An experimental and theoretical study on the electrostatic effect of an appended cationic group on electronic properties of aromatic systems

Viviana Grosso, Carlos Previtali and Carlos A. Chesta*
Departamento de Química, Universidad Nacional de Río Cuarto

D. Mariano A. Vera* and Adriana B. Pierini*
INFIQC, Departamento de Química Orgánica. Facultad de Ciencias Químicas, Universidad Nacional de Córdoba

Electronic Supporting Information (ESI). Supplementary Material

Table of Contents

Part 1. Experimental

Supplementary figures to the experimental section

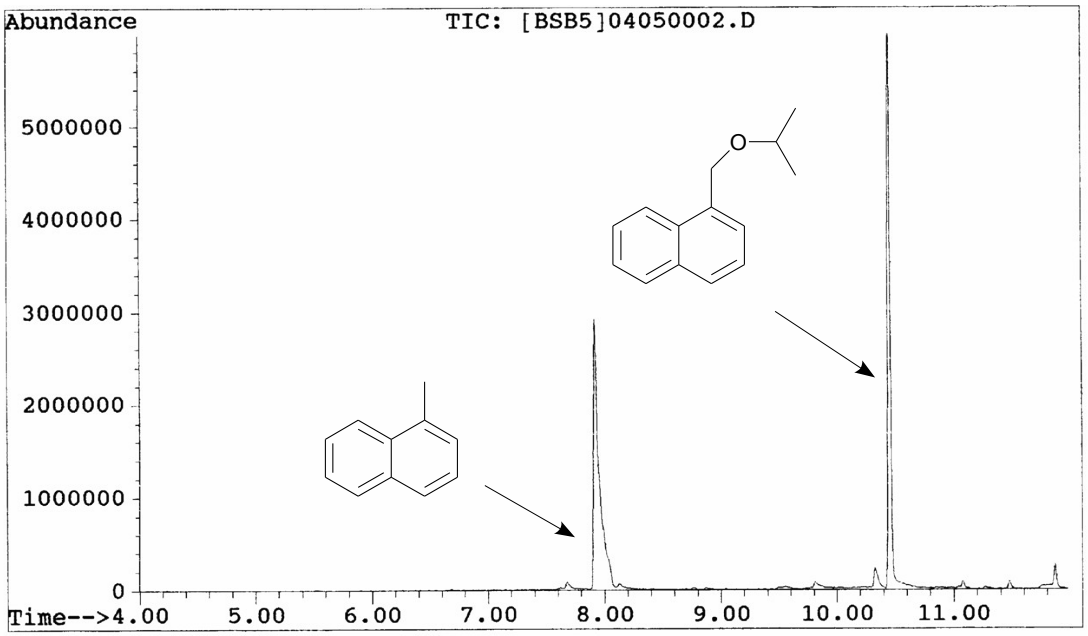


Figure S1. GC-mass chromatogram of a solution of **c1Naph** (1×10^{-3} M) in acetonitrile/2-propanol (9:1) after photolysis at 310 nm. Photoproducts were identified by comparison of the mass spectra of those of the authentic compounds. Photoreaction in the absence of the alcohol gave 1-methylnaphthalene and a large number of identified products

Part 2. Computational Supplementary Material

2.1 Koopmans theorem (KT) estimation to the vertical ionization potentials (*I*) and electron affinities (E_A)

As a first estimate to the actual change in the donor/acceptor capabilities of the aromatics systems in the absence of solvent, the KT values were discussed in the text. The following correlation between KT values and the experimental ones, for a family of compounds structurally related to our aromatics and **c*n*Ar** family, with known *I*'s and E_A's, were computed. The good linear correlation (correlation indexes of 0.981 and 0.984) and the values of the slopes obtained (-0.93 and -0.83), which are close to 1, indicate that the shifts from Δε(HOMO) and Δε(LUMO) are reasonably good estimations to the Δ*I*'s and ΔE_A's, respectively. Further highly correlated DFT thermodynamic calculations, by computing the total energy of the neutral, anionic and cationic species in each case, are also in agreement with these estimations, as checked for the shortest chain derivatives (see main text). The results for the aromatics species on Chart S1 are summarized in Table S1 and Figure S3.

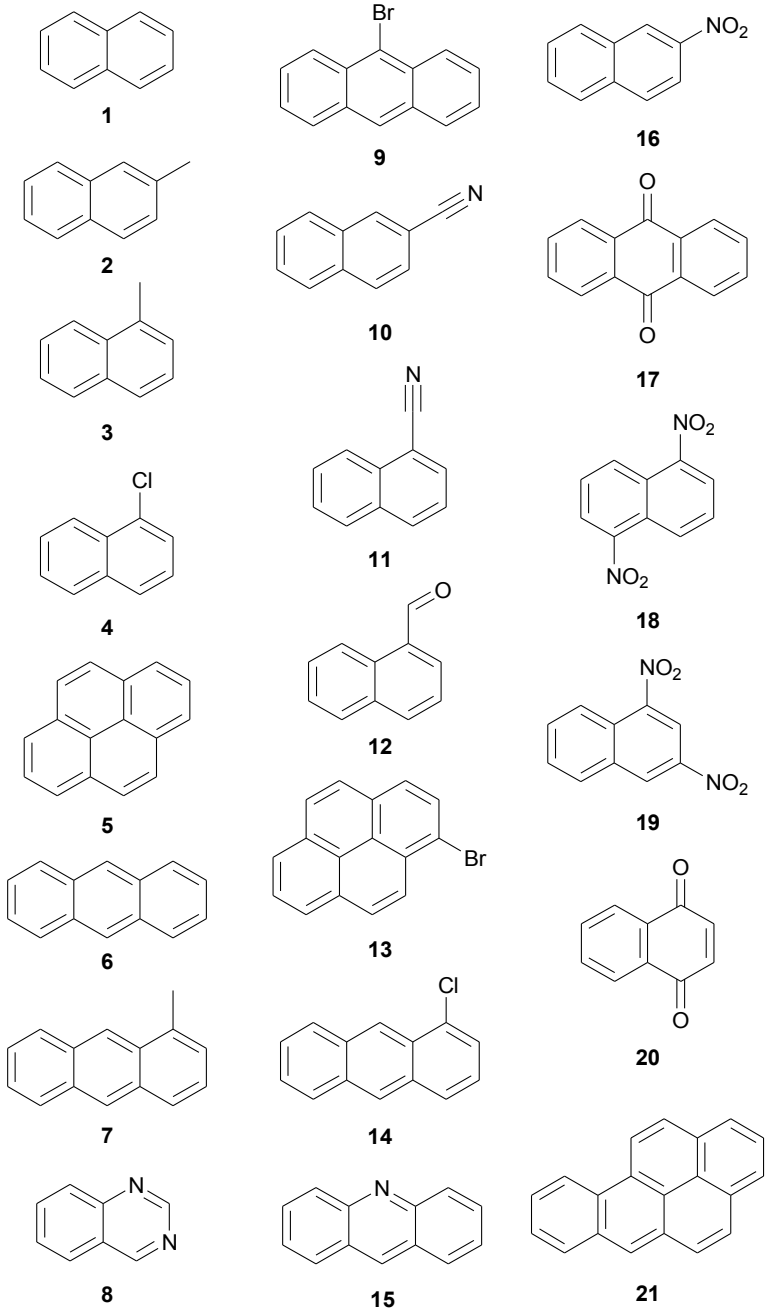


Chart S1

Table S1. Linear correlation between the experimental *I*'s and E_A's and HOMO and LUMO energies at the HF/6-31G* level

For ionization potentials

Compound (Chart S1)	HOMO energy /eV	*I*, experim. /eV	Reference
1	-7.805	8.145	Cockett, M.C.R.; Ozeki, H.; Okuyama, K.; Kimura, K., *J. Chem. Phys*., 1993, **98**, 7763.
2	-7.680	7.850	a) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289. b)Schafer, W.; Schw eig, A.; Vermeer, H.; Bickel-haupt, F.; De Graaf, H., *J. Electron Spectrosc. Relat. Phenom*., 1975, **6**, 91. c) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289
3	-7.685	7.900	Gotkis, I.; Lifshitz, C., *Org. Mass Spectrom.*, 1993, **28**, 372
4	-8.034	8.130	Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289
5	-7.040	7.500	Mautner, M., *J. Phys. Chem*., 1980, **84**, 2716
6	-6.896	7.436	a) Hager, J.W.; Wallace, S.C., *Anal. Chem*., 1988, **60**, 5. b) Stahl, D.; Maquin, F., *Chem. Phys. Lett*., 1984, **108**, 613. c) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289. Average
8	-8.829	9.010	a) Brogli, F.; Heilbronner, E.; Kobayashi, T., *Helv. Chim. Acta*, 1972, **55**, 274 b) Dew ar, M.J.S.; Worley, S.D., *J. Chem. Phys*., 1969, **51**, 263.
9	-7.080	7.530	Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289
10	-8.437	8.600	a) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289. b) Utsunomiya, C.; Kobayashi, T.; Nagakura, S., *Bull. Chem. Soc. Jpn*., 1975, **48**, 1852. Average
11	-8.394	8.600	a) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289. b) Utsunomiya, C.; Kobayashi, T.; Nagakura, S., *Bull. Chem. Soc. Jpn*., 1975, **48**, 1852. Average
12	-8.158	8.330	Wentw orth, W.E.; Kao, L.W.; Becker, R.S., *J. Phys. Chem*., 1975, **79**, 1161
15	-7.625	7.800	Jongsma, C.; Vermeer, H.; Bickelhaupt, F.; Schafer, W.; Schw eig, A., *Tetrahedron*, 1975, **31**, 2931
16	-8.577	8.650	a) Klasinc, L.; Kovac, B.; Gusten, H., *Pure Appl. Chem*., 1983, **55**, 289. b) Kotov, B.V.; Potapov, V.K., *Khim. Vys. Energ*., 1972, **6**, 375. Average
20	-9.671	9.660	Redchenko, V.V.; Freimanis, Y.F.; Dregeris, Y.Y., *J. Gen. Chem. USSR*, 1980, **50**, 1507
21	-6.742	7.110	a) Clar, E.; Schmidt, W., *Tetrahedron*, 1979, **35**, 1027. b) Akiyama, I.; Li, K.C.; LeBreton, P.R.; Fu, P.P.; Harvey, R.G., *J. Phys. Chem*., 1979, **83**, 2997.

For electron affinities

Compound (Chart S1)	LUMO energy /eV	E_A, experim. /eV	Reference
1	2.815	-0.200	a) Jordan, K.D.; Burrow , P.D.; *Acc. Chem. Res*. 1978, **11**, 341. b) Lyapustina, S.A.; Xu, S.K.; Nilles, J.M.; Bow en, K.H., *J. Chem. Phys*., 2000, **112**, 6643 c) Schiedt, J.; Knott, W.J.; Le Barbu, K.; Schlag, E.W.; Weinkauf, R., *J. Chem. Phys*., 2000, **113**, 9470.
4	2.438	0.277	Steelhammer, J.C.; Wentw orth, W.E., *J. Chem. Phys*., 1969, **51**, 1802
5	2.029	0.494	a) Lyons, L.E.; Morris, G.C.; Warren, L.J., J. Phys. Chem., 1968, 72, 3677. b) Becker, R.S.; Chen, E., J. Chem. Phys., 1966, 45, 2403. c) Wentw orth, W.E.; Becker, R.S., *J. Am. Chem. Soc*., 1962, **84**, 4263. Average
6	1.761	0.597	a) Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358 b) Scheidt, J.; Weinkauf, R., *Chem. Phys. Lett*., 1997, **266**, 201 c) Ruoff, R.S.; Kadish, K.M.; Boulas, P.; Chen, E.C.M., *J. Phys. Chem*., 1995, **99**, 8843
7	1.955	0.550	Chen, G.D.; Cooks, R.G., *J. Mass Spectrom*., 1995, **30**, 1167
8	2.058	0.570	Dillow , G.W.; Kebarle, P., *Can. J. Chem*., 1989, **67**, 1628.
10	1.877	0.650	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
11	1.801	0.676	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
12	1.832	0.681	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
13	1.718	0.720	Chen, G.D.; Cooks, R.G., *J. Mass Spectrom*., 1995, **30**, 1167
14	1.648	0.828	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
15	1.567	0.906	Kokubo, S.; Ando, N.; Koyasu, K.; Mitsui, M.; Nakajima, A., *J. Chem. Phys*., 2004, **121**, 11112.
16	1.392	1.184	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
17	0.939	1.591	Heinis, T.; Chow dhury, S.; Scott, S.L.; Kebarle, P., *J. Am. Chem. Soc*., 1988, **110**, 400
18	0.752	1.765	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
19	0.583	1.782	Heinis, T.; Chow dhury, S.; Kebarle, P., *Org. Mass Spectrom*., 1993, **28**, 358
20	0.753	1.800	Fukuda, E.K.; McIver, R.T., Jr., *J. Am. Chem. Soc*., 1985, **107**, 2291
21	1.704	0.815	Crocker, L.; Wang, T.B.; Kebarle, P., *J. Am. Chem. Soc*., 1993, **115**, 7818

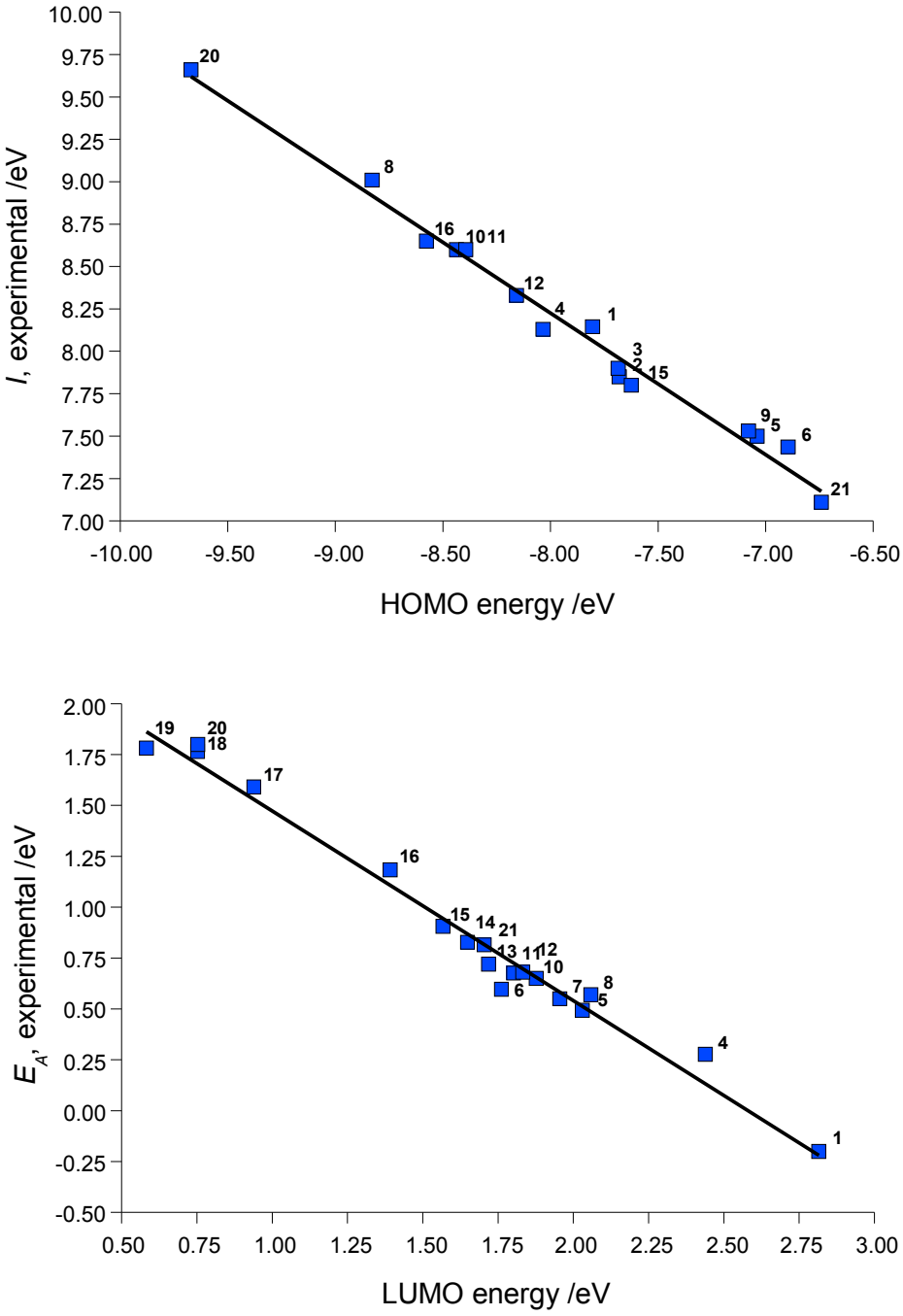


Figure S2. Correlation between experimental ionization potentials (top) and electron affinities (bottom) and their KT values for the set of compounds on Chart S1.

2.2. Whole conformers of the molecules and models used for evaluating the shifts in the gas phase electronic properties of the chromophores.

Pyrene derivatives. The **MePy** was exposed to a single point charge of +0.6 and +0.7 a.u. approaching the chromophore along an axis lying either on the plane or above the plane of the pyrene, with the same orientation found in the totally gauche and in the plane, C_s, conformers of the actual **c*n*Py** molecules, respectively, as shown in Figure S3.

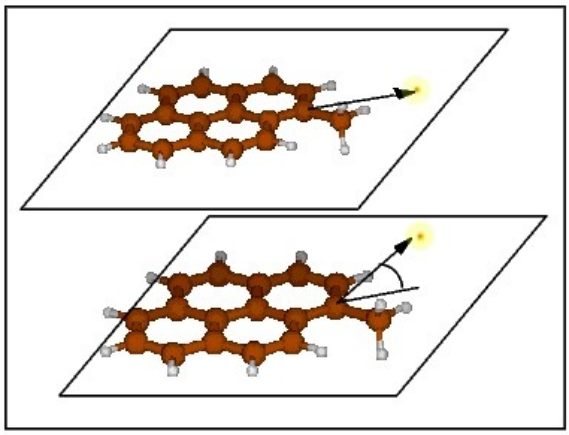


Figure S3: **MePy** exposed to a non bonded charge along the axis of the alkyl chain of the totally gauche (C_1) and plane (C_s) conformers

The shifts were not sensitively affected by these two different orientation, in contrast to the high sensitivity to the charge magnitude and distance. The results for these models are summarized toghether with the ones discussed on the main text on figure S4.
The whole summary of the shifts in the orbitals for the external (non bonded) charge models and for the actual **c*n*Py** different conformations are summarized on table S2.

Naphthalene derivatives. The complete summary of results for the naphthalene derivatives are shown on table S3.

Details on the changes in the total energies of the species and the changes in the shifts observed as a function of the dihedral θ, where the rotation about θ transforms the C_s into the C_1 conformer (0 to 90 degrees), are shown on Figure S5 for **c1Naph**.

Table S2. Summary of the shifts calculated in gas phase for the pyrene series. [a]

		r /Å	ε(HOMO)	ε(LUMO)	Δε(HOMO)	Δε(LUMO)
species	**MePy**	6.80	-6.93	2.04	0.00	0.00
	C1Py	1.68	-9.91	-1.10	-2.98	-3.14
	C4Py	5.17	-8.74	0.22	-1.81	-1.82
Cs Conformers						
	C1Py	1.68	-9.69	-0.87	-2.77	-2.91
	C4Py	5.17	-8.64	0.28	-1.71	-1.76
Models MePy + array of charges fitting the electrostatic potential of the TAA group						
		5.17	-8.11	0.83	-1.18	-1.21
		1.70	-8.70	0.22	-1.77	-1.82
MePy + single point charge above the pyrene plane, along the axis of the chain of the **c1Py** and **c4Py** salts	charge /a. u.					
	0.59	1.70	-8.78	0.09	-1.85	-1.95
		2.50	-8.52	0.40	-1.59	-1.64
		3.50	-8.27	0.68	-1.34	-1.36
		5.17	-7.94	1.02	-1.01	-1.02
	0.69	1.70	-9.08	-0.25	-2.15	-2.29
		2.50	-8.77	0.12	-1.85	-1.92
		3.50	-8.49	0.45	-1.56	-1.59
		5.17	-8.10	0.85	-1.17	-1.19
on the plane of pyrene, along the axis of the chain of the *Cs* conformers of the salts.						
	0.59	1.70	-8.80	0.13	-1.87	-1.91
		2.50	-8.49	0.46	-1.56	-1.59
		3.50	-8.26	0.69	-1.33	-1.35
		5.17	-7.96	1.00	-1.03	-1.04

a) All energies in eV

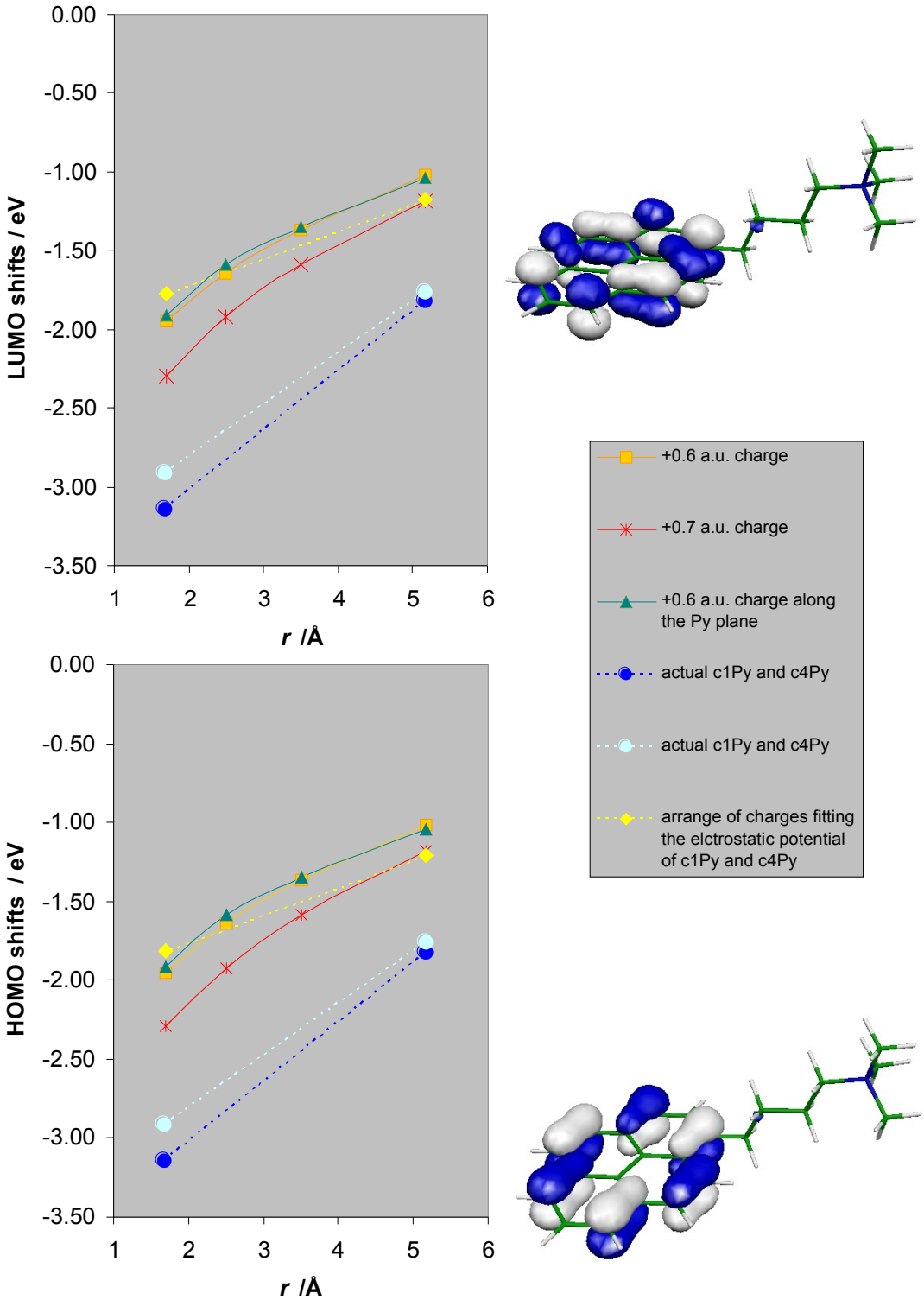
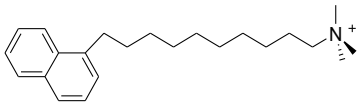
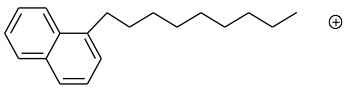
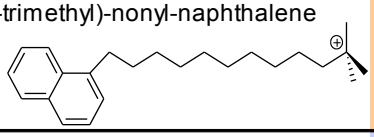


Figure S4: Summary of chromophore – external (non bonded) electric field obtained for the pyrene derivatives.

Table S3. Summary of results obtained for the naphthalene series in gas phase.[a]

species or models	distance cromophore-charged group in numbers of methylenes -CH_2-	$\varepsilon(\pi)$ /eV	$\varepsilon(\pi^*)$ /eV	$\Delta\varepsilon(\pi)$ /eV	$\Delta\varepsilon(\pi^*)$ /eV
MeNaph		-7.69	2.83	0.00	0.00
c1Naph	1	-11.09	-0.78	-3.40	-3.61
c1Naph, *Cs* conformer	1	-10.92	-0.50	-3.23	-3.33
MeNaph + array of charges equivalent to the field of the TAA group in the **c1Naph** species	1	-9.70	0.81	-2.01	-2.01
c7Naph folded	<2	-10.21	0.24	-2.52	-2.59
c8Naph folded	<2	-10.30	0.14	-2.61	-2.69
c2Naph	2	-10.50	-0.06	-2.81	-2.89
c2Naph, *Cs* conformer	2	-10.38	0.12	-2.69	-2.71
c3Naph	3	-10.07	0.41	-2.38	-2.42
c4Naph	4	-9.71	0.76	-2.02	-2.07
c4Naph, Cs conformer	4	-9.67	0.84	-1.98	-1.99
MeNaph + array of charges fitting the electrostatic potential of the TAA group in the **c4Naph** species	4	-8.97	1.55	-1.28	-1.28
MeNaph + array of charges fitting the electrostatic potential of the TAA group in the **c4Naph** species, including the polarized -(CH2)4- alkyl bridge	4	-9.63	0.89	-1.94	-1.93
c7Mnaf	7	-9.05	1.45	-1.36	-1.38
MeNaph + single point charge (+1.0) at the position of the N atom of the TAA in **c7Naph** salt (at 10.29Å)	7	-8.95	1.57	-1.27	-1.26
c8Mnaf	8	-8.90	1.60	-1.21	-1.23
c10Mnaf 	10	-8.68	1.82	-0.99	-1.01
point charge +1.0 + **MeNaph** 	10	-8.64	1.88	-0.95	-0.95
point charge +1.0 + 2-*n*-nonyl-naphthalene 	10	-8.70	1.79	-1.02	-1.04
Point charge +1.0 +(9-trimethyl)-nonyl-naphthalene 	10	-8.67	1.82	-0.99	-1.01
C16Naph	16	-8.32	2.18	-0.63	-0.65
point charge +1.0 + **MeNaph**	16	-8.32	2.20	-0.63	-0.63

a) all energies in eV

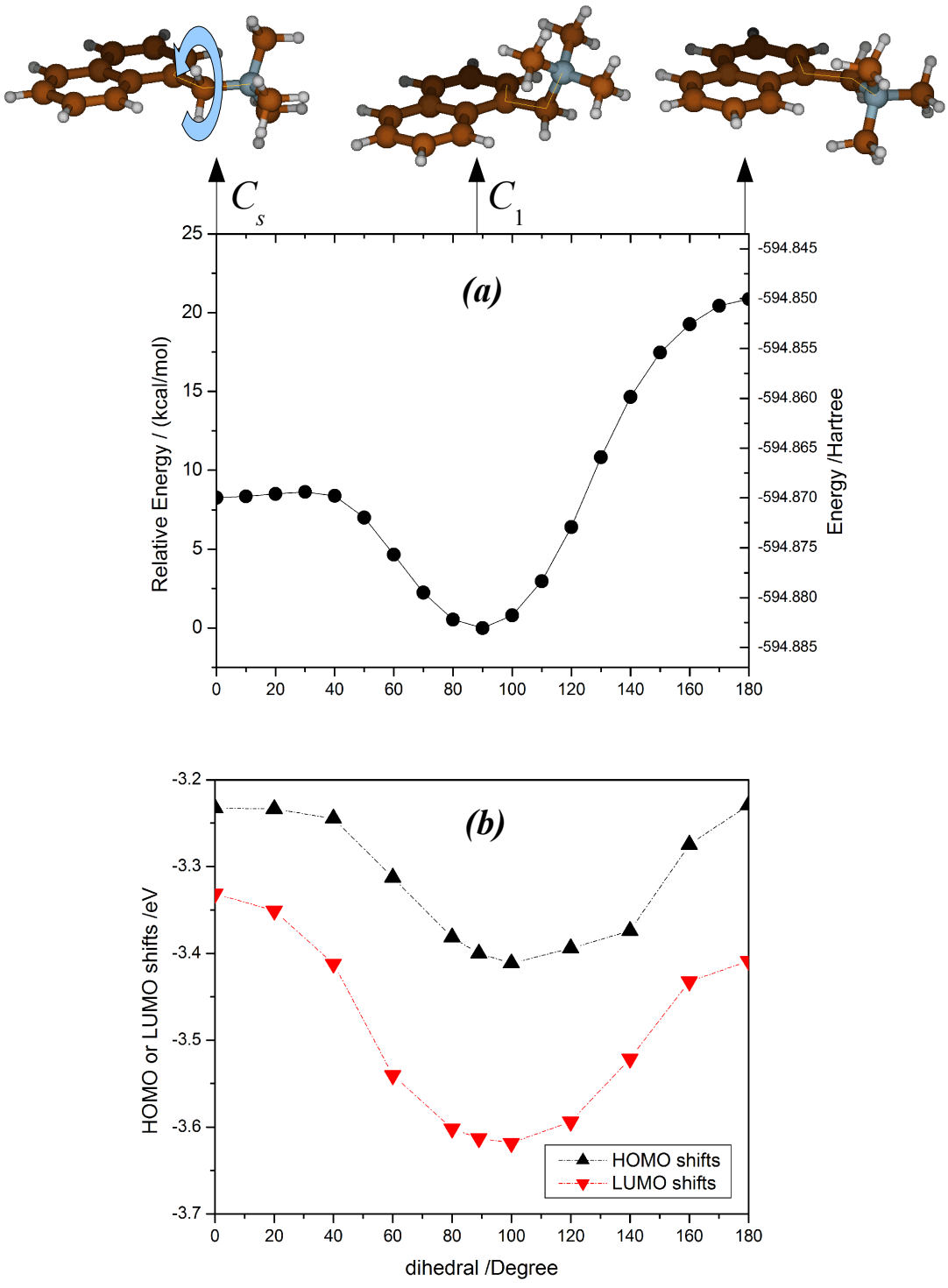


Figure S5: Energy profile (*a*), and changes in the HOMO and LUMO shifts (*b*), as a function of the selected dihedral, which interconverts plane and C_1 conformers.

2.3. Shifts on the orbital energies in acetonitrile.

Table S4. Summary of the shifts calculated in acetonitrile. [a]

	ε(HOMO)	ε(LUMO)	Δε(HOMO)	Δε(LUMO)
Mepy	-7.051	1.917	0.000	0.000
c1Py	-7.575	1.306	-0.524	-0.611
c4Py	-7.150	1.815	-0.099	-0.102
MeNaph	-7.782	2.736	0.000	0.000
c1Naph	-8.432	1.949	-0.650	-0.786
c1Naph (C_s conformer)	-8.360	2.132	-0.579	-0.604
c2Naph	-8.150	2.325	-0.369	-0.410
c2Naph (C_s conformer)	-8.101	2.435	-0.319	-0.300
c3Naph	-7.978	2.514	-0.196	-0.221
c4Naph	-7.870	2.622	-0.088	-0.114
c4Naph (C_s conformer)	-7.889	2.643	-0.107	-0.093

a) At the HF/6-31G* level, all energies in eV

2.4. DFT thermodynamic calculations for the shortest chain derivatives. Total energies in atomic units for each substrate and oxidized/reduced product both in gas phase and in acetonitrile.

Table S5. Suplementary information to main text Table 2: B3LYP Total energies for all species on the thermodynamic cycles on Chart2.

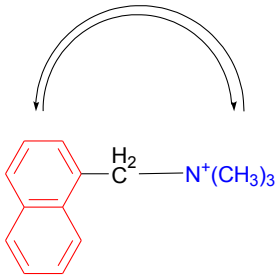
gas phase	Ar or Salt	(Ar)·- or (salt)·-	(Ar)·+ or (salt)·+
MeNaph	-425.22428	-425.21116	-424.94070
c1Naph	-598.87564	-598.99638	-598.46943
MePy	-655.10924	-655.12061	-654.85195
c1Py [b]	-828.76381	-828.89138	-828.39916
MePy [b]	-655.26107	-655.27497	-655.00232
c1Py	-828.96125	-829.09119	-828.59526
MeAnt	-578.86063	-578.87681	-578.60541
c1Ant	-870.45202	-870.58670	-870.08520
Acetonitrile			
MeNaph	-425.21997	-425.27122	-424.99500
c1Naph	-598.92935	-599.00486	-598.68084
MePy	-655.10482	-655.17617	-654.89975
c1Py	-828.81446	-828.90437	-828.59150
MeAnt	-578.85552	-578.93205	-578.65362
c1Ant	-870.49034	-870.58923	-870.26982

a) B3LYP/6-31+G*All energies in Hartree; b) B3LYP/6-311++G(2d,p)//B3LYP/6-31+G*

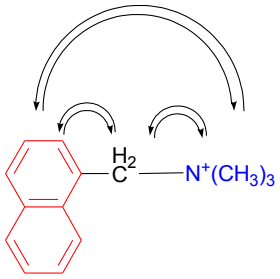
2.5 NBO analysis details

An alternative evaluation of the importance of the orbital coupling between the chromophore π system, the bridge and the TAA group is shown for the **c1Naph** species, for which the effect is expected to be maximum. The actual **c1Naph** molecule, *i.e.* the unaltered Fock matrix, has been compared to different models in which specific interactions between natural bonding orbitals with high and low occupancy have been suppressed by setting their non-diagonal Fock matrix elements (in NBO basis) to zero; in NBO terminology, the comparison of the system before and after specific *deletions*.[30] **c1Naph** has been compared to three models which have been setup by deleting:

I. The direct, "through space" interactions between the chromophore and the TAA group, *i.e.* setting to zero the non-diagonal elements involving the bonding and antibonding π orbitals with the antibonding and bonding σ orbitals respectively, of the TAA



II. The above deletions (I) plus the interaction between the cromophore and the -CH_2-bridge and with the TAA group. As previously, each deletion involves a couple of a highly occupied bonding orbital with a slightly occupied antibonding one.



III. The same as in I+II, but also including the more diffuse Rydberg orbitals with non-negligible occupation.§

The models are compared to c1Naph in terms of their canonical HOMO and LUMOs. The results are summarized on Table S6. The contribution of the orbital interactions to the overall effect is again below 0.3 eV, fairly smaller in comparison to the overall shifts in gas phase, as previously discussed on the main text.

§ Only the Rydberg orbitals of the C1 of the naphthalene and those in the -CH_2-TAA, having an occupation number >0.0005 e

Table S6. Variation in the shifts of **c1Naph** and the models described above (i.e. after deletion of orbital interactions)				
	ε(π) /eV	ε(π*) /eV	Δε(π) /eV	Δε(π*) /eV
MeNaph	-7.69	2.83	0	0
c1Naph	-11.09	-0.78	-3.40	-3.61
model I	-11.07	-0.76	-3.38	-3.59
model II	-10.97	-0.62	-3.28	-3.44
model III	-10.91	-0.56	-3.22	-3.39

The same procedure as in model I was applied in the case of the folded conformers of **c7** and **c8Naph** in order to check that the TAA group is not close enough to the chromophore for allowing direct orbital coupling (see main text).
Independently, the same fact can be ensured by the direct inspection of the off-diagonal Fock matrix elements (perturbational analysis).[30] For example, for the selected conformer of **c7Naph**, it has been found that even the closest σ*(CH) NBOs of the TAA (C42 – H50 and C42 – H51, see Figure S6) the interaction was smaller than 0.01 eV with any π orbital in the chromophore.

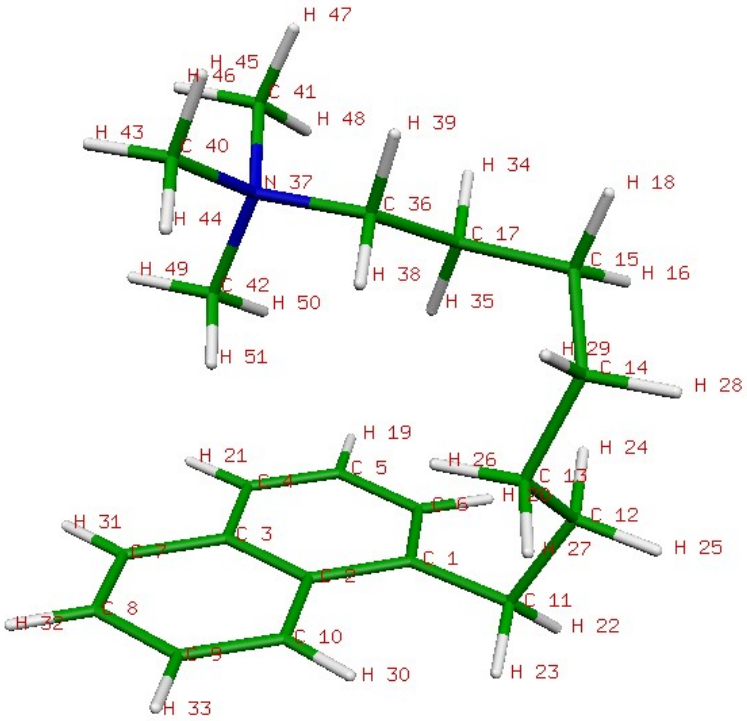


Figure S6: 3D structure of the folded **c7Naph**

2.6 Cartesian coordinates of main compounds

c1-c16Naph series at HF level

c1Naph- Cs conformer
33

C	1.094275	-0.064589	-1.871512
C	1.097608	-0.005159	-0.451276
C	2.345862	0.037965	0.204128
C	3.538763	0.021053	-0.559041
C	3.499778	-0.036069	-1.913674
C	2.256659	-0.079426	-2.575660
C	-0.102278	0.013054	0.343802
C	0.000389	0.071020	1.697725
C	1.256772	0.113863	2.345041
C	2.396139	0.097822	1.619879
C	-1.392205	-0.037259	-0.473005
N	-2.758837	-0.025359	0.221260
C	-2.992632	1.262090	0.992041
C	-3.806405	-0.084696	-0.882565
C	-2.961177	-1.249361	1.097180
H	3.353003	0.130072	2.101490
H	-0.857793	0.086737	2.331946
H	1.287340	0.159028	3.414443
H	4.476791	0.054490	-0.041218
H	4.405484	-0.048679	-2.484684
H	2.231665	-0.124480	-3.645823
H	0.173184	-0.098858	-2.414988
H	-1.395743	-0.940888	-1.066445
H	-1.417701	0.813258	-1.139868
H	-3.992298	1.236218	1.397914
H	-2.270774	1.357968	1.779212
H	-2.892613	2.088257	0.305089
H	-4.784001	-0.077890	-0.426228
H	-3.688378	0.776391	-1.521493
H	-3.666136	-0.992906	-1.447475
H	-3.961614	-1.214701	1.500481
H	-2.839808	-2.127268	0.481549
H	-2.238044	-1.261083	1.888916

c1Naph
33

C	-2.098598	-0.459795	-1.946201
C	-2.085926	-0.488351	-0.528106
C	-0.854185	-0.523260	0.165144
C	0.357901	-0.496174	-0.604862
C	0.289302	-0.511960	-1.970445
C	-0.942115	-0.485298	-2.655937
C	-3.305083	-0.504058	0.200256
C	-3.309371	-0.571873	1.555255
C	-2.082559	-0.636888	2.253636
C	-0.899061	-0.610978	1.585038
H	-3.046202	-0.437682	-2.453289
C	1.721603	-0.535190	0.039724
H	1.194174	-0.554444	-2.551524
H	-0.953171	-0.490951	-3.729674
H	-4.230205	-0.469303	-0.346131
H	-4.235099	-0.588797	2.099577
H	-2.088118	-0.715775	3.325466
H	0.006576	-0.685548	2.156007
N	2.391087	0.823479	0.291365
C	3.693885	0.565495	0.975743
C	2.660738	1.535736	-0.993382

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 C     1.555091     1.705635     1.160262
 H     2.417123    -1.067984    -0.591923
 H     1.707328    -1.027838     0.998347
 H     2.076135     2.640821     1.300684
 H     0.605135     1.879121     0.683296
 H     1.405463     1.227217     2.114441
 H     4.192635     1.506065     1.154661
 H     3.509586     0.067296     1.915313
 H     4.309024    -0.059006     0.345668
 H     3.194099     2.448731    -0.775621
 H     3.264896     0.905198    -1.628172
 H     1.726563     1.762651    -1.478189

c2Naph- Cs conformer
   36

 C     0.644487     0.014400     0.109607
 C     0.623659    -0.070379     1.543604
 C     1.847841    -0.071569     2.244071
 C     3.071032     0.010408     1.524586
 C     3.068639     0.089511     0.174269
 C     1.841201     0.091101    -0.533885
 C     1.843414    -0.154715     3.659767
 C     0.677286    -0.233240     4.352267
 C    -0.551259    -0.232286     3.656845
 C    -0.577371    -0.153621     2.298752
 C    -0.690357     0.014015    -0.624074
 C    -0.546655     0.107817    -2.139001
 N    -1.850567     0.110993    -2.918964
 C    -2.702410     1.285240    -2.557060
 C    -1.503617     0.207969    -4.371977
 C    -2.622504    -1.150703    -2.700563
 H     3.990314     0.151664    -0.374292
 H     1.897228     0.155686    -1.605092
 H     3.996682     0.008526     2.071246
 H    -1.223934    -0.892439    -0.361814
 H    -1.280696     0.846915    -0.259482
 H    -0.040132     1.019623    -2.419410
 H     0.017158    -0.729908    -2.522298
 H    -1.530141    -0.155308     1.803653
 H     2.785142    -0.154592     4.178636
 H     0.683203    -0.295793     5.424815
 H    -1.471957    -0.294685     4.208005
 H    -3.474473    -1.154273    -3.363615
 H    -1.986130    -1.995420    -2.917722
 H    -2.962383    -1.198109    -1.679831
 H    -3.555391     1.310848    -3.218324
 H    -3.040647     1.190358    -1.539096
 H    -2.123433     2.189349    -2.671296
 H    -2.413115     0.212453    -4.953147
 H    -0.955333     1.121501    -4.544254
 H    -0.897643    -0.641363    -4.648138

c2Naph
   36

 C     1.357550    -0.654926    -1.234537
 C     1.353503    -0.541514     0.183650
 C     2.597034    -0.414038     0.840101
 C     3.792286    -0.390072     0.074546
 C     3.759649    -0.492184    -1.279004
 C     2.519125    -0.631624    -1.941101
 C     2.638713    -0.318511     2.256415
 C     1.496931    -0.350743     2.986356
 C     0.249501    -0.470574     2.332089
 C     0.159240    -0.559193     0.975603
 C    -1.214948    -0.639757     0.333394
 C    -1.624388     0.758008    -0.141615
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 N    -2.958967     0.865822    -0.862712
 H     1.528275    -0.287449     4.058270
 H    -0.644736    -0.498289     2.931080
 H     3.593801    -0.226222     2.741311
 H    -1.917696    -1.004545     1.071284
 H    -1.212498    -1.350317    -0.482965
 H    -1.692725     1.422465     0.707809
 H    -0.887868     1.159122    -0.822000
 H     0.433610    -0.782600    -1.768357
 H     4.731095    -0.291960     0.589385
 H     4.669682    -0.475602    -1.849705
 H     2.498998    -0.727575    -3.011654
 C    -3.192111     2.310794    -1.172855
 C    -2.942779     0.101105    -2.145972
 C    -4.078594     0.374137    -0.004785
 H    -3.873331     0.273344    -2.665744
 H    -2.117893     0.446376    -2.750844
 H    -2.835987    -0.951040    -1.941166
 H    -5.014035     0.569813    -0.507172
 H    -3.972551    -0.685568     0.157764
 H    -4.054741     0.897198     0.939483
 H    -4.128855     2.413327    -1.699547
 H    -3.228198     2.868906    -0.249859
 H    -2.383813     2.674545    -1.788683

c3Naph
   39

 C     1.090598     1.121309    -0.274588
 C     1.098808     1.149829     1.158854
 C     2.337397     1.240752     1.830367
 C     3.541088     1.312624     1.079631
 C     3.509928     1.298647    -0.275019
 C     2.270595     1.201390    -0.950031
 C     2.362732     1.266793     3.249564
 C     1.214504     1.211159     3.972242
 C    -0.029304     1.131904     3.306198
 C    -0.084295     1.101590     1.947901
 C    -0.199624     0.969733    -1.054919
 C    -0.676063    -0.495782    -1.097698
 C    -1.987591    -0.593864    -1.870784
 N    -2.579462    -1.985311    -2.016340
 H     4.418644     1.362839    -0.844933
 H     2.270197     1.195930    -2.026594
 H     4.476534     1.385555     1.604785
 H    -0.037336     1.317424    -2.069772
 H    -0.979248     1.599128    -0.638232
 H     0.098776    -1.088624    -1.568700
 H    -0.794358    -0.860005    -0.085240
 H    -2.754177    -0.000110    -1.391417
 H    -1.860888    -0.223940    -2.879315
 H    -1.045882     1.059311     1.470681
 H     3.314136     1.336081     3.746010
 H     1.244139     1.235003     5.046110
 H    -0.936943     1.104162     3.881995
 C    -3.851091    -1.863279    -2.794870
 C    -1.651272    -2.891898    -2.758619
 C    -2.892600    -2.580982    -0.681552
 H    -4.290345    -2.842395    -2.911436
 H    -4.532239    -1.218492    -2.260815
 H    -3.632992    -1.442834    -3.764716
 H    -3.401092    -3.521342    -0.832241
 H    -1.979566    -2.748567    -0.135407
 H    -3.531407    -1.903690    -0.134818
 H    -2.149176    -3.834752    -2.927887
 H    -1.397083    -2.437846    -3.704630
 H    -0.760092    -3.054756    -2.176210
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c4Naph
42

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.434090
C	1.235615	0.000000	2.117284
C	2.448233	0.007085	1.377808
C	2.426814	0.018379	0.023038
C	1.189703	0.015109	-0.663120
C	1.249467	-0.000604	3.536996
C	0.093489	0.003283	4.249167
C	-1.146802	0.012494	3.571753
C	-1.190891	0.010168	2.212905
C	-1.290493	-0.048151	-0.793475
C	-1.870785	-1.467572	-0.889302
C	-3.186048	-1.504919	-1.681527
C	-3.694717	-2.941218	-1.759550
N	-4.995769	-3.161807	-2.512795
C	-6.122572	-2.415430	-1.875190
C	-4.869787	-2.744960	-3.942404
C	-5.306923	-4.624686	-2.468125
H	3.342814	0.032186	-0.539005
H	1.198350	0.028727	-1.739537
H	3.381932	0.009727	1.911303
H	-1.095471	0.318132	-1.796405
H	-2.030072	0.621747	-0.366186
H	-1.137850	-2.112543	-1.365648
H	-2.033237	-1.866008	0.107173
H	-3.912054	-0.864885	-1.192048
H	-3.012659	-1.102834	-2.673754
H	-2.964732	-3.571322	-2.248858
H	-3.863111	-3.334085	-0.766224
H	-2.147783	0.029659	1.725745
H	2.198894	-0.000727	4.042262
H	0.114900	0.005742	5.323661
H	-2.059873	0.027838	4.139562
H	-6.229618	-4.806719	-2.997926
H	-4.502690	-5.171643	-2.936031
H	-5.409333	-4.933087	-1.438903
H	-7.041467	-2.678634	-2.377118
H	-6.183284	-2.691692	-0.833217
H	-5.953559	-1.355645	-1.966606
H	-5.777227	-3.011490	-4.463066
H	-4.722787	-1.679432	-3.998064
H	-4.029705	-3.257741	-4.386276

c7Naph- Folded conformer
51

C	-1.951785	-0.114841	-1.682008
C	-2.221310	-0.207597	-0.287867
C	-2.281087	-1.495016	0.288741
C	-2.063195	-2.636897	-0.526371
C	-1.802478	-2.511614	-1.852952
C	-1.750200	-1.226407	-2.438448
C	-2.564334	-1.632986	1.673679
C	-2.781654	-0.538886	2.442901
C	-2.718933	0.751942	1.867491
C	-2.442682	0.937473	0.546653
C	-2.345454	2.348011	0.000557
C	-0.893142	2.835246	-0.118062
C	-0.057999	1.949102	-1.054126
C	1.361981	2.499502	-1.146358
C	2.114877	2.577372	0.102115
C	2.290668	1.224546	0.712339
C	2.937067	0.278716	-0.331726
N	3.122745	-1.119066	0.287411
C	1.832004	-1.647232	0.684310

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 C     3.727441    -2.003874    -0.689295
 C     3.983616    -1.022183     1.450174
 H     1.628514     3.230673     0.811375
 H     3.090087     2.981653    -0.125747
 H    -3.004425    -0.640723     3.489391
 H    -2.899581     1.605633     2.497976
 H    -2.609430    -2.619710     2.098839
 H    -2.884913     3.015643     0.664874
 H    -2.836370     2.421512    -0.964800
 H    -0.433311     2.803811     0.865632
 H    -0.876000     3.846438    -0.512143
 H    -0.054072     0.934620    -0.670553
 H    -0.527157     1.926820    -2.031696
 H     1.347920     3.510569    -1.529606
 H     1.961067     1.883868    -1.803234
 H    -1.918101     0.847840    -2.156832
 H    -2.112045    -3.610402    -0.071832
 H    -1.641885    -3.382524    -2.461826
 H    -1.555467    -1.132211    -3.491798
 H     2.935487     1.313283     1.573680
 H     1.333288     0.837198     1.018024
 H     2.289929     0.205887    -1.205802
 H     3.906459     0.675387    -0.629810
 H     3.858743    -2.992306    -0.251476
 H     3.080897    -2.076637    -1.562568
 H     4.696833    -1.607204    -0.987379
 H     4.114916    -2.010613     1.887992
 H     4.953008    -0.625511     1.152090
 H     3.529468    -0.357660     2.183713
 H     1.963305    -2.635663     1.122129
 H     1.377856    -0.982710     1.417850
 H     1.185461    -1.719995    -0.188964

c7Naph
   51

 C     3.727985     1.466808    -0.662010
 C     4.206241     0.206511    -0.205795
 C     5.438568     0.178069     0.483030
 C     6.145848     1.389952     0.700668
 C     5.658122     2.575818     0.254394
 C     4.428170     2.610946    -0.441116
 C     5.957701    -1.060728     0.944413
 C     5.279268    -2.212346     0.722362
 C     4.044443    -2.184925     0.032301
 C     3.499230    -1.022661    -0.423707
 C     2.153471    -1.054931    -1.121085
 C     0.984632    -0.679747    -0.197601
 C    -0.367152    -0.704643    -0.913727
 C    -1.533400    -0.353294     0.012443
 C    -2.887437    -0.376342    -0.700911
 C    -4.047759    -0.023199     0.241368
 C    -5.367407    -0.062604    -0.523229
 H     5.672331    -3.152930     1.064031
 H     3.527551    -3.114066    -0.135668
 H     6.898126    -1.068771     1.466383
 H     1.987548    -2.057546    -1.502893
 H     2.157764    -0.402586    -1.988989
 H     0.966220    -1.372455     0.640077
 H     1.152673     0.306032     0.226753
 H    -0.348459    -0.007068    -1.749079
 H    -0.532703    -1.691234    -1.342413
 H    -1.554522    -1.051720     0.846263
 H    -1.369468     0.633192     0.440856
 H     2.799768     1.520790    -1.198352
 H     7.083386     1.351129     1.226748
 H     6.202997     3.487193     0.422284
 H     4.049112     3.551136    -0.800267
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 H    -2.870705     0.324159    -1.532482
 H    -3.055179    -1.362409    -1.127533
 H    -4.058484    -0.728991     1.064484
 H    -3.873618     0.962501     0.658323
 N    -6.620919     0.264816     0.270652
 H    -5.348714     0.643800    -1.341840
 H    -5.533489    -1.048397    -0.935670
 C    -7.789009     0.169184    -0.659394
 C    -6.821457    -0.706479     1.388732
 C    -6.563816     1.652550     0.822607
 H    -7.510322     1.879506     1.289688
 H    -5.776257     1.720070     1.554182
 H    -6.379102     2.345562     0.015559
 H    -8.693474     0.398228    -0.116579
 H    -7.657895     0.874883    -1.465442
 H    -7.844442    -0.833282    -1.055504
 H    -7.770334    -0.501045     1.860935
 H    -6.821898    -1.709303     0.988662
 H    -6.029431    -0.597720     2.110447

c8Naph- Folded conformer
   54

 C    -2.022876     1.335562     0.632603
 C    -2.226102     0.194824    -0.216850
 C    -2.452647    -1.073267     0.371219
 C    -2.460393    -1.204632     1.784540
 C    -2.244331    -0.120357     2.571496
 C    -2.030114     1.147876     1.985892
 C    -2.677401    -2.203600    -0.462502
 C    -2.670782    -2.089916    -1.816014
 C    -2.439361    -0.827723    -2.412301
 C    -2.229609     0.272260    -1.640594
 C    -1.836078     2.752692     0.106362
 C    -0.376736     3.242462     0.064282
 C     0.475629     2.581908    -1.020887
 C     1.949075     3.009193    -1.035669
 C     2.770973     2.652592     0.213914
 C     2.684455     1.190709     0.675494
 C     3.125399     0.191316    -0.402344
 C     3.318478    -1.266559     0.028034
 N     2.094774    -2.162740     0.146794
 H     3.947799    -1.765153    -0.695692
 H     3.812558    -1.317590     0.988866
 H    -2.263599    -0.209850     3.642821
 H    -1.899678     1.996584     2.634565
 H    -2.660736    -2.168639     2.219100
 H    -2.390713     3.414804     0.762047
 H    -2.287357     2.868474    -0.871254
 H    -0.383198     4.316431    -0.103132
 H     0.067568     3.089908     1.043720
 H     0.406578     1.501140    -0.928097
 H     0.048608     2.821254    -1.991657
 H     2.006620     4.084747    -1.177246
 H     2.421714     2.575339    -1.913572
 H    -2.073479     1.217651    -2.120799
 H    -2.878042    -3.153573     0.002301
 H    -2.861367    -2.946902    -2.436812
 H    -2.449600    -0.736959    -3.483506
 H     2.464081     3.278085     1.045672
 H     3.811013     2.903748     0.021817
 H     1.674051     0.990817     1.008050
 H     3.322791     1.069195     1.547658
 H     2.487790     0.246701    -1.275313
 H     4.110078     0.491887    -0.749805
 C     2.587115    -3.539750     0.460365
 C     1.176876    -1.734052     1.247713
 C     1.328556    -2.214291    -1.136477
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 H     1.741660    -4.204360     0.550434
 H     3.232863    -3.877923    -0.335496
 H     3.133663    -3.516727     1.391050
 H     0.431107    -2.499656     1.390159
 H     1.750099    -1.603252     2.152917
 H     0.685803    -0.817677     0.977770
 H     0.539274    -2.943379    -1.039737
 H     0.888827    -1.252956    -1.339422
 H     1.999051    -2.496477    -1.934636

c8Naph
   54

 C     4.095354    -1.000194    -0.420268
 C     4.800261     0.230247    -0.202146
 C     6.050007     0.200357     0.454527
 C     6.588433    -1.041291     0.885025
 C     5.911352    -2.193893     0.663946
 C     4.659404    -2.164994     0.005523
 C     6.754844     1.413824     0.671388
 C     6.248057     2.602573     0.255054
 C     5.000187     2.639353    -0.407717
 C     4.302059     1.493711    -0.627225
 C     2.733247    -1.031583    -1.085274
 C     1.582931    -0.678632    -0.130234
 C     0.215406    -0.703409    -0.815578
 C    -0.934070    -0.374561     0.139200
 C    -2.303917    -0.397368    -0.542132
 C    -3.447940    -0.068682     0.420142
 C    -4.819319    -0.094071    -0.270980
 C    -5.913330     0.240196     0.738507
 H    -5.747298     1.221593     1.161290
 N    -7.339282     0.257545     0.213367
 H    -5.910173    -0.477553     1.547380
 H     6.318493    -3.136625     0.982631
 H     4.144010    -3.094973    -0.162283
 H     7.541785    -1.050526     1.383065
 H     2.565476    -2.029658    -1.478132
 H     2.712947    -0.366771    -1.943507
 H     1.588718    -1.383286     0.697660
 H     1.753342     0.302091     0.304915
 H     0.211000     0.005789    -1.641570
 H     0.048260    -1.685061    -1.255355
 H    -0.931180    -1.084309     0.963941
 H    -0.767737     0.606713     0.579034
 H     3.359254     1.548840    -1.137184
 H     7.705783     1.373897     1.172852
 H     6.791089     3.515213     0.422389
 H     4.605274     3.582070    -0.742356
 H    -2.310688     0.314073    -1.365293
 H    -2.473577    -1.378470    -0.980789
 H    -3.444455    -0.780404     1.242256
 H    -3.281777     0.912975     0.857378
 H    -4.815330     0.621445    -1.085701
 H    -4.978293    -1.077211    -0.699822
 C    -8.242490     0.603548     1.354795
 C    -7.508384     1.286844    -0.856829
 C    -7.735446    -1.081687    -0.318518
 H    -8.552045     1.336886    -1.128707
 H    -7.182776     2.244534    -0.479267
 H    -6.924628     1.012692    -1.719436
 H    -9.263640     0.622013     1.005322
 H    -8.134590    -0.140571     2.129126
 H    -7.970165     1.574593     1.739315
 H    -8.781242    -1.053860    -0.585326
 H    -7.147707    -1.314097    -1.190623
 H    -7.573039    -1.826592     0.445997
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c10Naph
60

C	5.303323	-0.977639	-0.372091
C	5.976473	0.274172	-0.175524
C	7.214402	0.291700	0.503664
C	7.772690	-0.924564	0.978896
C	7.125432	-2.097939	0.778689
C	5.885757	-2.116539	0.097082
C	7.887294	1.526891	0.698425
C	7.360947	2.691425	0.240067
C	6.124469	2.680792	-0.444681
C	5.456946	1.513458	-0.644095
C	3.955660	-1.059110	-1.061916
C	2.776878	-0.707991	-0.141369
C	1.425376	-0.784376	-0.854012
C	0.246120	-0.457572	0.064232
C	-1.107951	-0.531489	-0.644049
H	7.547375	-3.021805	1.131810
H	5.394414	-3.062363	-0.053170
H	8.716593	-0.897915	1.494155
H	3.819429	-2.071171	-1.430485
H	3.937958	-0.418833	-1.938695
H	2.781620	-1.389242	0.706001
H	2.914812	0.288044	0.270157
H	1.423138	-0.098892	-1.700008
H	1.291741	-1.781492	-1.270191
H	0.247605	-1.143718	0.909058
H	0.379871	0.539015	0.480809
H	4.521649	1.532149	-1.170023
H	8.829638	1.523142	1.217529
H	7.879782	3.620883	0.391363
H	5.713396	3.604459	-0.811474
C	-2.284318	-0.205108	0.278267
H	-1.111561	0.155607	-1.488211
H	-1.243277	-1.527998	-1.060403
C	-3.638554	-0.279437	-0.430154
H	-2.282299	-0.892137	1.122165
H	-2.150785	0.791551	0.694224
C	-4.810928	0.047741	0.497949
H	-3.644177	0.408815	-1.272796
H	-3.775550	-1.275968	-0.844786
C	-6.165463	-0.029730	-0.221850
H	-4.808882	-0.640913	1.339490
H	-4.677627	1.044719	0.911118
C	-7.289655	0.305609	0.753653
H	-6.160015	0.663020	-1.056036
H	-6.291586	-1.027840	-0.626408
N	-8.703228	0.274074	0.197127
H	-7.287686	-0.389327	1.582219
H	-7.156184	1.301932	1.152384
C	-9.639993	0.629397	1.308355
C	-8.872334	1.269235	-0.905000
C	-9.055696	-1.088498	-0.305666
H	-9.910399	1.286197	-1.201129
H	-8.578364	2.244597	-0.547302
H	-8.262699	0.985898	-1.746468
H	-10.653109	0.613571	0.936168
H	-9.532202	-0.090290	2.105430
H	-9.399442	1.616912	1.671457
H	-10.095436	-1.093031	-0.596322
H	-8.442870	-1.330693	-1.157597
H	-8.893528	-1.807965	0.482855

c16Naph
78

C	8.822406	-0.897557	-0.072351

C	9.368494	0.428488	-0.075089
C	10.490234	0.707070	0.735830
C	11.058501	-0.325043	1.529008
C	10.534541	-1.574464	1.509004
C	9.408644	-1.854536	0.699572
C	11.040139	2.016014	0.742680
C	10.507631	3.003930	-0.021483
C	9.390425	2.729711	-0.842427
C	8.840834	1.486425	-0.867062
C	7.591166	-1.250311	-0.882847
C	6.288065	-0.815886	-0.194456
C	5.046590	-1.163124	-1.029379
C	3.789962	-0.728459	-0.281221
C	2.452753	-0.999470	-0.973555
H	10.967626	-2.359429	2.101799
H	9.013054	-2.855754	0.697048
H	11.914318	-0.099257	2.139760
H	7.567681	-2.325589	-1.028764
H	7.644981	-0.812416	-1.874648
H	6.226074	-1.303516	0.774286
H	6.312278	0.252205	-0.002887
H	5.115415	-0.664088	-1.989870
H	5.033838	-2.231331	-1.216516
H	3.730007	-1.230972	0.674403
H	3.812214	0.337018	-0.097749
H	7.999930	1.304543	-1.509827
H	11.894493	2.211897	1.365908
H	10.933211	3.990732	-0.011312
H	8.979281	3.511836	-1.455275
C	1.309345	-0.502411	-0.086735
H	2.425604	-0.476124	-1.928171
H	2.341973	-2.069500	-1.142918
C	-0.027864	-0.773423	-0.779068
H	1.336504	-1.025758	0.867881
H	1.420136	0.567618	0.082629
C	-1.171272	-0.276363	0.107752
H	-0.055013	-0.250076	-1.733684
H	-0.138644	-1.843453	-0.948432
C	-2.508480	-0.547375	-0.584581
H	-1.144113	-0.799711	1.062368
H	-1.060481	0.793666	0.277115
C	-3.651889	-0.050316	0.302239
H	-2.535630	-0.024028	-1.539198
H	-2.619261	-1.617405	-0.753945
C	-4.989097	-0.321327	-0.390095
H	-3.624730	-0.573663	1.256854
H	-3.541098	1.019714	0.471602
C	-6.132506	0.175732	0.496725
H	-5.016247	0.202019	-1.344711
H	-5.099878	-1.391357	-0.559459
C	-7.469714	-0.095280	-0.195608
H	-6.105347	-0.347615	1.451341
H	-6.021715	1.245761	0.666088
C	-8.613123	0.401780	0.691212
H	-7.496864	0.428067	-1.150225
H	-7.580495	-1.165310	-0.364972
C	-9.950331	0.130768	-0.001122
H	-8.585964	-0.121568	1.645827
H	-8.502332	1.471809	0.860575
C	-11.093740	0.627827	0.885698
H	-9.977481	0.654115	-0.955738
H	-10.061112	-0.939262	-0.170486
N	-12.434444	0.356107	0.191555
H	-11.066581	0.104480	1.840314
H	-10.982949	1.697857	1.055062
C	-13.547959	0.840172	1.055190
C	-12.471591	1.072164	-1.114578
C	-12.586018	-1.107938	-0.040173

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 H   -13.423368     0.879268    -1.607356
 H   -12.360804     2.142193    -0.945206
 H   -11.657748     0.718373    -1.745777
 H   -14.499737     0.647275     0.562412
 H   -13.520801     0.316824     2.009806
 H   -13.437169     1.910201     1.224553
 H   -13.537796    -1.300834    -0.532952
 H   -11.772174    -1.461720    -0.671377
 H   -12.558863    -1.631277     0.914446
```

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MeNaph
   21

 C    -0.316330     0.046571    -1.711479
 C    -0.282539     0.004925    -0.292836
 C     0.974426     0.002595     0.347022
 C     2.152917     0.041761    -0.439865
 C     2.085944     0.081111    -1.794577
 C     0.830168     0.083455    -2.438973
 C    -1.471675    -0.034641     0.501666
 C    -1.362116    -0.073280     1.856088
 C    -0.101637    -0.075261     2.496130
 C     1.036361    -0.038385     1.763946
 C    -2.836680    -0.033151    -0.160896
 H     1.997898    -0.039721     2.239404
 H    -2.248370    -0.102973     2.459353
 H    -0.058814    -0.106475     3.566809
 H     3.102540     0.039528     0.059437
 H     2.982127     0.110448    -2.381805
 H     0.787305     0.114712    -3.509648
 H    -1.261994     0.048932    -2.212621
 H    -3.617669    -0.065789     0.587790
 H    -2.979746     0.862075    -0.756951
 H    -2.956311    -0.894936    -0.809117
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Anthracene and pyrene derivatives at the B3LYP level

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MeAnt
   27

 C    -0.267592     0.011324    -2.954079
 C    -0.244033     0.019477    -1.524247
 C     1.027031     0.010048    -0.833081
 C     2.209816    -0.031823    -1.643030
 C     2.145366    -0.047331    -3.012327
 C     0.890161    -0.020129    -3.682640
 C    -1.429108     0.033742    -0.785197
 C    -1.417425     0.019555     0.611388
 C    -0.152441     0.010140     1.313643
 C     1.061033     0.031786     0.582983
 C    -2.636947     0.011389     1.358216
 C    -2.631098    -0.020041     2.726116
 C    -1.392229    -0.047173     3.426167
 C    -0.201880    -0.031706     2.746321
 C     2.388031     0.059724     1.311969
 H     2.764479    -0.951836     1.517779
 H     0.857891    -0.028556    -4.768707
 H     3.062100    -0.083547    -3.594938
 H    -1.235094     0.025383    -3.450612
 H     3.182705    -0.068452    -1.166432
 H    -2.382720     0.045967    -1.309143
 H    -3.574853     0.025308     0.807817
 H     0.722079    -0.068243     3.311975
 H    -3.565124    -0.028415     3.281255
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H	-1.392418	-0.083412	4.512369
H	2.313395	0.580229	2.269227
H	3.155445	0.581679	0.736201

c1Ant
48

C	0.949920	1.048668	-2.221612
C	1.133709	0.836158	-0.815550
C	2.501387	0.770334	-0.349738
C	3.581792	0.874720	-1.279979
C	3.351186	1.061214	-2.615367
C	2.013429	1.162663	-3.082658
C	0.072271	0.697736	0.126123
C	0.352534	0.639683	1.521103
C	1.729210	0.571972	1.961127
C	2.755227	0.611574	1.014952
C	-0.644757	0.673896	2.549805
C	-0.314619	0.611473	3.880561
C	1.039271	0.494277	4.296916
C	2.031476	0.481330	3.355604
C	-1.349007	0.689014	-0.366292
N	-2.027581	-0.694542	-0.693101
C	-1.157765	-1.603556	-1.572424
C	-0.061790	-2.411265	-0.881882
C	-2.395030	-1.387003	0.618965
C	-3.143043	-2.713987	0.507449
C	-3.329225	-0.379710	-1.441684
C	-3.198681	0.203971	-2.845584
H	1.277160	0.435589	5.354259
H	-1.100077	0.663137	4.629156
H	3.075472	0.418304	3.650373
H	-1.690905	0.790413	2.292460
H	3.786548	0.547041	1.354071
H	4.596222	0.814067	-0.895212
H	-0.045731	1.162741	-2.636217
H	4.176953	1.147530	-3.314363
H	1.829349	1.344024	-4.137736
H	-1.435727	1.251397	-1.290363
H	-2.034159	1.145512	0.348543
H	-1.459970	-1.507257	1.164464
H	-3.006707	-0.667255	1.167684
H	-1.856916	-2.280787	-2.069295
H	-0.722220	-0.957355	-2.332787
H	-3.878219	-1.319943	-1.493069
H	-3.886698	0.299873	-0.790633
H	0.468302	-2.956447	-1.670195
H	0.667339	-1.788232	-0.365697
H	-0.452987	-3.154775	-0.183967
H	-3.203509	-3.134618	1.516528
H	-4.169193	-2.599500	0.149700
H	-2.633882	-3.450599	-0.118460
H	-4.214704	0.337124	-3.231457
H	-2.719455	1.185805	-2.872223
H	-2.678115	-0.465094	-3.535166

MePy
29

C	-1.064490	-0.000172	-3.084561
C	-1.069864	-0.000018	-1.679629
C	0.173183	-0.000134	-0.977153
C	1.399513	-0.000404	-1.711825
C	1.354794	-0.000549	-3.114930
C	0.135674	-0.000435	-3.791450
C	2.639986	-0.000515	-0.985674

C	2.659152	-0.000370	0.374917
C	1.442471	-0.000099	1.139823
C	0.190550	0.000020	0.451296
C	-1.035417	0.000289	1.188098
C	-1.002238	0.000437	2.603989
C	0.238655	0.000318	3.248359
C	1.437733	0.000056	2.540892
C	-2.284514	0.000252	-0.915928
C	-2.268221	0.000399	0.446360
C	-2.272448	0.000726	3.422320
H	0.264493	0.000434	4.335602
H	2.383888	-0.000030	3.076938
H	3.604180	-0.000456	0.913093
H	3.568771	-0.000720	-1.551164
H	2.287848	-0.000754	-3.673334
H	0.122133	-0.000551	-4.878112
H	-2.012351	-0.000083	-3.617476
H	-3.230760	0.000339	-1.452070
H	-3.207240	0.000602	0.990236
H	-2.043230	0.000810	4.492145
H	-2.892290	0.882909	3.217259
H	-2.892562	-0.881312	3.217457

c1Py

41

C	-3.689496	-0.409250	-3.038443
C	-3.678900	-0.448824	-1.646212
C	-2.465060	-0.443036	-0.939728
C	-1.233474	-0.397074	-1.657117
C	-1.255245	-0.362949	-3.084858
C	-2.491866	-0.367105	-3.750388
C	-0.009950	-0.330325	-3.796558
C	1.180455	-0.335912	-3.135461
C	1.231827	-0.367182	-1.702267
C	0.011117	-0.390144	-0.956541
C	0.035620	-0.413148	0.478183
C	1.296663	-0.390796	1.137736
C	2.477744	-0.412613	0.374436
C	2.454593	-0.393611	-1.010616
C	-2.413373	-0.496223	0.489598
C	-1.228222	-0.479099	1.163362
C	1.421879	-0.411303	2.629633
N	1.564704	0.991777	3.325977
C	0.398922	1.883658	2.997120
C	1.615373	0.766238	4.812137
C	2.833849	1.668650	2.886889
H	3.438076	-0.463376	0.882681
H	3.384790	-0.411927	-1.570972
H	2.117354	-0.318927	-3.685126
H	-0.034583	-0.306425	-4.882690
H	-2.506661	-0.339884	-4.836610
H	-4.634895	-0.414087	-3.572208
H	-4.614273	-0.486972	-1.094241
H	-3.348609	-0.559355	1.039985
H	-1.254328	-0.543156	2.246381
H	0.566849	-0.871165	3.126609
H	2.323244	-0.943981	2.943357
H	1.734541	1.726802	5.316403
H	0.685906	0.292999	5.132069
H	2.461370	0.117641	5.045099
H	0.543889	2.843102	3.496790
H	0.353501	2.019799	1.917518
H	-0.519677	1.415083	3.349639
H	2.913797	2.628672	3.399677
H	3.683195	1.036000	3.149900
H	2.798855	1.816989	1.808470

Main pyrene derivatives at HF level and MePy plus external (non bonded) electric filed as array of charges.

MePy

C	-0.277522	-0.487588	-1.601967
C	-0.277522	-0.487588	-0.154226
C	0.970920	-0.487588	0.507404
C	2.190422	-0.487328	-0.248130
C	2.149961	-0.487242	-1.657847
C	0.861676	-0.487398	-2.307225
C	3.437528	-0.487308	0.416197
C	4.607481	-0.487034	-0.335043
C	4.558835	-0.486844	-1.719070
C	3.342728	-0.486925	-2.376453
C	1.028613	-0.487780	1.918666
C	2.319939	-0.487732	2.569040
C	3.456025	-0.487510	1.862191
C	-1.463546	-0.487907	0.595635
C	-1.377465	-0.487941	1.979668
C	-0.158815	-0.487957	2.635048
C	-2.822077	-0.487830	-0.069020
H	-2.962390	0.387784	-0.695740
H	-2.282805	-0.488283	2.560774
H	-0.131140	-0.488145	3.710692
H	2.345944	-0.487912	3.644616
H	4.410002	-0.487476	2.359375
H	5.558213	-0.487018	0.168599
H	5.472967	-0.486632	-2.285415
H	3.311786	-0.486858	-3.451893
H	0.833418	-0.487461	-3.382766
H	-1.217281	-0.487801	-2.120421
H	-2.962883	-1.363914	-0.694979
H	-3.609043	-0.487281	0.675202

c1Py

C	0.253048	-1.624447	-0.612607
C	0.342267	-0.184045	-0.480612
C	-0.858682	0.523203	-0.212418
C	-2.094318	-0.184428	-0.040847
C	-2.132396	-1.588191	-0.152952
C	-0.907421	-2.278183	-0.460506
C	-3.283608	0.521921	0.238622
C	-4.470871	-0.184199	0.406458
C	-4.497808	-1.563733	0.298113
C	-3.337377	-2.262274	0.017924
C	-0.854607	1.932771	-0.116866
C	-2.086626	2.629146	0.164807
C	-3.234000	1.960479	0.336576
C	1.538299	0.542671	-0.620644
C	1.502480	1.935502	-0.565707
C	0.338780	2.623375	-0.312026
C	2.862303	-0.113081	-0.913771
N	3.751262	-0.418515	0.304262
C	4.133591	0.835164	1.019316
C	3.070487	-1.331214	1.270291
C	4.992692	-1.081001	-0.195153
H	2.405007	2.495925	-0.737731
H	0.346576	3.697209	-0.273770
H	-2.060395	3.701393	0.233111
H	-4.145781	2.489659	0.547263
H	-5.377312	0.353069	0.620345

H	-5.423661	-2.092710	0.428625
H	-3.363202	-3.333573	-0.071711
H	-0.939613	-3.346647	-0.578814
H	1.126022	-2.193427	-0.866996
H	2.754827	-1.054982	-1.426197
H	3.468892	0.530149	-1.534870
H	5.638575	-1.301951	0.641303
H	4.728324	-1.996711	-0.701772
H	5.498633	-0.417955	-0.880582
H	3.735815	-1.509157	2.101935
H	2.161003	-0.868954	1.615468
H	2.845432	-2.264545	0.780049
H	4.809761	0.581645	1.821960
H	4.625791	1.501754	0.327311
H	3.249079	1.302791	1.417245

c4Py

C	-1.772141	2.910469	0.011561
C	-2.732345	1.921205	0.175703
C	-2.395114	0.584660	-0.131619
C	-1.096901	0.263416	-0.596144
C	-0.146264	1.284324	-0.744334
C	-0.506870	2.589921	-0.440304
C	-3.382161	-0.443881	0.031445
C	-3.068234	-1.784274	-0.272209
C	-1.741667	-2.083254	-0.751677
C	-0.817486	-1.125284	-0.902931
C	-4.064770	2.222616	0.648276
C	-4.981542	1.260133	0.800681
C	-4.675395	-0.119180	0.497007
C	-5.616997	-1.131390	0.648883
C	-5.299617	-2.445047	0.348480
C	-4.036016	-2.770866	-0.108899
C	1.276116	1.011581	-1.193074
C	2.174247	0.537998	-0.039977
C	3.616417	0.271542	-0.496397
C	4.454830	-0.176881	0.696749
N	5.917600	-0.484232	0.423042
C	6.636148	0.721558	-0.089870
C	6.546365	-0.900460	1.715371
C	6.060307	-1.602295	-0.558146
H	0.216406	3.377474	-0.565284
H	-2.018304	3.933424	0.234122
H	-4.303318	3.246419	0.874964
H	-5.969588	1.497396	1.152617
H	-6.602492	-0.885993	1.002797
H	-6.040000	-3.214654	0.470054
H	-3.795765	-3.792840	-0.343451
H	-1.507109	-3.104615	-0.995408
H	0.153061	-1.395103	-1.274123
H	1.297439	0.281791	-1.995760
H	1.691363	1.925159	-1.607398
H	2.171072	1.294042	0.740171
H	1.757542	-0.362841	0.399974
H	3.608016	-0.489210	-1.269412
H	4.021688	1.177382	-0.933942
H	4.456336	0.587016	1.462118
H	4.043087	-1.079755	1.126477
H	7.588591	-1.124692	1.546002
H	6.456874	-0.094622	2.427764
H	6.039734	-1.777253	2.088804
H	7.687255	0.489823	-0.173878
H	6.248454	0.990404	-1.058097
H	6.495975	1.536906	0.603858
H	7.106131	-1.855269	-0.646699
H	5.506457	-2.457466	-0.200871
H	5.682440	-1.292966	-1.518144

MODEL1: Mepy plus array of charges reproducing the of the TAA group in c1Py

array of charges at C1M configuration with best ESP fitting charge from g98

atom	x	y	z
C	-0.277522	-0.487588	-1.601967
C	-0.277522	-0.487588	-0.154226
C	0.970920	-0.487588	0.507404
C	2.190422	-0.487328	-0.248130
C	2.149961	-0.487242	-1.657847
C	0.861676	-0.487398	-2.307225
C	3.437528	-0.487308	0.416197
C	4.607481	-0.487034	-0.335043
C	4.558835	-0.486844	-1.719070
C	3.342728	-0.486925	-2.376453
C	1.028613	-0.487780	1.918666
C	2.319939	-0.487732	2.569040
C	3.456025	-0.487510	1.862191
C	-1.463546	-0.487907	0.595635
C	-1.377465	-0.487941	1.979668
C	-0.158815	-0.487957	2.635048
C	-2.822077	-0.487830	-0.069020
H	-2.962390	0.387784	-0.695740
H	-2.282805	-0.488283	2.560774
H	-0.131140	-0.488145	3.710692
H	2.345944	-0.487912	3.644616
H	4.410002	-0.487476	2.359375
H	5.558213	-0.487018	0.168599
H	5.472967	-0.486632	-2.285415
H	3.311786	-0.486858	-3.451893
H	0.833418	-0.487461	-3.382766
H	-1.217281	-0.487801	-2.120421
H	-2.962883	-1.363914	-0.694979
H	-3.609043	-0.487281	0.675202

charge/a.u.	x	y	z
0.190954	-3.449915	0.924588	-0.251609
-0.394123	-3.669232	1.591484	1.088303
-0.275069	-2.563595	1.813049	-1.097294
-0.467986	-4.787245	0.756554	-0.939768
0.209070	-5.236239	1.729307	-1.070276
0.202492	-4.629385	0.290660	-1.900197
0.201054	-5.421176	0.135891	-0.325186
0.163871	-3.026674	2.785487	-1.168090
0.148249	-1.598035	1.884852	-0.627162
0.149410	-2.467075	1.378590	-2.078666
0.187756	-4.141905	2.546889	0.918860
0.188313	-4.310304	0.964610	1.688996
0.185155	-2.715841	1.723367	1.569670

MODEL4 MePy plus field generated by TAA in the C4Py salt

atom	x	y	z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.392539
C	1.228367	0.000000	2.085350
C	2.441001	-0.000026	1.359935
C	2.401268	-0.000021	-0.029842
C	1.190626	-0.000010	-0.702408
C	3.689102	-0.000063	2.090337
C	3.708249	-0.000101	3.428238
C	2.484766	-0.000078	4.198657
C	1.246230	-0.000017	3.519804
C	0.035199	-0.000017	4.247737

C	0.065396	-0.000030	5.650512
C	1.295350	-0.000118	6.291095
C	2.485601	-0.000140	5.585557
C	-1.221054	0.000041	2.160884
C	-1.204846	0.000026	3.500661
C	-1.205067	0.000014	6.471048
H	1.325812	-0.000141	7.366452
H	3.421266	-0.000190	6.116875
H	4.642954	-0.000138	3.961031
H	4.607285	-0.000069	1.529798
H	3.323274	-0.000031	-0.584324
H	1.177293	-0.000010	-1.777679
H	-0.937167	0.000008	-0.528440
H	-2.156917	0.000124	1.630091
H	-2.133902	0.000102	4.038092
H	-1.813822	-0.876122	6.268582
H	-0.973819	0.000598	7.529209
H	-1.814353	0.875577	6.267747

charge/a.u.	x	y	z
0.248285	-4.902790	3.009028	8.385566
-0.328743	-6.037805	2.247886	7.780948
-0.475473	-4.712456	2.574719	9.802771
-0.370908	-5.245630	4.465409	8.374869
0.212870	-6.150415	4.620345	8.942814
0.205020	-4.435140	5.022680	8.819212
0.204122	-5.394620	4.786078	7.355130
0.168461	-5.604222	2.814371	10.362149
0.166656	-4.541215	1.511905	9.836661
0.180756	-3.866520	3.098983	10.221387
0.178120	-6.941735	2.484303	8.321877
0.190247	-6.144746	2.537437	6.746329
0.179438	-5.843318	1.190776	7.849909