Supporting Information

A New Luminescence Process of Polycyclic Aromatic Hydrocarbons with Carbonyl Groups: Photophysical Properties of Secondary *N*-Alkyl and Tertiary *N,N*-Dialkyl Carboxamides of Naphthalene, Anthracene, and Pyrene

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1. Materials and instruments used in this study.

Materials. Pyrene-1-carboxylic acid chloride and anthracene-9-carboxylic acid chloride were obtained by the reaction of corresponding carboxylic acid and oxaryldichloride with DMF as a catalyst.[103] Pyrene and anthracene were used after purification by recrystallization with ethanol two times. EPA, organic glass solvent, was prepared by mixing ethanol, diethylether and isopentane in 1:3:3 volume ratio. *N*-benzylpyrene-1-carboxamide, (**Py 1a**) *N*-*n*-butylpyrene-1-carboxamide (**Py 1b**), *N*-tert-butylpyrene-1-carboxamide (**Py 1c**), *N,N*-diethylpyrene-1-carboxamide (**Py 2a**) and *N*-benzyl-*N*-tert-butylpyrene-1-carboxamide (**Py 2c**) were prepared as described in a previous report.[83]

Instrumentals. All photophysical measurements performed in solutions were carried out using dilute solutions with optical density (O.D.) around 0.1 at the maximum absorption wavelength in 1 cm path length quarz cells. In addition, all samples solutions were deaerated by bubbling with algon gas for 15 min before the measurements. Absolute Quantum Yields were measured by a Hamamatsu Photonics C9920-02 Absolute PL Quantum Yield Measurement system. Fluorescence lifetimes of *N*-alkyl or *N,N*-dialkylpyrene-1-carboxamides were measured using a Hamamatsu Photonics OB 920 Fluorescence Lifetime Spectrometer equipped with flash lamp. In addition,

HORIBA Jobin Yvon FluoroCube Fluorescence Lifetime Imaging and Time Correlated Single Photon Counting system equipped with LEDs lamps (269 nm and 371 nm) were also used in measurements of *N*-alkyl or *N,N*-dialkylnaphthalene-2-carboxamides and *N*-alkyl or *N,N*-dialkylanthracene-9-carboxamides.

2. Optimized structures of Nap 1, Nap 2, Anth 1, Anth 2, Py 1a and Py 2a in the ground states.

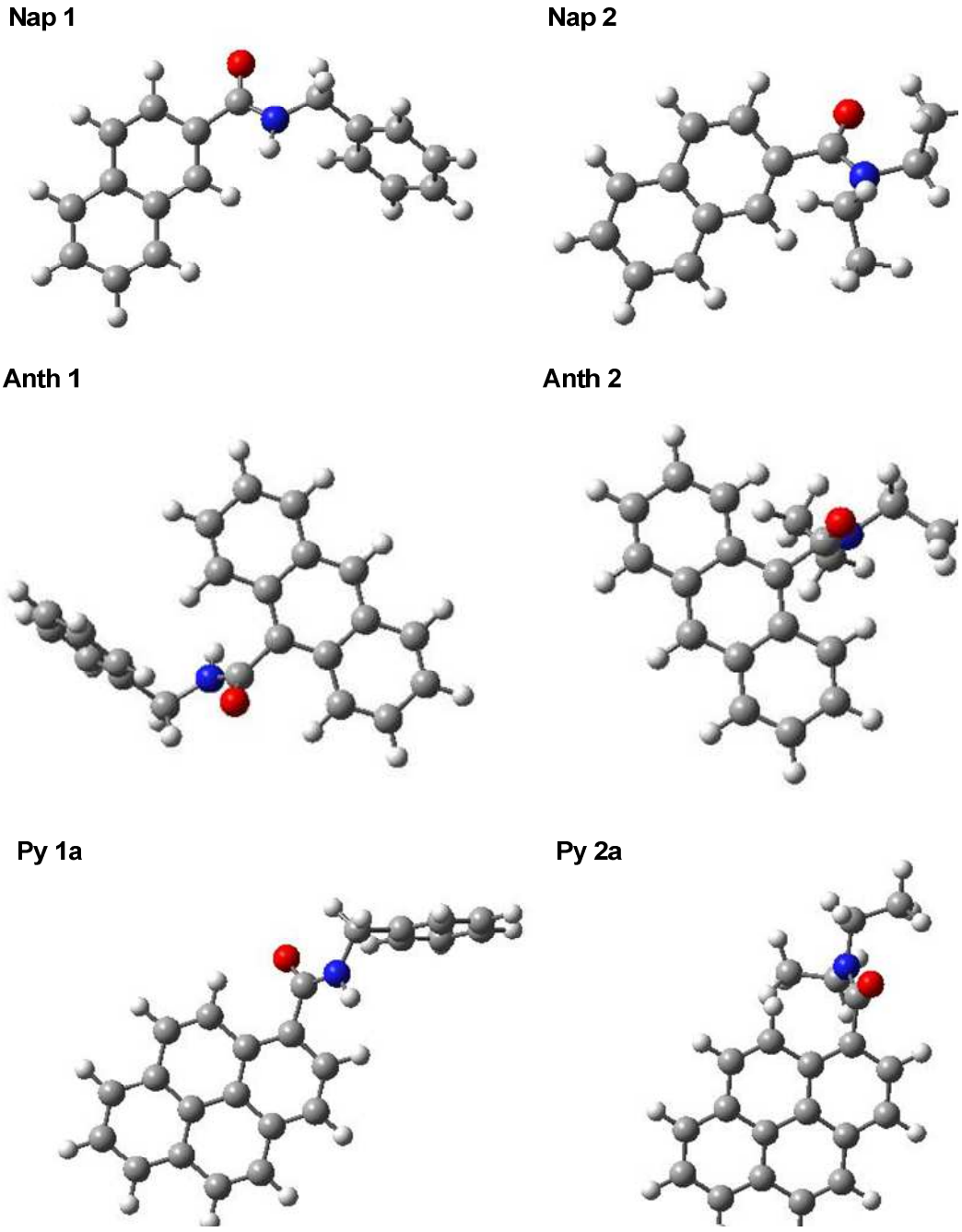
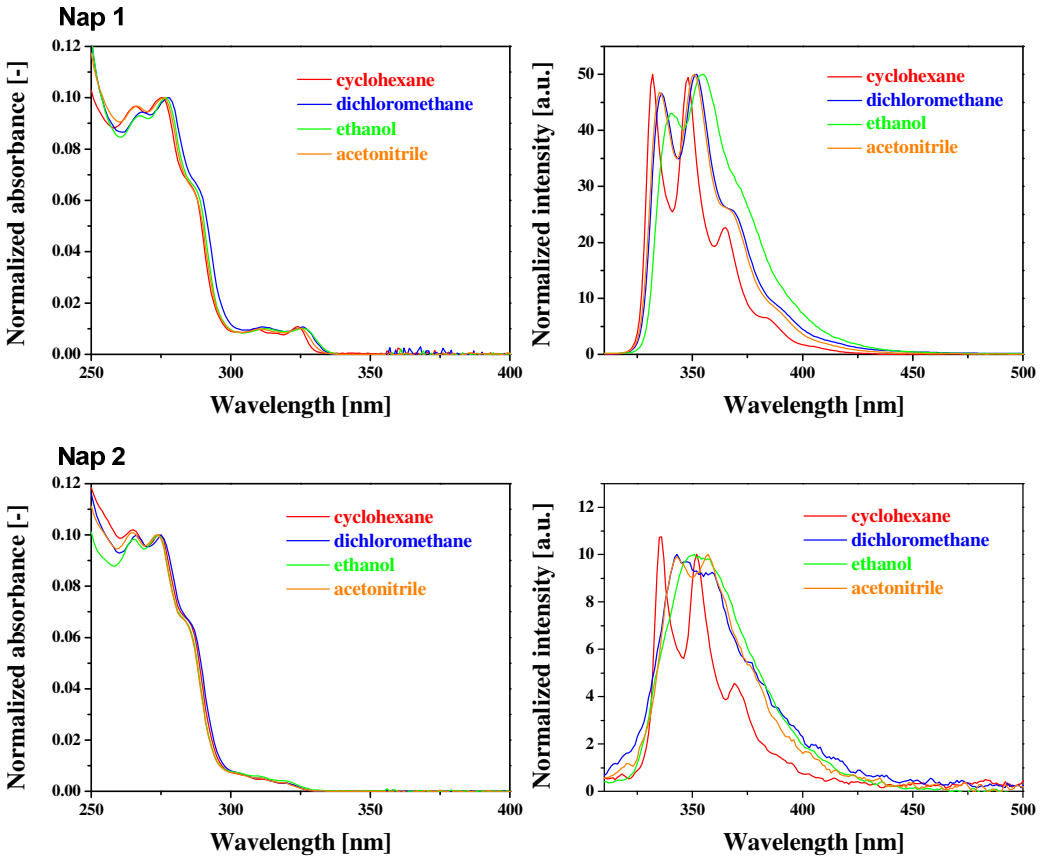
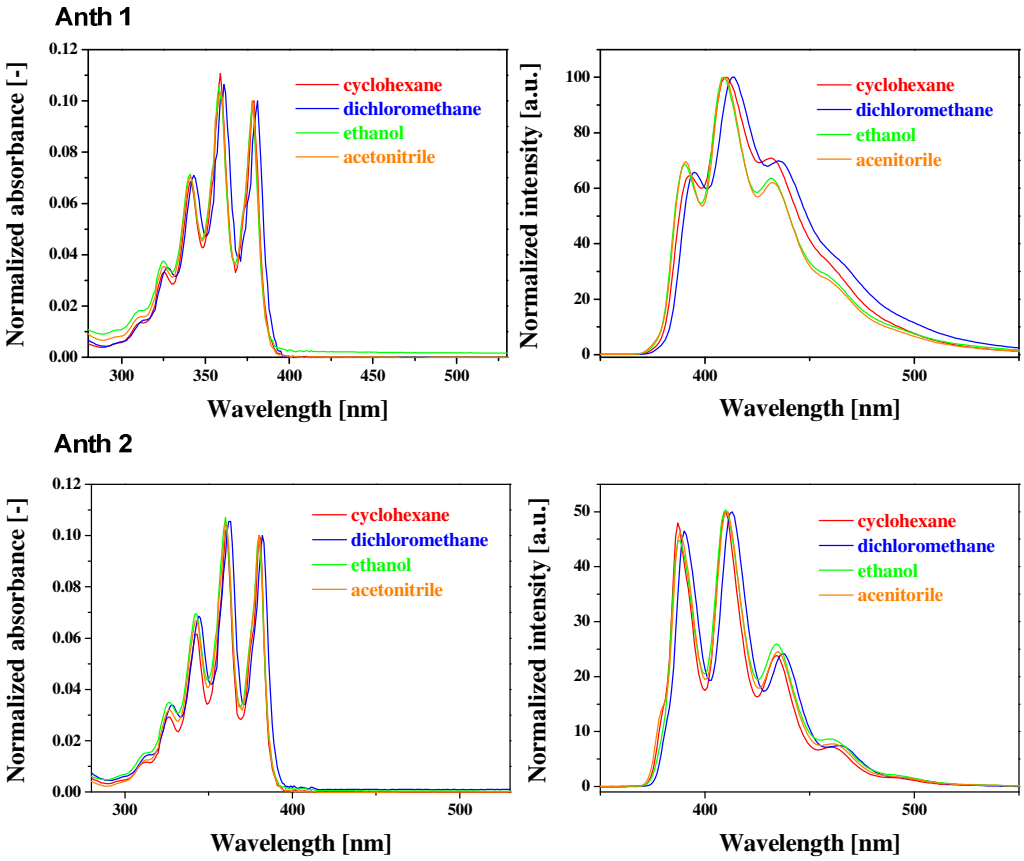


Figure S1. Optimized structures of **Nap 1**, **Nap 2**, **Anth 1**, **Anth 2**, **Py 1a** and **Py 2a** in the ground states (DFT at ωB97X-D 6-31G(d,p)).

3. Sovent polarity dependence of Nap 1, Nap 2, Anth 1, Anth 2, Py 1 and Py 2.

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Normalized absorbance [-]
Wavelength [nm]
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dichloromethane
ethanol
acetonitrile
Normalized intensity [a.u.]
Wavelength [nm]
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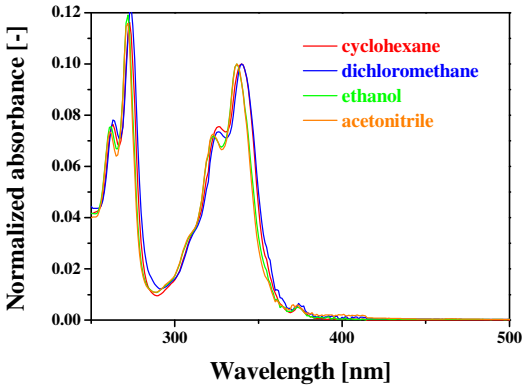
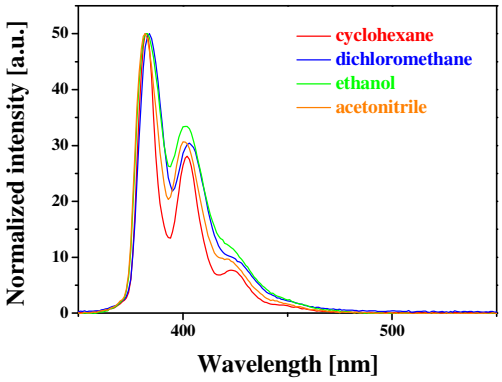
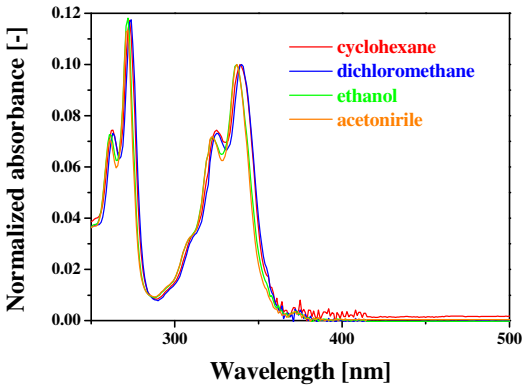
dichloromethane
ethanol
acenitorile
Anth 2
Normalized absorbance [-]
Wavelength [nm]
cyclohexane
dichloromethane
ethanol
acetonitrile
Normalized intensity [a.u.]
Wavelength [nm]
cyclohexane
dichloromethane
ethanol
acenitorile

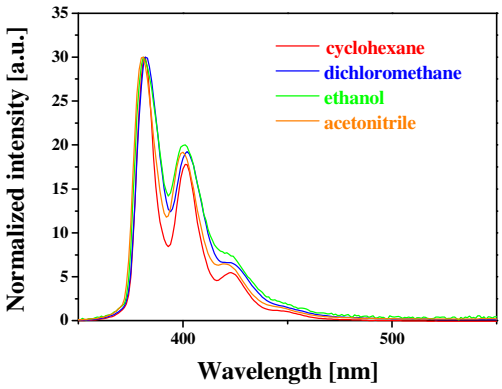
Py 1a



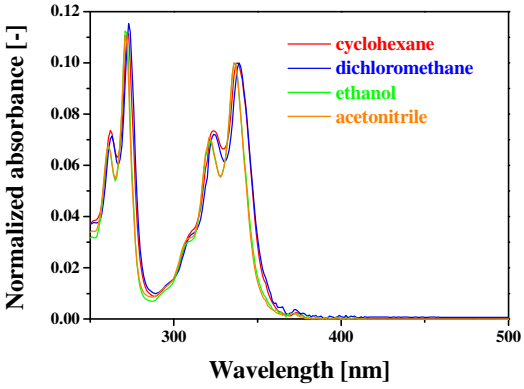


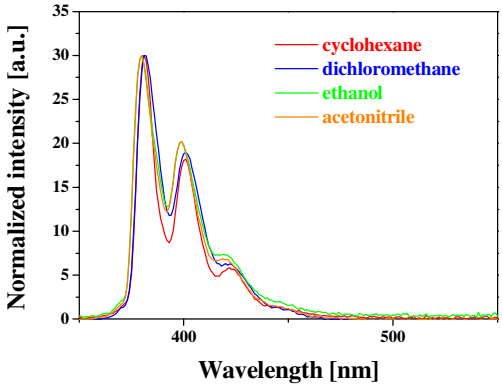
Py 1b



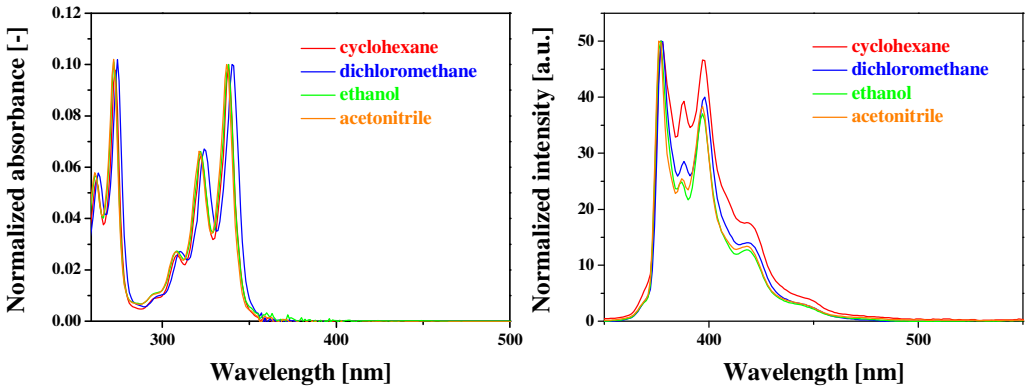


Py 1c

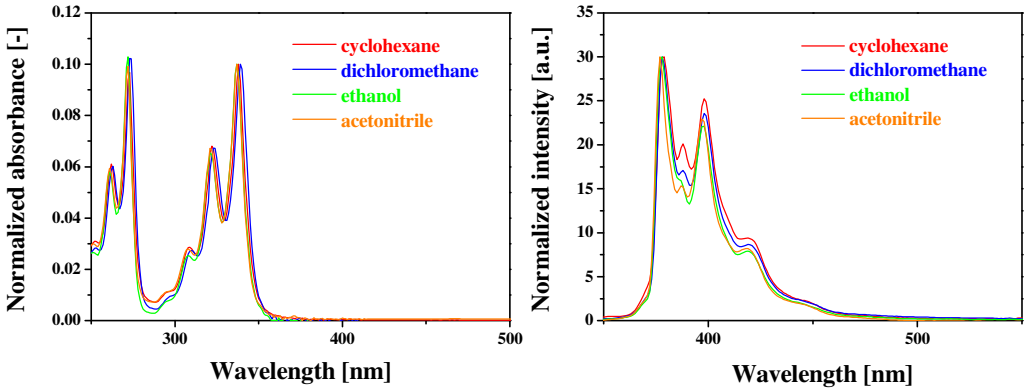




Py 2a


Normalized absorbance [-]
Wavelength [nm]
cyclohexane
dichloromethane
ethanol
acetonitrile
Normalized intensity [a.u.]
Wavelength [nm]
cyclohexane
dichloromethane
ethanol
acetonitrile

Py 2b


Normalized absorbance [-]
Wavelength [nm]
cyclohexane
dichloromethane
ethanol
acetonitrile
Normalized intensity [a.u.]
Wavelength [nm]
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dichloromethane
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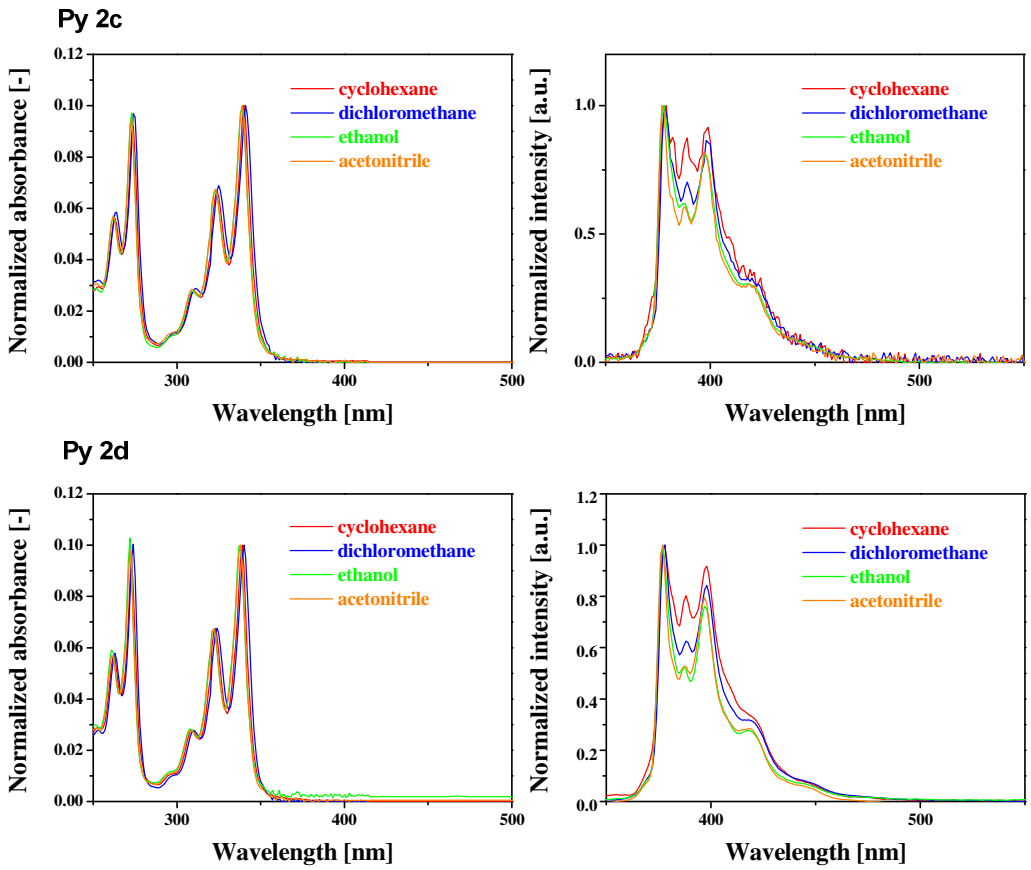


Figure S2. UV-Vis and fluorescence spectra of *N*-alkyl and *N,N*-dialkyl carboxamides in several solvents (room temperature, $\lambda_{ex} = \lambda_{em}$).

Table S1. Photophysical parameters of *N*-alkyl and *N,N*-dialkyl carboxamides in several solvents.

entry	solvent	λ_{abs} [nm]	λ_{em} [nm]	Stokes shift [nm]
Nap 1	cyclohexane	277	332, 348, 365	55
	dichloromethane	278	337, 353, 370	59
	ethanol	277	341, 354	64
	acetonitrile	276	335, 351, 368	59
Nap 2	cyclohexane	274	336, 352, 369	62
	dichloromethane	275	343, 359	58
	ethanol	274	351	77
	acetonitrile	274	343, 357	69
Anth 1	cyclohexane	379	393, 410, 431	14
	dichloromethane	381	395, 413, 436	14

	ethanol	378	390, 409, 432	12
	acetonitrile	378	391, 409, 433	13
Anth 2	cyclohexane	380	387, 410, 434, 462	7
	dichloromethane	382	390, 413, 437, 465	8
	ethanol	380	388, 410, 434, 462	8
	acetonitrile	379	388, 410, 435, 463	9
Py 1a	cyclohexane	340	383, 402, 424	43
	dichloromethane	340	384, 403, 428	44
	ethanol	337	383, 402, 425	46
	acetonitrile	337	382, 401, 423	45
1b	cyclohexane	339	382, 401, 423	43
	dichloromethane	340	382, 402, 424	42
	ethanol	337	381, 401, 423	44
	acetonitrile	337	381, 400, 422	44
1c	cyclohexane	338	381, 401, 422	43
	dichloromethane	339	381, 401, 423	42
	ethanol	336	380, 399, 421	44
	acetonitrile	336	380, 399, 420	44
2a	cyclohexane	338	377, 388, 397	39
	dichloromethane	341	378, 389, 399, 423	37
	ethanol	339	378, 387, 398	39
	acetonitrile	339	377, 388, 397, 420	38
2b	cyclohexane	339	378, 388, 398, 422	39
	dichloromethane	340	378, 388, 398, 420	38
	ethanol	340	377, 387, 397, 419	37
	acetonitrile	338	377, 387, 398, 420	39
2c	cyclohexane	338	377, 388, 397, 419	39
	dichloromethane	340	377, 388, 398, 420	37
	ethanol	338	377, 387, 397, 419	39
	acetonitrile	337	376, 387, 397, 419	39
2d	cyclohexane	338	379, 388, 398, 420	41
	dichloromethane	339	378, 388, 398, 420	39
	ethanol	337	378, 387, 398, 419	41
	acetonitrile	337	377, 387, 397, 419	40

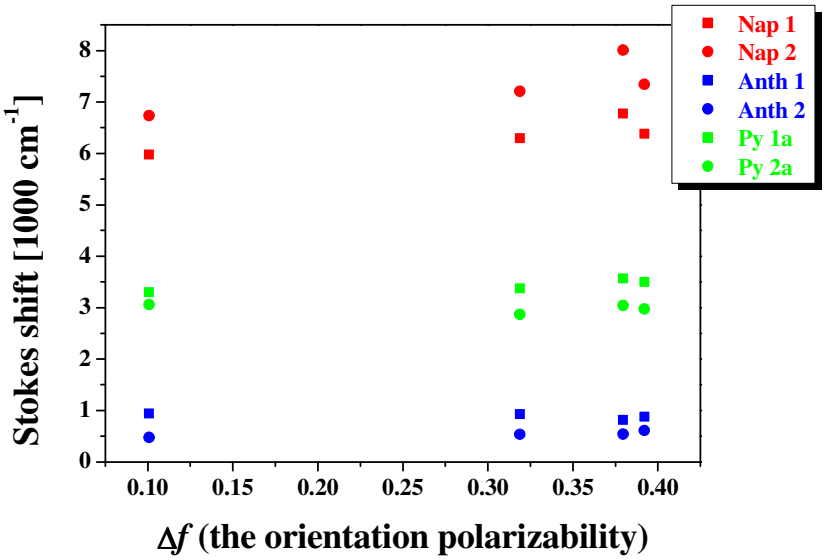


Figure S3. Lippert-Mataga plot for **Nap 1**, **Nap 2**, **Anth 1**, **Anth 2**, **Py 1a** and **Py 2a**. Δf, the orientation polarizability, is defined by $\Delta f = (\varepsilon - 1)/(2\varepsilon + 1) - 1/2\{(n^2-1)/(2n^2+1)\}$. The colored points represent cyclohexane, dichloromethane, ethanol, and acetonitrile in the order of increasing Δf. Solvent properties (the values of dielectric constant (ε) and refractive index (n)) used to calculate Δf are available from ref 91.

Table S2. The changes in dipole moments of **Nap 1**, **Nap 2**, **Anth 1**, **Anth 2**, **Py 1 and Py 2**.

entry	slope	ρ [Å]	$(\mu_e - \mu_g)^{2a}$
Nap 1	1995	4.7	20.9
Nap 2	3123	4.6	29.9
Anth 1	-295	5.0	N.D.[b]
Anth 2	357	4.8	3.7
Py 1a	749	5.1	7.8
Py 2a	-248	4.9	N.D.[b]

[a]$(\mu_e - \mu_g)^2$: The change in dipole moment, were obtained by Lippert-Mataga equation defined by $\nu_a - \nu_e = 2(\mu_e - \mu_g)^2 \Delta f/hc\ \rho^3$ + constant. $\nu_a - \nu_e$, h, c, and ρ mean Stokes shift, Planck's constant, Speed of light, and molecular radius calculated by optimized structures in the ground states, respectively.

[b]N.D.: Not determined because of negative slope.

4. Solvent viscosity dependence of Nap 1, Nap 2, Anth 1, Anth 2, Py 1a and Py 2a.

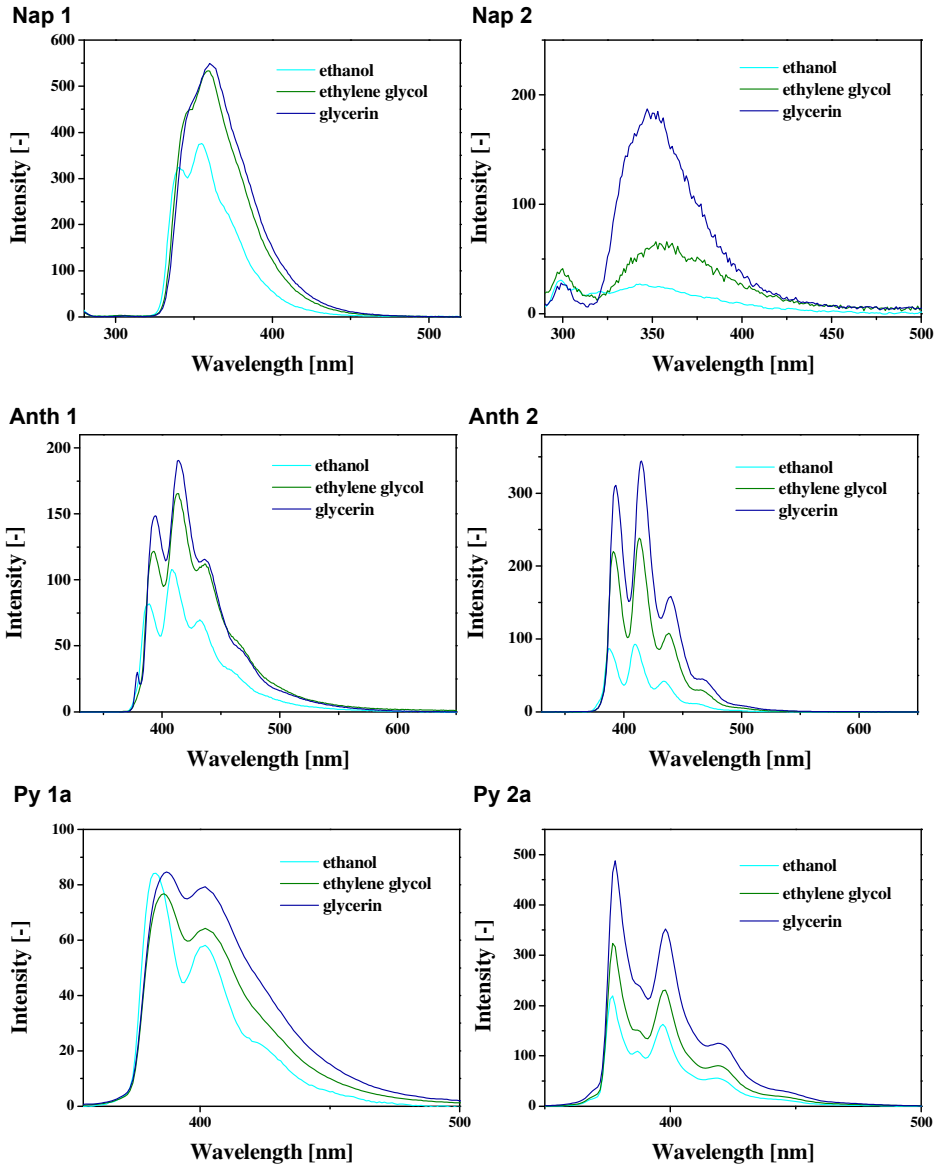


Figure S4. UV-Vis and fluorescence spectra of *N*-alkyl and *N,N*-dialkyl carboxamides in viscous solvents (room temperature, $\lambda_{ex} = \lambda_{em}$).

Table S3. Photophysical parameters of *N*-alkyl and *N,N*-dialkyl carboxamides in viscous solvents.

entry	Solvent	λ_{ex}[nm]	λ_{em} [nm]	Φ_{fl}	τ [ns]	k_r^*	k_{nr}^*
Nap1	ethanol	277	341, 354	0.28	9.19	3.0×10^7	7.8×10^7
	ethylene glycol	278	346, 358	0.28	11.3	2.5×10^7	6.4×10^7
	glycerin	279	361	0.40	10.5	3.9×10^7	5.6×10^7
Nap2	ethanol	274	298, 343	0.0020	0.51(0.17), 1.58 (0.65), 6.70 (0.18)		
	ethylene glycol	275	300, 355	0.0050	1.40 (0.05), 0.12 (0.73), 9.82 (0.22)		
	glycerin	276	301, 351	0.010	0.29 (0.31), 0.97 (0.63), 6.0 (0.06)		
Anth 1	ethanol	379	388, 408, 432	0.10	1.54	6.6×10^7	5.8×10^8
	ethylene glycol	380	392, 413, 436	0.17	2.58	6.6×10^7	3.2×10^8
	glycerin	380	394, 415, 438	0.25	4.79	5.2×10^7	1.6×10^8
Anth 2	ethanol	380	388, 410, 434, 462	0.062	1.15	5.4×10^7	8.2×10^8
	ethylene glycol	382	391, 413, 438, 467	0.19	2.79	6.8×10^7	2.9×10^8
	glycerin	383	393, 415, 440, 468	0.30	4.69	6.4×10^7	1.5×10^8
Py 1a	ethanol	337	383, 401	0.61	27.1	2.3×10^7	1.4×10^7
	ethylene glycol	339	386, 402	0.88	20.7	4.3×10^7	5.3×10^6
	glycerin	340	387, 402	0.91	17.5	5.2×10^7	5.2×10^6
Py 2a	ethanol	337	377, 387, 397, 419	0.061	30.4	2.0×10^6	3.1×10^7
	ethylene glycol	339	377, 387, 398, 420	0.15	28.1	5.3×10^6	3.0×10^7
	glycerin	338	378, 389, 398, 420	0.23	38.6	6.1×10^6	2.0×10^7

*k_r, k_{nr}: Not determined in **Nap 2** because its fluorescence lifetimes were multicomponent.

5. Fluorescence spectra of naphthalene, anthracene and pyrene at 298 K and 78 K.

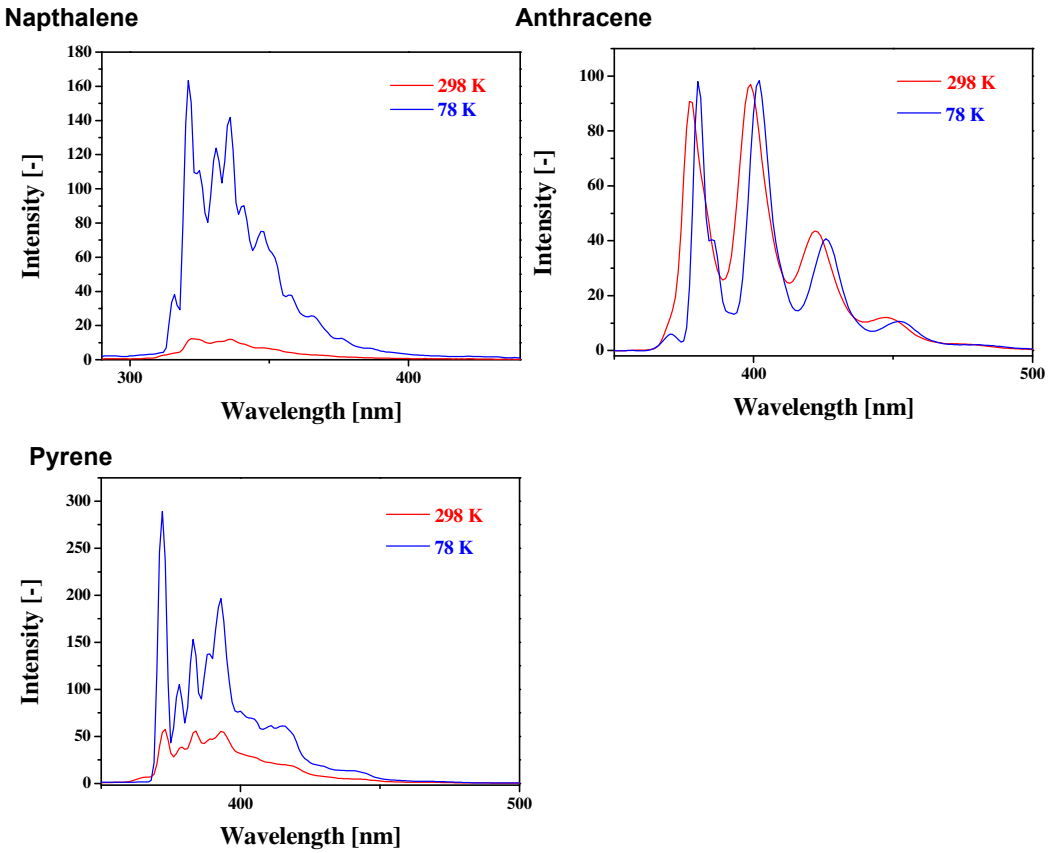
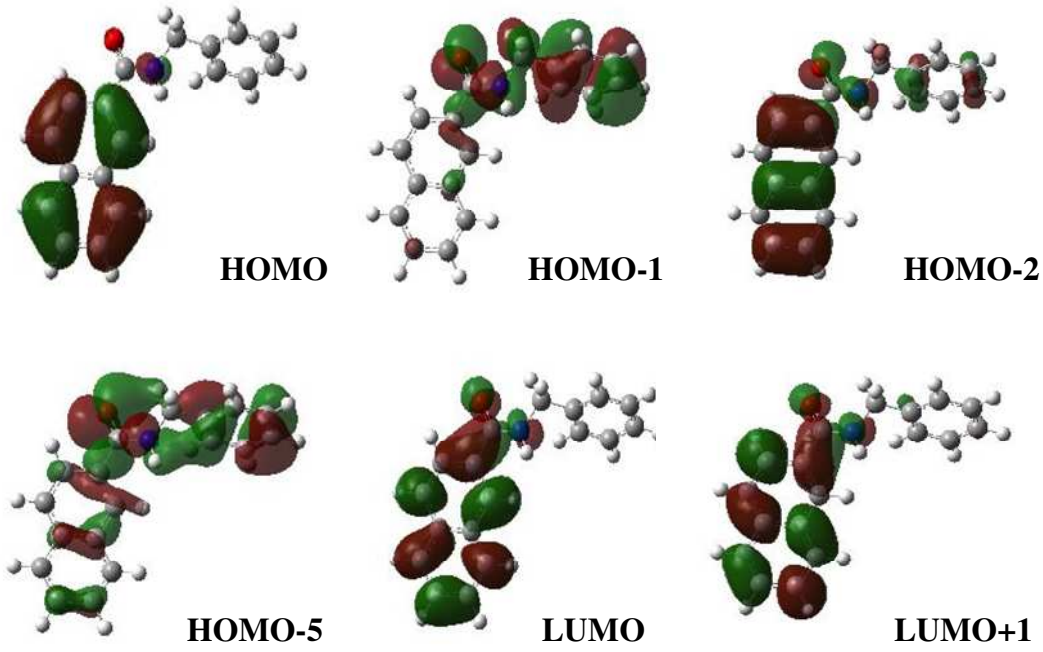


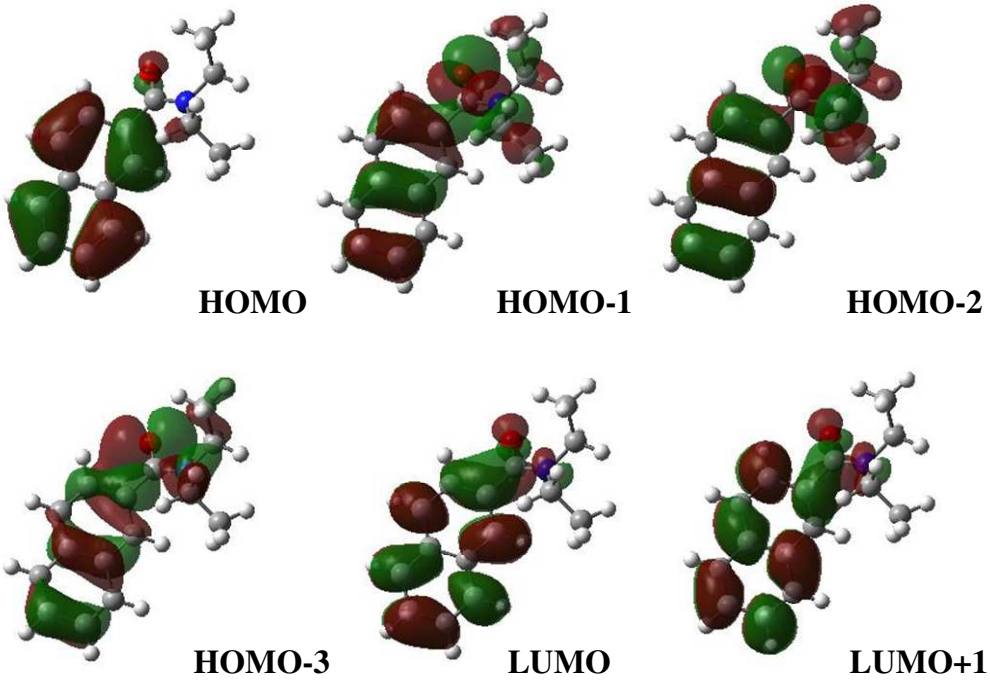
Figure S5. Fluorescence spectra of naphthalene, anthracene and pyrene at 298 K and 78 K (EPA solvent, $\lambda_{ex} = \lambda_{abs}$).

6. Frontier orbitals of Nap 1, Nap 2, Anth 1, Anth 2, Py 1a and Py 2a.

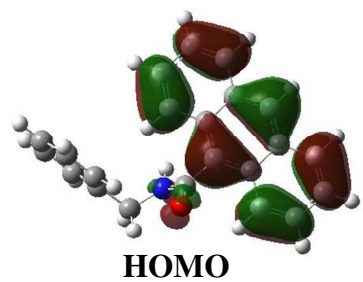
Nap 1



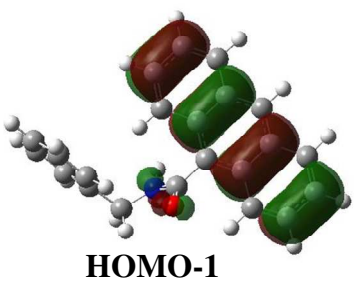
Nap 2



Anth 1



HOMO



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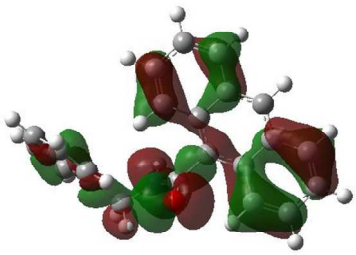

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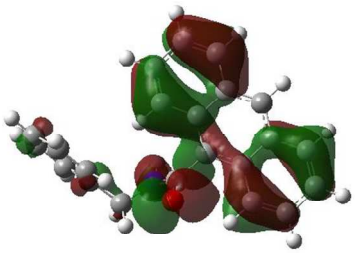

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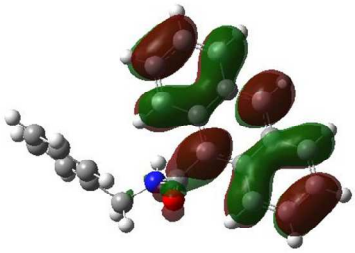
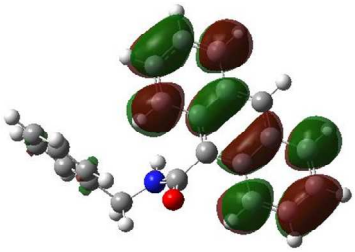
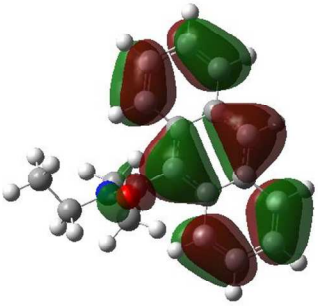


LUMO



LUMO+4

Anth 2



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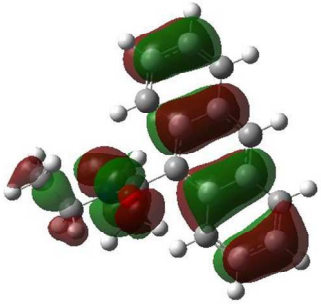

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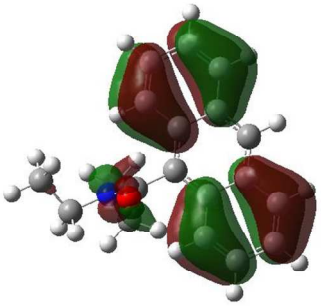

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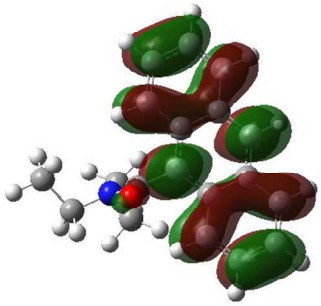
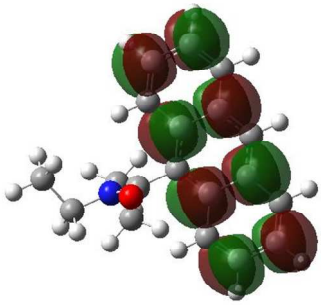
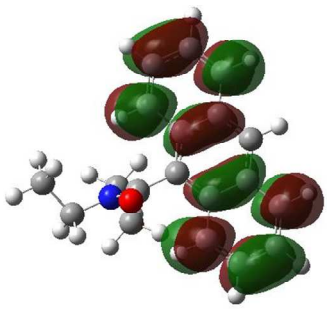


LUMO

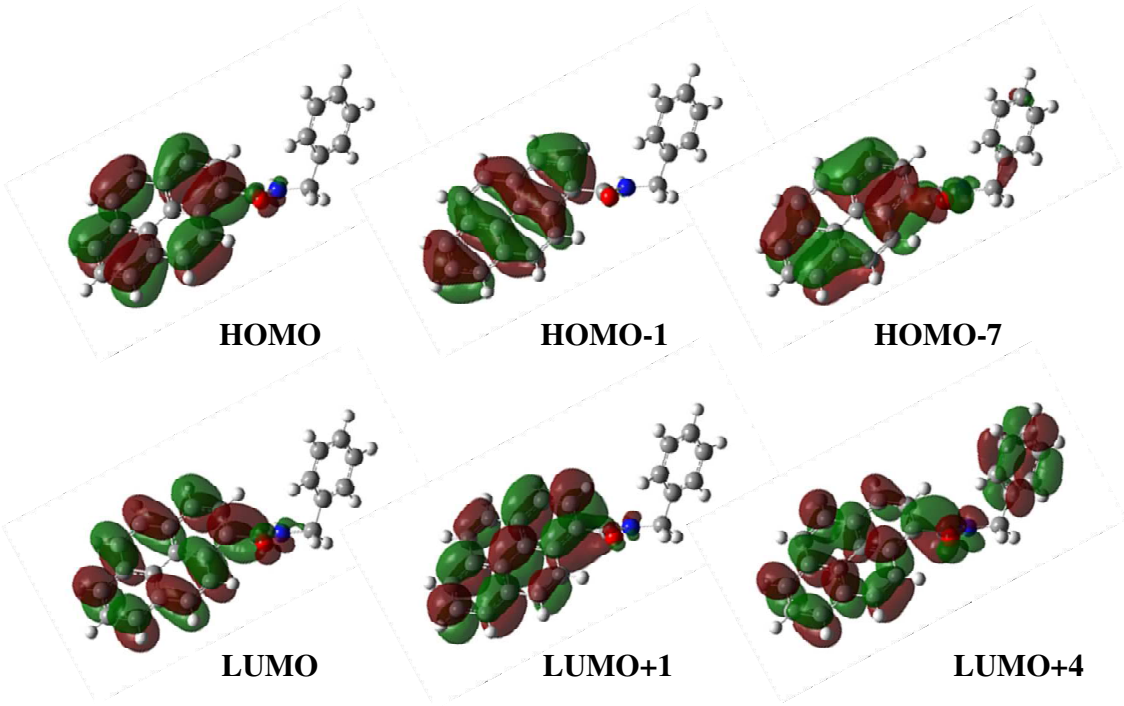


LUMO+1



LUMO+2

Py 1a



Py 2a

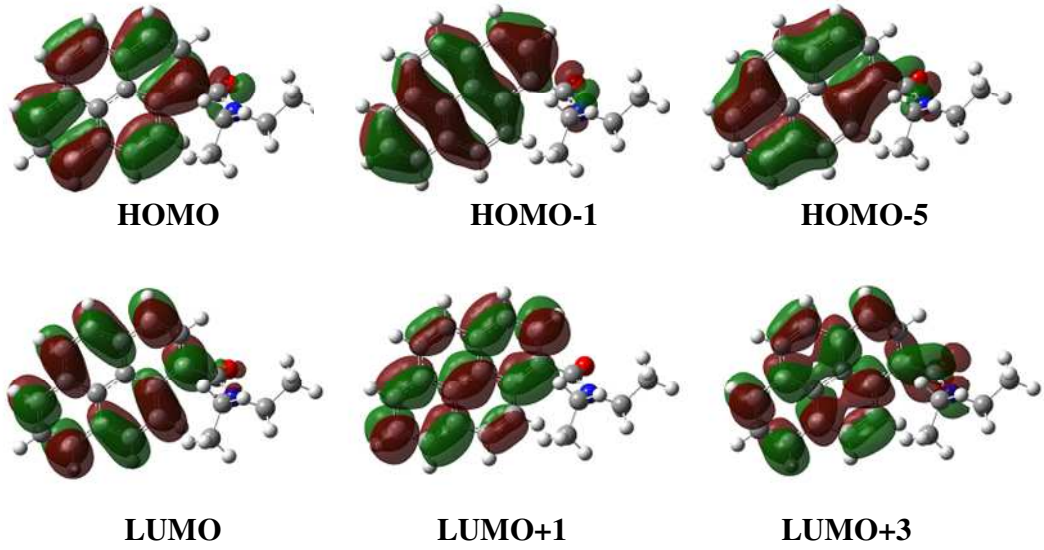


Figure S6. Frontier orbitals of **Nap 1**, **Nap 2**, **Anth 1**, **Anth 2**, **Py 1a** and **Py 2a** (TD-DFT at ωB97X-D 6-31G(d.p)).

6. Optimized structures of Nap 1, Nap 2, Anth 1, Anth 2, Py 1a and Py 2a in the excited states.

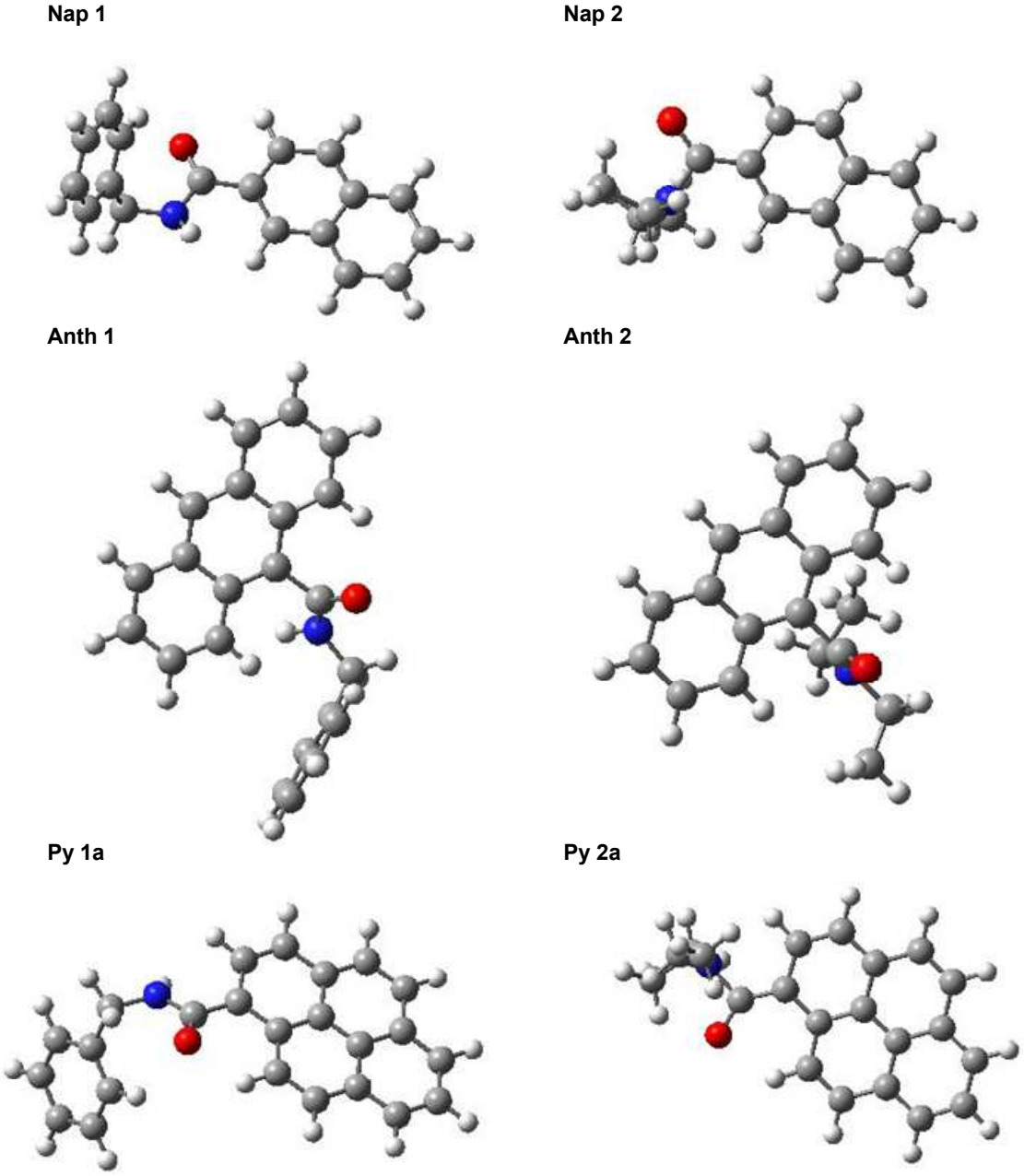
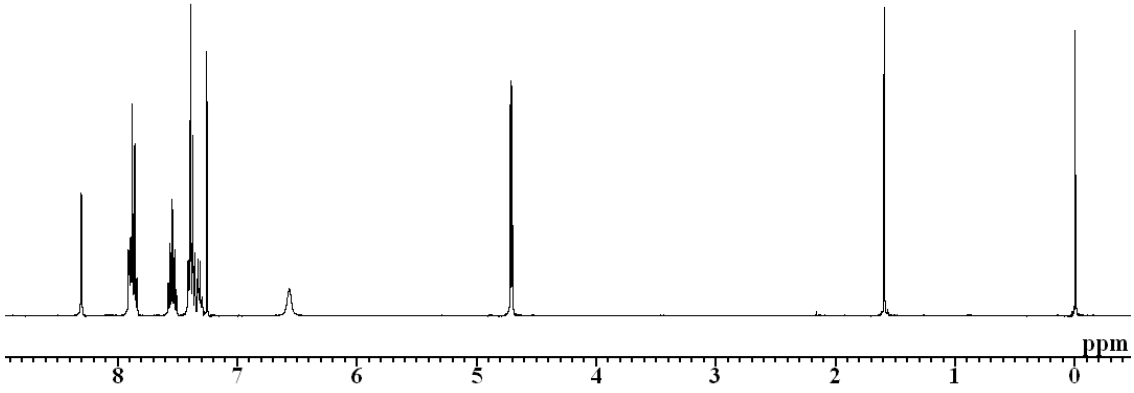


Figure S7. Optimized structures of **Nap 1**, **Nap 2**, **Anth 1**, **Anth 2**, **Py 1a** and **Py 2a** in the excited states (DFT at ωB97X-D 6-31G(d,p)).

7. ^{1}H NMR and ^{13}C NMR spectra of Nap 1, Nap 2, Anth 1, Anth 2 and Py 2b and Py 2d.

(a)



(b)

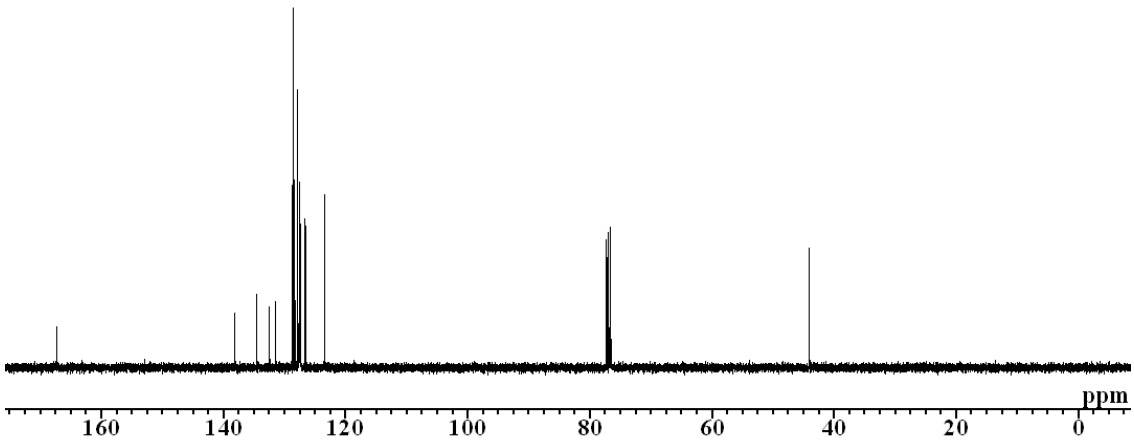


Figure S8. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Nap 1** ($CDCl_3$, room temperature).

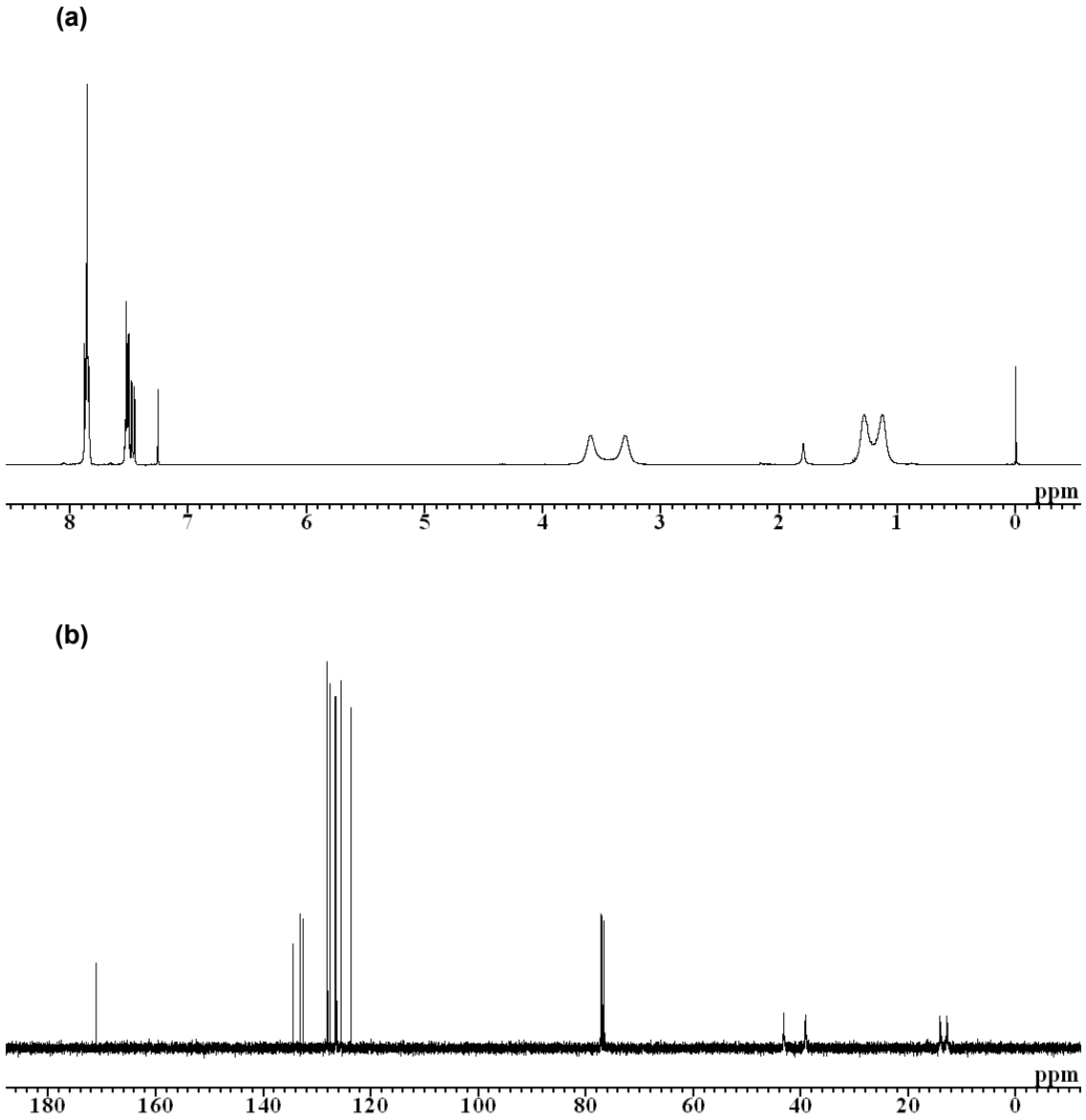


Figure S9. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Nap 2** ($CDCl_3$, room temperature).

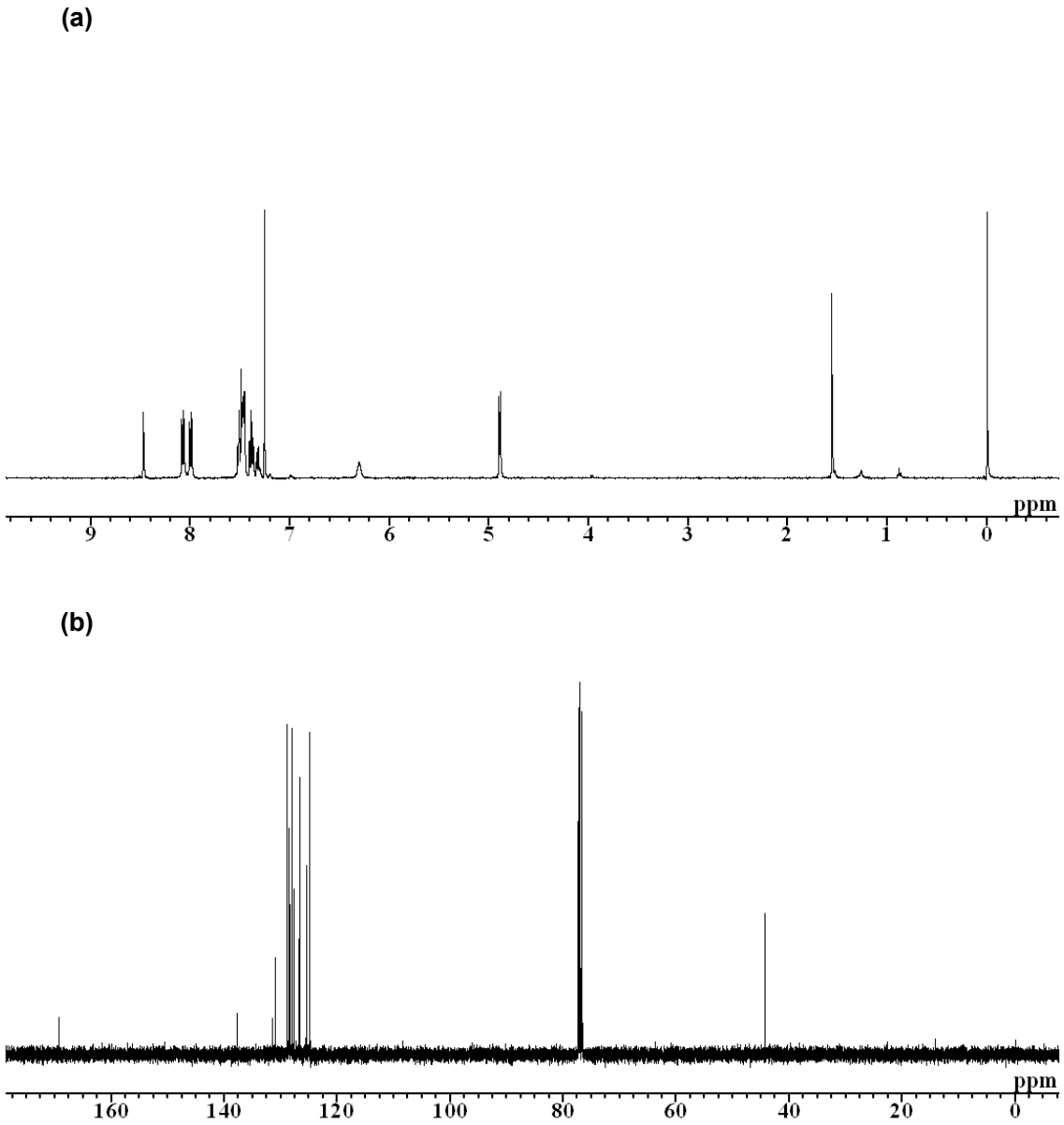


Figure S10. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Anth 1** ($CDCl_{3,}$ room temperature).

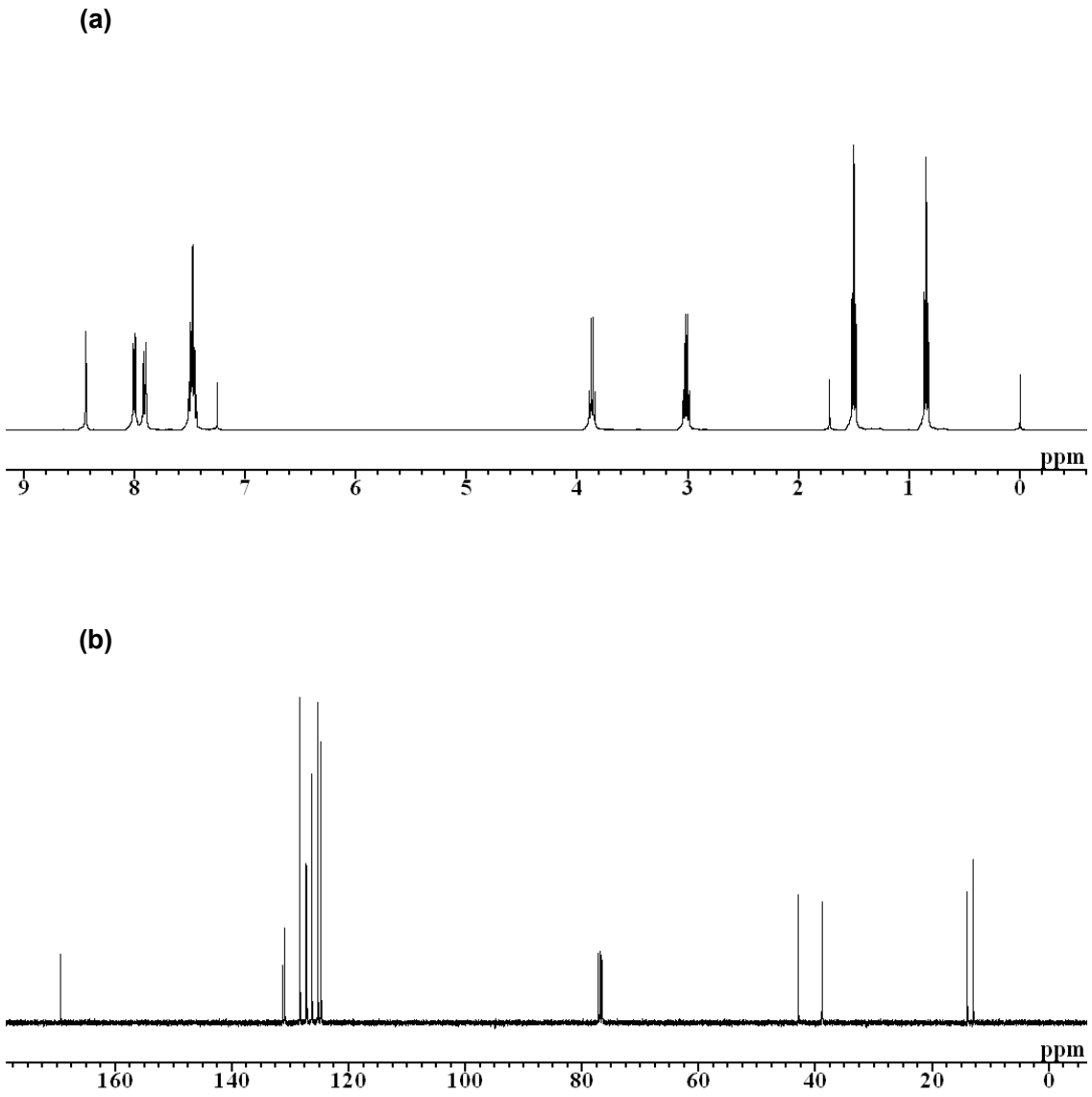


Figure S11. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Anth 2** ($CDCl_{3,}$ room temperature).

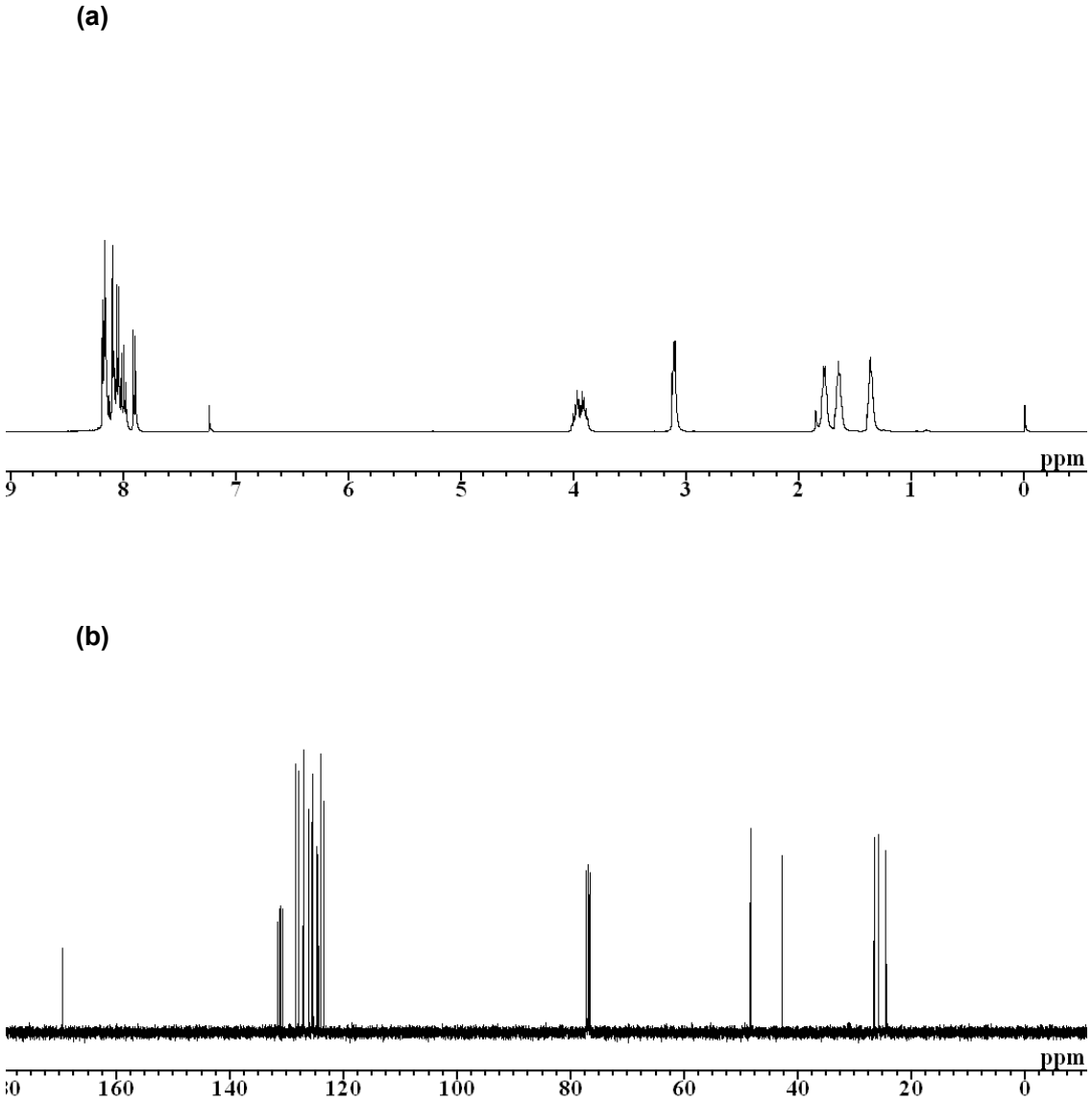


Figure S12. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Py 2b** ($CDCl_3$, room temperature).

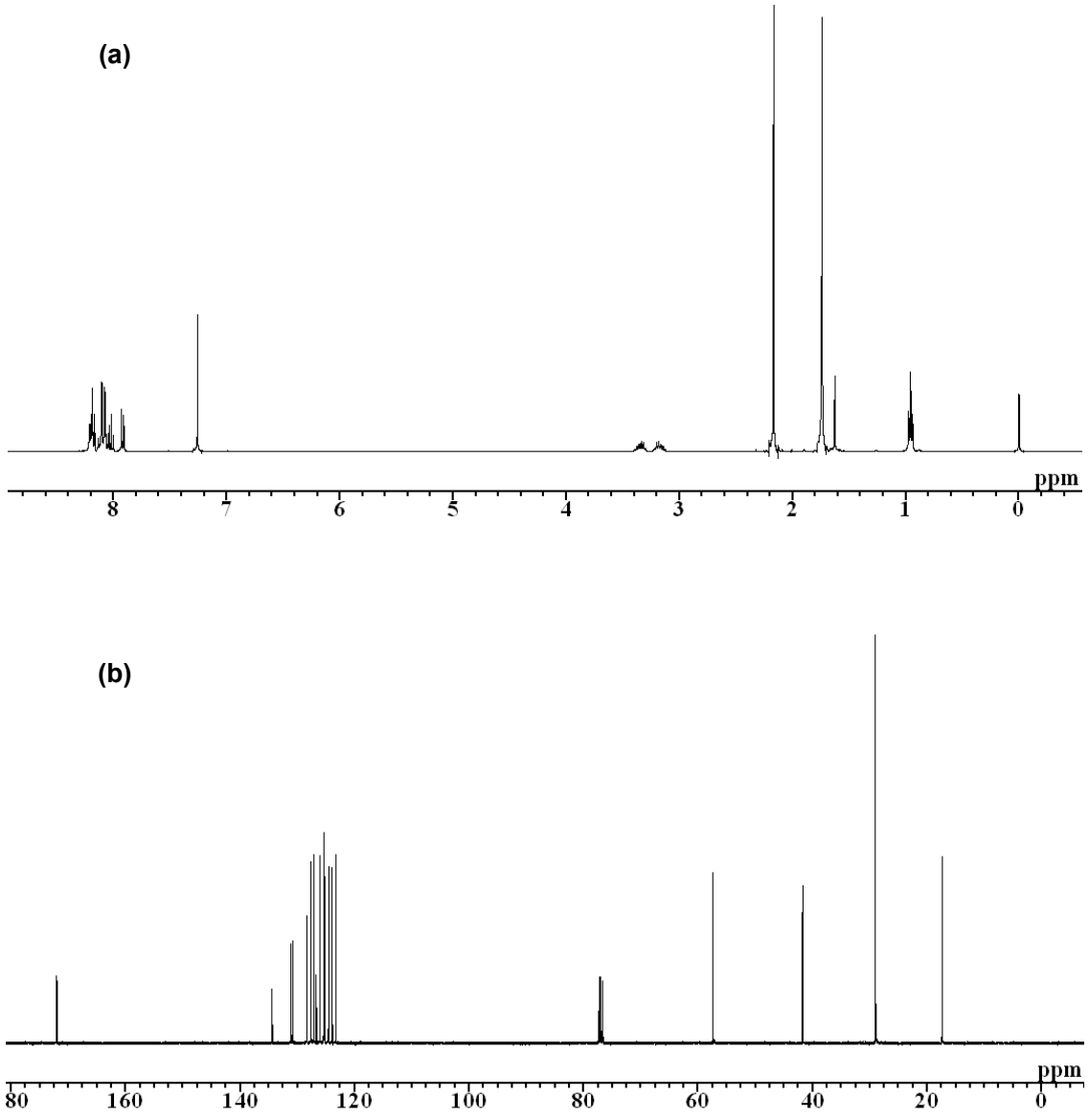


Figure S13. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **Py 2d** ($CDCl_3$, room temperature).

8. Atom coordinates and absolute energies of Nap 1, Nap 2, Anth 1, Anth 2, Py 1a and Py 2a in theoretical calculations.

Nap 1 (ground)

E(RwB97XD) = -824.705711089 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	1.101732	1.166185	0.06173
2	1	0	0.532218	-0.89434	-0.120057
3	6	0	1.350169	-0.179509	-0.067203
4	6	0	3.473301	1.620531	0.173429
5	6	0	2.67741	-0.678912	-0.088978
6	6	0	2.183436	2.072514	0.202272
7	6	0	3.759305	0.236926	0.024054
8	6	0	2.956634	-2.064373	-0.218647
9	1	0	1.9542	3.123655	0.336524
10	1	0	5.911733	0.438616	0.080917
11	1	0	4.300304	2.317963	0.271588
12	6	0	4.249636	-2.517451	-0.243165
13	1	0	2.126907	-2.761116	-0.300218
14	1	0	4.4532	-3.578515	-0.34468
15	6	0	5.326348	-1.60602	-0.135979
16	1	0	6.345993	-1.977075	-0.156296
17	6	0	5.086682	-0.262789	-0.004772
18	6	0	-0.286103	1.736964	0.116676
19	8	0	-0.53029	2.767128	0.727781
20	7	0	-1.240634	1.031056	-0.554369
21	1	0	-0.957786	0.273261	-1.154061
22	6	0	-2.638282	1.40759	-0.542297
23	1	0	-2.928748	1.843319	-1.506124
24	1	0	-2.72872	2.19875	0.207558
25	6	0	-3.542345	0.239885	-0.211649
26	6	0	-5.237714	-1.893901	0.430628
27	6	0	-4.706326	0.013984	-0.944382
28	6	0	-3.232835	-0.618156	0.846346

29	6	0	-4.073848	-1.677808	1.165491
30	6	0	-5.552721	-1.044678	-0.624645
31	1	0	-4.953295	0.67114	-1.774295
32	1	0	-2.324716	-0.449725	1.418405
33	1	0	-3.822582	-2.335813	1.991526
34	1	0	-6.455105	-1.208468	-1.205265
35	1	0	-5.893718	-2.721956	0.67936

Nap 1(excited)

E(TD-KS) = -824.548856311 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	0.882499	0.833416	-0.440418
2	1	0	1.154438	-1.166933	-1.292062
3	6	0	1.600587	-0.380669	-0.689558
4	6	0	2.870382	1.680458	0.714649
5	6	0	2.910597	-0.57501	-0.228891
6	6	0	1.561368	1.847123	0.241898
7	6	0	3.582783	0.47284	0.507345
8	6	0	3.633971	-1.761984	-0.460125
9	1	0	1.036491	2.783137	0.402017
10	1	0	5.374488	1.081155	1.514833
11	1	0	3.350346	2.492909	1.252161
12	6	0	4.952792	-1.930893	0.019604
13	1	0	3.165444	-2.567893	-1.01751
14	1	0	5.464511	-2.866387	-0.183507
15	6	0	5.590038	-0.93148	0.734054
16	1	0	6.60011	-1.062009	1.101894
17	6	0	4.889845	0.276634	0.968523
18	6	0	-0.498119	1.097259	-0.86288
19	8	0	-0.998623	2.223339	-0.806092
20	7	0	-1.201193	0.012343	-1.349467
21	1	0	-0.904787	-0.898613	-1.031783
22	6	0	-2.615252	0.140092	-1.662834
23	1	0	-2.844411	-0.514153	-2.510515
24	1	0	-2.764755	1.173945	-1.980141

25	6	0	-3.523116	-0.18822	-0.495453
26	6	0	-5.154001	-0.807643	1.693164
27	6	0	-4.300895	-1.344927	-0.49587
28	6	0	-3.56973	0.660887	0.615327
29	6	0	-4.379204	0.35134	1.701391
30	6	0	-5.114844	-1.655177	0.591773
31	1	0	-4.273789	-2.009027	-1.356639
32	1	0	-2.964061	1.562458	0.610042
33	1	0	-4.410575	1.018578	2.557268
34	1	0	-5.717057	-2.558405	0.57676
35	1	0	-5.787267	-1.046138	2.541982

Nap 2 (ground)

E(RwB97XD) = -711.634982226 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	-0.22227	-0.704032	-0.177813
2	1	0	0.112594	1.283693	-0.886985
3	6	0	0.560273	0.385169	-0.472785
4	6	0	1.730776	-1.942095	0.533746
5	6	0	1.963536	0.356764	-0.269367
6	6	0	0.382653	-1.891104	0.310754
7	6	0	2.559808	-0.823008	0.253985
8	6	0	2.788185	1.472596	-0.5677
9	1	0	-0.247697	-2.754278	0.493719
10	1	0	4.415439	-1.748647	0.868297
11	1	0	2.187968	-2.848981	0.919217
12	6	0	4.140191	1.42077	-0.350163
13	1	0	2.328387	2.37082	-0.970609
14	1	0	4.762267	2.279736	-0.580144
15	6	0	4.733313	0.248309	0.174431
16	1	0	5.80521	0.219199	0.341816
17	6	0	3.962007	-0.846112	0.468294
18	6	0	-1.696818	-0.752793	-0.468465
19	8	0	-2.160361	-1.7286	-1.047179
20	7	0	-2.48316	0.309092	-0.104205

21	6	0	-3.899203	0.215925	-0.457474
22	1	0	-4.304378	1.232218	-0.475638
23	1	0	-3.96279	-0.187374	-1.469207
24	6	0	-2.133527	1.290757	0.918113
25	1	0	-1.173746	1.016217	1.356403
26	1	0	-2.875455	1.223823	1.724539
27	6	0	-4.699927	-0.664021	0.499673
28	1	0	-4.638646	-0.297952	1.529561
29	1	0	-4.31948	-1.686549	0.465263
30	1	0	-5.754764	-0.675253	0.210571
31	6	0	-2.080729	2.725088	0.398967
32	1	0	-3.038153	3.035038	-0.029065
33	1	0	-1.316807	2.839982	-0.374223
34	1	0	-1.844545	3.410177	1.218183

Nap 2 (excited)

E(TD-KS) = -711.507714541 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	0.236253	0.731059	0.033525
2	1	0	0.040672	-1.407209	-0.259267
3	6	0	-0.479655	-0.461828	-0.135112
4	6	0	-1.857738	1.961167	0.161169
5	6	0	-1.894721	-0.471293	-0.153422
6	6	0	-0.500455	1.958616	0.178643
7	6	0	-2.607833	0.752878	-0.003379
8	6	0	-2.641122	-1.667186	-0.319301
9	1	0	0.060129	2.878752	0.304387
10	1	0	-4.548919	1.681729	0.093466
11	1	0	-2.400632	2.896014	0.274178
12	6	0	-4.015013	-1.648773	-0.333861
13	1	0	-2.105403	-2.605814	-0.435309
14	1	0	-4.566495	-2.57541	-0.461762
15	6	0	-4.716331	-0.434987	-0.183953
16	1	0	-5.801292	-0.430465	-0.196691
17	6	0	-4.017723	0.740348	-0.022367

18	6	0	1.64257	0.784358	0.066626
19	8	0	2.472182	1.735206	0.183801
20	7	0	2.407247	-0.438823	-0.079136
21	6	0	2.971412	-0.736491	-1.387843
22	1	0	3.010209	-1.828281	-1.478103
23	1	0	2.265611	-0.354119	-2.126153
24	6	0	3.055479	-1.010523	1.094169
25	1	0	3.974401	-0.44082	1.278974
26	1	0	3.353052	-2.030909	0.830502
27	6	0	4.360827	-0.129454	-1.596884
28	1	0	5.090716	-0.558068	-0.905345
29	1	0	4.310056	0.948136	-1.436957
30	1	0	4.695264	-0.336178	-2.615817
31	6	0	2.158969	-0.985459	2.321842
32	1	0	1.213855	-1.497847	2.131597
33	1	0	1.940611	0.041297	2.619206
34	1	0	2.670469	-1.485286	3.147515

Anth 1 (ground)

E(RwB97XD) = -978.290074672 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	1	0	-0.014184	4.950229	-0.092311
2	6	0	0.220301	3.891742	-0.045962
3	1	0	2.320896	4.18107	-0.264552
4	6	0	1.510413	3.468011	-0.142846
5	6	0	-0.56458	1.610074	0.188811
6	6	0	1.835776	2.076272	-0.080658
7	6	0	-0.829579	2.945351	0.130201
8	6	0	0.77854	1.117588	0.072102
9	6	0	3.154798	1.633826	-0.163371
10	1	0	-1.853034	3.293052	0.227335
11	1	0	-1.380281	0.911822	0.343457
12	6	0	3.479684	0.28004	-0.083775
13	1	0	3.951359	2.363441	-0.288449

14	6	0	4.835611	-0.167646	-0.16502
15	6	0	2.434082	-0.688267	0.077068
16	1	0	2.018988	-2.808919	0.311765
17	6	0	1.099127	-0.251212	0.126076
18	6	0	5.139352	-1.492616	-0.090024
19	1	0	5.618061	0.575805	-0.287807
20	1	0	6.171412	-1.822297	-0.152002
21	6	0	4.102818	-2.455499	0.076195
22	1	0	4.360327	-3.507469	0.145544
23	6	0	2.797902	-2.071502	0.157385
24	6	0	-0.002923	-1.272303	0.247584
25	8	0	-0.139158	-1.99652	1.224039
26	7	0	-0.816574	-1.34208	-0.84412
27	1	0	-0.707558	-0.631272	-1.551422
28	6	0	-2.058006	-2.100712	-0.82402
29	1	0	-1.899064	-2.938027	-0.141606
30	1	0	-2.235959	-2.504128	-1.824936
31	6	0	-3.231369	-1.256972	-0.372523
32	6	0	-5.31332	0.411801	0.468847
33	6	0	-3.358617	-0.909312	0.976625
34	6	0	-4.158536	-0.765314	-1.289631
35	6	0	-5.197296	0.063967	-0.872598
36	6	0	-4.391428	-0.077086	1.39287
37	1	0	-2.633855	-1.290531	1.690481
38	1	0	-4.06899	-1.032495	-2.339765
39	1	0	-5.913827	0.438785	-1.596752
40	1	0	-4.480398	0.187392	2.441821
41	1	0	-6.12111	1.058877	0.795712

Anth 1(excited)

E(TD-KS) = -978.167926776 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	1	0	0.219278	4.90943	0.065398
2	6	0	-0.032421	3.855287	0.01732
3	1	0	-2.146382	4.194768	0.292443

4	6	0	-1.367992	3.451399	0.145294
5	6	0	0.61771	1.539249	-0.231784
6	6	0	-1.732383	2.097357	0.086779
7	6	0	0.952628	2.903799	-0.185972
8	6	0	-0.703517	1.099601	-0.053933
9	6	0	-3.079718	1.686506	0.141083
10	1	0	1.988855	3.197305	-0.314907
11	1	0	1.406285	0.821431	-0.430141
12	6	0	-3.467424	0.33594	0.017332
13	1	0	-3.853402	2.445805	0.226432
14	6	0	-4.81958	-0.038515	0.01849
15	6	0	-2.457776	-0.68083	-0.111064
16	1	0	-2.125892	-2.782472	-0.383369
17	6	0	-1.082359	-0.28464	-0.036966
18	6	0	-5.207356	-1.377906	-0.113523
19	1	0	-5.574555	0.734334	0.13262
20	1	0	-6.260274	-1.638747	-0.110799
21	6	0	-4.2371	-2.356638	-0.247453
22	1	0	-4.519119	-3.398616	-0.354604
23	6	0	-2.874734	-2.012303	-0.248158
24	6	0	-0.027565	-1.334287	0.077851
25	8	0	0.039695	-2.310896	-0.665342
26	7	0	0.843198	-1.158102	1.118157
27	1	0	0.797253	-0.281055	1.614641
28	6	0	2.084422	-1.911717	1.202471
29	1	0	1.889101	-2.886618	0.751861
30	1	0	2.330056	-2.063392	2.25751
31	6	0	3.215464	-1.203233	0.48683
32	6	0	5.193902	0.238404	-0.868362
33	6	0	3.272567	-1.22151	-0.910856
34	6	0	4.159696	-0.46057	1.194055
35	6	0	5.146713	0.256417	0.52158
36	6	0	4.254665	-0.503052	-1.58312
37	1	0	2.530497	-1.792765	-1.461359
38	1	0	4.123285	-0.44132	2.280603
39	1	0	5.877225	0.829203	1.084333

40	1	0	4.289487	-0.523167	-2.667831
41	1	0	5.961299	0.797219	-1.394575

Anth 2 (ground)

E(RwB97XD) = -865.222574128 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	1	0	-0.795538	5.211801	0.407498
2	6	0	-0.661536	4.148569	0.236597
3	1	0	-2.713349	3.675051	0.569082
4	6	0	-1.723211	3.300037	0.325972
5	6	0	0.82745	2.317395	-0.307142
6	6	0	-1.563508	1.896197	0.103855
7	6	0	0.633212	3.647583	-0.084224
8	6	0	-0.262092	1.391889	-0.223808
9	6	0	-2.635569	1.009325	0.205872
10	1	0	1.468481	4.336752	-0.155563
11	1	0	1.81505	1.944612	-0.560407
12	6	0	-2.472961	-0.358646	-0.010488
13	1	0	-3.620012	1.393392	0.462025
14	6	0	-3.567679	-1.273297	0.098887
15	6	0	-1.176008	-0.86946	-0.347653
16	1	0	-0.064454	-2.665832	-0.865148
17	6	0	-0.091168	0.01465	-0.430434
18	6	0	-3.390119	-2.606568	-0.11325
19	1	0	-4.546624	-0.878453	0.355539
20	1	0	-4.228266	-3.290435	-0.026702
21	6	0	-2.103901	-3.1139	-0.459448
22	1	0	-1.981564	-4.176897	-0.640311
23	6	0	-1.0353	-2.276781	-0.576115
24	6	0	1.267693	-0.519907	-0.81328
25	8	0	1.564696	-0.690579	-1.989109
26	7	0	2.12919	-0.803084	0.204451
27	6	0	1.821393	-0.632048	1.619679
28	1	0	2.729267	-0.265188	2.111888

29	1	0	1.069881	0.150781	1.730418
30	6	0	3.451733	-1.308367	-0.148082
31	1	0	3.802363	-1.93588	0.677382
32	1	0	3.346714	-1.939253	-1.032804
33	6	0	1.339395	-1.91904	2.283927
34	1	0	1.170678	-1.755917	3.352287
35	1	0	2.076522	-2.720688	2.175768
36	1	0	0.401259	-2.253272	1.833153
37	6	0	4.43976	-0.179761	-0.428166
38	1	0	4.52982	0.488911	0.434053
39	1	0	4.100354	0.400846	-1.28949
40	1	0	5.432013	-0.581333	-0.65315

Anth 2 (excited)

E(TD-KS) = -865.099620487 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	1	0	-0.33948	5.268461	0.373453
2	6	0	-0.277765	4.199434	0.199554
3	1	0	-2.372149	3.864059	0.612223
4	6	0	-1.42832	3.406188	0.330301
5	6	0	0.999377	2.227831	-0.373343
6	6	0	-1.386436	2.022077	0.110555
7	6	0	0.927231	3.614312	-0.150952
8	6	0	-0.133862	1.413391	-0.249888
9	6	0	-2.529828	1.202952	0.232323
10	1	0	1.82127	4.219192	-0.257991
11	1	0	1.947169	1.782878	-0.659836
12	6	0	-2.502626	-0.191034	0.010416
13	1	0	-3.477167	1.668959	0.493504
14	6	0	-3.646927	-0.991128	0.13622
15	6	0	-1.258565	-0.810311	-0.361838
16	1	0	-0.31841	-2.660469	-0.929233
17	6	0	-0.091995	0.001195	-0.429228
18	6	0	-3.59972	-2.373377	-0.103049

19	1	0	-4.58324	-0.524515	0.428728
20	1	0	-4.500928	-2.96819	0.000837
21	6	0	-2.405443	-2.967571	-0.474638
22	1	0	-2.359632	-4.033369	-0.671024
23	6	0	-1.241022	-2.190501	-0.605121
24	6	0	1.213455	-0.648012	-0.790844
25	8	0	1.468082	-0.897955	-1.964898
26	7	0	2.072329	-0.939112	0.222579
27	6	0	1.776238	-0.704077	1.631068
28	1	0	2.711971	-0.408837	2.118968
29	1	0	1.098503	0.147035	1.715246
30	6	0	3.349118	-1.55704	-0.117914
31	1	0	3.65412	-2.184815	0.725354
32	1	0	3.189325	-2.204774	-0.982266
33	6	0	1.174856	-1.925774	2.320271
34	1	0	1.003595	-1.7198	3.3808
35	1	0	1.841367	-2.790599	2.245721
36	1	0	0.218719	-2.189094	1.859752
37	6	0	4.420186	-0.51786	-0.435983
38	1	0	4.566361	0.168125	0.404568
39	1	0	4.123042	0.061389	-1.313781
40	1	0	5.376896	-1.00239	-0.651358

Py 1a (ground)

E(RwB97XD) = -1054.50906853 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	-6.178592	-0.91423	0.142606
2	6	0	-5.13261	-1.827991	0.163203
3	6	0	-3.804111	-1.393992	0.109629
4	6	0	-3.530902	-0.004259	0.03343
5	6	0	-4.605839	0.924051	0.013939
6	6	0	-5.919491	0.449266	0.069185
7	6	0	-2.696714	-2.310242	0.132427
8	6	0	-2.179153	0.457906	-0.024272

9	6	0	-1.103988	-0.47383	-0.002235
10	6	0	-1.415349	-1.879897	0.081838
11	6	0	0.21504	0.013794	-0.09063
12	6	0	0.447741	1.388409	-0.16267
13	6	0	-0.598729	2.297136	-0.160682
14	6	0	-1.921221	1.853178	-0.101607
15	6	0	-3.029891	2.7716	-0.114712
16	6	0	-4.306569	2.330043	-0.060852
17	1	0	-5.134276	3.033423	-0.072913
18	1	0	-2.814921	3.834793	-0.170539
19	1	0	-2.9104	-3.373299	0.198342
20	1	0	-7.204088	-1.266713	0.185049
21	1	0	-5.339196	-2.892747	0.22239
22	1	0	-6.740633	1.160262	0.05472
23	1	0	-0.595469	-2.585041	0.127544
24	1	0	1.470623	1.753999	-0.18586
25	1	0	-0.393869	3.362785	-0.201866
26	6	0	1.39513	-0.917287	-0.074917
27	8	0	1.508481	-1.846272	0.715759
28	7	0	2.342287	-0.639084	-1.014529
29	1	0	2.201661	0.150167	-1.624096
30	6	0	3.625896	-1.318117	-1.040645
31	1	0	3.477052	-2.269385	-0.52426
32	1	0	3.891795	-1.533641	-2.079931
33	6	0	4.721157	-0.516895	-0.369656
34	6	0	4.640474	-0.247734	1.000199
35	6	0	5.802488	-0.022632	-1.095407
36	6	0	5.625501	0.505193	1.626834
37	1	0	3.801706	-0.641113	1.568046
38	6	0	6.793196	0.730085	-0.467628
39	1	0	5.87382	-0.228211	-2.160719
40	6	0	6.704962	0.996645	0.893857
41	1	0	5.555419	0.705732	2.691361
42	1	0	7.631433	1.108542	-1.044252
43	1	0	7.474927	1.58301	1.385222

Py 1a (excited)

E(TD-KS) = -1054.37355989 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	5.449649	-2.100632	-0.373155
2	6	0	4.261506	-2.555736	0.173013
3	6	0	3.148122	-1.678639	0.319622
4	6	0	3.261846	-0.320434	-0.102144
5	6	0	4.493791	0.137418	-0.664703
6	6	0	5.572935	-0.77833	-0.78799
7	6	0	1.93103	-2.105518	0.874224
8	6	0	2.163589	0.563347	0.035097
9	6	0	0.930148	0.105462	0.5961
10	6	0	0.851335	-1.239215	1.009912
11	6	0	-0.189129	1.024929	0.689829
12	6	0	0.003264	2.35965	0.27817
13	6	0	1.197457	2.802444	-0.239226
14	6	0	2.310347	1.919484	-0.396176
15	6	0	3.529193	2.348782	-0.94335
16	6	0	4.603454	1.48279	-1.079659
17	1	0	5.538876	1.832438	-1.504821
18	1	0	3.624317	3.382562	-1.263243
19	1	0	1.831249	-3.135187	1.205139
20	1	0	6.290597	-2.778034	-0.479504
21	1	0	4.16125	-3.587172	0.497552
22	1	0	6.507078	-0.426624	-1.216168
23	1	0	-0.070992	-1.586427	1.455693
24	1	0	-0.800959	3.074389	0.416971
25	1	0	1.313166	3.843238	-0.527745
26	6	0	-1.50295	0.602188	1.215179
27	8	0	-1.663772	-0.335048	2.002802
28	7	0	-2.578434	1.353087	0.783975
29	1	0	-2.476307	1.83951	-0.093444
30	6	0	-3.933892	0.987744	1.160003
31	1	0	-3.861389	0.495359	2.13157

32	1	0	-4.519547	1.904716	1.284899
33	6	0	-4.608543	0.075864	0.155899
34	6	0	-4.159052	-1.238602	-0.008177
35	6	0	-5.66265	0.53377	-0.632612
36	6	0	-4.755261	-2.072343	-0.94607
37	1	0	-3.339712	-1.592057	0.610954
38	6	0	-6.263245	-0.302219	-1.571863
39	1	0	-6.02088	1.553226	-0.510131
40	6	0	-5.809175	-1.606571	-1.730992
41	1	0	-4.400673	-3.091762	-1.063693
42	1	0	-7.084621	0.067183	-2.178079
43	1	0	-6.274847	-2.260381	-2.461796

Py 2a(ground)

E(RwB97XD) = -941.43996326 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	-3.840768	-4.818532	1.620024
2	6	0	-2.466721	-4.662308	1.483688
3	6	0	-1.939548	-3.582268	0.76932
4	6	0	-2.825232	-2.641998	0.18097
5	6	0	-4.228379	-2.809887	0.321464
6	6	0	-4.714202	-3.903166	1.045438
7	6	0	-0.52287	-3.392242	0.601219
8	6	0	-2.306881	-1.529176	-0.550376
9	6	0	-0.902792	-1.355558	-0.680609
10	6	0	-0.029221	-2.337617	-0.087357
11	6	0	-0.416948	-0.246034	-1.390077
12	6	0	-1.303291	0.645035	-1.990942
13	6	0	-2.674525	0.478133	-1.865542
14	6	0	-3.199015	-0.597985	-1.143963
15	6	0	-4.616502	-0.795221	-0.98689
16	6	0	-5.105977	-1.845428	-0.28924
17	1	0	-6.177896	-1.981936	-0.178562
18	1	0	-5.289169	-0.07628	-1.445683

19	1	0	0.150452	-4.125166	1.036371
20	1	0	-4.234524	-5.662119	2.177724
21	1	0	-1.788663	-5.382703	1.93224
22	1	0	-5.787344	-4.03166	1.154242
23	1	0	1.042496	-2.221848	-0.212542
24	1	0	-0.907848	1.481484	-2.558624
25	1	0	-3.352334	1.186985	-2.332155
26	6	0	1.063608	-0.033044	-1.583198
27	8	0	1.604521	-0.341039	-2.637103
28	7	0	1.757722	0.502681	-0.535851
29	6	0	1.141186	1.077965	0.655015
30	1	0	1.550848	2.086819	0.790832
31	1	0	0.072023	1.196778	0.473256
32	6	0	1.363344	0.251021	1.918474
33	1	0	2.42869	0.091229	2.110332
34	1	0	0.941563	0.769927	2.784066
35	1	0	0.879098	-0.724446	1.83316
36	6	0	3.187534	0.72786	-0.726613
37	1	0	3.659538	0.730804	0.260771
38	1	0	3.586909	-0.118365	-1.288606
39	6	0	3.482512	2.028354	-1.469264
40	1	0	3.067661	2.892165	-0.939949
41	1	0	4.561826	2.17743	-1.565153
42	1	0	3.048509	1.987469	-2.470552

Py 2a (excited)

E(TD-KS) = -941.313797871 A.U.

center number	atomic number	atomic type	coodinates [Å]		
			X	Y	Z
1	6	0	5.167334	-1.303177	0.073641
2	6	0	4.044225	-2.115491	0.131255
3	6	0	2.757751	-1.560236	0.079935
4	6	0	2.611751	-0.151237	-0.032516
5	6	0	3.77183	0.673054	-0.09084
6	6	0	5.036175	0.076736	-0.036179

7	6	0	1.574492	-2.36495	0.137067
8	6	0	1.306813	0.434618	-0.086258
9	6	0	0.153801	-0.393262	-0.027212
10	6	0	0.335894	-1.808258	0.085871
11	6	0	-1.146265	0.21625	-0.07823
12	6	0	-1.22351	1.633706	-0.195817
13	6	0	-0.096529	2.414784	-0.250787
14	6	0	1.188979	1.848543	-0.19776
15	6	0	2.371237	2.651016	-0.254767
16	6	0	3.607461	2.096241	-0.204179
17	1	0	4.496656	2.718302	-0.248311
18	1	0	2.25689	3.728572	-0.340569
19	1	0	1.6847	-3.442214	0.222796
20	1	0	6.156994	-1.74784	0.114739
21	1	0	4.150891	-3.193103	0.217094
22	1	0	5.919734	0.707202	-0.080589
23	1	0	-0.544252	-2.438188	0.12957
24	1	0	-2.195055	2.114471	-0.246904
25	1	0	-0.193239	3.493608	-0.340429
26	6	0	-2.335952	-0.531389	-0.015903
27	8	0	-2.614812	-1.764483	0.069047
28	7	0	-3.613029	0.154467	-0.06271
29	6	0	-4.394495	0.275334	1.163174
30	1	0	-5.145705	1.05168	0.981418
31	1	0	-4.933476	-0.666667	1.318488
32	6	0	-3.534568	0.601809	2.373166
33	1	0	-2.958121	1.515649	2.215873
34	1	0	-4.181305	0.740684	3.242403
35	1	0	-2.840311	-0.212807	2.5855
36	6	0	-4.325868	0.176657	-1.333335
37	1	0	-4.872873	1.126386	-1.370194
38	1	0	-3.567373	0.188989	-2.11691
39	6	0	-5.282959	-1.001425	-1.520415
40	1	0	-6.09015	-0.982578	-0.783813
41	1	0	-5.730652	-0.947931	-2.51513
42	1	0	-4.729246	-1.935572	-1.417915