0.652690
C	-4.341420	4.857590	-0.905470
C	-2.710105	3.022444	-0.795938
C	-3.354042	5.721876	-1.353090
H	-5.348112	5.231775	-0.770680
H	-3.610347	6.760017	-1.550018
C	-6.063424	0.434312	0.067628
H	-7.052578	0.858873	0.159664
C	-4.645083	-1.547750	0.071584
H	-4.565093	-2.623184	0.138124
C	-5.908548	-0.952482	0.165809
C	2.640607	5.324014	1.188596
H	1.897564	6.067956	1.461784
C	2.266748	4.015035	0.934680
H	1.221748	3.746273	1.036047
C	-2.051275	5.261632	-1.575253
H	-1.286602	5.929880	-1.961206
C	-1.754257	3.936241	-1.295416
H	-0.750270	3.577111	-1.492339

ν-DABNA_radical_2 (S_0, C_1 symmetry)

E(B3LYP) = -3151.4878046 hartree

H(B3LYP) = -3150.403590 hartree

B	-3.324534	1.562429	-0.518276
B	1.826589	1.706230	0.409697
N	-3.088293	-1.299195	-0.182648
N	1.743268	-1.164673	0.079476
N	4.474168	2.864734	0.410869
N	-6.028794	2.585500	-0.537993
N	-7.953452	-1.746086	0.085884
N	6.586612	-1.463700	-0.260424
C	3.003069	-0.537851	0.074708
C	0.524017	-0.465860	0.057166
C	0.500983	0.958817	0.152616
C	3.080548	0.872125	0.244734
C	-0.673328	-1.189206	-0.050609
C	-0.748786	1.562202	-0.049450
C	-1.963923	0.889384	-0.252396
C	-1.909098	-0.534183	-0.156884
C	-4.382148	-0.742380	-0.171802
C	-4.535663	0.663644	-0.344353
H	-0.642748	-2.267235	-0.054166
H	-0.779908	2.643026	-0.049192
C	-5.853963	1.203584	-0.361478
C	-5.493840	-1.572003	-0.001012

C	4.367772	1.475952	0.244103
C	-6.966603	0.371905	-0.211485
H	-7.980064	0.746311	-0.240131
C	-6.795559	-1.014233	-0.005555
H	-5.384632	-2.643056	0.084688
C	-2.977824	-2.735234	-0.132033
C	-2.979544	-3.471167	-1.319434
C	-2.876948	-3.390230	1.098784
C	-2.880850	-4.862628	-1.274915
H	-3.061277	-2.946988	-2.266882
C	-2.777014	-4.781455	1.138996
H	-2.873807	-2.803508	2.012626
C	-2.779657	-5.518978	-0.046814
H	-2.884562	-5.432732	-2.199837
H	-2.697487	-5.288532	2.096668
H	-2.704317	-6.602387	-0.013578
C	1.711727	-2.605381	0.043296
C	1.684113	-3.278865	-1.180924
C	1.718814	-3.325977	1.240245
C	1.663252	-4.673903	-1.205188
H	1.681417	-2.704751	-2.102475
C	1.697572	-4.721062	1.211693
H	1.742993	-2.786917	2.182612
C	1.669883	-5.396173	-0.010174
H	1.645157	-5.195577	-2.157991
H	1.704928	-5.279330	2.143870
H	1.656096	-6.482430	-0.031411
C	-7.366711	3.112339	-0.432391
C	-8.188439	3.178087	-1.561292
C	-7.838436	3.556122	0.805242
C	-9.481930	3.689696	-1.449383
H	-7.807818	2.827568	-2.515992
C	-9.132556	4.067639	0.913096
H	-7.187255	3.497247	1.672218
C	-9.955202	4.135120	-0.213141
H	-10.119576	3.738716	-2.327729
H	-9.497209	4.411961	1.876916
H	-10.962947	4.532276	-0.127773
C	5.781002	3.461120	0.290176
C	6.619448	3.550825	1.404904
C	6.206411	3.948997	-0.947932
C	7.883254	4.128837	1.278615
H	6.275168	3.166017	2.360122
C	7.470430	4.528250	-1.069874
H	5.542830	3.871411	-1.803999
C	8.309931	4.618457	0.042254
H	8.534365	4.194939	2.145804
H	7.798645	4.907283	-2.033801
H	9.294565	5.067600	-0.054261
C	-8.044933	-2.930429	0.756366
C	-7.221882	-3.340221	1.844907
C	-9.125816	-3.780824	0.389277
C	-7.460156	-4.543854	2.495570
H	-6.433240	-2.681114	2.190436
C	-9.334024	-4.992865	1.028367
H	-9.768328	-3.450097	-0.420796
C	-8.502473	-5.384553	2.086735
H	-6.832970	-4.830687	3.335990
H	-10.154041	-5.634441	0.716461
H	-8.676558	-6.326736	2.599048
C	7.748868	-1.180576	0.507617
C	9.021355	-1.204578	-0.085656
C	7.642632	-0.877925	1.875114
C	10.158288	-0.940909	0.676153
H	9.111812	-1.430406	-1.143389
C	8.783563	-0.598501	2.624413
H	6.662986	-0.864256	2.341852
C	10.048652	-0.632325	2.033513
H	11.134842	-0.964028	0.199271
H	8.681934	-0.368155	3.681966
H	10.936581	-0.421579	2.622898
C	6.603682	-2.529247	-1.201049

C	7.211587	-3.754215	-0.881751
C	6.017099	-2.371439	-2.467426
C	7.238444	-4.790411	-1.813290
H	7.660747	-3.886371	0.097405
C	6.032847	-3.419626	-3.385312
H	5.553022	-1.424562	-2.723878
C	6.646665	-4.633476	-3.068342
H	7.713759	-5.731425	-1.548335
H	5.575651	-3.278486	-4.361445
H	6.664285	-5.445497	-3.789824
C	-4.986269	3.467479	-0.880945
C	-3.635122	3.018788	-0.935814
C	-5.296867	4.812506	-1.184527
C	-4.304062	5.687915	-1.596886
H	-6.317009	5.167273	-1.114166
H	-4.570734	6.715174	-1.833270
C	3.388325	3.697157	0.749531
C	3.634100	5.056434	1.048009
C	2.061543	3.182713	0.809132
C	2.599881	5.885634	1.454874
H	4.636517	5.458929	0.979014
H	2.816832	6.925371	1.687532
C	5.524588	0.705718	0.050292
H	6.504751	1.158734	0.013524
C	4.162285	-1.310553	-0.068095
H	4.116250	-2.385474	-0.165909
C	5.412369	-0.680024	-0.091523
C	-2.980731	5.252844	-1.732974
H	-2.209546	5.929479	-2.090109
C	-2.671978	3.942023	-1.403159
H	-1.650685	3.601430	-1.531309
C	1.298912	5.388340	1.589696
H	0.494938	6.029148	1.940667
C	1.054468	4.061678	1.268211
H	0.050543	3.673431	1.397960

ν-DABNA_radical_3 (S_0, C_1 symmetry)

E(B3LYP) = -2865.036667 hartree

H(B3LYP) = -2864.055589 hartree

B	-4.300361	-0.388530	0.320210
B	0.770416	-1.515933	-0.349593
N	-3.544312	2.341628	-0.241664
N	1.192822	1.343195	-0.266005
N	3.168953	-3.116241	-0.152879
N	-7.133115	-0.942763	0.249778
N	6.001297	0.817888	0.240613
C	2.319673	0.507912	-0.157852
C	-0.131944	0.873531	-0.238218
C	-0.406693	-0.527245	-0.210933
C	2.148830	-0.903340	-0.207653
C	-1.183757	1.801866	-0.248544
C	-1.749454	-0.881507	-0.012790
C	-2.830710	0.009263	0.073240
C	-2.518442	1.384153	-0.143092
C	-4.911672	2.020035	-0.266608
C	-5.327979	0.685191	0.008244
H	-0.962514	2.853409	-0.339889
H	-1.971619	-1.935460	0.081060
C	-6.715688	0.366365	-0.027287
C	-5.863242	3.022949	-0.560587
C	3.307799	-1.720939	-0.108426
C	-7.673657	1.358315	-0.347529
H	-8.734209	1.145217	-0.386618
C	-7.171308	2.610585	-0.583451
H	-5.578472	4.045235	-0.773863
C	-3.181068	3.726025	-0.412089
C	-3.073401	4.555791	0.706578
C	-2.948579	4.238724	-1.691538
C	-2.732784	5.899537	0.544274
H	-3.259491	4.141948	1.693107

C	-2.608184	5.582694	-1.849441
H	-3.037289	3.580714	-2.550750
C	-2.500227	6.414293	-0.732607
H	-2.650577	6.543398	1.415622
H	-2.428828	5.979502	-2.844868
H	-2.236342	7.460911	-0.857427
C	1.416814	2.765389	-0.340680
C	1.474381	3.530702	0.827275
C	1.584087	3.374067	-1.586945
C	1.699224	4.905462	0.746104
H	1.344490	3.042026	1.788145
C	1.807910	4.749420	-1.664011
H	1.538680	2.764244	-2.484308
C	1.865933	5.516180	-0.498552
H	1.747146	5.497796	1.655585
H	1.938649	5.220507	-2.634389
H	2.042873	6.586482	-0.559784
C	-8.532697	-1.249185	0.091870
C	-9.419395	-1.055571	1.155154
C	-8.999658	-1.737429	-1.130802
C	-10.773516	-1.351572	0.992633
H	-9.040615	-0.675036	2.099057
C	-10.354608	-2.033154	-1.289226
H	-8.297463	-1.881162	-1.946502
C	-11.242502	-1.840555	-0.228797
H	-11.461117	-1.200095	1.820153
H	-10.715375	-2.412811	-2.241165
H	-12.297046	-2.070633	-0.353579
C	4.346825	-3.918628	0.062978
C	5.169750	-4.263970	-1.012740
C	4.663057	-4.349258	1.353883
C	6.307824	-5.041580	-0.794948
H	4.911449	-3.920246	-2.009821
C	5.801745	-5.127476	1.567743
H	4.013617	-4.071725	2.178771
C	6.624972	-5.474275	0.494496
H	6.947145	-5.307008	-1.632308
H	6.045190	-5.461418	2.572607
H	7.511960	-6.078966	0.662276
C	7.114379	0.272685	-0.455296
C	8.354290	0.121591	0.186255
C	6.992824	-0.118063	-1.798913
C	9.446360	-0.398474	-0.506085
H	8.454886	0.413704	1.226699
C	8.085604	-0.653697	-2.477399
H	6.039321	0.001943	-2.303224
C	9.320273	-0.793340	-1.839432
H	10.398215	-0.507789	0.007392
H	7.973041	-0.948860	-3.517588
H	10.172218	-1.203681	-2.374231
C	6.184183	1.935861	1.099125
C	7.006090	3.006710	0.712026
C	5.550457	1.984023	2.351591
C	7.195078	4.092635	1.564778
H	7.493504	2.980418	-0.257377
C	5.731681	3.082166	3.189905
H	4.919594	1.156473	2.659704
C	6.557638	4.141070	2.806292
H	7.835227	4.912176	1.248201
H	5.234877	3.100825	4.156655
H	6.703216	4.991804	3.466050
C	-6.276638	-1.951133	0.736117
C	-4.874259	-1.729593	0.837081
C	-6.829739	-3.187674	1.138028
C	-6.022899	-4.172230	1.688056
H	-7.891691	-3.371889	1.036586
H	-6.473301	-5.112087	1.997943
C	1.959388	-3.772903	-0.456744
C	1.964666	-5.176219	-0.623663
C	0.747359	-3.041129	-0.612127
C	0.808620	-5.844973	-0.996611
H	2.876573	-5.741237	-0.479208

H	0.841422	-6.923916	-1.127302
C	4.578971	-1.152028	0.062465
H	5.461176	-1.766153	0.171316
C	3.594269	1.074440	-0.032166
H	3.738084	2.145117	-0.022299
C	4.711455	0.239079	0.088974
C	-4.652443	-3.952995	1.867045
H	-4.026681	-4.710835	2.329905
C	-4.107231	-2.750429	1.443160
H	-3.049769	-2.574163	1.604991
C	-0.378595	-5.141274	-1.227115
H	-1.275571	-5.660366	-1.552961
C	-0.389409	-3.768242	-1.032561
H	-1.304573	-3.223705	-1.235831

ν-DABNA_radical_4 (S_0, C_1 symmetry)

E(B3LYP) = -3151.491673 hartree

H(B3LYP) = -3150.407683 hartree

B	2.951714	2.370763	0.292267
B	-2.205806	1.834223	-0.420374
N	3.075982	-0.516959	-0.001708
N	-1.731648	-1.006815	-0.161097
N	-4.975671	2.636354	-0.274262
N	5.598138	3.651049	0.343320
N	7.947286	-0.496151	-0.186592
N	-6.476784	-1.950234	0.330143
C	-3.062159	-0.551439	-0.096285
C	-0.614924	-0.154336	-0.159990
C	-0.782081	1.263852	-0.230653
C	-3.330124	0.840032	-0.223216
C	0.668411	-0.712453	-0.092365
C	0.380697	2.025136	-0.067315
C	1.684994	1.521494	0.083450
C	1.811053	0.098630	-0.007074
C	4.279813	0.199647	0.028741
C	4.253455	1.601091	0.177685
H	0.779849	-1.784952	-0.099636
H	0.266317	3.099365	-0.053647
C	5.500593	2.301522	0.204555
C	5.510122	-0.492904	-0.065030
C	-4.683831	1.269421	-0.156667
C	6.721420	1.604324	0.065849
H	7.644383	2.172054	0.060476
C	6.722928	0.209489	-0.059490
H	5.534988	-1.570402	-0.148876
C	3.143822	-1.957546	-0.057853
C	3.185983	-2.694297	1.128376
C	3.179832	-2.609182	-1.293137
C	3.265466	-4.086588	1.077096
H	3.157843	-2.171058	2.079496
C	3.259861	-4.001518	-1.339285
H	3.147930	-2.021060	-2.205284
C	3.302237	-4.741128	-0.155709
H	3.300753	-4.658357	2.000271
H	3.292507	-4.507133	-2.300229
H	3.366707	-5.824998	-0.194203
C	-1.509469	-2.431563	-0.157208
C	-1.367460	-3.118889	1.051299
C	-1.447640	-3.123435	-1.369282
C	-1.164133	-4.499352	1.044806
H	-1.421554	-2.567215	1.984924
C	-1.243374	-4.503981	-1.371494
H	-1.562200	-2.574300	-2.299091
C	-1.101988	-5.193229	-0.165448
H	-1.058219	-5.032285	1.985560
H	-1.197195	-5.040162	-2.315396
H	-0.946240	-6.268536	-0.168392
C	-6.338045	3.057065	-0.060931
C	-7.244222	3.078709	-1.124794
C	-6.748218	3.442227	1.217770

C	-8.561017	3.486362	-0.906780
H	-6.910812	2.775350	-2.112649
C	-8.065473	3.850964	1.431499
H	-6.031331	3.419612	2.033107
C	-8.972848	3.873387	0.370326
H	-9.264540	3.499895	-1.734517
H	-8.381834	4.150625	2.426791
H	-9.998490	4.190246	0.538083
C	8.050589	-1.594037	-1.085549
C	7.504657	-1.511192	-2.376638
C	8.708032	-2.772332	-0.698351
C	7.609004	-2.588826	-3.253845
H	7.004997	-0.598515	-2.685706
C	8.823595	-3.838118	-1.589144
H	9.127813	-2.843779	0.300046
C	8.272070	-3.756504	-2.869399
H	7.183809	-2.506337	-4.250858
H	9.337385	-4.742388	-1.273219
H	8.359533	-4.591042	-3.559390
C	9.078799	-0.105030	0.581820
C	10.357303	-0.076361	0.002181
C	8.935140	0.253588	1.931816
C	11.465108	0.293738	0.762025
H	10.475387	-0.343407	-1.043101
C	10.046512	0.640793	2.678096
H	7.951335	0.228806	2.389327
C	11.318300	0.658581	2.102021
H	12.447172	0.311159	0.296541
H	9.915936	0.917965	3.720862
H	12.183164	0.954692	2.688795
C	-7.702404	-1.799836	-0.374878
C	-8.928862	-2.025002	0.270636
C	-7.705137	-1.432713	-1.730537
C	-10.126859	-1.894087	-0.429425
H	-8.935688	-2.303250	1.319640
C	-8.908781	-1.286986	-2.417185
H	-6.760506	-1.264204	-2.237503
C	-10.126827	-1.520754	-1.774834
H	-11.066580	-2.072572	0.086937
H	-8.891452	-1.004040	-3.466650
H	-11.062915	-1.414236	-2.315718
C	-6.309867	-3.042675	1.225337
C	-6.744219	-4.329492	0.869313
C	-5.715727	-2.848658	2.482779
C	-6.595313	-5.392810	1.757767
H	-7.198578	-4.487953	-0.103546
C	-5.555258	-3.921397	3.357604
H	-5.385458	-1.854435	2.766258
C	-5.997028	-5.198482	3.004543
H	-6.938089	-6.382143	1.465720
H	-5.095852	-3.752385	4.328223
H	-5.878070	-6.030830	3.692481
C	4.477930	4.402155	0.540775
C	3.128742	3.892012	0.581916
C	4.721318	5.789504	0.748843
C	3.686531	6.659410	1.036094
H	5.751780	6.126884	0.691733
H	3.886817	7.714969	1.201336
C	-4.023868	3.610305	-0.636712
C	-4.454935	4.934119	-0.880105
C	-2.646918	3.272684	-0.775920
C	-3.557388	5.897340	-1.314848
H	-5.494703	5.204782	-0.748018
H	-3.916268	6.905952	-1.504728
C	-5.722229	0.349311	0.053116
H	-6.750382	0.670428	0.137461
C	-4.103920	-1.472468	0.062419
H	-3.914703	-2.534196	0.125807
C	-5.425011	-1.013114	0.146981
C	2.375774	6.165353	1.133133
H	1.558143	6.836356	1.384066
C	2.117871	4.812181	0.910626

H	1.095317	4.467215	1.021092
C	-2.213454	5.573320	-1.533177
H	-1.518439	6.318741	-1.909236
C	-1.785504	4.282672	-1.262095
H	-0.749096	4.029206	-1.455417

DABNA-1_radical (S_0, C_1 symmetry)

E(B3LYP) = -1058.580527 hartree

H(B3LYP) = -1058.223425 hartree

B	1.400666	0.397123	-0.037004
N	-1.477326	0.024693	-0.009729
N	2.905631	-2.119923	-0.189652
C	1.550543	-2.145512	-0.178524
C	0.737564	-0.967158	-0.095470
C	-0.664408	-1.109423	-0.078067
C	-1.252561	-2.403293	-0.122747
C	-0.442720	-3.532824	-0.213295
C	0.943441	-3.424315	-0.250580
H	-2.328043	-2.521539	-0.095415
H	-0.911663	-4.512256	-0.256230
H	1.585686	-4.295857	-0.322590
C	3.572640	-0.938933	-0.041292
C	4.989363	-1.058253	0.014685
C	2.951344	0.355334	0.092925
C	5.788550	0.045428	0.245974
H	5.409840	-2.051509	-0.109518
C	3.806796	1.439007	0.362441
C	5.192442	1.301989	0.439024
H	6.869175	-0.060459	0.295698
H	5.810872	2.170548	0.650750
C	-0.976884	1.338133	-0.075132
C	0.428113	1.592301	-0.133009
C	-1.895017	2.415250	-0.097128
C	0.822724	2.941715	-0.300509
C	-1.446538	3.717951	-0.225577
H	-2.958785	2.228291	-0.028403
C	-0.076976	3.992025	-0.348324
H	-2.171365	4.527738	-0.247273
H	0.270729	5.012787	-0.479840
C	-2.905670	-0.164352	0.091189
C	-3.503113	-0.257523	1.350211
C	-3.681866	-0.257877	-1.067022
C	-4.882693	-0.445178	1.449387
H	-2.884362	-0.182563	2.239408
C	-5.060820	-0.446105	-0.962555
H	-3.200469	-0.181840	-2.037456
C	-5.662241	-0.539599	0.294591
H	-5.346899	-0.518083	2.428864
H	-5.663802	-0.519424	-1.863231
H	-6.735825	-0.685866	0.373963
H	3.383608	2.420947	0.545295
H	1.877769	3.157354	-0.420503

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*m*CP (S_0, C_2 symmetry)

E(B3LYP) = -1264.792563 hartree

H(B3LYP) = -1264.353956 hartree

N	0.31171	2.41889	0.41989
N	-0.31171	-2.41889	0.41989
C	0.00000	0.00000	0.43462
C	-0.15162	-1.20304	1.13342
C	-0.15991	-1.20145	2.53436
C	0.00000	0.00000	3.22328
C	0.15991	1.20145	2.53436
C	0.15162	1.20304	1.13342
H	0.00000	0.00000	-0.64976
H	-0.30296	-2.13416	3.06979
H	0.00000	0.00000	4.30954
H	0.30296	2.13416	3.06979

C	-0.46986	3.57052	0.58084
C	1.28005	2.67523	-0.56059
C	-1.57150	3.78768	1.41300
C	0.00000	4.57237	-0.30580
C	2.30287	1.85061	-1.03674
C	1.11658	4.00274	-1.03113
C	-2.18803	5.03626	1.36014
H	-1.94078	3.01111	2.07468
C	-0.63769	5.81794	-0.33876
C	3.15301	2.36948	-2.01124
H	2.43783	0.84233	-0.65969
C	1.98409	4.49884	-2.01127
C	-1.72682	6.04522	0.49751
H	-3.04555	5.22918	1.99908
H	-0.28851	6.59575	-1.01288
C	2.99644	3.67797	-2.49933
H	3.95442	1.74620	-2.39842
H	1.87018	5.51415	-2.38214
H	-2.22877	7.00839	0.48146
H	3.67484	4.05118	-3.26117
C	-1.28005	-2.67523	-0.56059
C	0.46986	-3.57052	0.58084
C	-2.30287	-1.85061	-1.03674
C	-1.11658	-4.00274	-1.03113
C	1.57150	-3.78768	1.41300
C	0.00000	-4.57237	-0.30580
C	-3.15301	-2.36948	-2.01124
H	-2.43783	-0.84233	-0.65969
C	-1.98409	-4.49884	-2.01127
C	2.18803	-5.03626	1.36014
H	1.94078	-3.01111	2.07468
C	0.63769	-5.81794	-0.33876
C	-2.99644	-3.67797	-2.49933
H	-3.95442	-1.74620	-2.39842
H	-1.87018	-5.51415	-2.38214
C	1.72682	-6.04522	0.49751
H	3.04555	-5.22918	1.99908
H	0.28851	-6.59575	-1.01288
H	-3.67484	-4.05118	-3.26117
H	2.22877	-7.00839	0.48146

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*m*CP_radical (S_0, C_1 symmetry)

E(B3LYP) = -747.833796 hartree

H(B3LYP) = -747.574581 hartree

N	-0.273419	-0.020810	0.002062
C	-2.352038	-0.814201	-1.021953
C	-3.726372	-0.815137	-0.985527
C	-4.514641	-0.135096	-0.082897
C	-3.835864	0.617746	0.888462
C	-2.440909	0.642915	0.923135
C	-1.690202	-0.064762	-0.026903
H	-1.781443	-1.341071	-1.780984
H	-5.599848	-0.175307	-0.105773
H	-4.401396	1.170862	1.634465
H	-1.922345	1.201732	1.695447
C	0.513185	1.138334	-0.040601
C	0.579496	-1.131534	0.043796
C	0.119358	2.476260	-0.125705
C	1.881314	0.766419	-0.021328
C	0.263478	-2.490434	0.123604
C	1.923659	-0.680276	0.034712
C	1.120067	3.444921	-0.171235
H	-0.928756	2.754040	-0.162103
C	2.866420	1.759675	-0.067123
C	1.318640	-3.399104	0.175495
H	-0.766792	-2.829416	0.150468
C	2.964597	-1.614391	0.088252
C	2.480775	3.095147	-0.138375
H	0.838356	4.492389	-0.236646
H	3.919202	1.489787	-0.051833

C	2.656744	-2.970247	0.154612
H	1.098132	-4.461386	0.236313
H	3.999965	-1.283643	0.082225
H	3.236365	3.874765	-0.173363
H	3.456255	-3.704500	0.194830

NPD (S_0, C_2 symmetry)

E(B3LYP) = -1805.486483 hartree

H(B3LYP) = -1804.818189 hartree

N	1.481512	-4.780387	0.459840
N	-1.481512	4.780387	0.459840
C	-1.189372	2.632869	1.642776
C	-0.772036	1.305669	1.639633
C	-0.217338	0.707626	0.494696
C	-0.094073	1.512050	-0.652643
C	-0.496162	2.842186	-0.657142
C	-1.053959	3.426061	0.492101
H	-1.636273	3.055787	2.536621
H	-0.920529	0.708670	2.535315
H	0.361968	1.099634	-1.548364
H	-0.370271	3.444270	-1.551687
C	0.217338	-0.707626	0.494696
C	0.772036	-1.305669	1.639633
C	0.094073	-1.512050	-0.652643
C	1.189372	-2.632869	1.642776
H	0.920529	-0.708670	2.535315
C	0.496162	-2.842186	-0.657142
H	-0.361968	-1.099634	-1.548364
C	1.053959	-3.426061	0.492101
H	1.636273	-3.055787	2.536621
H	0.370271	-3.444270	-1.551687
C	1.395756	-5.606044	1.611015
C	0.269522	-5.542027	2.451900
C	2.412548	-6.525935	1.913140
C	0.177673	-6.367459	3.569540
H	-0.530228	-4.845323	2.221867
C	2.301144	-7.359776	3.025203
H	3.287591	-6.584893	1.274575
C	1.189372	-7.284976	3.864647
H	-0.700854	-6.301137	4.206353
H	3.099577	-8.065624	3.239401
H	1.109552	-7.932125	4.733337
C	-1.395756	5.606044	1.611015
C	-2.412548	6.525935	1.913140
C	-0.269522	5.542027	2.451900
C	-2.301144	7.359776	3.025203
H	-3.287591	6.584893	1.274575
C	-0.177673	6.367459	3.569540
H	0.530228	4.845323	2.221867
C	-1.189372	7.284976	3.864647
H	-3.099577	8.065624	3.239401
H	0.700854	6.301137	4.206353
H	-1.109552	7.932125	4.733337
C	2.252014	-5.216327	-0.665163
C	1.824387	-6.344369	-1.441087
C	3.400923	-4.530881	-1.015363
C	2.634811	-6.756005	-2.551888
C	0.624590	-7.057084	-1.173077
C	4.177858	-4.930322	-2.125080
H	3.703680	-3.673714	-0.421615
C	2.225109	-7.877174	-3.323337
C	3.811189	-6.026671	-2.870927
C	0.254635	-8.134135	-1.947671
H	-0.002996	-6.740294	-0.347899
H	5.076394	-4.372354	-2.373720
C	1.064659	-8.555041	-3.029057
H	2.847870	-8.187213	-4.159250
H	4.411646	-6.345442	-3.719379
H	-0.668380	-8.664233	-1.728907
H	0.763552	-9.409723	-3.628825

C	-2.252014	5.216327	-0.665163
C	-1.824387	6.344369	-1.441087
C	-3.400923	4.530881	-1.015363
C	-2.634811	6.756005	-2.551888
C	-0.624590	7.057084	-1.173077
C	-4.177858	4.930322	-2.125080
H	-3.703680	3.673714	-0.421615
C	-2.225109	7.877174	-3.323337
C	-3.811189	6.026671	-2.870927
C	-0.254635	8.134135	-1.947671
H	0.002996	6.740294	-0.347899
H	-5.076394	4.372354	-2.373720
C	-1.064659	8.555041	-3.029057
H	-2.847870	8.187213	-4.159250
H	-4.411646	6.345442	-3.719379
H	0.668380	8.664233	-1.728907
H	-0.763552	9.409723	-3.628825

NPD_radical_1 (S_0, C_1 symmetry)

E(B3LYP) = -1573.810849 hartree

H(B3LYP) = -1573.241196 hartree

N	-4.192368	-0.484941	-0.225227
N	5.758980	-0.832638	0.116810
C	3.623400	-1.859792	0.311946
C	2.241683	-1.824188	0.277820
C	1.541520	-0.635005	-0.024598
C	2.311214	0.516758	-0.293180
C	3.695173	0.502029	-0.230138
C	4.400004	-0.690498	0.094056
H	4.152300	-2.779916	0.540951
H	1.683681	-2.727821	0.505657
H	1.809538	1.431485	-0.596355
H	4.253871	1.394101	-0.493584
C	0.067284	-0.602452	-0.079569
C	-0.680813	-1.726782	-0.476042
C	-0.655666	0.556607	0.262615
C	-2.068934	-1.699912	-0.533581
H	-0.164870	-2.629231	-0.791208
C	-2.043075	0.590342	0.223519
H	-0.122122	1.437465	0.608162
C	-2.778037	-0.539875	-0.176356
H	-2.610361	-2.577674	-0.870214
H	-2.570880	1.492053	0.517202
C	-4.985268	-1.641146	0.008360
C	-4.653646	-2.535235	1.042126
C	-6.131677	-1.891299	-0.761575
C	-5.443808	-3.656115	1.283337
H	-3.777469	-2.343936	1.653437
C	-6.925357	-3.007711	-0.499656
H	-6.397450	-1.209497	-1.562580
C	-6.586849	-3.900371	0.517717
H	-5.170096	-4.335349	2.086605
H	-7.809894	-3.182754	-1.106585
H	-7.204819	-4.771730	0.714142
C	-4.812471	0.696699	-0.745709
C	-5.755510	1.428161	0.049426
C	-4.483830	1.138908	-2.013973
C	-6.364874	2.597121	-0.518555
C	-6.096850	1.060544	1.378909
C	-5.072625	2.303720	-2.553922
H	-3.762764	0.574342	-2.597341
C	-7.306456	3.326959	0.256512
C	-6.001962	3.011961	-1.827640
C	-7.007909	1.796676	2.103313
H	-5.628629	0.188796	1.821201
H	-4.795687	2.625225	-3.554071
C	-7.625430	2.937007	1.536678
H	-7.768663	4.207742	-0.183040
H	-6.466658	3.903016	-2.242419
H	-7.253870	1.501146	3.119628

H	-8.346307	3.505634	2.117847
C	6.616035	0.170023	0.414634
C	7.995447	0.016175	-0.033492
C	6.300370	1.294699	1.213048
C	8.961078	1.015819	0.298973
C	8.397958	-1.091696	-0.811189
C	7.269897	2.249046	1.547723
H	5.299616	1.383330	1.620970
C	10.293415	0.866803	-0.166900
C	8.570982	2.130708	1.092766
C	9.704861	-1.214604	-1.244223
H	7.654278	-1.842933	-1.052543
H	6.991813	3.088017	2.180414
C	10.660042	-0.225807	-0.924061
H	11.023212	1.632422	0.086123
H	9.315943	2.879221	1.350730
H	10.000037	-2.077174	-1.835773
H	11.684081	-0.328589	-1.273148

NPD_radical_2 (S_0, C_1 symmetry)

E(B3LYP) = -1420.164112 hartree

H(B3LYP) = -1419.643981 hartree

N	-3.081504	0.498976	0.234156
N	6.678007	-1.369052	-0.366401
C	4.844704	0.308853	-0.381210
C	3.482703	0.539156	-0.314752
C	2.555782	-0.509196	-0.113847
C	3.074633	-1.821991	-0.018836
C	4.429208	-2.070131	-0.112408
C	5.373477	-1.012467	-0.263715
H	5.518201	1.133943	-0.586738
H	3.114322	1.550459	-0.462164
H	2.395642	-2.652172	0.152212
H	4.820014	-3.080304	-0.039058
C	1.108630	-0.245461	-0.026152
C	0.612311	0.967984	0.488023
C	0.156962	-1.194795	-0.448479
C	-0.750089	1.221687	0.583126
H	1.306636	1.712517	0.866717
C	-1.206261	-0.946296	-0.372168
H	0.490856	-2.130627	-0.886888
C	-1.688093	0.269044	0.147123
H	-1.094201	2.156861	1.011849
H	-1.911730	-1.689688	-0.728995
C	-3.623864	1.809988	0.143972
C	-3.131184	2.722439	-0.806068
C	-4.684706	2.203338	0.974203
C	-3.680125	3.998327	-0.906385
H	-2.320945	2.424528	-1.464069
C	-5.238058	3.477641	0.853236
H	-5.073335	1.508535	1.711321
C	-4.738997	4.385568	-0.081093
H	-3.285164	4.688984	-1.646991
H	-6.060275	3.762101	1.504692
H	-5.169558	5.378902	-0.168427
C	7.715047	-0.494461	-0.150301
C	8.931003	-0.766470	-0.829136
C	7.698224	0.587676	0.770069
C	10.047266	0.037498	-0.647691
H	8.949979	-1.613626	-1.507750
C	8.833161	1.366676	0.967266
H	6.805570	0.770509	1.359120
C	10.007284	1.110664	0.251587
H	10.960950	-0.177552	-1.195755
H	8.805761	2.177686	1.690795
H	10.887650	1.728100	0.406672
C	-3.927477	-0.579548	0.651698
C	-5.004403	-1.018977	-0.186582
C	-3.690297	-1.204094	1.862301
C	-5.839225	-2.088953	0.281064

C	-5.268264	-0.458806	-1.465532
C	-4.504308	-2.271372	2.302051
H	-2.865502	-0.860085	2.479068
C	-6.914732	-2.529555	-0.536879
C	-5.563508	-2.697498	1.534455
C	-6.314920	-0.916884	-2.234489
H	-4.631949	0.337933	-1.833309
H	-4.294789	-2.741144	3.258977
C	-7.152019	-1.956991	-1.765107
H	-7.546489	-3.336443	-0.172990
H	-6.200020	-3.511248	1.872930
H	-6.499116	-0.477933	-3.211264
H	-7.977218	-2.305264	-2.380313

NPD_radical_3 (S_0, C_1 symmetry)

E(B3LYP) = -1133.708307 hartree

H(B3LYP) = -1133.291367 hartree

N	-0.983942	0.467128	0.253076
C	6.946599	0.611565	-0.460407
C	5.559848	0.791420	-0.365731
C	4.696952	-0.297298	-0.141952
C	5.253987	-1.583355	-0.016695
C	6.637010	-1.788675	-0.113443
C	7.419787	-0.675777	-0.330101
H	7.603674	1.458153	-0.641382
H	5.142989	1.787268	-0.493743
H	4.603376	-2.430715	0.184671
H	7.057645	-2.785143	-0.007211
C	3.230570	-0.093630	-0.039273
C	2.691769	1.038474	0.594517
C	2.322920	-1.026412	-0.570534
C	1.318217	1.232187	0.700521
H	3.359663	1.763179	1.052264
C	0.948825	-0.836526	-0.482961
H	2.699809	-1.898847	-1.097306
C	0.421612	0.298054	0.156220
H	0.935280	2.105416	1.218314
H	0.271947	-1.562924	-0.921647
C	-1.572742	1.759478	0.241678
C	-1.097854	2.751400	-0.635579
C	-2.660523	2.059899	1.076470
C	-1.691046	4.010930	-0.661253
H	-0.265848	2.527262	-1.295516
C	-3.257481	3.319387	1.029875
H	-3.035337	1.304833	1.759446
C	-2.776841	4.305109	0.167489
H	-1.308752	4.763170	-1.346566
H	-4.099753	3.530470	1.683729
H	-3.241551	5.286419	0.138327
C	-1.781316	-0.666039	0.613630
C	-2.853428	-1.095001	-0.237027
C	-1.501856	-1.357520	1.778146
C	-3.638842	-2.224827	0.171420
C	-3.158262	-0.466006	-1.474275
C	-2.266545	-2.482604	2.158308
H	-0.681487	-1.021635	2.405211
C	-4.708553	-2.655114	-0.659570
C	-3.320440	-2.900942	1.379276
C	-4.197488	-0.915829	-2.258096
H	-2.559115	0.377087	-1.798529
H	-2.023825	-3.003818	3.080199
C	-4.986408	-2.015993	-1.845758
H	-5.302941	-3.507917	-0.339995
H	-3.919430	-3.759365	1.673025
H	-4.412992	-0.423632	-3.202587
H	-5.806582	-2.357288	-2.471579

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benzene_radical (S_0, C_1 symmetry)

E(B3LYP) = -231.561281 hartree

H(B3LYP) = -231.468342 hartree

C	1.214182	0.632581	0.000010
C	-0.000006	1.324735	0.000004
C	-1.214170	0.632605	-0.000016
C	-1.226370	-0.771791	0.000016
C	-0.000010	-1.400162	0.000002
C	1.226377	-0.771778	-0.000017
H	2.154646	1.179101	0.000019
H	0.000022	2.411306	0.000006
H	-2.154658	1.179083	-0.000023
H	-2.162896	-1.323299	0.000010
H	2.162871	-1.323339	-0.000009

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carbzole_radical (S_0, C_1 symmetry)

E(B3LYP) = -516.823712 hartree

H(B3LYP) = -516.650609 hartree

N	0.000008	-1.703411	0.000060
C	1.093076	-0.865580	-0.000055
C	-1.093079	-0.865576	0.000069
C	2.439388	-1.255719	-0.000113
C	0.732339	0.520883	-0.000026
C	-2.439380	-1.255722	0.000064
C	-0.732343	0.520879	0.000090
C	3.419217	-0.259019	-0.000056
H	2.697904	-2.310199	-0.000252
C	1.712549	1.497459	0.000091
C	-3.419217	-0.259021	-0.000003
H	-2.697895	-2.310202	0.000184
C	-1.712555	1.497456	-0.000069
C	3.063146	1.095349	0.000067
H	4.469641	-0.535679	-0.000104
H	1.460000	2.554870	0.000111
C	-3.063151	1.095345	-0.000097
H	-4.469639	-0.535689	0.000020
H	-1.460003	2.554866	-0.000101
H	3.842214	1.852752	0.000201
H	-3.842219	1.852747	-0.000254

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diphenylamine_radical (S_0, C_1 symmetry)

E(B3LYP) = -518.014341 hartree

H(B3LYP) = -517.818275 hartree

N	-0.000012	-1.132632	0.000076
C	1.202565	-0.481646	0.026908
C	1.433848	0.812271	0.573266
C	2.327309	-1.210426	-0.447507
C	2.716207	1.346084	0.605231
H	0.606655	1.359841	1.012091
C	3.597122	-0.653856	-0.437550
H	2.150074	-2.209069	-0.834370
C	3.801407	0.629157	0.087935
H	2.876379	2.327627	1.044165
H	4.438639	-1.221639	-0.825603
H	4.799418	1.057711	0.111765
C	-1.202557	-0.481657	-0.026883
C	-1.433821	0.812278	-0.573182
C	-2.327359	-1.210431	0.447496
H	-0.606613	1.359866	-1.011967
C	-3.597137	-0.653846	0.437467
H	-2.150150	-2.209066	0.834393
H	-4.438715	-1.221595	0.825445
C	-3.801403	0.629173	-0.088049
H	-4.799428	1.057700	-0.111962
C	-2.716164	1.346125	-0.605198
H	-2.876283	2.327700	-1.044097

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naphthalene_radical (S_0, C_1 symmetry)

E(B3LYP/6-31G(d)) = -385.205071 hartree

H(B3LYP/6-31G(d)) = -516.650609 hartree

C	1.228177	-1.412893	0.000060
C	2.477201	0.605365	0.000028
C	-0.014271	-0.763072	0.000021
C	1.302827	1.325094	-0.000015
H	3.435297	1.119680	0.000028
C	0.035727	0.678110	-0.000018
C	-1.274980	-1.418699	0.000017
H	1.329439	2.411949	-0.000048
C	-1.192132	1.393622	-0.000058
C	-2.440515	-0.686427	-0.000024
H	-1.298106	-2.504466	0.000043
C	-2.398475	0.730065	-0.000062
H	-1.161820	2.480933	-0.000090
H	-3.401182	-1.194121	-0.000029
H	-3.327741	1.293350	-0.000096
C	2.451085	-0.820568	0.000067
H	3.376246	-1.390910	0.000101

N-phenyl-1-naphthylamine_radical

(S_0, C_1 symmetry)

E(B3LYP) = -671.661699 hartree

H(B3LYP) = -671.416101 hartree

N	0.712303	-0.700302	0.252395
C	-0.267856	0.219175	0.209722
C	-1.633760	-0.275246	0.044688
C	-0.087349	1.613559	0.407276
C	-2.722899	0.648916	0.041033
C	-1.901892	-1.648792	-0.132508
C	-1.172913	2.495431	0.421386
H	0.910542	1.988377	0.605162
C	-4.041294	0.158336	-0.143826
C	-2.465732	2.036606	0.228903
C	-3.198189	-2.100169	-0.303565
H	-1.064527	-2.337531	-0.125467
H	-0.995158	3.553595	0.594717
C	-4.276439	-1.190381	-0.313335
H	-4.866248	0.866903	-0.148906
H	-3.302821	2.730109	0.235211
H	-3.388324	-3.162383	-0.432060
H	-5.291052	-1.553815	-0.452628
C	2.045717	-0.403694	0.074214
C	2.544380	0.570317	-0.828196
C	2.982768	-1.210630	0.765295
C	3.914805	0.741436	-0.997389
H	1.846095	1.148262	-1.424957
C	4.347807	-1.009411	0.612092
H	2.597745	-1.977185	1.430775
C	4.824325	-0.032022	-0.270239
H	4.277353	1.479888	-1.708079
H	5.048403	-1.625656	1.169572
H	5.893000	0.110963	-0.403414