

Emission Color Tuning and Deep Blue Dopant Materials Based on 1,6-Bis(*N*-phenyl-*p*-R-phenylamino)pyrene

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Experimental Section Aniline, 4-Bromobenzonitrile, 4-Bromofluorobenzene, 4-Bromotoluene, 4-*tert*-Butylbromobenzene, 4-Bromoanisole, diphenylamine, 4-Bromotriphenylamine, and pyrene were purchased and used as received. 4-Bromo-*N*-methyl-*N*-phenylbenzenamine¹ and 1,6-dibromopyrene² were prepared using the method reported in the literature. Electronically-tuned *N*-phenyl-*p*-R-phenylamine (**1R**) is well characterized in literatures.³

Synthesis of 2F. A procedure analogous to the preparation of **2CN** was used, but instead starting from 4-fluoro-*N*-phenylbenzenamine (1.14 g, 6.12 mmol). **2F** was obtained as a pale yellow powder. Yield: 40% (0.64 g). ¹H NMR (CDCl₃): δ 8.08 (d, 2H), 8.07 (d, 2H), 7.89 (d, 2H), 7.76 (d, 2H), 7.17 (t, 4H), 7.05 (m, 4H), 6.96 (d, 4H), 6.90 (m, 6H). ¹³C NMR (CDCl₃): 149.1, 141.3, 129.6, 129.4, 128.3, 128.0, 127.9, 126.7, 126.4, 124.5, 124.4, 123.1, 121.7, 121.4, 116.2, 116.1. HRMS(FAB) calcd for C₄₀H₂₆F₂N₂: 572.2064. Found: 572.2052 [M]⁺. Anal. Calcd for C₄₀H₂₆F₂N₂: C, 83.90; H, 4.58; N, 4.89 Found: C, 84.01; H, 4.62; N, 4.78.

Synthesis of 2H. A procedure analogous to the preparation of **2CN** was used, but instead starting from diphenylamine (1.03 g, 6.12 mmol). **2H** was obtained as a pale yellow powder. Yield: 62% (0.92 g). ¹H NMR (CDCl₃): δ 8.10 (d, 2H), 8.07 (d, 2H), 7.88 (d, 2H), 7.78 (d, 2H), 7.18 (t, 8H), 7.05 (d, 8H), 6.93 (t, 8H). ¹³C NMR (CDCl₃): 148.8, 141.3, 129.7, 129.4, 128.5, 128.2, 127.9, 126.7, 126.3, 123.3, 122.3, 122.0. HRMS(FAB) calcd for C₄₀H₂₈N₂: 536.2252. Found: 537.2261 [M]⁺. Anal. Calcd for C₄₀H₂₈N₂: C, 89.52; H, 5.26; N, 5.22. Found: C, 88.92; H, 5.24; N, 5.18.

Synthesis of 2Me. A procedure analogous to the preparation of **2CN** was used, but instead starting from 4-methyl-*N*-phenylbenzenamine (1.12 g, 6.12 mmol). **2Me** was obtained as a yellow powder. Yield: 63% (0.99 g). ¹H NMR (CDCl₃): δ 8.10 (d, 2H), 8.05 (d, 2H), 7.87 (d, 2H), 7.76 (d, 2H), 7.15 (t, 4H), 6.97-7.02 (m, 12H), 6.89 (t, 2H), 2.27 (s, 6H). ¹³C NMR (CDCl₃): 149.2, 146.3, 141.4, 131.9, 130.2, 129.4, 129.3, 128.5, 128.1, 127.8, 126.7, 126.2, 123.2, 123.0, 121.5, 121.3, 21.0. HRMS(FAB) calcd for C₄₂H₃₂N₂: 564.2565. Found: 564.2514 [M]⁺. Anal. Calcd for C₄₂H₃₂N₂: C,

89.33; H, 5.71; N, 4.96. Found: C, 89.14; H, 5.67; N, 4.82.

Synthesis of 2^tBu. A procedure analogous to the preparation of **2CN** was used, but instead starting from 4-*tert*-butyl-N-phenylbenzenamine (1.38 g, 6.12 mmol). **2^tBu** was obtained as a yellow powder. Yield: 87% (1.57 g). ¹H NMR (CDCl₃): δ 8.13 (d, 2H), 8.08 (d, 2H), 7.90 (d, 2H), 7.81 (d, 2H), 7.21 (d, 4H), 7.18 (t, 4H), 7.03 (d, 8H), 6.91 (t, 2H), 1.29 (s, 18H). ¹³C NMR (CDCl₃): 149.1, 146.0, 145.1, 141.4, 129.6, 129.3, 128.6, 128.3, 127.9, 126.7, 126.3, 126.2, 123.3, 122.3, 121.5, 121.4, 34.4, 31.7. HRMS(FAB) calcd for C₄₈H₄₄N₂: 648.3504. Found: 648.3514 [M]⁺. Anal. Calcd for C₄₈H₄₄N₂: C, 88.85; H, 6.83; N, 4.32. Found: C, 88.71; H, 6.79; N, 4.25.

Synthesis of 2OMe. A procedure analogous to the preparation of **2CN** was used, but instead starting from 4-methoxy-N-phenylbenzenamine (1.22 g, 6.12 mmol). **2OMe** was obtained as a yellow powder. Yield: 75% (1.24 g). ¹H NMR (CDCl₃): δ 8.11 (d, 2H), 8.05 (d, 2H), 7.87 (d, 2H), 7.76 (d, 2H), 7.14 (t, 4H), 7.09 (d, 4H), 6.90 (d, 4H), 6.85 (t, 2H), 6.78 (d, 4H), 3.76 (s, 6H). ¹³C NMR (CDCl₃): 155.6, 149.7, 142.0, 141.6, 129.4, 129.3, 128.3, 127.8, 127.7, 126.7, 126.2, 125.5, 123.2, 120.7, 120.3, 114.8, 55.7. HRMS(FAB) calcd for C₄₂H₃₂N₂O₂: 596.2464. Found: 596.2426 [M]⁺. Anal. Calcd for C₄₂H₃₂N₂O₂: C, 84.54; H, 5.41; N, 4.69. Found: C, 84.27; H, 5.32; N, 4.65.

Synthesis of 2NPh₂. A procedure analogous to the preparation of **2CN** was used, but instead starting from *N*¹,*N*¹,*N*⁴-triphenylbenzene-1,4-diamine (2.06 g, 6.12 mmol). **2NPh₂** was obtained as a yellow powder. Yield: 61% (1.48 g). ¹H NMR (CDCl₃): δ 8.13 (d, 2H), 8.10 (d, 2H), 7.91 (d, 2H), 7.83 (d, 2H), 7.20 (t, 8H), 7.17 (t, 4H), 7.06 (d, 8H), 7.00 (d, 4H), 6.92-6.95 (m, 8H), 6.89 (t, 2H). ¹³C NMR (CDCl₃): 149.0, 148.1, 144.0, 142.3, 141.2, 129.6, 129.3, 128.5, 128.2, 127.8, 126.7, 126.3, 125.8, 123.9, 123.8, 123.3, 122.5, 121.4, 121.3. HRMS(FAB) calcd for C₆₄H₄₆N₄: 870.3722. Found: 870.3704 [M]⁺. Anal. Calcd for C₆₄H₄₆N₄: C, 88.25; H, 5.32; N, 6.43. Found: C, 88.19; H, 5.27; N, 6.31.

Synthesis of 2NMePh. A procedure analogous to the preparation of **2CN** was used, but instead starting from *N*¹-methyl-*N*¹,*N*⁴-diphenylbenzene-1,4-diamine (1.68 g, 6.12 mmol). **2NMePh** was obtained as an orange powder. Yield: 73% (1.51 g). ¹H NMR (CDCl₃): δ 8.14 (d, 2H), 8.09 (d, 2H), 7.91 (d, 2H), 7.82 (d, 2H), 7.21 (t, 4H), 7.17 (t, 4H), 7.05 (d, 4H), 6.99 (d, 4H), 6.93 (d, 8H), 6.88 (t, 2H), 6.84 (t, 2H), 3.26 (s, 6H). ¹³C NMR (CDCl₃): 149.4, 149.2, 143.9, 143.4, 141.3, 129.6, 129.3, 129.3, 128.5, 128.1, 127.8, 126.7, 126.3, 124.3, 123.3, 121.2, 121.1, 120.1, 118.6, 40.5. HRMS(FAB) calcd for C₅₄H₄₂N₄: 746.3409. Found: 746.3436 [M]⁺. Anal. Calcd for C₅₄H₄₂N₄: C, 86.83; H, 5.67; N, 7.50. Found: C, 86.71; H, 5.59; N, 7.42.

Fabrication of the OLED devices. OLED devices were fabricated with **2CN** as the dopant materials. An ITO-coated glass (20 Ω/sq) substrate was first cleaned using conventional procedures. After insertion into a fabrication chamber, the sample was exposed to an UV ozone treatment, and organic layers were deposited onto the ITO layer by thermal evaporation, and LiF and Al were deposited successively onto the underlying organic layers. The characteristics of each OLED device were measured using a photoresearch PR650 spectrometer and a KEITHLEY 306 source measure unit.

Reference

1. Rao, H.; Jin, Y.; Fu, H.; Jiang, Y.; Zhao, Y. *Chem. Eur. J.* **2006**, *12*, 3636.
2. Grimshaw, J.; Trocha-Grimshaw, J. J. *Chem. Soc. Perkin Trans. I* **1972**, 1622.
3. (a) Hartwig, J. F.; Driver, M. S.; Louie, J.; Hamann, B. U.S. Patent 5817877, 1998; *Chem Abstr.* **1998**, *129*, 275692. (b) Wolfe, J. P.; Buchwald, S. L. *J. Org. Chem.* **2000**, *65*, 1144 (c) Kung, A. C.; McIlroy, S. P.; Falvey, D. E. *J. Org. Chem.* **2005**, *70*, 5283. (d) Hill, L. L.; Moore, L. R.; Huang, R.; Craciun, R.; Vincent, A. J.; Dixon, D. A.; Chou, J.; Woltermann, C. J.; Shaughnessy, K. H. *J. Org. Chem.* **2006**, *71*, 5117.

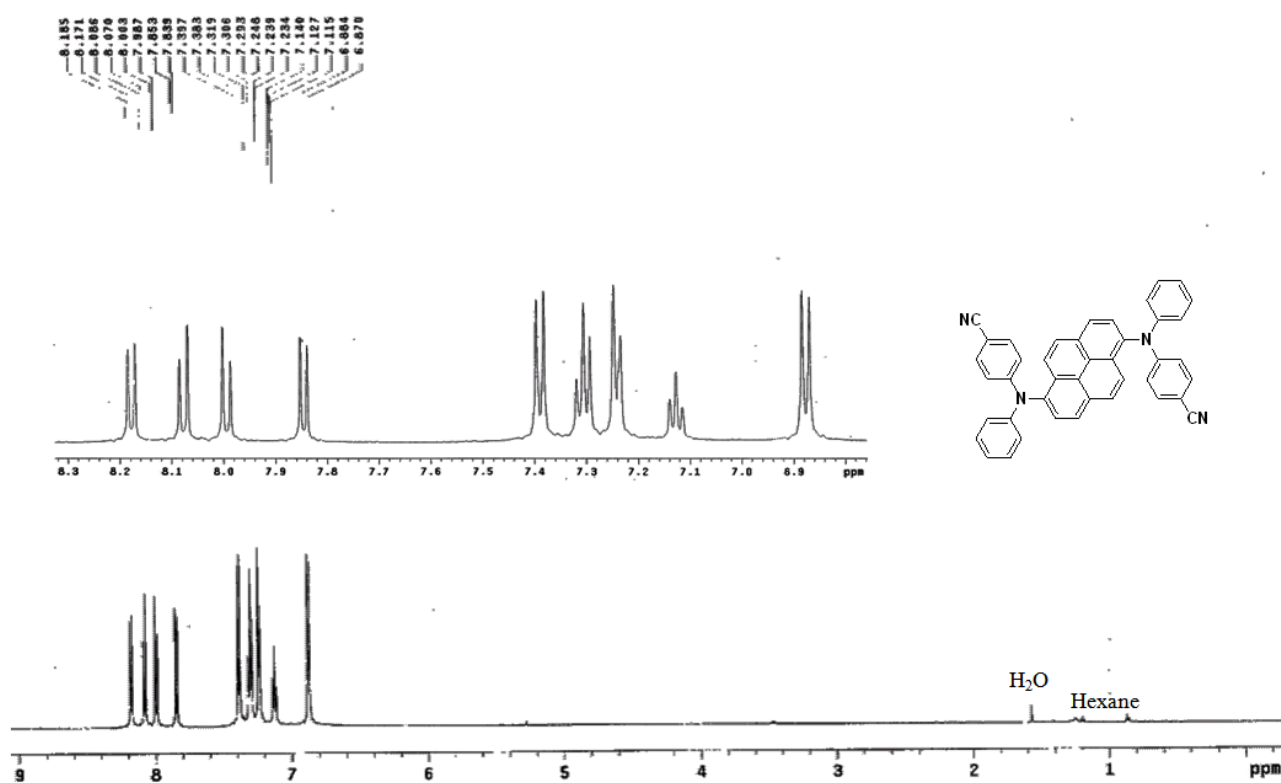


Figure S1 (a). $^1\text{H-NMR}$ spectrum of **2CN** in CDCl_3 .

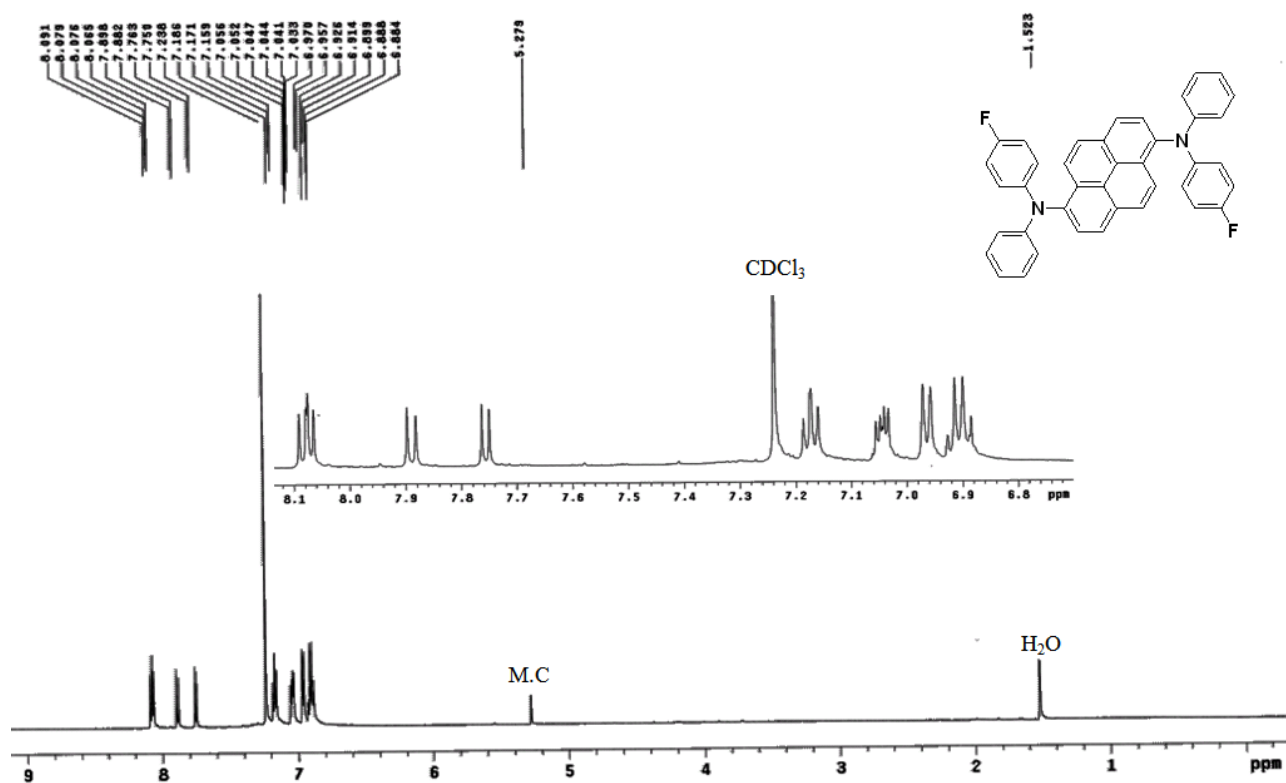


Figure S1 (b). $^1\text{H-NMR}$ spectrum of **2F** in CDCl_3 .

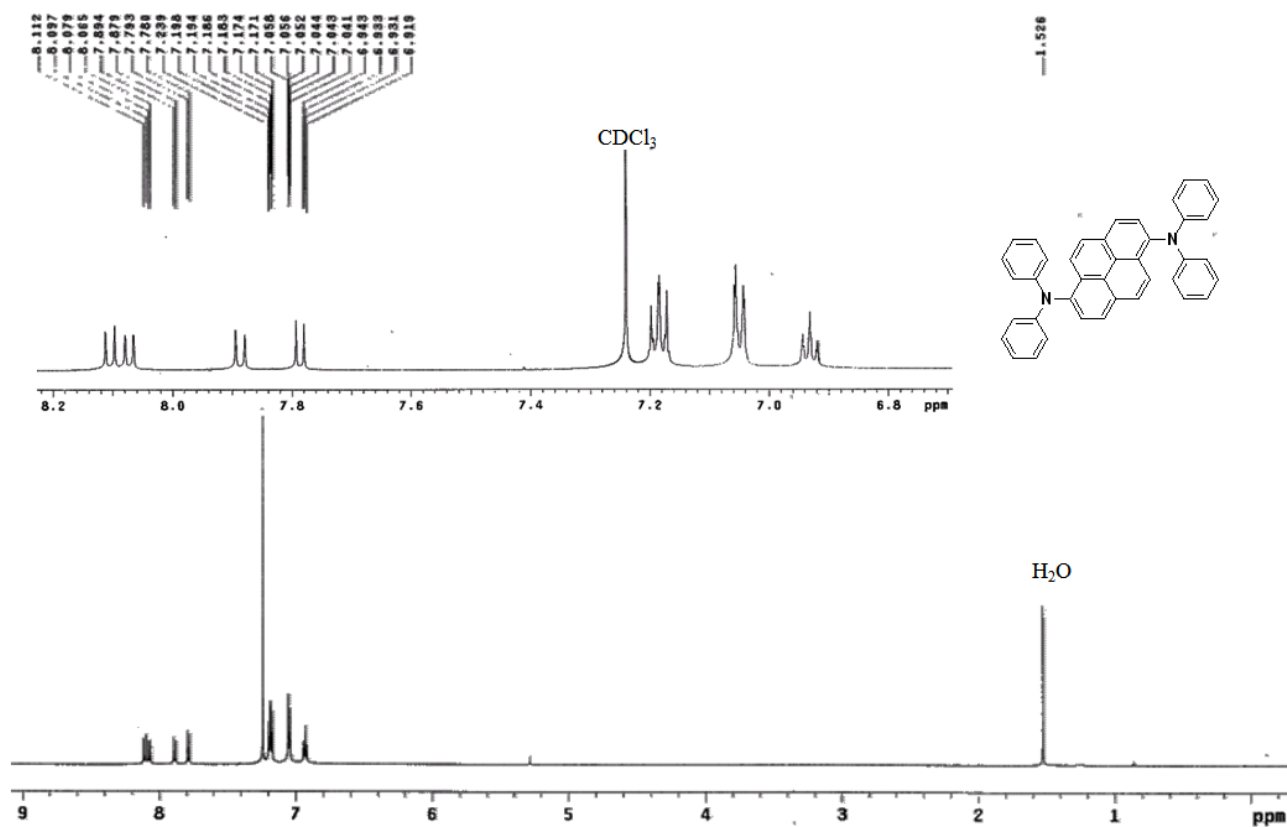


Figure S1 (c). ¹H-NMR spectrum of **2H** in CDCl₃.

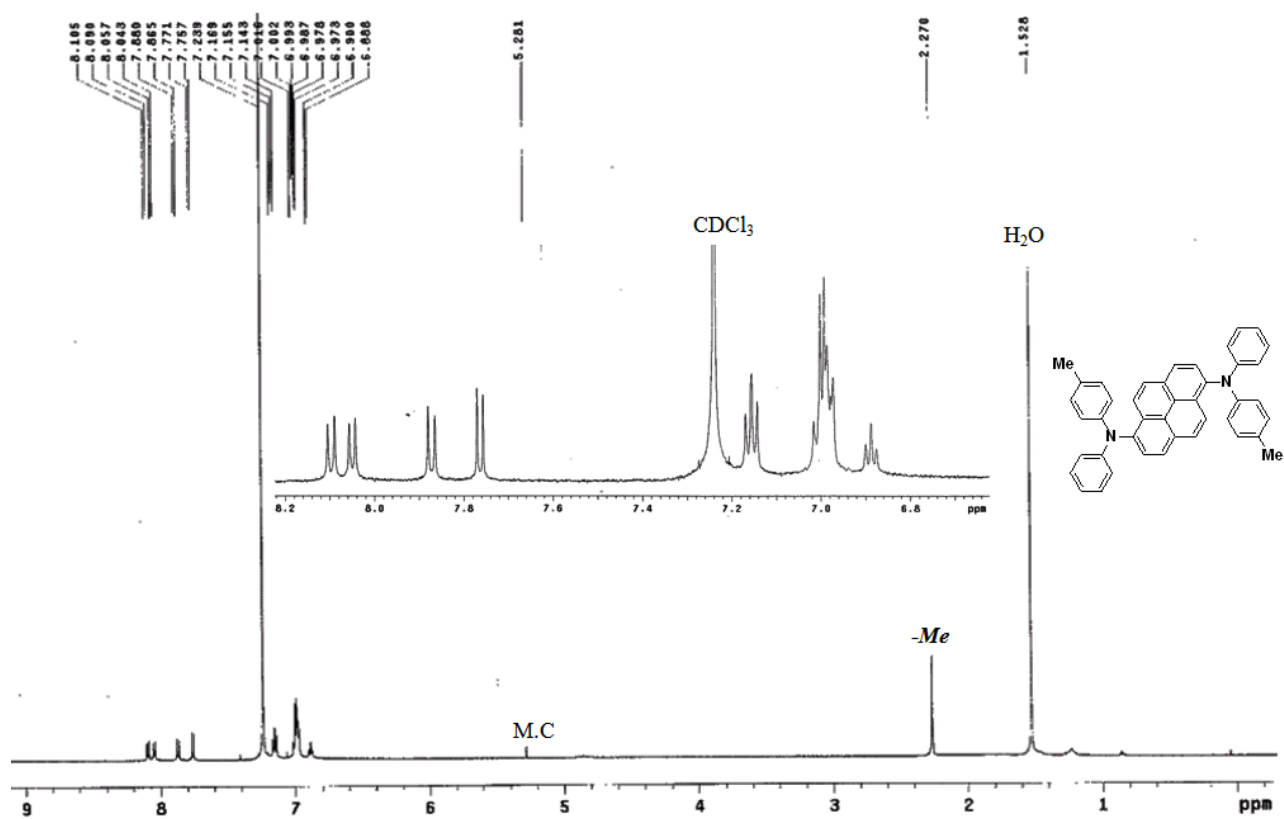


Figure S1 (d). ¹H-NMR spectrum of **2Me** in CDCl₃.

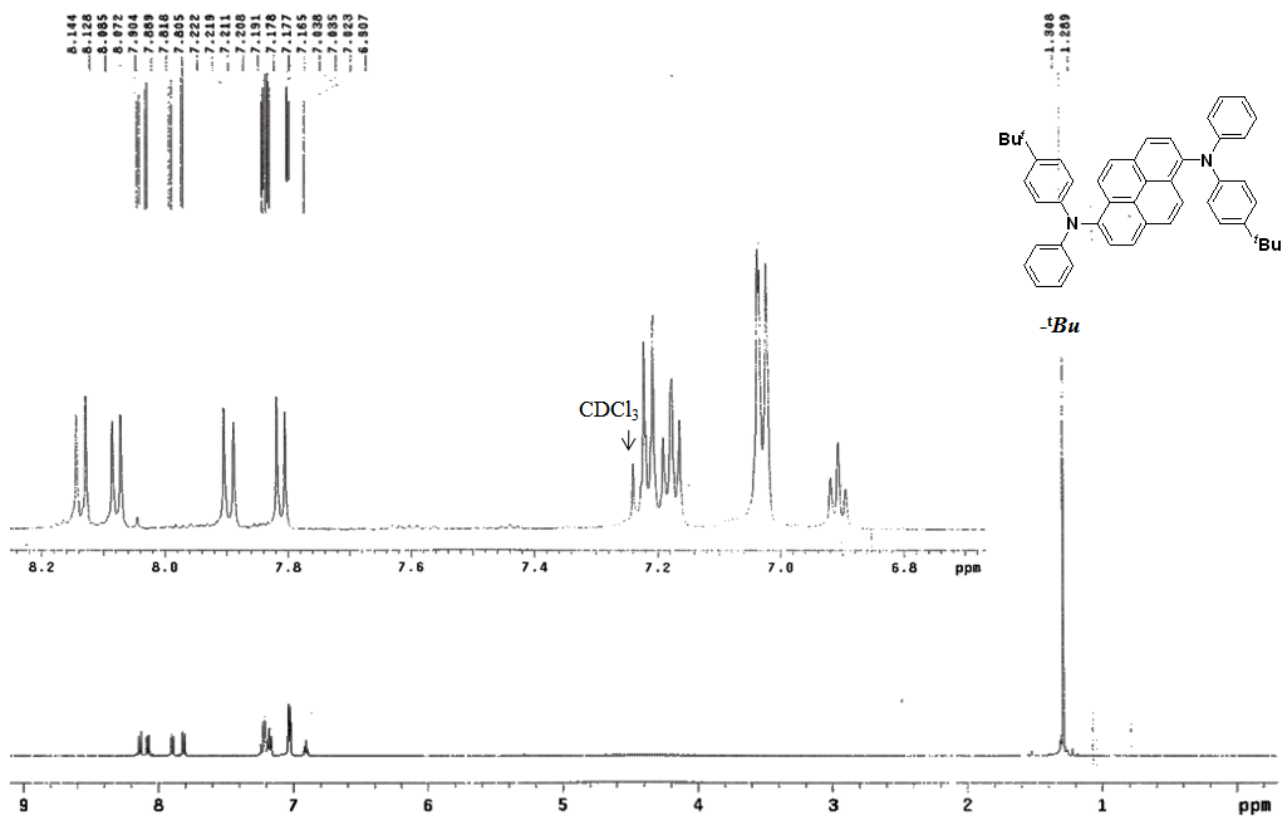


Figure S1 (e). ^1H -NMR spectrum of **2'Bu** in CDCl_3 .

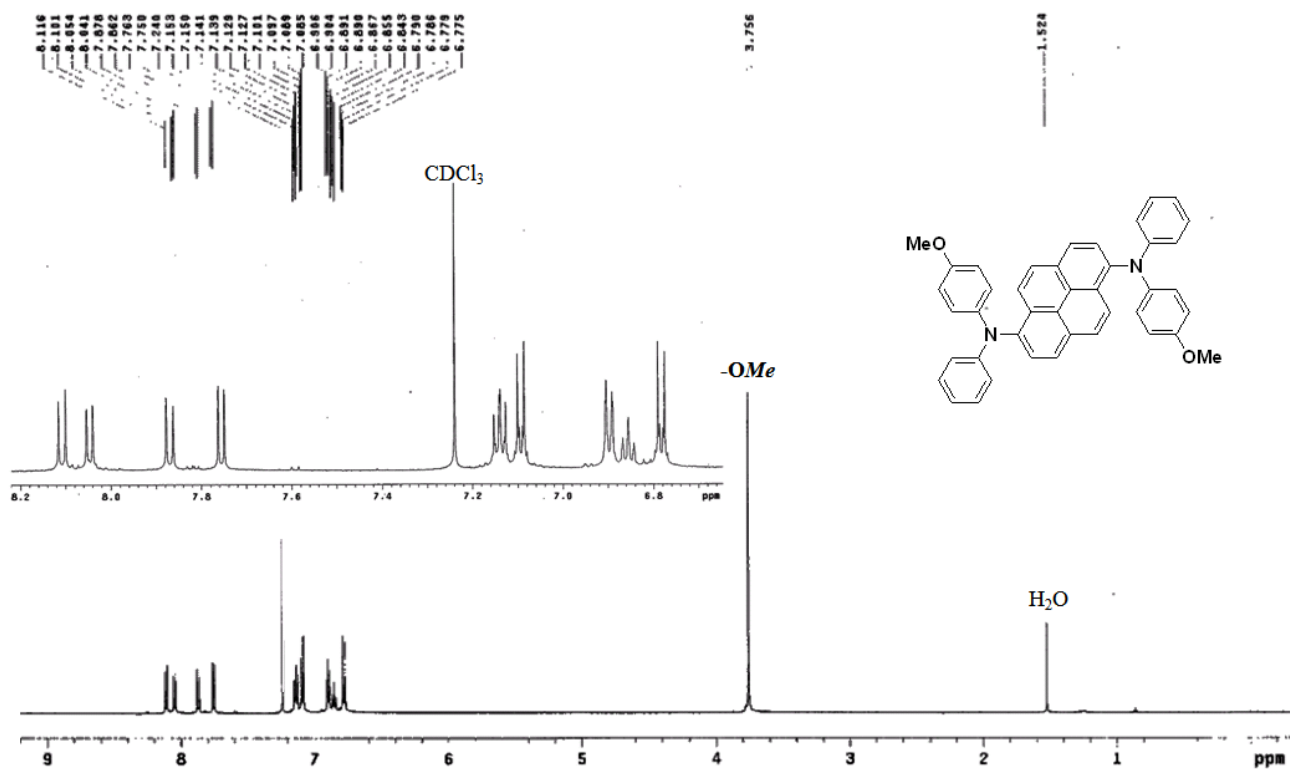


Figure S1 (f). ^1H -NMR spectrum of **2OMe** in CDCl_3 .

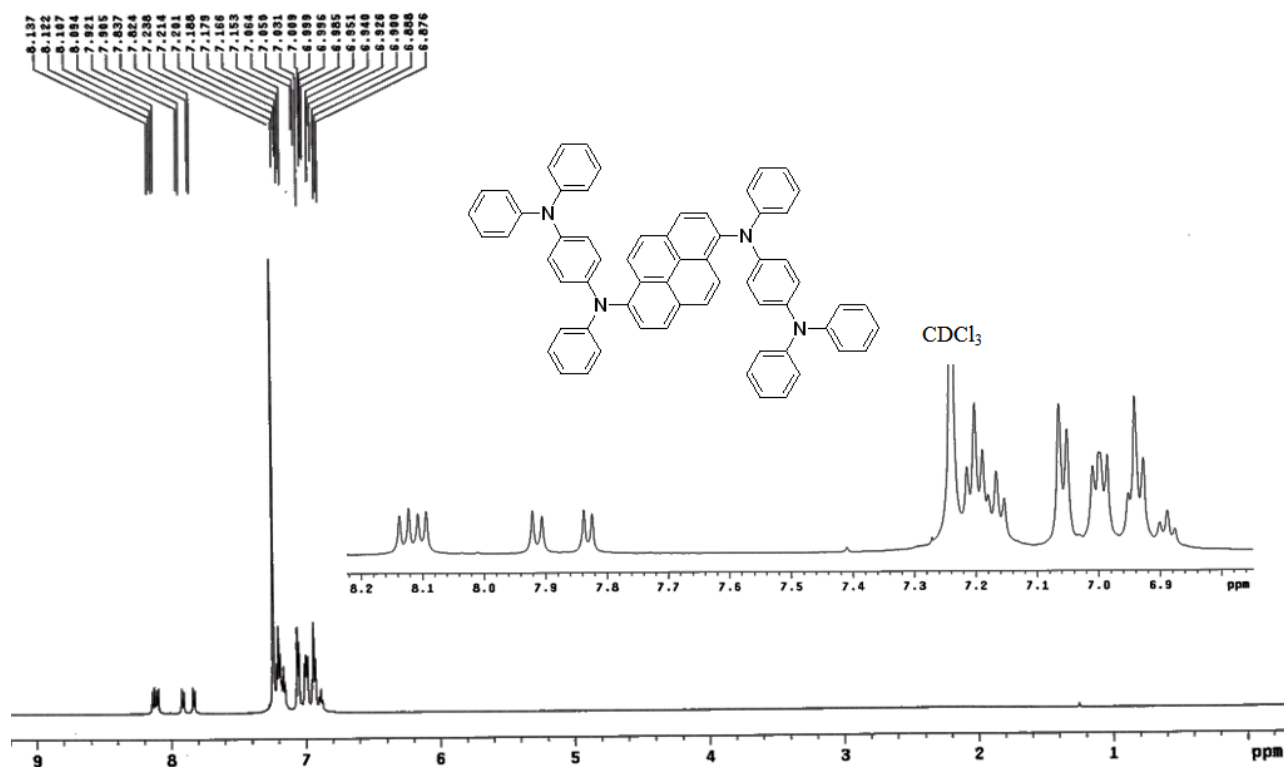


Figure S1 (g). ¹H-NMR spectrum of 2NPh₂ in CDCl₃.

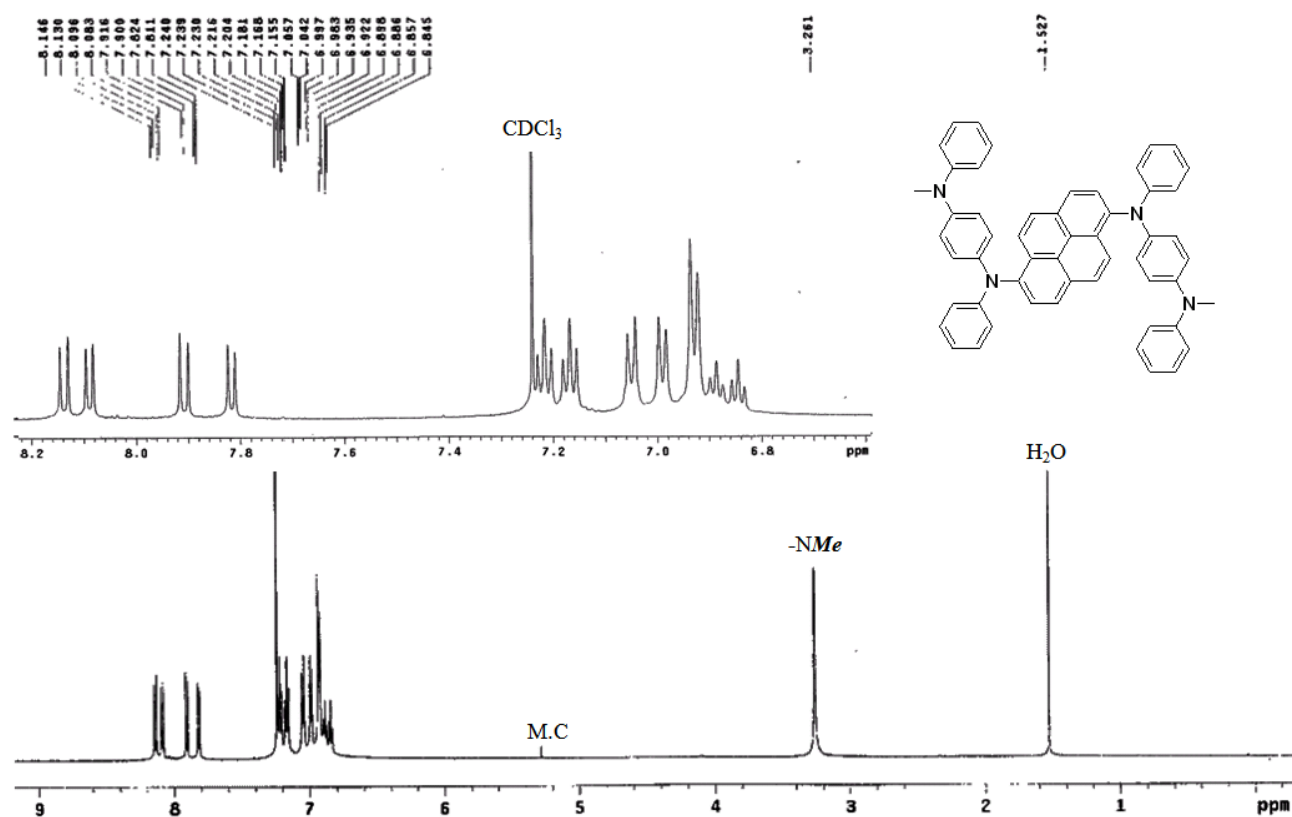


Figure S1 (h). ¹H-NMR spectrum of 2NMePh in CDCl₃.

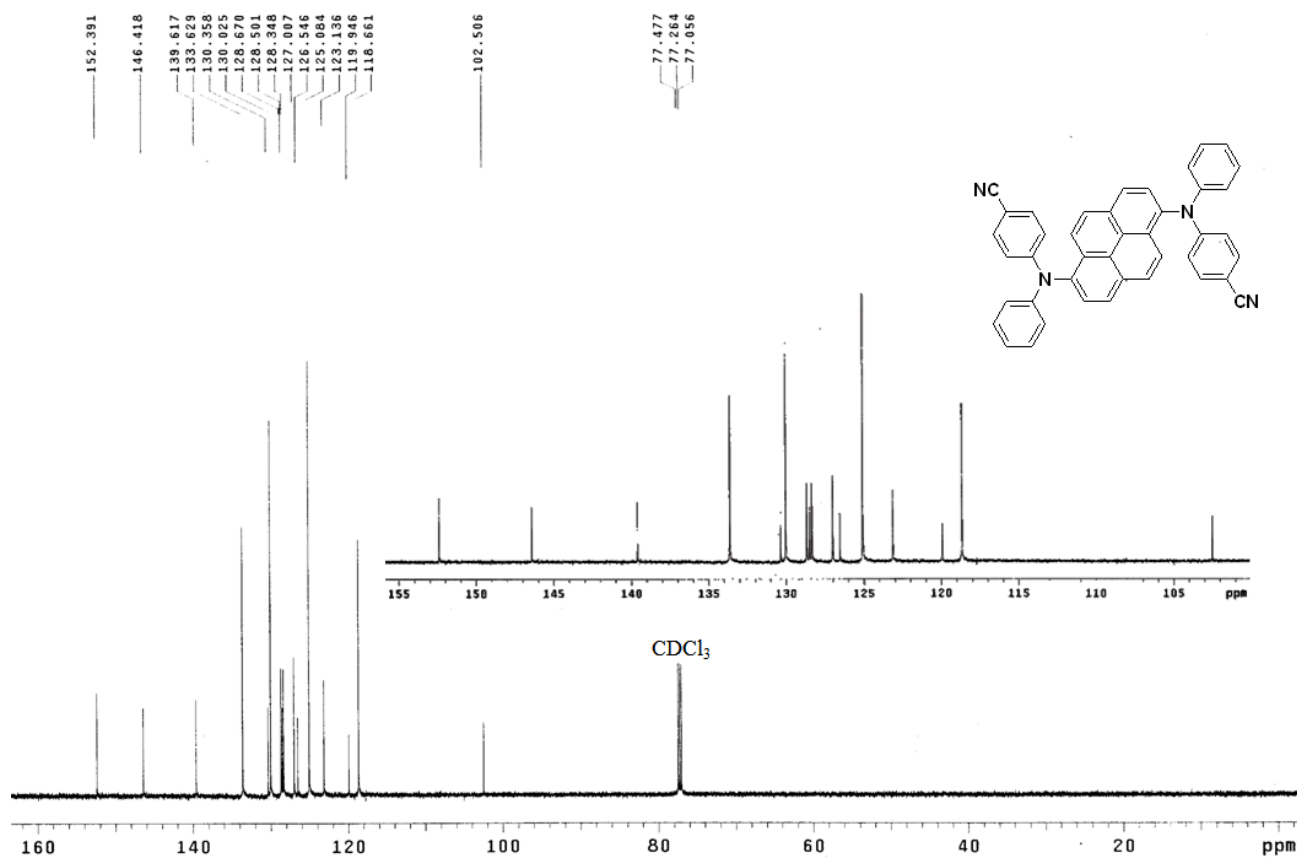


Figure S2 (a). ¹³C-NMR spectrum of **2CN** in CDCl₃.

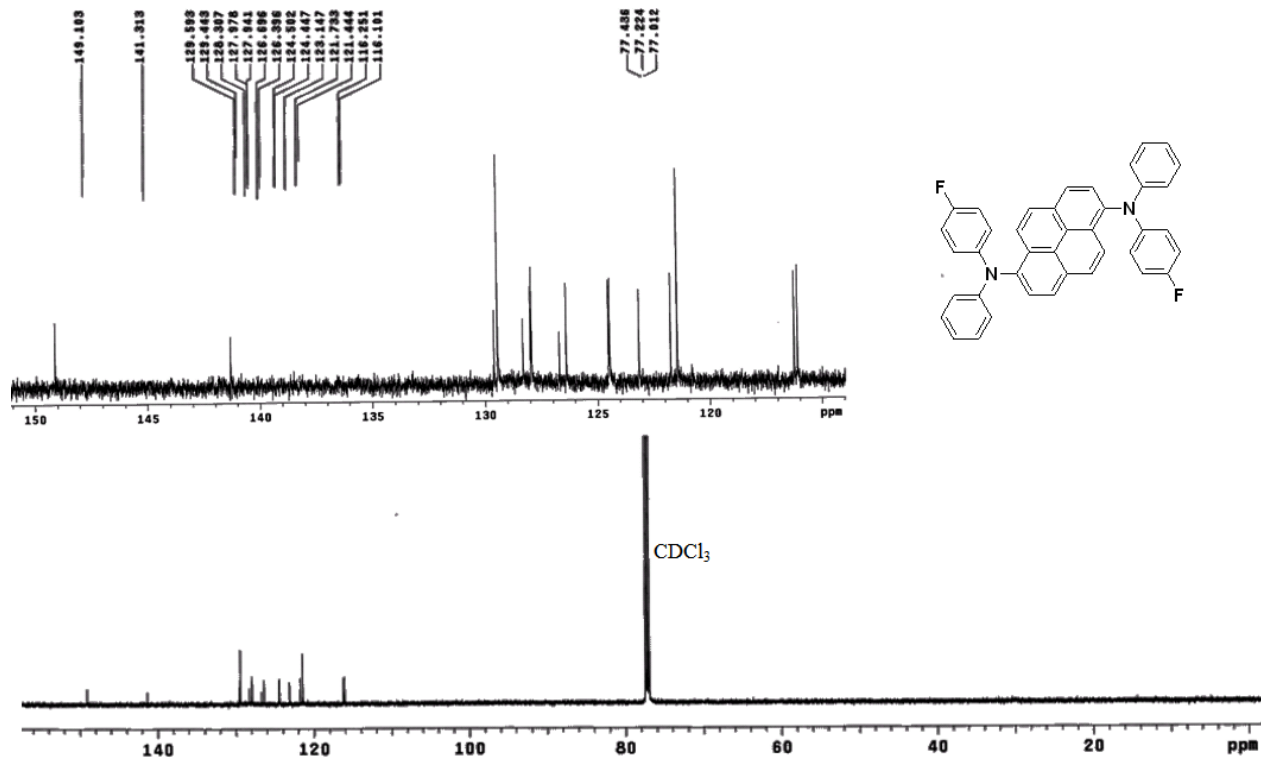


Figure S2 (b). ¹³C-NMR spectrum of **2F** in CDCl₃.

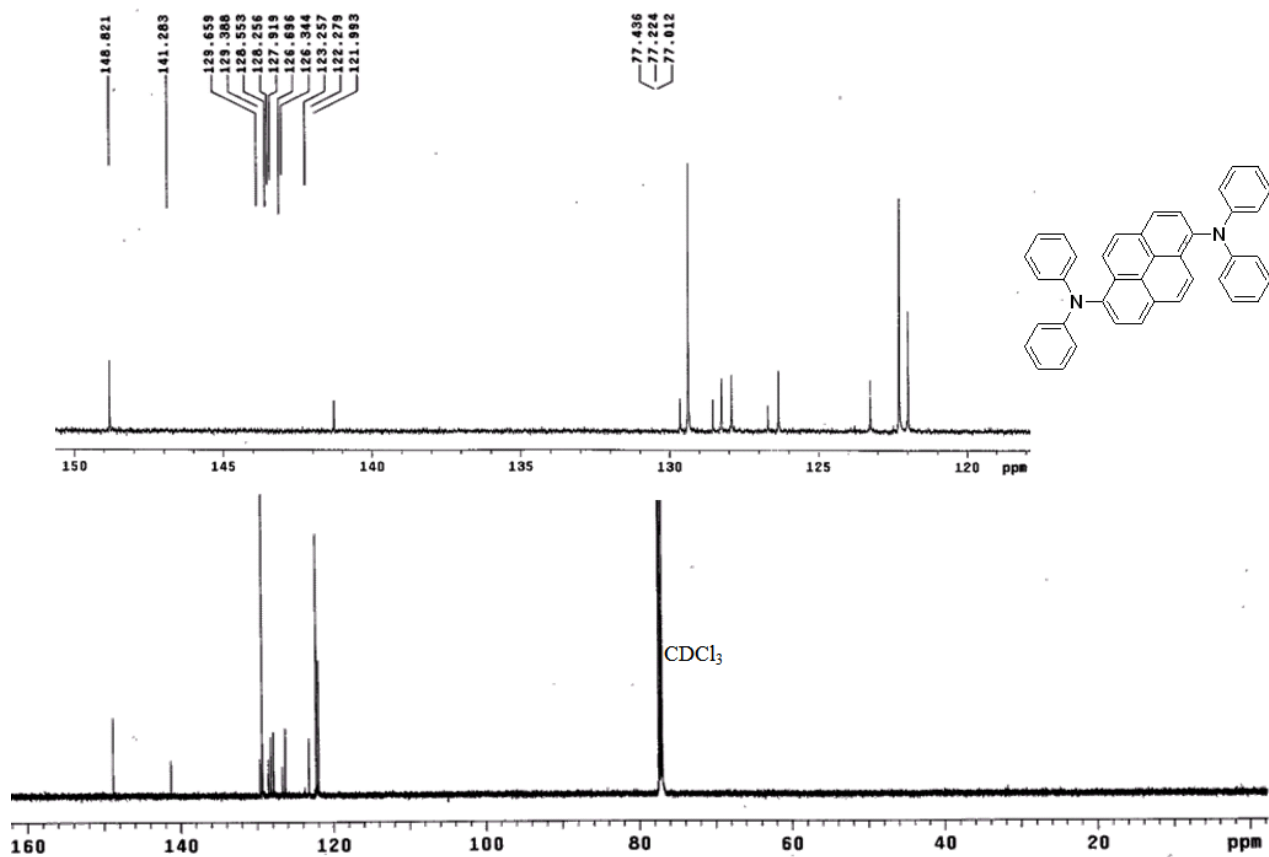


Figure S2 (c). ¹³C-NMR spectrum of **2H** in CDCl₃.

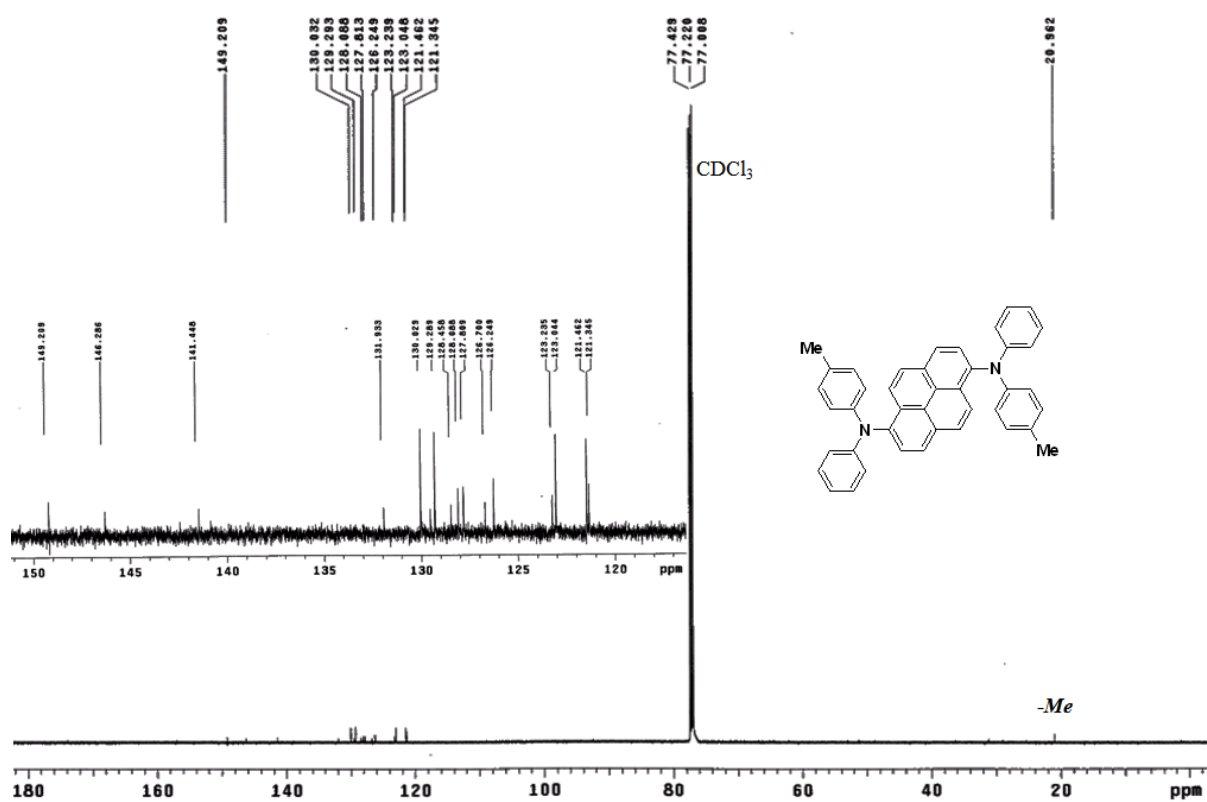


Figure S2 (d). ¹³C-NMR spectrum of **2Me** in CDCl₃.

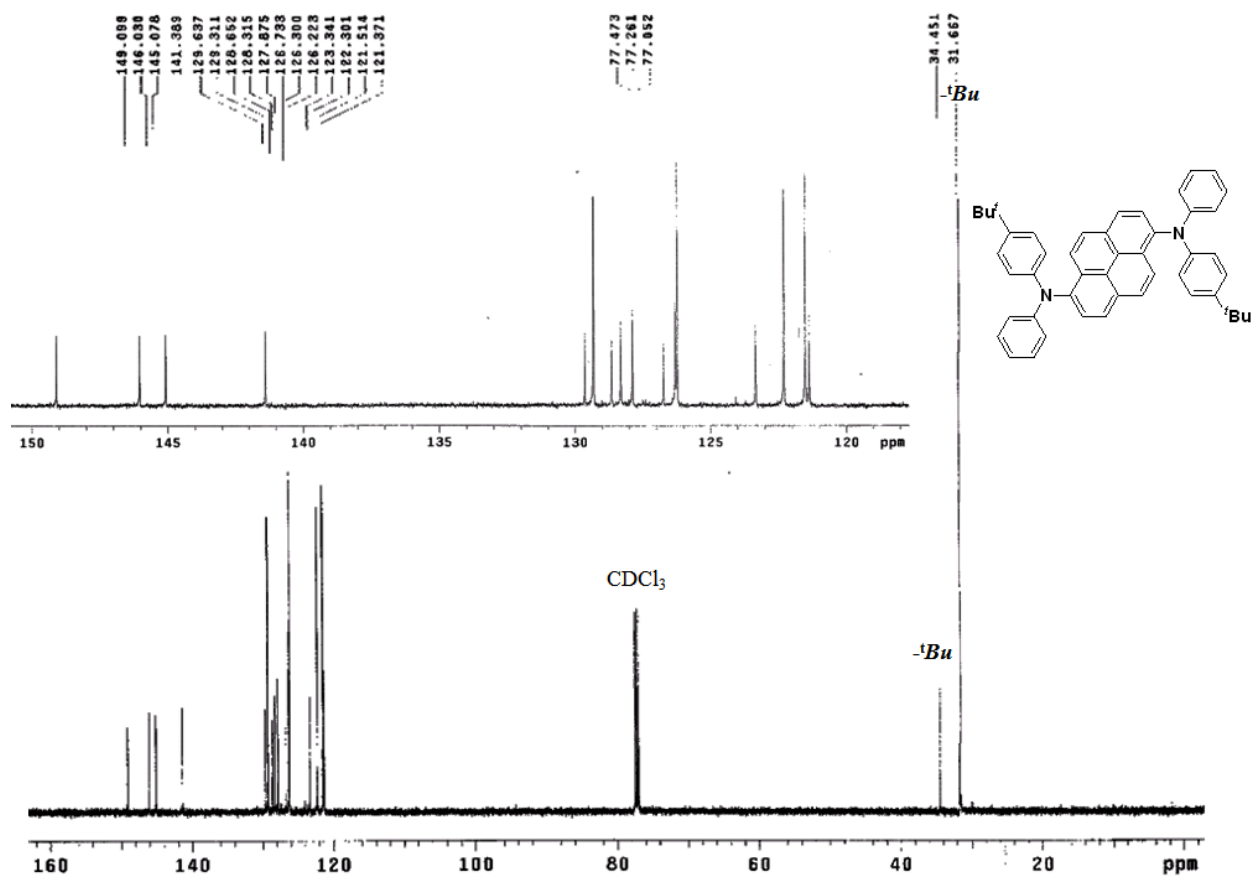


Figure S2 (e). ¹³C-NMR spectrum of **2'Bu** in CDCl₃.

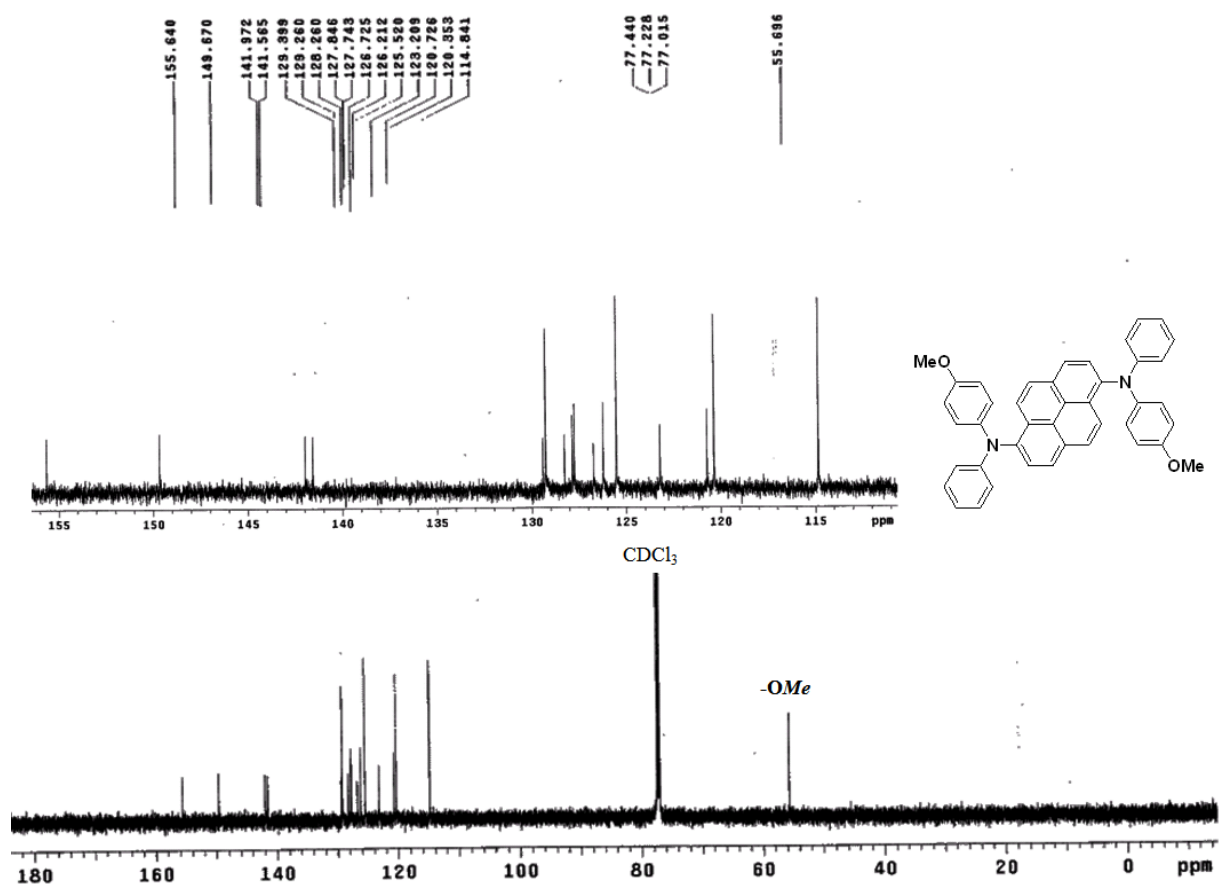


Figure S2 (f). ¹³C-NMR spectrum of **2OMe** in CDCl₃.

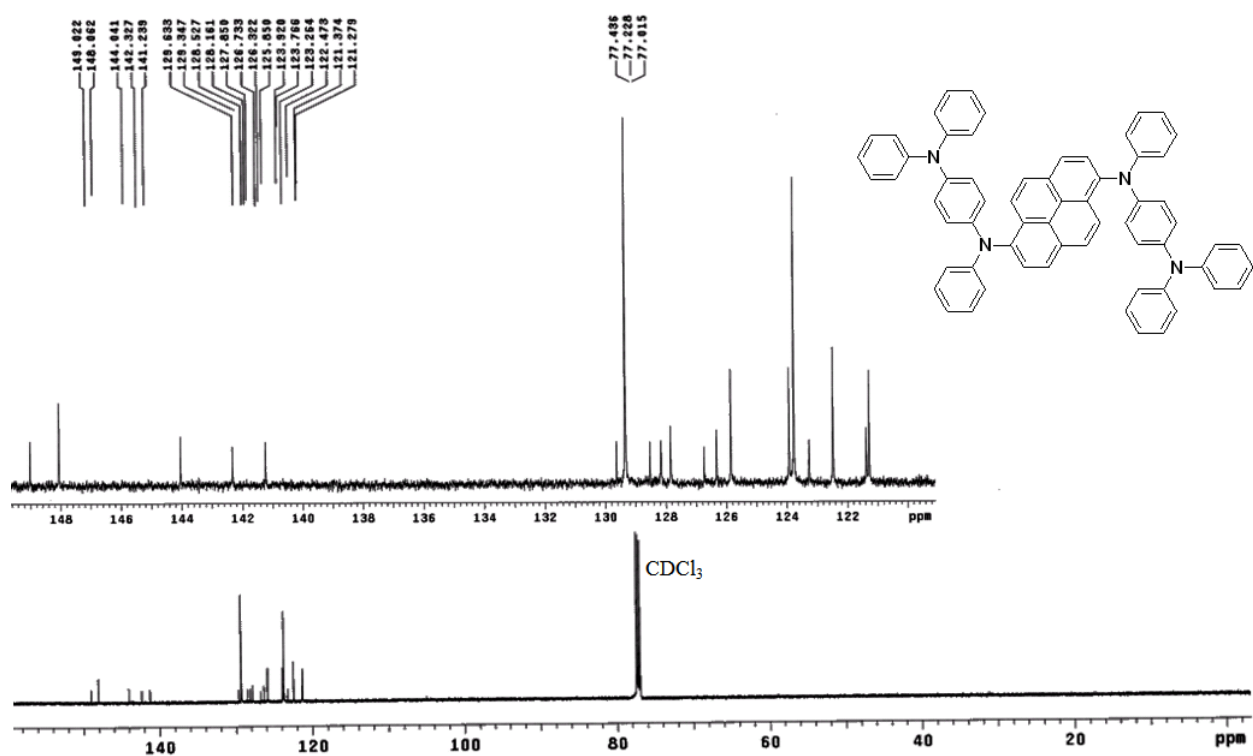


Figure S2 (g). ¹³C-NMR spectrum of 2NPh₂ in CDCl₃.

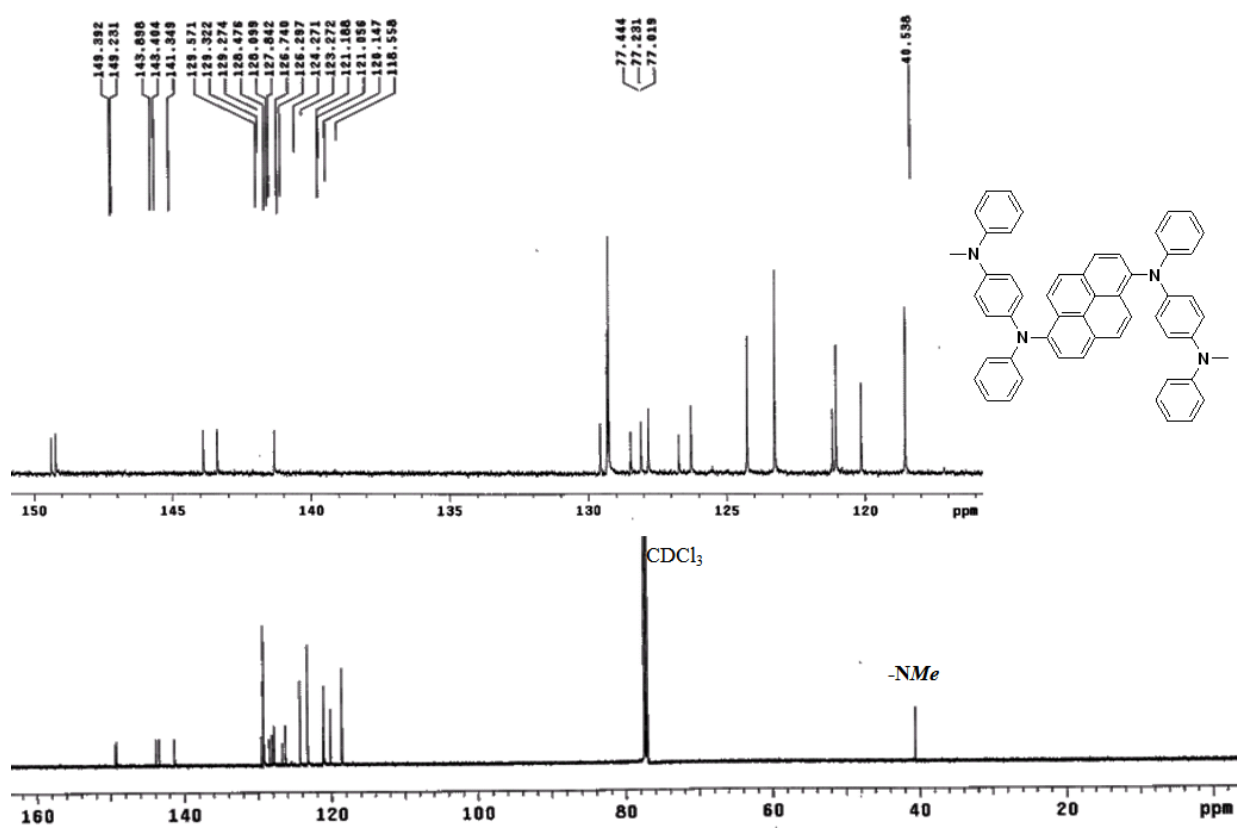


Figure S2 (h). ¹³C-NMR spectrum of 2NMePh in CDCl₃.

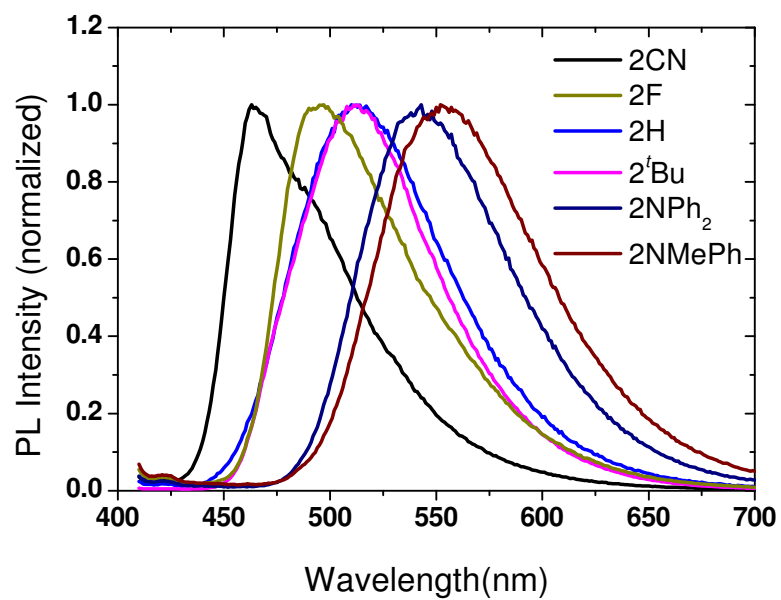


Figure S3. PL spectra in a solid film of **2R**.

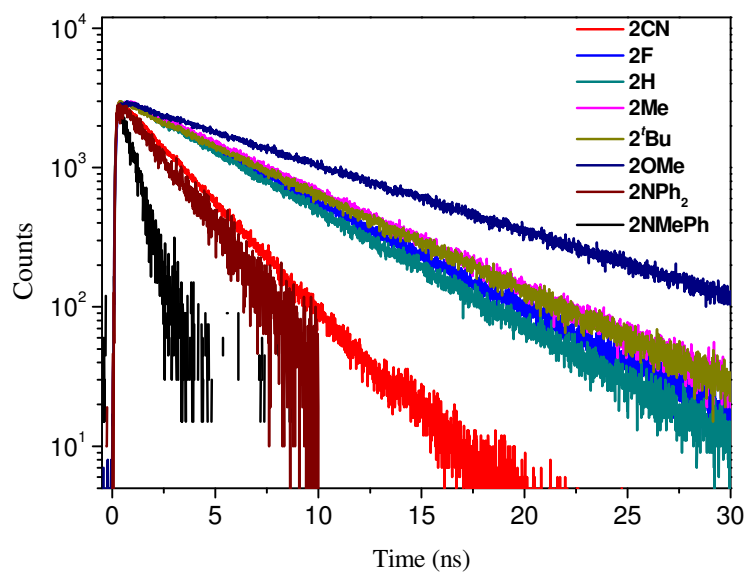


Figure S5. Fluorescence lifetimes (τ_F) of **2R**

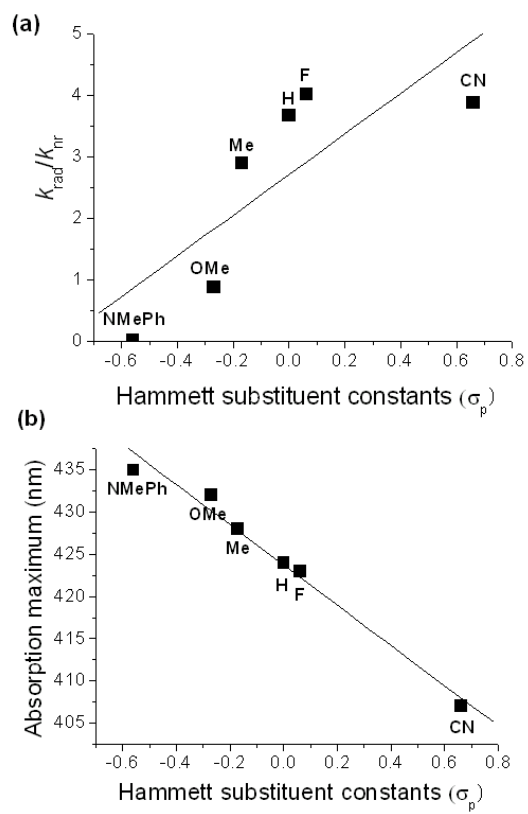


Figure S4. (a) Plot of the $k_{\text{rad}}/k_{\text{nr}}$ versus Hammett substituent constants (σ_p); (b) plot of the absorption maximum versus Hammett substituent constants (σ_p).

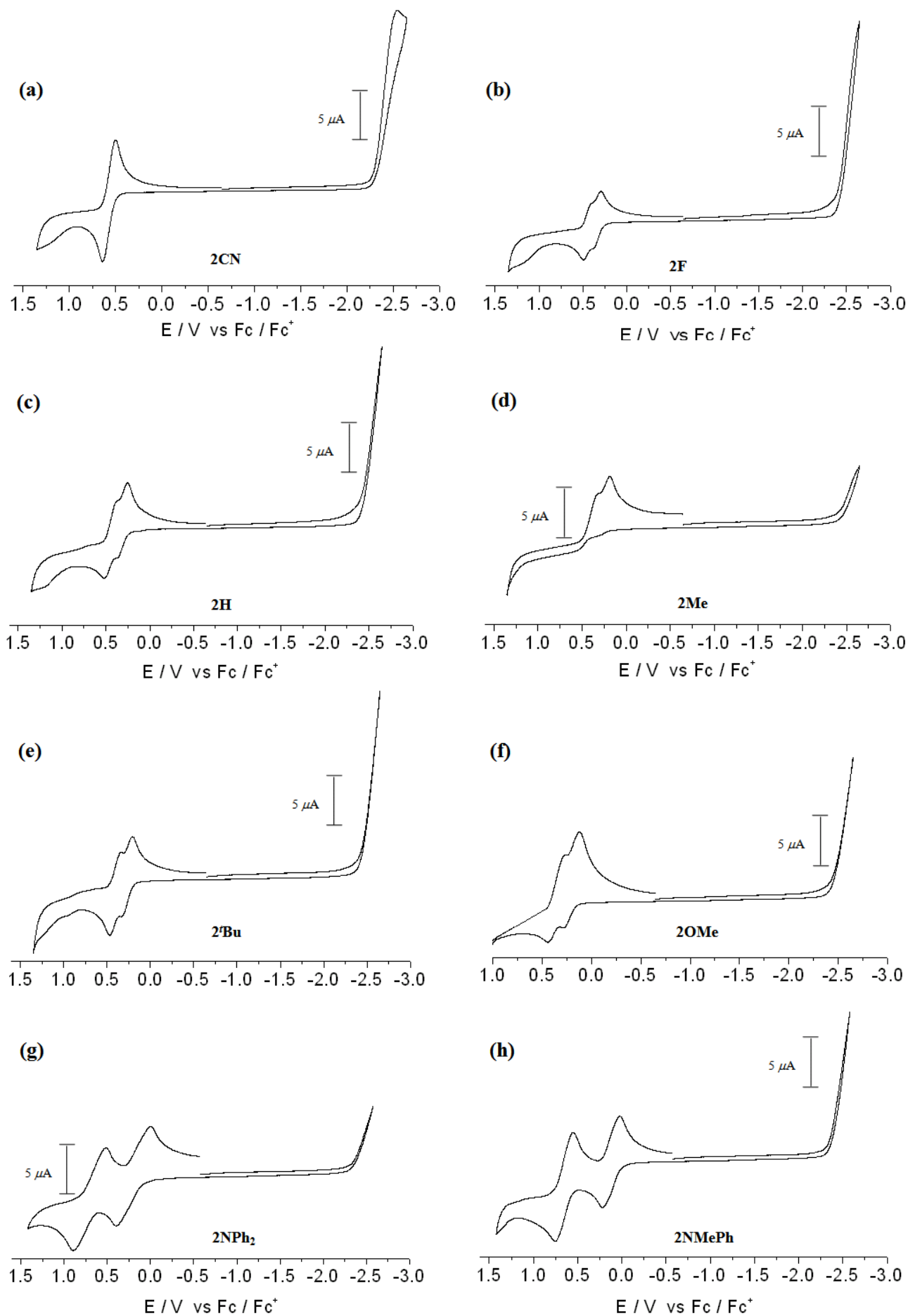


Figure S6. Cyclic voltammograms of **2R**.

Table S1. Oxidation and reduction potentials of **2R**

Entry	oxidation (V) ^a					reduction (V) ^a		E_g^{opt} (eV) ^c	HOMO (eV) ^d	LUMO (eV) ^d
	E_{pa1}	E_{pa2}	E_{pc1}	E_{pc2}	$E_{\text{onset}}^{\text{ox}}$	E_{pc}	$E_{\text{onset}}^{\text{red}}$			
2CN	0.64	- ^b	0.50	- ^b	0.51	-2.54	-2.30	2.80	-5.31	-2.51
2F	0.38	0.49	0.40	0.29	0.26	- ^b	- ^b	2.71	-5.06	-2.35
2H	0.37	0.51	0.36	0.25	0.24	- ^b	- ^b	2.71	-5.04	-2.33
2Me	0.31	- ^b	0.33	0.18	0.20	- ^b	- ^b	2.68	-5.00	-2.32
2'Bu	0.33	0.46	0.33	0.20	0.20	- ^b	- ^b	2.68	-5.00	-2.32
2OMe	0.28	0.44	0.26	0.12	0.15	- ^b	- ^b	2.63	-4.95	-2.32
2NPh₂	0.40	0.89	0.52	0.00	0.07	- ^b	- ^b	2.54	-4.87	-2.33
2NMePh	0.21	0.75	0.55	0.02	0.01	- ^b	- ^b	2.54	-4.81	-2.27

^a E_{pa} = anodic peak potential; E_{pc} = cathodic peak potential; E_{onset} = onset potential. ^b It was difficult to measure this value. ^c Optical bandgap E_g^{opt} from the absorption edge. ^d The HOMO and LUMO levels were determined using the following equations: E_{HOMO} (eV) = $-e(E_{\text{onset}}^{\text{ox}} + 4.8)$, E_{LUMO} (eV) = $-e(E_{\text{HOMO}} - E_g^{\text{opt}})$.

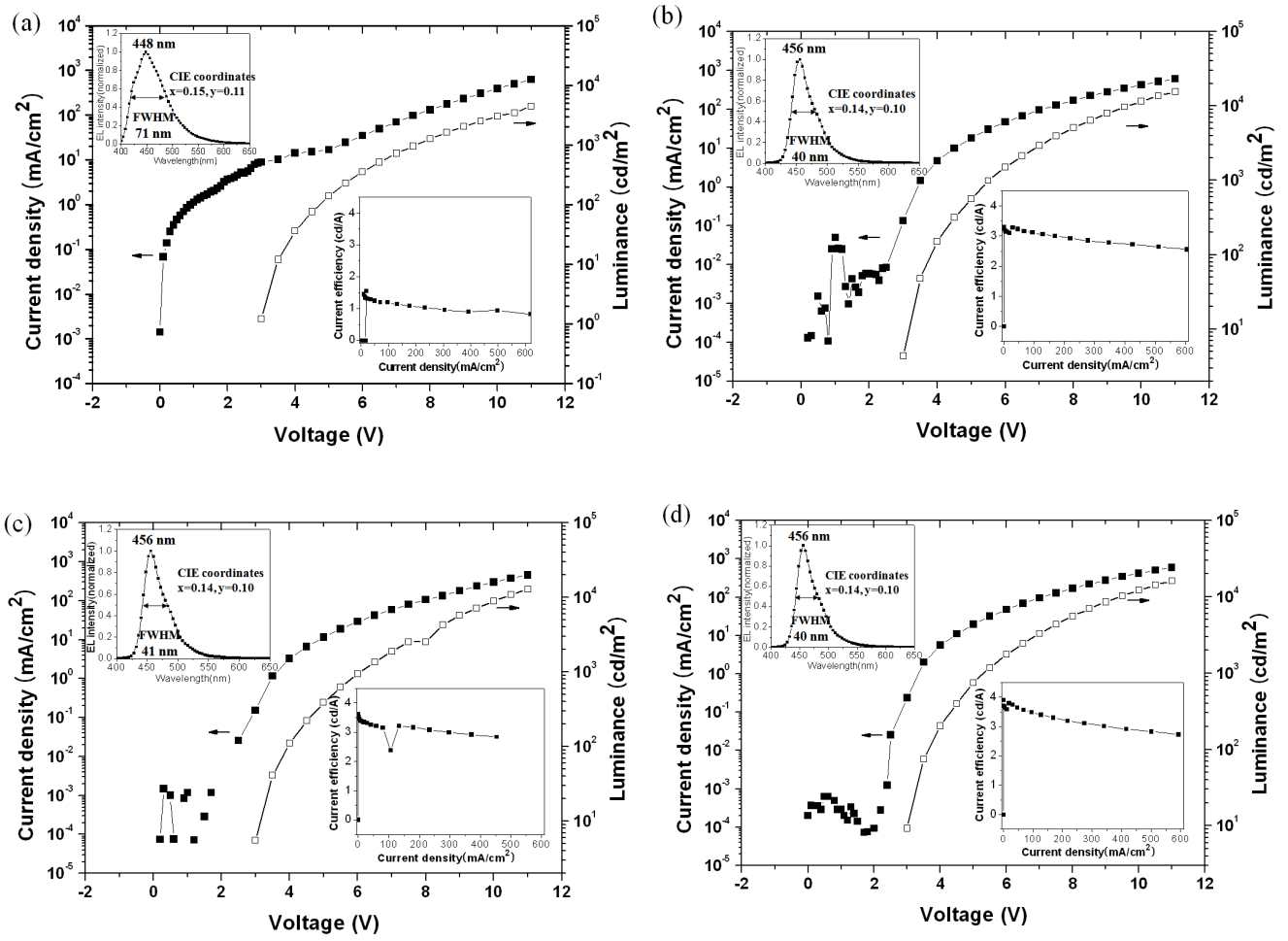


Figure S7. The I - V - L curves of the 2CN device (0 %, (a); 5 %, (b); 7 %, (c); 9 %, (d) doping). (Insets: Current efficiency and EL spectrum)

Theoretical Calculation

The HOMO and LUMO levels of compound **2R** were calculated using the double numerical plus d-functions (DND), and the geometries were optimized under the same conditions. No atom was omitted from the detailed study of the bond lengths and angles of the optimized structure.

Task parameters

Calculate energy

Symmetry on

Electronic parameters

Spin_polarization: restricted

Charge: 0

Basis: dnd

Pseudopotential: none

Functional: pwc

Harris: off

Aux_density: octupole

Integration_grid: medium

Occupation: fermi

Cutoff_Global: 3.3000 angstrom

Scf_density_convergence: 1.0000e-005

Scf_charge_mixing: 0.2000

Scf_iterations: 50

Scf_diis: 6 pulay

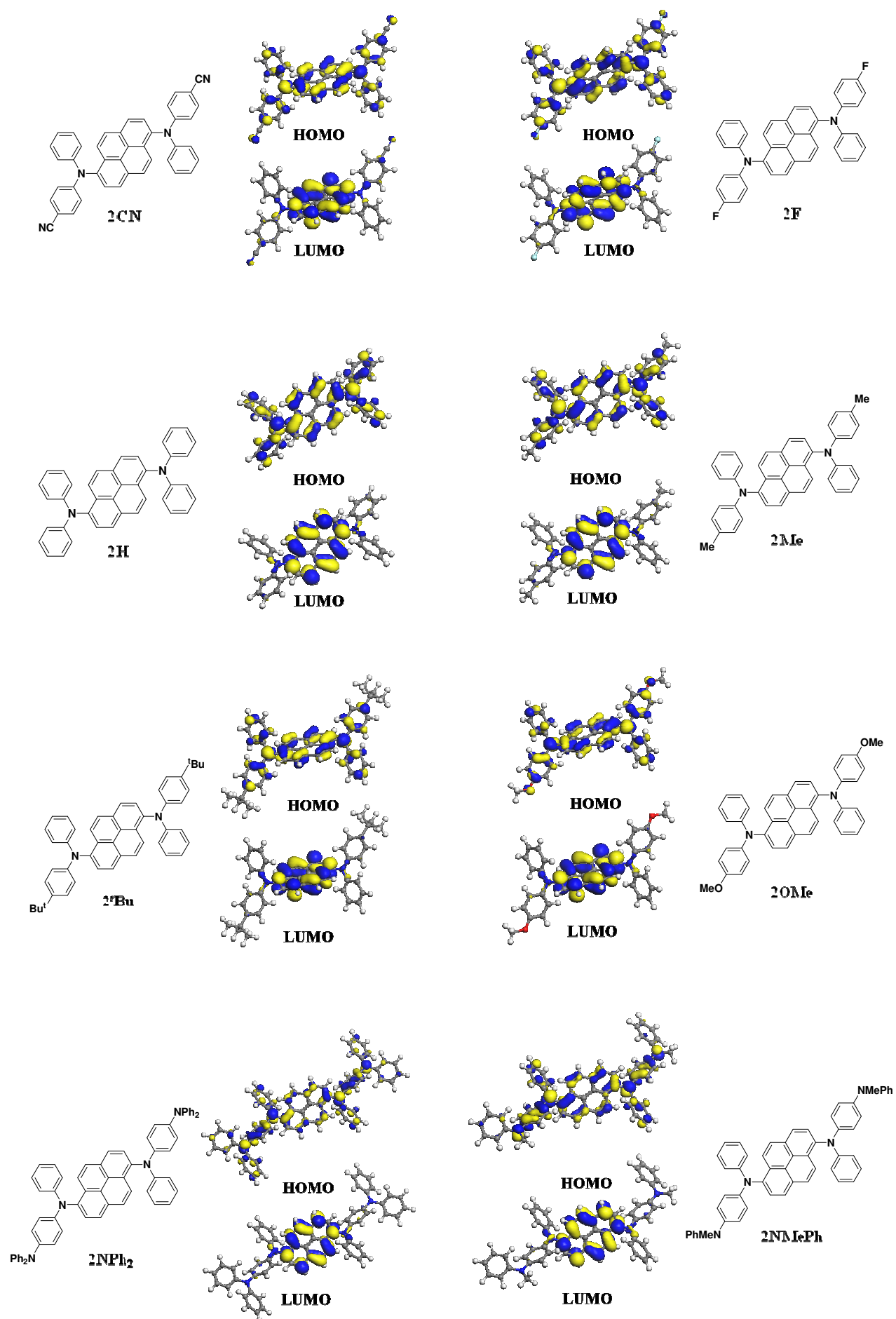


Figure S7. Representative HOMO-LUMO orbital diagram of **2R** obtained from the *Dmol*³ calculation.

Table S2 (a). Optimized Modeling Coordinates for **2CN**.

ATOM	X	Y	Z
C	-3.97737111131090	-2.18963504163056	-2.81708099777452
C	-2.98707013782839	-3.76467701809807	-0.92474869667989
C	-0.66579136971406	-3.14263258896938	0.27408329769291
C	0.67254344052716	-0.92664374427365	-0.55203742156313
C	-0.35857613881962	0.63588354549753	-2.50681453948961
C	-2.69967608930146	-0.02476723814351	-3.58851189213003
C	1.03954734212451	2.80700550341991	-3.31683341077091
C	3.30693199609721	3.43699782583305	-2.24426431025741
C	4.36829799511843	1.95878373982314	-0.23497741297668
C	3.03022849864569	-0.25756588004602	0.59074836107814
C	4.06086520194494	-1.82002379419171	2.54584425879437
C	2.66386872720559	-3.99256590775318	3.35410630083014
C	0.39645340864705	-4.62259469054218	2.28147106746117
C	6.68766720065262	2.58311881181260	0.96673727545185
C	7.67648777591690	1.00923861817974	2.86102207559389
C	6.40029482350490	-1.15729889817848	3.63005613392904
N	8.05080694529410	4.84499127640816	0.29165973864723
N	-4.35290657456256	-6.02413592448679	-0.24741372139225
C	6.88331068999240	7.25757397449890	0.72141811137873
C	10.62803097566801	4.64502368551356	-0.40629594701360
C	-6.92445232753020	-5.81490931241743	0.46933121822184
C	-3.19358803536745	-8.43913753815795	-0.68252541422557
C	7.28551993796480	9.27258046048872	-0.97000294707325
C	6.07771380429975	11.58860101463765	-0.58710316442070
C	4.42926703411242	11.92490518149880	1.45558159399105
C	4.02531773766249	9.92358759754814	3.13547645880596
C	5.24957320781131	7.60952026621174	2.78598248925197
C	12.40728404776572	6.52190301200325	0.25553096059366
C	14.93322709240146	6.27206024231911	-0.42261298566110
C	15.78056157667023	4.13257585619369	-1.77028768601688
C	14.00492295538589	2.25877081364291	-2.43990314709146
C	11.47690931704801	2.51669760870209	-1.77980178809318
C	-8.71821739833699	-7.67655426593061	-0.19596489962829
C	-11.23743275151637	-7.42146413875765	0.50469088152199
C	-12.06285656056449	-5.29143513335892	1.88143526153526
C	-10.27322445685335	-3.43091436657914	2.55063425531778
C	-7.75202282766180	-3.69374988776444	1.86721559211937
C	-3.59820588479507	-10.45666898737885	1.00548209586655
C	-2.39644748511154	-12.77476397326368	0.61586517398833
C	-0.75094758974832	-13.11094494131983	-1.42898991787044
C	-0.34453930229605	-11.10720928082718	-3.10548916215724
C	-1.56301922138632	-8.79115577741353	-2.74978226065362
H	-5.76690362078608	-2.70774977787460	-3.69635356564754
H	-3.49246830226499	1.15953968628462	-5.07922141797570
H	0.25944322846489	3.96317749932855	-4.83678211336912
H	4.32905143352027	5.08999483732114	-2.91346886739364
H	3.44473965393220	-5.14980654756495	4.87285054112916
H	-0.62500529926449	-6.27674302145137	2.94902452741829
H	9.46437160328296	1.52863759907024	3.74276351773688
H	7.19268133872556	-2.34110675916507	5.12137481677055
H	8.52747943581700	9.00408914585858	-2.59062039525002
H	6.40427168221508	13.13014500094568	-1.91750270474799
H	3.47589795149961	13.73027413447337	1.73664430032934
H	2.75989922126858	10.16538943895125	4.74536079738527
H	4.93018952395143	6.05866697122702	4.10141377161512
H	11.80145936662471	8.16826727754467	1.32849181645069
H	16.28638232922180	7.72370148710871	0.12535715379677
H	14.62280283064677	0.61125507561256	-3.50916675945411
H	10.12613144073059	1.06697791113570	-2.33347414778732
H	-8.12788005269104	-9.31641852933702	-1.28764222096769
H	-12.60211859637399	-8.86204205564780	-0.04354647843803
H	-10.87442512367541	-1.79107005301144	3.64090500625920
H	-6.39010984975697	-2.25475411572656	2.42143967058379
H	-4.83680464079425	-10.18956146816744	2.62878631507387
H	-2.72501030197425	-14.31821437008867	1.94355947121221
H	0.19807603173527	-14.91793586890420	-1.71434392578721
H	0.91827763003130	-11.34859162948670	-4.71746149314713
H	-1.24197857841689	-7.23841469138338	-4.06261795316149
C	18.38440515095591	3.85880222225171	-2.41827145591811

C	-14.65772333293382	-5.01468487274471	2.56333866106843
N	20.52282555324281	3.63297932103617	-2.93494010948062
N	-16.78786700313437	-4.78373559430689	3.11161946016289

Table S2 (b). Optimized Modeling Coordinates for **2F**.

ATOM	X	Y	Z
C	-3.91465140735800	-2.12915624105708	-3.00219468937115
C	-2.98935417798608	-3.73441400662827	-1.09894707695526
C	-0.68646554421878	-3.14320947700191	0.15599527779211
C	0.68611374524445	-0.92398923275779	-0.60629462957213
C	-0.28457021377082	0.66824169254267	-2.56846089601106
C	-2.59981453456801	0.03153609728350	-3.71905577155289
C	1.14513044332332	2.84294307520470	-3.31160811961406
C	3.38435334789364	3.45050508361763	-2.16749547522276
C	4.38735257795799	1.93921514958784	-0.15298573964969
C	3.01268587056092	-0.27771963909372	0.61225825184383
C	3.98197604884462	-1.86826801461345	2.57660169820752
C	2.55060505904915	-4.04129438372254	3.32169813084475
C	0.31396405893751	-4.65145095775920	2.17400926668931
C	6.69444091449903	2.52560749352663	1.09645177297571
C	7.61742343723771	0.92311899497997	3.00283294059042
C	6.29789823141038	-1.23268820857544	3.72632949748334
N	8.14012084815199	4.72483889890143	0.41479643779097
N	-4.42764737630686	-5.94157895659705	-0.42697792797694
C	7.10863626820416	7.19832290442240	0.75592994905290
C	10.75041046533291	4.39273225407008	-0.20177936581694
C	-7.04032738554205	-5.62338483832532	0.18363293622016
C	-3.37838313236750	-8.40920495474973	-0.76166266568938
C	7.81032311983304	9.18472936249884	-0.87462821065234
C	6.80336837551509	11.60254549835577	-0.54987059922725
C	5.05250398814037	12.08253951513514	1.37707009887736
C	4.33127901055107	10.10851486199337	2.98107383085364
C	5.34867911020026	7.68760232106352	2.69023603047420
C	12.62065296028806	6.02730701909509	0.75812012273451
C	15.16437331053713	5.68097215950631	0.14132482932691
C	15.82944844570393	3.66713651191874	-1.41488611512217
C	14.03581366017510	2.00095788970057	-2.37832278169603
C	11.49379639347084	2.37909524693387	-1.77861473962023
C	-8.89956963732498	-7.28229055097472	-0.75708346244604
C	-11.44516203531114	-6.94853003673604	-0.14018707813938
C	-12.12395262127944	-4.92437546027445	1.39643525253639
C	-10.34237390103421	-3.23220193555622	2.33707787251522
C	-7.79865728110452	-3.59773668091604	1.73840463312711
C	-4.06565364322375	-10.39714273160457	0.87317004884142
C	-3.02961793947307	-12.80468206058279	0.56170995827774
C	-1.26554194385576	-13.27173846806934	-1.35659847844680
C	-0.56219304597461	-11.29693639104838	-2.96733668977568
C	-1.61018406237081	-8.88723454830984	-2.69113888681466
H	-5.69022600094176	-2.61291114541700	-3.92802977826195
H	-3.34308443541159	1.23671749206778	-5.21899013153799
H	0.41330733360447	4.02267088331688	-4.83780441740822
H	4.43116898487572	5.10868676848924	-2.78358370114452
H	3.27926154714144	-5.21794821970062	4.85180085347697
H	-0.73338385720219	-6.30907559483285	2.79081700961261
H	9.39474932883863	1.40561684596263	3.92611547057952
H	7.03899794053641	-2.43579012983452	5.22898976850649
H	9.14680397268536	8.81756835096119	-2.39776779140165
H	7.37277227245252	13.11281026541138	-1.83385244903672
H	4.25870062997052	13.96894552549767	1.62043713995856
H	2.97626306812984	10.45312926200563	4.49773017133866
H	4.78843964608613	6.16832619655963	3.96161435945193
H	12.07353083731851	7.58033446099414	1.99106174358331
H	16.62339910613550	6.93499495651372	0.87429816809488
F	18.34035822579682	3.31208192119675	-2.01947343383216
H	14.62872983569534	0.45328691429733	-3.59908706030770
H	10.06481084653693	1.10540301067704	-2.53547830030628
H	-8.34330825079438	-8.84271538437157	-1.97649041314309

H	-12.89573042399807	-8.22057337167551	-0.85855015999869
F	-14.63670156220567	-4.58263629556891	2.00146423614658
H	-10.94463903924413	-1.67614109583269	3.54254129569557
H	-6.37880981665282	-2.30479249504370	2.47959516627015
H	-5.41121098293525	-10.03838084971440	2.39030214488594
H	-3.58669269247375	-14.31650849730810	1.84917011925110
H	-0.44708474433797	-15.14903382721409	-1.58758684020034
H	0.80144991005724	-11.63271388367959	-4.47821405501841
H	-1.06380264779157	-7.36643074652980	-3.96663209253984

Table S2 (c). Optimized Modeling Coordinates for **2H**.

ATOM	X	Y	Z
C	-3.93620886441998	-2.10711888237648	-2.97976991415822
C	-3.01203615248353	-3.71405143095403	-1.07712329134186
C	-0.70951687324627	-3.12323026817692	0.17893407740831
C	0.66712115676014	-0.90718038721708	-0.58496294753893
C	-0.30177358688327	0.68586019124163	-2.54778606577137
C	-2.61899726540529	0.05210617244517	-3.69626255832709
C	1.13316753586850	2.85591136987035	-3.29430429621970
C	3.37677648910576	3.45714665836475	-2.15519226777708
C	4.37856612059530	1.94481479171060	-0.14089603157189
C	2.99726791636054	-0.26648636434440	0.62936200804360
C	3.96562917142161	-1.85907648500724	2.59290225466376
C	2.52841758619436	-4.02635408992560	3.34247628186032
C	0.28883315433961	-4.63141577146693	2.19791561364040
C	6.69207574650907	2.52215844855124	1.10022656705080
C	7.61417209540952	0.91714157581784	3.00527551176246
C	6.28691969741188	-1.23105173787654	3.73608973827714
N	8.14746319192776	4.71342743242714	0.41332556946158
N	-4.44482786294621	-5.92735979740721	-0.41392022091969
C	7.12709229730117	7.18898535945796	0.75714424170739
C	10.75356259842927	4.36704675453873	-0.21794004852486
C	-7.06288124227741	-5.62509026890997	0.18548594118710
C	-3.37547372136381	-8.38441942783678	-0.75436570368650
C	7.83079291289843	9.17328548344206	-0.87601193615120
C	6.83642670388405	11.59518965437655	-0.54750213366520
C	5.09684112420965	12.08446826977380	1.38754793860068
C	4.37385519021296	10.11383676728809	2.99481045036719
C	5.37854671537567	7.68829017003466	2.69981951951435
C	12.63259801172073	6.00562122695250	0.71554081935533
C	15.16719592641989	5.63027307335435	0.08012023030225
C	15.88150288311698	3.60710414969367	-1.46812381966620
C	14.02108757250360	1.96305271428745	-2.38341872487907
C	11.47979447719633	2.33682932628663	-1.78038637298022
C	-8.90173622911427	-7.31620518983997	-0.73676082613344
C	-11.44811738744665	-6.98048625037275	-0.12753239675226
C	-12.21910197951404	-4.94665440154287	1.37905848193416
C	-10.39924863483936	-3.25064820232807	2.28187965648501
C	-7.84582079928072	-3.58550789655434	1.70815011408651
C	-4.05216168466187	-10.38648644315353	0.86883347509416
C	-2.98847990753271	-12.78112200783383	0.55483330915958
C	-1.20932545457228	-13.22361207585094	-1.35624344993052
C	-0.51931656237529	-11.23693300966316	-2.95723975836792
C	-1.59560434910550	-8.83993413459369	-2.67914523729524
H	-5.71214699595676	-2.59162301401208	-3.90446456278121
H	-3.36098303309625	1.25825160534294	-5.19641101105407
H	0.40235866105820	4.03615120494528	-4.82085294478823
H	4.42997988982937	5.10960768494228	-2.77601781032707
H	3.25663378888651	-5.20395112222773	4.87226864154294
H	-0.76327656927890	-6.28498013920897	2.81731248922483
H	9.39715717818285	1.39541095861568	3.91992782694489
H	7.02722525669278	-2.43651775187141	5.23753538216427
H	9.16053554096098	8.79835618386006	-2.40303523100999
H	7.40767929154367	13.10315905236636	-1.83360247228545
H	4.31251622977109	13.97469318419863	1.63311960220945
H	3.02811894823948	10.46487056127777	4.51835762992385
H	4.81777583570876	6.17170140426614	3.97422487793951

H	12.08988916459212	7.56861797004657	1.93945334011727
H	16.59673996679224	6.91694025989224	0.82561112437082
H	17.86321577739417	3.31141870858510	-1.95197456715572
H	14.54730990656637	0.38326424468164	-3.59981656829127
H	10.03690027386191	1.06394778820660	-2.51438296631953
H	-8.32020614671564	-8.88707035000684	-1.93226478414327
H	-12.84416681460010	-8.30837138347909	-0.86462541406177
H	-14.21087073011195	-4.68511279095317	1.84058046174652
H	-10.96604196395224	-1.66201793473000	3.46868617079154
H	-6.43565221724397	-2.27256122799005	2.43521148057724
H	-5.40998642339872	-10.04501605608448	2.37891456643960
H	-3.53658219364877	-14.30353925211021	1.83368093560389
H	-0.36860981920426	-15.09098967041156	-1.58792688885763
H	0.85415018782967	-11.55307485512753	-4.46358420920873
H	-1.05944187232184	-7.30953475330574	-3.94734243154978

Table S2 (d). Optimized Modeling Coordinates for **2Me**.

ATOM	X	Y	Z
C	-3.89980173348765	-2.16134599460722	-2.99493421042084
C	-2.96482023220188	-3.76394016096961	-1.09382148396932
C	-0.66440738532272	-3.15897459467844	0.16093314727453
C	0.69710742728757	-0.93293982795224	-0.60180437951694
C	-0.28293281332666	0.65409079026046	-2.56343296218152
C	-2.59672933368128	0.00609259041055	-3.71122810264451
C	1.13681185380329	2.83389605106555	-3.30915125455361
C	3.37320030524640	3.45359768467187	-2.16565226281661
C	4.38329201949828	1.95141238875134	-0.14806945839853
C	3.02128243690422	-0.27431909771879	0.61531873511285
C	4.00035149812993	-1.86082307004745	2.57781382334615
C	2.58211819804996	-4.04228801872660	3.32143231251938
C	0.34663399189601	-4.66283934311859	2.17664914794551
C	6.68199952649964	2.55779892515356	1.10913112095794
C	7.61417838630779	0.95745890726102	3.01356413778505
C	6.31202223533092	-1.21065945192816	3.72865826745841
N	8.11054918731583	4.77119338185982	0.43987080367294
N	-4.38937301454933	-5.98005657351713	-0.42585991686851
C	7.03156599728614	7.22797845587042	0.73211651426619
C	10.73461092251556	4.46798711045325	-0.14340232052941
C	-7.01099339745037	-5.68125839254301	0.16899155930167
C	-3.31061780485880	-8.43527122842607	-0.73530786106936
C	7.73165572042431	9.21178985132517	-0.90355432403666
C	6.65226777940453	11.60540624891173	-0.64423450602609
C	4.83300848525505	12.06816192508644	1.22376725751471
C	4.12168408708049	10.10019907871664	2.83905821214174
C	5.21148983311433	7.70461329360028	2.615271110532176
C	12.57738260485196	6.13947827437319	0.79950135297852
C	15.12687902205482	5.78346583250104	0.21967827152696
C	15.94551537516816	3.74986159551374	-1.27730593117976
C	14.09191005925307	2.08299166612562	-2.19146274505440
C	11.53309033428240	2.43181600177859	-1.65822041669826
C	-8.85295772453548	-7.35861759260779	-0.76457911592288
C	-11.39839287652105	-7.01953134637898	-0.15938178228139
C	-12.21454180014360	-4.99565496972834	1.35223734959828
C	-10.36082076118007	-3.32891751959021	2.26637113904981
C	-7.80515778590668	-3.65983941007612	1.70571077812559
C	-3.99850936853685	-10.42711226104826	0.89588838355924
C	-2.92133754335892	-12.81957237679291	0.61567953296299
C	-1.11760407653594	-13.27261274608162	-1.26969231721874
C	-0.41747309689701	-11.29642580027749	-2.87961783670976
C	-1.50448739997025	-8.90147310175890	-2.63420691887437
H	-5.67454924685884	-2.65534861918132	-3.91682586229770
H	-3.34701724271608	1.20903126578859	-5.20993940164590
H	0.39936706964479	4.00831877811470	-4.83704633487592
H	4.41157103963480	5.11602497754425	-2.78440794865764
H	3.31969283284941	-5.21690618314132	4.84910893672219
H	-0.69095910885360	-6.32641540806126	2.79365556722497
H	9.38730381735479	1.45303207565869	3.93758261405463

H	7.06105617880096	-2.41235630512152	5.22900431372847
H	9.12138313307728	8.85511679143534	-2.38094964462895
H	7.21868235637936	13.11209617192381	-1.93404819427647
H	3.98054261410004	13.93502517965953	1.41256157435418
H	2.71604438865983	10.43021880450185	4.31305080683569
H	4.65417398885462	6.18925483213572	3.89246517416354
H	12.00350034990585	7.71114638483975	1.99847132003516
H	16.51847507904813	7.10187644573450	0.98835919485140
C	18.71324646998574	3.38040050760251	-1.90476795566496
H	14.65796898788144	0.48072106433953	-3.36372081728354
H	10.13259928350641	1.11686395396073	-2.40136934483423
H	-8.27889353242723	-8.93264352002968	-1.96011155021568
H	-12.78812514765989	-8.35223232179295	-0.90601475312058
C	-14.98957831726793	-4.59416942450085	1.92448297321877
H	-10.92257280932779	-1.74985417002391	3.47127107424559
H	-6.40234621192043	-2.35431927258648	2.46111569134111
H	-5.37691156559533	-10.07820984947071	2.38564046454587
H	-3.47804236357338	-14.33316195633873	1.90158088531200
H	-0.26762651926355	-15.13885983466467	-1.47537917367926
H	0.97624349737020	-11.61905108631711	-4.36632839215985
H	-0.95714020683976	-7.37930103621915	-3.90756740426132
H	19.22989753586720	4.33867553277485	-3.68554375773583
H	19.17372821414780	1.36488286014451	-2.13525983912231
H	19.93867781843639	4.15097420895964	-0.41139276702957
H	-16.01787615945459	-6.40086655636456	2.00356557569278
H	-15.90902869054542	-3.42661658135033	0.45817682064097
H	-15.25801822945774	-3.62230092467920	3.74376652200307

Table S2 (e). Optimized Modeling Coordinates for **2'Bu**.

ATOM	X	Y	Z
C	-3.83909821046285	-2.31535405530355	-3.02899821701846
C	-2.95381891188576	-3.80726485737016	-1.01920895116521
C	-0.69575780378636	-3.12309865253177	0.26983095848768
C	0.69735741348747	-0.95589511164943	-0.59279397449063
C	-0.21473709502382	0.50317787796919	-2.68337992456874
C	-2.50539829747332	-0.20168425212161	-3.84491056015823
C	1.24553047551609	2.61617440574786	-3.53438709912033
C	3.45209455871753	3.29762598688235	-2.36800029257798
C	4.38762969873532	1.93156374110432	-0.22125329400145
C	2.99071381136657	-0.23168985076785	0.64592174610706
C	3.90166597854557	-1.68909095055081	2.73798430172307
C	2.44088155846185	-3.80122065528677	3.58966345532581
C	0.23820482520295	-4.48704292917370	2.41862220987390
C	6.65235639811116	2.60677767834064	1.05920840799745
C	7.53384333760882	1.11940051255132	3.07393347597273
C	6.19326220614336	-0.98598380722256	3.89885758285190
N	8.08052848030923	4.79837488685747	0.31637788737519
N	-4.36277044415761	-6.01563564157930	-0.29262869004865
C	6.97109368603218	7.25306001216030	0.49193687424001
C	10.70726744909174	4.49434904123048	-0.23867082410647
C	-7.00418278103219	-5.74781086925824	0.21392306337014
C	-3.22281957951618	-8.45745164504352	-0.46728118473994
C	7.68590904897675	9.18325496416105	-1.20138200781340
C	6.55825398027515	11.56368331272061	-1.07133278499075
C	4.67810396116174	12.07001255088818	0.72295581365198
C	3.95554253524177	10.15619072082686	2.39735029987803
C	5.09239173003328	7.77516471614465	2.30282067732611
C	12.52901667094996	6.23519985112707	0.62033584270141
C	15.07840612965414	5.88874222359086	0.05324619508350
C	15.95222854407925	3.80166526627000	-1.35046438020191
C	14.11308017348203	2.07356615063061	-2.17568583359713
C	11.54557342286819	2.40919259745265	-1.65205513419286
C	-8.79291251406248	-7.48849422485372	-0.69438891452731
C	-11.36201233025585	-7.18778814425846	-0.15009733484162
C	-12.27006390578300	-5.14357857528509	1.27825688105010
C	-10.45255724946650	-3.40395441496212	2.15451956874028
C	-7.88242321262108	-3.69207254417918	1.65714751902162

C	-3.94533644758385	-10.40756166667486	1.19956455237433
C	-2.78763059877408	-12.77382942621610	1.07447644077571
C	-0.86816560241789	-13.24466481541083	-0.68799013368245
C	-0.13977100013091	-11.31217670154438	-2.33743861934275
C	-1.30641136067608	-8.94509417524599	-2.24826690514768
H	-5.58826387956010	-2.86503520381759	-3.96814823303801
H	-3.21157050287699	0.90874229499227	-5.43382361015309
H	0.56395979628229	3.68684814875252	-5.16141753699269
H	4.52661397942422	4.90533422834996	-3.06528605709942
H	3.12030708106979	-4.86964698102604	5.21905954306829
H	-0.83416291743303	-6.09651400921591	3.11503414046870
H	9.28836310348533	1.66437348401399	4.00599828702979
H	6.89703823693082	-2.09445872645278	5.49017056423852
H	9.12234301190357	8.79164912821299	-2.62427945999522
H	7.13588428022305	13.02661789153525	-2.40570650250685
H	3.78812368727954	13.92708110173213	0.80763885382345
H	2.50075161588950	10.51900372955365	3.81482002399186
H	4.52238924911768	6.30365539543374	3.62485093811980
H	11.93664057537680	7.85964779683593	1.73835534906977
H	16.42292696025526	7.28285969490960	0.75969790609887
C	18.80338528743007	3.49734107068240	-1.90716269408932
H	14.65968564154955	0.42768200969549	-3.28319556765010
H	10.17095147363440	1.04113143906385	-2.34591578901001
H	-8.17159898753524	-9.08715075755110	-1.83394194079682
H	-12.66946074428343	-8.59067954216595	-0.89722772128115
C	-15.09809915457531	-4.75411615174566	1.90070391821945
H	-11.04357079014257	-1.78860437237861	3.29092113465594
H	-6.52975854870279	-2.32307273992684	2.39200418341220
H	-5.41597261277979	-10.04488346912009	2.59437759030571
H	-3.37288570742057	-14.25295609120740	2.38741214892847
H	0.04512621388948	-15.09047024895049	-0.76835273458832
H	1.34551281965372	-11.64743184174930	-3.72935632661980
H	-0.72892173949982	-7.45874333672269	-3.54993946765026
C	19.74913138870945	5.80344190249094	-3.46843106343385
C	19.38839867175928	1.06665402530596	-3.43017036817565
C	20.29075971689596	3.36726924484557	0.62673338577565
C	-16.79356036811402	-6.83928620722077	0.74048686716423
C	-15.98828846240255	-2.15795168743877	0.84485891847858
C	-15.47018049515748	-4.79148776676684	4.81877007731490
H	19.45408217681319	7.59279559285209	-2.45263658281484
H	18.73804962804343	5.92584297282819	-5.28225050692225
H	21.78523451070732	5.62432646050751	-3.86853268285150
H	18.43281783668224	1.06548790366012	-5.27775304000298
H	18.81890023938272	-0.64690258955498	-2.39637099466718
H	21.43518338186153	0.93943010744634	-3.78287735402229
H	22.33071472245645	3.16663923691402	0.25843879934521
H	19.67073521035309	1.73881711687649	1.76298619811993
H	20.01542412415618	5.08241829222779	1.76713852734945
H	-16.30597707515639	-8.72559719648456	1.46981414189048
H	-16.65127949610486	-6.88220905903002	-1.33431335588422
H	-18.78247155045475	-6.47096175555865	1.22714327213427
H	-17.99712445591204	-1.84347611554401	1.29361646350021
H	-15.76243966438019	-2.08904529416292	-1.22238397232204
H	-14.90102984986669	-0.58406711531048	1.65817880870844
H	-14.87695885674750	-6.62010821233952	5.61488124650737
H	-17.47381363989759	-4.48788563364188	5.29766875969935
H	-14.35946734840003	-3.30169894005572	5.75017595598998

Table S2 (f). Optimized Modeling Coordinates for **2OMe**.

ATOM	X	Y	Z
C	-3.95610115340213	-2.22228320116464	-2.86173412250806
C	-2.95325953783496	-3.82464675290964	-0.99533020366417
C	-0.63725606114102	-3.18786007517163	0.21537534057391
C	0.67178786188198	-0.93673586632843	-0.56266829508751
C	-0.37319950475842	0.64578804987344	-2.49485457055892
C	-2.70222587030575	-0.03148715526659	-3.59410435707297
C	0.99536960634360	2.85141825876981	-3.25717130069578

C	3.24661410570328	3.49864479651549	-2.15889883140070
C	4.32180340786512	2.00142478055482	-0.17155293566546
C	3.01130750432535	-0.24813216880881	0.60858942227147
C	4.05608778721807	-1.83043244537242	2.54116452401090
C	2.68777651034854	-4.03636786393523	3.30301174413311
C	0.43796338215251	-4.68493396050078	2.20275948247619
C	6.64014477246268	2.63549301167298	1.03603991217076
C	7.64138649864927	1.03469491660883	2.90460493881873
C	6.38527928648283	-1.15370821634029	3.64018554972889
N	8.01092070762319	4.87621432922069	0.34511491665317
N	-4.31750252348546	-6.07248163076035	-0.31352360535175
C	6.90827329747134	7.31278542428116	0.69621675212171
C	10.62051933321842	4.61690519383190	-0.32910641359010
C	-6.92823392272961	-5.82557925036027	0.35953978387007
C	-3.20322959380170	-8.50321648431803	-0.67120560324780
C	7.54441033839018	9.33360644071032	-0.92157218044734
C	6.42661896731854	11.70270115683523	-0.60012435252059
C	4.64581895407655	12.10580057730634	1.31756004750460
C	4.00201216299241	10.10290893464152	2.91824002145786
C	5.12862505529499	7.73122524459249	2.63108751583450
C	12.48122696556607	6.24745121015706	0.62924087281954
C	15.02329120330289	5.97145525829209	-0.05389127955243
C	15.75044150030506	4.01115454271184	-1.68256563931381
C	13.90339596045204	2.35414630217481	-2.63028478663277
C	11.37700750547892	2.66268432623894	-1.97677852078811
C	-8.78092288588025	-7.46633229920641	-0.59716965800977
C	-11.32457386617300	-7.20070596811876	0.08436344779948
C	-12.06219553814542	-5.24101837795922	1.70900155853802
C	-10.22308930277161	-3.57496451923927	2.65655217630169
C	-7.69512418126227	-3.87306846396795	2.00473101514749
C	-3.82909740375388	-10.53247840845984	0.94028930733387
C	-2.69388030872474	-12.89257256125210	0.61360138980497
C	-0.90889321041034	-13.27895621842225	-1.30348755184905
C	-0.27703426188436	-11.26813232940529	-2.89908352946782
C	-1.42079847101382	-8.90551105531470	-2.60661951204343
H	-5.74273746483869	-2.74075073982759	-3.74691619656573
H	-3.50571033509820	1.16752801025951	-5.06848827436316
H	0.20551088705349	4.02242206874718	-4.76156319957685
H	4.24651492002611	5.18012793456449	-2.78953905019524
H	3.47731609080094	-5.20719178332386	4.80769903744313
H	-0.56089139884026	-6.36761422304243	2.83181048695304
H	9.42931945700485	1.55198066779636	3.78788219728830
H	7.18800904190411	-2.35212283446277	5.11545616053200
H	8.90346027728071	9.02269509259827	-2.43698123365973
H	6.93656914939845	13.23979809033757	-1.87754629209743
H	3.76687418187662	13.95522220776632	1.55403243415712
H	2.62791825048109	10.38811252413820	4.43011044155872
H	4.63050898449613	6.18643159453306	3.89709640156711
H	11.93781245312841	7.76097538817142	1.91459198983329
H	16.40961254524228	7.27977774624152	0.72006820441860
H	14.49010028494598	0.84700611033947	-3.90538912262622
H	9.95625650060590	1.38190173551593	-2.74000054690186
H	-8.23038544198774	-8.97949287123761	-1.87976266494203
H	-12.70407305491622	-8.51797583683851	-0.68660292919780
H	-10.81685970819966	-2.06924123649355	3.93006837701107
H	-6.28074887422949	-2.58549807149027	2.76833438799326
H	-5.19185825074839	-10.23476161003266	2.45501304758757
H	-3.19410524584896	-14.43688716762857	1.88611391917484
H	-0.01742691637468	-15.12196886351630	-1.54349453515809
H	1.10018932432833	-11.54021425406402	-4.41043004567724
H	-0.93252505196507	-7.35385623677353	-3.86785650860836
O	18.20477875348445	3.55128728457329	-2.47361611060519
O	-14.51943309195884	-4.79039446949668	2.49658214873376
C	20.15169285139594	5.19401127997328	-1.53248274953869
C	-16.45957416577396	-6.43947607427844	1.55259330377800
H	19.83659998723437	7.16477876337149	-2.13584307096544
H	21.91851912795939	4.49332912958466	-2.35413229930422
H	20.27266664371632	5.11552337620054	0.54671545957663
H	-16.14622978582735	-8.40704745443282	2.16765953935520
H	-16.56885018110459	-6.37168587986367	-0.52759498954599
H	-18.23148247524646	-5.73606857032098	2.36070064716400

Table S2 (g). Optimized Modeling Coordinates for **2NPh₂**.

ATOM	X	Y	Z
C	-3.86110299215478	-1.69109132014042	-3.12019286980225
C	-3.13977198581205	-3.35747834891457	-1.18182084609151
C	-0.82163467762093	-2.96110675784982	0.13227502162117
C	0.78784059383383	-0.91119814904924	-0.63525129604844
C	0.03215472747641	0.72731839381017	-2.65304046044910
C	-2.31705226146522	0.31225071606957	-3.83772869003527
C	1.70164449568545	2.71415596077668	-3.41277546754098
C	3.96153355287310	3.11923929888176	-2.22057849623482
C	4.75059717367557	1.57681787871882	-0.13359604789693
C	3.14784607689686	-0.48256256465381	0.62416954331927
C	3.90529614621114	-2.12306467676782	2.63941106588561
C	2.24077734414787	-4.11731353794724	3.39171041830511
C	-0.02514190280395	-4.51526171051053	2.20748836903617
C	7.05005048754832	1.99831149644814	1.20562136837961
C	7.77882693923447	0.32433451119434	3.13581672478175
C	6.24982133111920	-1.69857646862974	3.83131421123549
N	8.60528345715374	4.14955802930431	0.64757177748063
N	-4.73658809911850	-5.46652198726922	-0.57489659189987
C	7.56561536530930	6.64169426095777	0.86086725146630
C	11.27543290267480	3.85478056191455	0.33648663503632
C	-7.39762025103444	-5.07992752359093	-0.25524807426193
C	-3.79202447317484	-7.98843712224351	-0.84514010405680
C	8.38841264590603	8.57611781342418	-0.77560228903191
C	7.36890109667587	11.00197285933463	-0.59682853220859
C	5.48461888147508	11.54184341908172	1.18271781026591
C	4.64485853856804	9.61957030293187	2.79176573905476
C	5.67999070756658	7.19331437808017	2.65196236413588
C	12.97436626309078	5.56368268306387	1.46905073033051
C	15.56233958100752	5.38952400215493	1.02717910164396
C	16.55668938152996	3.49497819681996	-0.55169190025898
C	14.87358532333834	1.71313039847180	-1.59213857060528
C	12.27688307321189	1.89104439415893	-1.15555923709480
C	-9.16534667596082	-6.65108967311561	-1.47472141103776
C	-11.74752192484250	-6.36324836042996	-1.05349481727908
C	-12.66565729629111	-4.48821563273563	0.59609721197767
C	-10.90547540449752	-2.85342755353591	1.74270453295945
C	-8.31700329714955	-3.14068688726684	1.31818022160375
C	-4.71202442794235	-9.93305107575128	0.72620772050828
C	-3.78971665459332	-12.39218350708311	0.48431479241623
C	-1.91299990313188	-12.96022779142703	-1.29396207740093
C	-0.97884091081120	-11.03040934845942	-2.84004278023985
C	-1.91244586566765	-8.56798044674981	-2.63472382133052
H	-5.64870076789784	-2.01799818889706	-4.08926568422814
H	-2.90207732241216	1.55714751539334	-5.37477728623305
H	1.13802566646734	3.91674608561960	-4.99156200813476
H	5.18907325175387	4.64007131805231	-2.85517870226470
H	2.81103829613367	-5.32806729287821	4.96179407278436
H	-1.25408158827689	-6.03713755392128	2.83804544555039
H	9.55541267235539	0.66435109983009	4.12116065751031
H	6.83956263257889	-2.94724896153824	5.36343522184043
H	9.83087749590595	8.15756886709831	-2.18457668321041
H	8.02985628496003	12.47198388045172	-1.88380070731496
H	4.67758008372646	13.43409368338581	1.30678821363938
H	3.18216953344280	10.01071155160184	4.19269409702252
H	5.02975439546272	5.71320971178905	3.92649548316490
H	12.25641839752484	7.04968072861689	2.69853391426508
H	16.84013516668243	6.74242551867655	1.90865435129581
H	15.59851352540520	0.21586525207181	-2.80585743243802
H	10.99946032294254	0.53525551595806	-2.03603607451495
H	-8.50723914998949	-8.11916310890386	-2.75886740056872
H	-13.07908400200517	-7.60549932208078	-2.01423271684095
H	-11.56979832662136	-1.37768411057962	3.01603907429643
H	-6.98157742548047	-1.89356011473954	2.27038487765505
H	-6.15085613017861	-9.49759734815852	2.13358793605856
H	-4.52242318103998	-13.86961091333527	1.72321567404883
H	-1.18784810489046	-14.88217430810042	-1.46826546030844
H	0.47702829004744	-11.44181071563258	-4.24234466107511
H	-1.19482612080770	-7.08295737515536	-3.86637917552590
N	19.20605735011747	3.46076547822494	-1.11190596645399

N	-15.31294913049948	-4.32480760564151	1.12621487440668
C	20.43391439826532	5.81229655251057	-1.66779896788405
C	20.61238296431944	1.16113276887169	-1.10347166144442
C	-16.58656331539816	-1.94898849374260	1.22031539873712
C	-16.70455768803111	-6.62302673182312	1.49402420940384
C	22.77992111144783	6.41636566485338	-0.57030194392491
C	23.94955237554610	8.72078242754138	-1.11209526220966
C	22.79201707073966	10.47259406281296	-2.72210011240340
C	20.45499808020077	9.88154640502142	-3.81090700023018
C	19.28682793911426	7.56980796649227	-3.30265837101691
C	22.65250666951057	0.81240803123414	-2.78222803051972
C	24.04266884956339	-1.43022271472315	-2.75105458868714
C	23.41411647011160	-3.38787859418530	-1.08664473878360
C	21.37705323874087	-3.05949216813855	0.56767069871710
C	19.99518399895538	-0.80982933364068	0.57661898844568
C	-18.60182969542195	-1.57366209089214	2.92184243849527
C	-19.89691202136704	0.72443642729900	2.97394264318534
C	-19.19244197354237	2.70744438490472	1.37089697967772
C	-17.16926294740582	2.35604120048021	-0.29600485017712
C	-15.88009447401547	0.05317505445380	-0.38586009909858
C	-19.04012403853881	-7.01067233109200	0.28038281689360
C	-20.36303869493845	-9.26870374403508	0.63393073464531
C	-19.37786419883371	-11.17983436598891	2.17478210987237
C	-17.05242560872578	-10.80254718331117	3.38057872578363
C	-15.73077521122911	-8.54074812134748	3.05813773339462
H	23.67468556338670	5.06975773190269	0.70474207390036
H	25.76396747393718	9.16306194983255	-0.23643289326623
H	23.70300917728031	12.27789748008551	-3.12262831859652
H	19.53829675765773	11.21940342257838	-5.08573656815533
H	17.47785431654874	7.10791683624030	-4.17122356925201
H	23.14382488332205	2.30925575603038	-4.10672683488130
H	25.61630175552526	-1.65564575555981	-4.06561745874790
H	24.49893977369291	-5.14105374244510	-1.07600791073220
H	20.86626355905801	-4.55821227137395	1.88929342873357
H	18.43366600056920	-0.56415254834704	1.89477137627333
H	-19.15298551250461	-3.09946742513803	4.18822431837044
H	-21.45807389897524	0.97036227660619	4.29947750312304
H	-20.20385350086584	4.50259086818559	1.42324903950682
H	-16.59934844646942	3.87807711125265	-1.56548212790119
H	-14.33099991689967	-0.21233777779306	-1.71532821231613
H	-19.80351112845013	-5.53935554890679	-0.94132105811387
H	-22.16680147141363	-9.54635797025899	-0.32701314317446
H	-20.40899723680996	-12.94623662013527	2.43346650558369
H	-16.26969231721874	-12.26832469256441	4.60227494551056
H	-13.92812371465789	-8.24255587727589	4.00762087769030

Table S2 (h). Optimized Modeling Coordinates for **2NMePh**.

ATOM	X	Y	Z
C	-3.77914493516583	-1.72072828802173	-3.05598957966313
C	-3.02710748177971	-3.34824376567805	-1.09459216530569
C	-0.73028956106361	-2.87094210595964	0.23222694116819
C	0.81240459949149	-0.76695387616265	-0.53139309717228
C	0.02242788948159	0.83418350977861	-2.56714464507322
C	-2.29295979538807	0.32305510802621	-3.77812480998095
C	1.61663443084915	2.88809994045193	-3.30903806562790
C	3.84106383554792	3.39245550141140	-2.08870348050143
C	4.66433949086456	1.88131337231048	0.00750230909226
C	3.13453747468144	-0.23821232552594	0.75472824008467
C	3.93361336149210	-1.84228602461200	2.78409198078036
C	2.33791565235711	-3.89439991734429	3.52826268761157
C	0.09955723701774	-4.38301562815524	2.32516623899935
C	6.93914015391685	2.38356474968593	1.35796013761370
C	7.71625111146982	0.74025166051236	3.29541661736277
C	6.25187969451386	-1.32898998227231	3.99245359943985
N	8.45171934036733	4.56051385385926	0.78092806637545
N	-4.60535430336412	-5.45784704831435	-0.45285500416338
C	7.40922770478460	7.03832432687217	1.01743030125212

C	11.10707411060718	4.23969155551549	0.35136038968668
C	-7.27169128311978	-5.03808727320198	-0.16981321977972
C	-3.65831863785922	-7.97963354963131	-0.60365529822623
C	8.30267843234945	9.02812355388000	-0.51485534040311
C	7.27607133001654	11.44902470920995	-0.29908725237946
C	5.31684184159504	11.93485896804232	1.41343125844224
C	4.41081836738839	9.96160827302202	2.92194407363545
C	5.44895387244820	7.53997190462534	2.74737979891858
C	12.90034940975580	5.81926548829377	1.53008635760397
C	15.46783292618693	5.55831049971587	1.03827991037138
C	16.37395520283430	3.69329319009291	-0.64785168560399
C	14.58228021447518	2.05725816188152	-1.75057341490489
C	11.99926016541905	2.33541631570201	-1.26481107904883
C	-9.05464813149508	-6.50770352297265	-1.47010042028061
C	-11.64410374302536	-6.10433515667943	-1.15350084346452
C	-12.55888722976730	-4.19888915972192	0.47343093936577
C	-10.75052145272768	-2.71338278500182	1.76574964856744
C	-8.17269698266455	-3.12735404553442	1.44974656758216
C	-4.66693995999270	-9.88447363425273	0.96384530284085
C	-3.72563936194359	-12.34573078860183	0.85441219646717
C	-1.74579842280691	-12.96239201727921	-0.79151843362035
C	-0.73523986683366	-11.07552882925471	-2.34284964412152
C	-1.68219657769132	-8.61164294492328	-2.26936757761073
H	-5.55449196037072	-2.10253957330847	-4.02820385779168
H	-2.90720905511829	1.54021817902518	-5.32643060486081
H	1.02146774836132	4.06391867810948	-4.89649081275213
H	5.01570152650270	4.96271320344621	-2.70450104953764
H	2.93695310055102	-5.07603642254203	5.10996349391545
H	-1.07902178768580	-5.94458552031054	2.95428566856946
H	9.48436017381117	1.13639643908868	4.27506831516789
H	6.87736273921946	-2.55611841627704	5.52823708257846
H	9.80556461257194	8.65832795987820	-1.87237057223629
H	7.99402381596286	12.95971993508984	-1.50681043840598
H	4.50668689491494	13.82387956756659	1.56703845909458
H	2.88935474883455	10.30711938209566	4.27150090341721
H	4.74750564220631	6.02347951299947	3.94961158633478
H	12.26608067680605	7.26767067536008	2.84895378378225
H	16.81264725204224	6.79135182440476	1.99175645981919
H	15.18163387054158	0.58404782498619	-3.05520002563194
H	10.65215174228361	1.07634977541629	-2.18435979178414
H	-8.41401527716734	-7.98633175758067	-2.75238689662786
H	-12.95037322873315	-7.27491255562587	-2.22661107083336
H	-11.38517813133309	-1.25664317440028	3.07304416896859
H	-6.82223369094488	-1.97848907819974	2.49913105101540
H	-6.18975592325337	-9.41266919917028	2.26627644676342
H	-4.53189751005052	-13.78826980657271	2.08970180202628
H	-1.00457539582315	-14.88478590771544	-0.86397965118115
H	0.80051182355263	-11.52175833835057	-3.64553615996345
H	-0.89052892751669	-7.16066306270345	-3.49673205163657
N	19.00582304894677	3.45437617813605	-1.09178478817440
N	-15.17639600325736	-3.87252899251269	0.91360567147084
C	20.54560306095479	5.67415717971051	-1.34954610558600
C	-16.22472991045895	-1.44272375192768	1.48782772185094
C	23.04235431372057	5.67030030916063	-0.43141627292465
C	24.58565297309663	7.79216028552377	-0.72496571124072
C	23.66073082979408	9.97018089086613	-1.90665871547014
C	21.17396919844833	9.99338620611664	-2.80652518984100
C	19.63159652943996	7.86664026915802	-2.54593812904991
C	-18.21489317052805	-1.24255729948377	3.24481828951807
C	-19.30743665350602	1.09843648807410	3.78523087751987
C	-18.41135685391840	3.29461093073965	2.61592690642754
C	-16.41859452689794	3.11392381865587	0.88601022952442
C	-15.34205905943370	0.77278568058850	0.30894589121259
H	23.75943247630119	4.00153884140016	0.54319040981649
H	26.51355908503534	7.75241619494170	0.00793645477221
H	24.86351776394374	11.63054934224314	-2.12263739268343
H	20.42902305572982	11.67372380352703	-3.74296625322475
H	17.70564630104816	7.88961916687286	-3.27287189934295
H	-18.88423798313727	-2.93353528518957	4.21440083488947
H	-20.84718267123078	1.20467412048274	5.15324508377336
H	-19.25919698165505	5.12415098885434	3.04515223466233
H	-15.70648048965452	4.80875245393315	-0.04883596170162
H	-13.81693802903275	0.65151751807072	-1.06891046601359

C	19.92940873447001	1.14762818504957	-2.33533019332359
C	-16.92274249955285	-5.83939717911979	0.01629586615600
H	19.41349793100349	1.06990818093635	-4.36307695773508
H	19.15015318153984	-0.52601992927697	-1.38433407193128
H	21.99328110975409	1.08646301705024	-2.19961406735621
H	-16.25603604886003	-7.71175340266562	0.62221061920303
H	-17.11515637891487	-5.84081359688062	-2.06677411022024
H	-18.79491127927461	-5.50933716437360	0.83028543941976
