Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short-through long-chain [n]acenes

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14 Abstract

15

16 Vertical, well-to-well, and adiabatic ionization energies (IEs) and electron affinities (EAs) were
17 calculated for the $n=1-10$ [n]acenes using a wide range of semiempirical, Hartree-Fock, density
18 functional, and second order Moller-Plesset perturbation theory model chemistries. None of the model
19 chemistries examined was able to accurately predict the IEs or EAs for both short- through mid-length
20 [n]acenes, as well as for extrapolations to the polymeric limit, when compared to available
21 experimental and benchmark theoretical data. Provided a minimal basis set size is employed, basis set
22 effects on predicted IEs and EAs are not significant relative to the choice of model chemistry. The poor
23 IE/EA prediction performance for the parent [n]acenes likely extends to their substituted derivatives
24 and heteroatom substituted analogs. Consequently, caution should be exercised in the application of
25 non-high level calculations for estimating the IE/EA of these important classes of materials.

26

27 **Keywords:** [n]acenes; Ionization energies; Electron affinities; Benchmarking; Organic electronics

28

29 Introduction

30

31 The [n]acenes and their derivatives offer potential in the field of organic electronics [1-3].
32 Consequently, the molecular properties of these compounds are of interest, both in terms of
33 experimental measurements as well as the development and application of suitable theoretical methods.
34 Unique challenges exist for computational approaches in dealing with these molecules, as evidenced by
35 the various predictions for the multiplicities and open/closed shell natures of their ground states [4-18]
36 [19-21]. Notable high-level work by Deleuze and co-workers may have resolved controversies arising
37 from the prior application of lower-level theory, and their results indicate these molecules should be
38 ground state closed shell singlets [19-21] with positive singlet-triplet gaps that converge on a
39 vanishingly small energetic transition between these multiplicities at the polymer limit (i.e., as $n \rightarrow \infty$).
40 In concert with these efforts, it was recently shown that among the generally available semiempirical,
41 Hartree-Fock (HF), density functional theory (DFT), and second order Moller-Plesset perturbation
42 (MP2) methods, only the B2PLYP and mPW2PLYP functionals (which combine exact HF exchange
43 with an MP2-like correlation to the DFT calculation) appear to accurately describe the singlet-triplet
44 gaps of both the short- through mid-length [n]acenes (e.g., benzene through decacene) as well as
45 extrapolations to the polymeric limit [22, 23].

46

47 In the current study, we turn our attention to an examination of how well a broad range of
48 semiempirical, HF, DFT, and MP2 methods perform for predicting the ionization energies (IEs) and
49 electron affinities (EAs) of the [n]acenes. In particular, we give special regard as to whether the
50 theoretical approaches meet a required criteria of accurate IE/EA prediction for both short homologs as
51 well as at the polymeric limit. This type of criteria seems a basic standard to apply for theoretical
52 studies into the use of these types of compounds towards organic electronic and related applications.

Within this context, the goal of any reasonable theoretical method is to reproduce molecular energies and energy transitions within the bounds of experimental accuracy (generally taken to be ~ 1 kcal/mol = 4.2 kJ/mol). For IEs and EAs, which are commonly reported in units of electron volts (eV; 1 eV = 96.5 kJ/mol), this accuracy requirement means a required error for the computational approach of < 0.04 eV.

While high-level composite methods and similarly expensive theoretical approaches can achieve thermochemical accuracy for IEs and EAs (see, e.g., [24-31]), lower level methods generally have average errors in the range of tens of kJ/mol [32-34]. However, high-level methods are presently computationally impractical for mid- through longer-chain [n]acenes, necessitating a move to lower levels of theory to study these compounds. In addition, because of synthetic difficulties, experimental IE data are only available for the $n=1-6$ [n]acenes and EA data for the $n=1-5$ [n]acenes. Additional experimental challenges resulted in relatively large uncertainties for some of the IE/EA measurements, which led to the need for subsequent benchmark theoretical investigations [35, 36] that helped better constrain the actual IE/EA values. Thus, in the present work we provide comparisons of our model chemistry and basis set dependent IE/EA estimates for the $n=1-10$ [n]acenes with both the available experimental and benchmark theoretical datasets, and the findings herein should help guide the future development of theoretical methods better suited to model this important class of compounds.

Computational details

Geometry optimizations, frequency calculations, and single point energy (SPE) calculations employed Gaussian 09 (G09) [37] with various combinations of the following semiempirical, HF, DFT, and MP2 model chemistries and basis sets: model chemistries, AM1 [38-40], B1B95 [41], B1LYP [41-43],

77 B2PLYPD [44, 45], B3LYP [42, 43, 46], B3P86 [46, 47], B3PW91 [46, 48-50], B97D [51], B98 [52,
 78 53], BHandH [42, 43, 54-57], BHandHLYP [42, 43, 54-56, 58], BLYP [42, 43, 58], BMK [59], CAM-
 79 B3LYP [60], HCTH/147 [61-63], HCTH/407 [61-63], HF [64-66], HFB [58], HFS [54-56], HSE06
 80 [67-73], LC-wPBE [74-77], M05 [78], M052X [79], M06 [80], M062X [80], M06HF [81], M06L [80],
 81 MP2 [82-86], mPW1LYP [42, 43, 87], mPW1PBE [87-89], mPW2PLYPD [45, 90], mPW3PBE [87-
 82 89], O3LYP [42, 43, 91], OPBE [88, 89, 92, 93], OTPSS [92-94], PBE0 [88, 89, 95], PDDG [96-100],
 83 PM3 [101, 102], PM6 [103], tHCTH [104], tHCTHhyb [104], TPSSh [94], VSXC [105], wB97 [106],
 84 wB97X [106], wB97XD [107], X3LYP [108], and XAlpha [54-56]; basis sets, 6-31G(d) [109-114], 6-
 85 311++G(d,p) [115, 116], 6-311++G(2d,2p) [115, 116], SVP [117, 118], TZV [117, 118], TZVP [117,
 86 118], cc-pVDZ [119-122], and cc-pVTZ [119-122]. Structures were confirmed as true minima absent
 87 imaginary frequencies. Geometry visualizations were conducted with Gabedit 2.2.12 [123]. KyPlot
 88 v.2.b.15 [124] was employed for all statistical analyses.

90 **Results and discussion**

92 Geometry optimizations and frequency calculations were conducted on the neutral, cationic, and
 93 anionic forms of the $n=1-10$ [n]acenes (i.e., from benzene through decacene; Figure 1) at the B3LYP/6-
 94 31G(d) level of theory. The benzene anion yields one imaginary frequency at the B3LYP/6-31G(d)
 95 level. Thus, calculations for the well-to-well electron affinity (WWEA) and adiabatic electron affinity
 96 (AEA) of benzene used the B3LYP/6-311++G(d,p) geometries, which are absent imaginary
 97 frequencies, for both the neutral and anionic forms. B3LYP/6-31G(d) calculations on the decacene
 98 cation failed to converge; therefore, this compound was omitted from well-to-well ionization energy
 99 (WWIE) and adiabatic ionization energy (AIE) calculations. Due to computational expense, B3LYP/6-
 100 31G(d) frequency calculations could only be completed on the $n=1-7$ [n]acene cations and $n=2-6$

[n]acene anions (as noted, the benzene anion frequency calculation was completed at the B3LYP/6-311++G(d,p) level). No imaginary frequencies were observed. Consequently, WWIE/AIE and WWEA/AEA calculations for the n=8-9 [n]acene cations and n=7-10 [n]acene anions, respectively, make use of optimized B3LYP/6-31G(d) geometries for which corresponding frequency calculations were not conducted (and with the assumption of no imaginary frequencies), and also employ estimated zero-point energy and thermal corrections extrapolated from lower homologs.

Using the B3LYP/6-31G(d) optimized geometries for the neutral form of each compound, vertical ionization energies (VIEs) were calculated for the n=1-10 [n]acenes across a broad range of model chemistries (semiempirical, HF, DFT, and MP2 methods) at the x/TZVP//B3LYP/6-31G(d) level of theory (Table 1; semiempirical calculations are at the x//B3LYP/6-31G(d) level). Experimental VIEs are available for benzene through hexacenes, and range from 9.2 to 9.25 eV (benzene), 8.09 to 8.31±0.03 eV (naphthalene), 7.40 to 7.44±0.03 eV (anthracene), 6.97±0.02 to 7.01 eV (tetracene), 6.61±0.02 eV (pentacene), and 6.36±0.02 eV (hexacene). Deleuze et al. [35] have completed a suite of benchmark quality VIE calculations on these compounds using a focal point analysis (FPA) extrapolated to the CCSD(T)/cc-pV ∞ Z level and obtained the following values which are in good agreement with the experimental dataset: 9.45 eV (benzene), 8.24 eV (naphthalene), 7.47 eV (anthracene), 6.95 eV (tetracene), 6.57 eV (pentacene), and 6.43 eV (hexacene). Using a single exponential decay function regression having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)=\text{VIE}$ in eV; $c=\text{VIE}$ at the polymeric limit), we obtained VIE as $n\rightarrow\infty$ for the [n]acenes at 5.86 and 6.00 eV, respectively, using the experimental and benchmark theoretical datasets.

In comparison, extrapolated VIE at the [n]acene polymeric limit using the semiempirical, HF, DFT, and MP2 methods at the x/TZVP//B3LYP/6-31G(d) level of theory (semiempirical calculations are at the

125 x//B3LYP/6-31G(d) level) range from 3.50 eV (HF) to 6.46 eV (MP2), with the DFT and
126 semiempirical methods having VIE as $n \rightarrow \infty$ lying between these two end members. The AM1 (5.88
127 eV) and PM3 (6.04 eV) semiempirical methods have the best projected VIE agreement at the polymer
128 limit when compared with the experimental and benchmark theoretical data. However, both the AM1
129 and PM3 methods have poor agreement with the benchmark theoretical data for benzene through
130 hexacene (mean signed deviations [MSD], mean absolute deviations [MAD], and root mean squared
131 deviations [RMSD] of 0.11/0.27, 0.18/0.28, and 0.19/0.31 eV, respectively). Consequently, while these
132 methods may provide reasonable extrapolated VIEs at the polymeric limit for the [n]acenes, they have
133 unsatisfactory prediction performance for short- through mid-range chain lengths.

134
135 An analogous problem is observed when one uses the criteria of the lowest MSD/MAD/RMSD against
136 the benzene through hexacene benchmark theoretical dataset for assessing the quality of a VIE
137 prediction method. The LC-wPBE and M062X functionals have the best error metrics for the n=1-6
138 [n]acenes (equivalent MSD/MAD/RMSD of -0.06/0.06/0.09 eV for both methods), but the projected
139 VIEs at the polymeric limits (5.38 and 5.41 eV, respectively) are well below the experimental and
140 benchmark theoretical estimates. With the exception of the four semiempirical methods (AM1, PM3,
141 PM6, and PDDG) and the MP2 approach, all model chemistries underestimate the projected VIE at the
142 polymer limit based on comparisons with the experimental data and benchmark theoretical
143 calculations. As well, the MP2 method shows signs of beginning an upward VIE trend between n=8-
144 10, thereby forming a parabolic VIE versus acene length relationship. Overall, no single semiempirical,
145 HF, DFT, or MP2 method is able to adequately estimate the VIEs of short- through long-chain acenes.
146 These deficiencies are illustrated in Figure 2(a), which shows trends and extrapolations for the
147 benchmark theoretical estimates and those obtained at the M062X/TZVP//B3LYP/6-31G(d),
148 PM3//B3LYP/6-31G(d), and B2PLYPD/TZVP//B3LYP/6-31G(d) levels of theory.

For the semiempirical, HF, DFT, and MP2 VIEs, regression analyses were also conducted using the $n=1-6$ homologs and compared to the $n=1-10$ polymeric limit extrapolations in order to investigate the sensitivity of the $n=7-10$ datapoint inclusions on projected VIEs as $n \rightarrow \infty$. As shown in Table 1, the $n=1-6$ projected polymeric limit VIEs are generally about 0.2 to 0.3 eV higher than the corresponding $n=1-10$ projected polymeric limit VIEs. However, even with the reduced regression dataset (making the analysis directly comparable to that conducted on the available experimental and benchmark theoretical datasets, where only the $n=1-6$ data is available), none of the model chemistries examined meets the criteria of reliably reproducing $[n]$ acene VIEs for both short and long homologs. The basis set dependence of estimated VIEs was also considered at the B3LYP/y//B3LYP/6-31G(d) level with representative Pople, Ahlrichs, and Dunning type basis sets (Table 2). With the exception of the minimal 6-31G(d) basis set, the basis set effects on extrapolated VIEs are not significant. Thus, model chemistry effects on extrapolated VIEs for the $[n]$ acenes dominate any reasonable basis set size influences.

Analogous calculations were conducted for the WWIEs of the $n=1-9$ $[n]$ acenes at the x/TZVP//B3LYP/6-31G(d) level (Table 3). The geometry optimization with the B3LYP/6-31G(d) method failed to converge for decacene, resulting in its omission. Benchmark theoretical WWIEs were calculated from ref. [35] by subtracting the relaxation energies (E_{relax}) these authors calculated at the B3LYP/cc-pVTZ level from the corresponding FPA AIEs. Similar results and trends were obtained for the WWIEs as with the VIEs, including the relative insignificance of basis set effects (Table 4). Deleuze et al. [35] reported the following E_{relax} at the B3LYP/cc-pVTZ level for the $n=1-6$ $[n]$ acenes (values in eV): benzene, -0.15; naphthalene, -0.09; anthracene, -0.07; tetracene, -0.06; pentacene, -0.05; and hexacene, -0.04. Our values at the B3LYP/TZVP//B3LYP/6-31G(d) level are in excellent

173 agreement (-0.13, -0.08, -0.06, -0.05, -0.04, and -0.04 eV, respectively). Relaxation energies are
 174 predicted to decline with increasing acene chain length for all model chemistries (Table 5), but modest
 175 variations in the E_{relax} among the different methods are observed (values in eV): benzene, -0.23
 176 [HFB/MP2] to -0.08 [HF/BHandH]; naphthalene, -0.14 [AM1/PDDG] to -0.06 [BHandH/XAlpha];
 177 anthracene, -0.11 [AM1/PDDG] to -0.05 [M06L/MP2]; tetracene, -0.10 [PDDG] to -0.04 [HFB];
 178 pentacene, -0.09 [PDDG] to -0.02 [HFB]; hexacene, -0.09 [PDDG] to 0.00 [HFB]; heptacene, -0.08
 179 [PDDG] to +0.01 [HFB]; octacene, -0.08 [PDDG] to +0.02 [HFB]; and nonacene, -0.07 [PDDG] to
 180 +0.03 [HFB].

181
 182 Frequency calculations were completed at the B3LYP/6-31G(d) level on the neutral and cationic forms
 183 of benzene through heptacene in order to obtain the following zero-point vibrational energy (ZPVE)
 184 plus thermal (T) corrections (values in eV): benzene, -0.05; naphthalene, 0.00; anthracene, +0.02;
 185 tetracene, +0.02; pentacene, +0.03; hexacene, +0.04; and heptacene, +0.04. These values are in
 186 excellent agreement with the B3LYP/cc-pVDZ ZPVE corrections reported by Deleuze et al. [35]:
 187 benzene, -0.07; naphthalene, -0.01; anthracene, +0.01; tetracene, +0.02; pentacene, +0.03; and
 188 hexacene, +0.03. Owing to computational expense, ZPVE+T corrections were not calculated for
 189 octacene and nonacene, but based on the trend between benzene and heptacene, the ZPVE+T correction
 190 for these two longer acenes can be reliably approximated as +0.04 eV (all higher acenes beyond
 191 nonacene are also expected to have a ZPVE+T correction of about +0.04 eV). Applying the ZPVE+T
 192 corrections to the WWIE data in Table 3 yields the estimated AIEs in Table 6. As with the VIE and
 193 WWIE calculations, we find no HF, semiempirical, DFT, or MP2 model chemistry that meets the
 194 criteria of accurate AIE estimation for both short and long [n]acenes.

195
 196 The equivalent set of calculations with the same suite of model chemistries were conducted in order to

197 estimate vertical electron affinities (VEAs; Table 7) and the corresponding presence/absence of
 198 significant basis set effects (Table 8; although the anomalous performance of the 6-311++G(d,p) and 6-
 199 311++G(2d,2p) Pople-type basis sets is notable), WWEAs (Table 9) and the corresponding
 200 presence/absence of significant basis set effects (Table 10), relaxation energies from the anionic form
 201 of the neutral geometry to the optimized anionic geometry (Table 11), and AEAs (Table 12). ZPE+T
 202 corrections were calculated at the B3LYP/6-31G(d) level for benzene through hexacene, resulting in
 203 the following values (values in eV): benzene, 0.24; naphthalene, 0.16; anthracene, 0.13; tetracene, 0.11;
 204 pentacene, 0.10; and hexacene, 0.10. These values are in excellent agreement with those calculated by
 205 Deleuze et al. [36] at the B3LYP/cc-pVTZ level: benzene, 0.27; naphthalene, 0.16; anthracene, 0.14;
 206 tetracene, 0.13; pentacene, 0.12; and hexacene, 0.11. Due to computational expense, ZPE+T
 207 corrections could not be calculated for heptacene through decacene. However, the benzene through
 208 hexacene [n]acene ZPE+T corrections are well fit by a single exponential decay function regression
 209 having a y-axis offset of the general form $y = ae^{-bx} + c$ ($x=n$, $y(x)=\text{ZPE}+T$ in eV; $c=\text{ZPE}+T$ at the
 210 polymeric limit; $r=0.9992$, $a=0.311$, $b=0.771$, and $c=0.096$), indicating a reliably estimated ZPE+T
 211 correction of 0.10 eV for heptacene and all higher [n]acene homologs. As with the ionization energies,
 212 all semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation
 213 theory methods fail to accurately predict the electron affinities of short- through long-chain [n]acenes.

215 Conclusions

217 Vertical, well-to-well, and adiabatic ionization energies (IEs) and electron affinities (AEs) were
 218 calculated for the $n=1-10$ [n]acenes using a wide range of semiempirical, Hartree-Fock, density
 219 functional, and second order Moller-Plesset perturbation theory model chemistries. In comparison to
 220 available experimental and benchmark theoretical values, none of the model chemistries considered

221 met the required criteria of accurate IE/EA prediction for both short- through mid-length [n]acenes as
222 well as for extrapolations to the polymeric limit. Basis set influences of IE/EA predictive capacity were
223 minimal compared to the effects of changing model chemistry. One must also reasonably conclude the
224 poor IE/EA prediction performance of these theoretical methods on the parent [n]acenes also extends to
225 their substituted derivatives and heteroatom substituted analogs, thereby warranting caution in their
226 employment for such property prediction efforts on these important classes of materials.

227

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229

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233

234

235 **Figure Captions**

236

237 **Figure 1.** General structure of the polyacenes (**1**) and the individual members from benzene (**2**; n=1)
238 through decacene (**11**; n=10).

239

240 **Figure 2.** Trends in calculated VIEs for benzene through decacene at the x//B3LYP/6-31G(d) level of
241 theory (x=M062X/TZVP, PM3, and B2PLYPD/TZVP) along with benchmark theoretical calculations
242 from ref. [35] and corresponding associated extrapolations to the polymeric limit using a single
243 exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ (corresponding
244 regression statistics given in Table 1). Regression estimated VIEs at the polymeric limit are provided
245 along the right y-axis.

246

Figures

Figure 1.

Figure 2.

259 **Table 1.** Experimental, benchmark theoretical [35], and estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) vertical ionization energies (VIEs) for the [n]acenes (n=1-10). Error metrics (MSD=mean signed deviation; MAD=mean absolute deviation; and RMSD=root mean squared deviation) are between VIEs obtained at the x/TZVP//B3LYP/6-31G(d) level of theory and the benchmark theoretical [35] values for the n=1-6 [n]acenes. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ (x=n, y(x)=VIE in eV; c=VIE at the polymERIC limit). Values are in eV. Note that semiempirical method VIEs are at the x//B3LYP/6-31G(d) level of theory.

263

	[n]acene										error metrics		regression statistics (n=1-10)				regression statistics (n=1-6)	
	1	2	3	4	5	6	7	8	9	10	MSD	MAD	RMSD	a	b	c	r	r
expt.	9.2 [125] 9.22 [126] 9.23 [127, 128] 9.24 [129, 130-135] 9.24±0.02 [136] 9.25 [137, 138] 9.25±0.03 [139] 9.25±0.05 [140]	8.09 [141] 8.15 [130, 133, 138, 142] 8.15±0.02 [136] 8.18±0.03 [143] 8.31±0.03 [144]	7.40 [145, 146] 7.41 [130] 7.41±0.02 [136] 7.42±0.02 [147] 7.44±0.03 [144]	6.97±0.02 [136] 7.01 [148]	6.61±0.02 [136]	6.36±0.02 [136]	n/a ^a	n/a	n/a	n/a	n/a	n/a	n/a	4.91 ^b	0.376	5.86	0.9998	0.9998
benchmark theoretical [35]	9.45	8.24	7.47	6.95	6.57	6.43	n/a	n/a	n/a	n/a	n/a	n/a	n/a	5.31	0.433	6.00	0.9998	0.9998
HF	7.92	6.95	6.14	5.55	5.11	4.76	4.49	4.26	4.08	3.93	-1.45	1.45	1.45	5.69	0.253	3.50	0.9999	3.60
HFS	n/c ^c	6.88	6.07	5.53	5.15	4.86	4.64	4.46	4.31	4.19	-1.43	1.43	1.43	5.25	0.297	3.95	0.9996	4.34
HFB	8.16	6.82	6.02	5.48	5.09	4.80	4.58	4.40	4.25	4.13	-1.46	1.46	1.46	5.77	0.345	4.02	0.9991	4.24
XAlpha	8.57	7.21	6.41	5.88	5.50	5.21	4.99	4.81	4.66	4.54	-1.06	1.06	1.06	5.76	0.349	4.44	0.9989	4.79
BLYP	n/c	7.71	6.90	6.36	5.97	5.68	5.46	5.27	5.13	5.00	-0.61	0.61	0.61	5.27	0.294	4.76	0.9996	5.04
BHandHLYP	9.05	7.85	7.05	6.50	6.10	5.80	5.57	5.39	5.25	5.13	-0.46	0.46	0.47	5.61	0.322	4.95	0.9997	5.19
B1LYP	9.08	7.79	6.99	6.44	6.05	5.76	5.54	5.36	5.22	5.10	-0.50	0.50	0.51	5.70	0.340	4.97	0.9994	5.25
B97D	9.12	7.77	6.97	6.43	6.05	5.76	5.53	5.35	5.21	5.09	-0.50	0.50	0.51	5.77	0.347	4.98	0.9991	5.32
M06L	9.16	7.83	7.02	6.47	6.08	5.79	5.56	5.38	5.23	5.11	-0.46	0.46	0.47	5.79	0.342	4.99	0.9992	5.31
mPW1LYP	9.11	7.82	7.01	6.47	6.08	5.79	5.56	5.38	5.24	5.12	-0.47	0.47	0.48	5.71	0.339	4.99	0.9993	5.29
VSXC	9.14	7.80	6.99	6.45	6.07	5.78	5.55	5.37	5.23	5.11	-0.48	0.48	0.49	5.78	0.347	5.00	0.9991	5.33
BHandH	9.10	7.88	7.08	6.53	6.13	5.84	5.61	5.43	5.29	5.18	-0.42	0.42	0.43	5.62	0.328	5.01	0.9996	5.26
O3LYP	9.17	7.84	7.03	6.49	6.10	5.81	5.58	5.40	5.26	5.14	-0.45	0.45	0.46	5.77	0.344	5.02	0.9992	5.34
TPSSh	9.17	7.85	7.04	6.50	6.12	5.83	5.60	5.42	5.28	5.16	-0.43	0.43	0.44	5.74	0.344	5.04	0.9992	5.37
M05	9.01	7.81	7.03	6.51	6.13	5.84	5.63	5.45	5.32	5.20	-0.46	0.46	0.47	5.45	0.331	5.06	0.9995	5.31
OPBE	9.24	7.89	7.08	6.54	6.15	5.86	5.64	5.46	5.31	5.19	-0.39	0.39	0.41	5.80	0.347	5.08	0.9991	5.41
OTPSS	9.26	7.90	7.09	6.55	6.16	5.87	5.65	5.47	5.32	5.20	-0.38	0.38	0.39	5.82	0.349	5.10	0.9991	5.42
X3LYP	9.22	7.91	7.11	6.56	6.18	5.88	5.66	5.48	5.34	5.22	-0.37	0.37	0.39	5.73	0.342	5.10	0.9993	5.39
B98	9.23	7.92	7.11	6.57	6.18	5.89	5.67	5.49	5.35	5.23	-0.37	0.37	0.38	5.74	0.344	5.11	0.9993	5.41
HSE06	9.25	7.97	7.16	6.62	6.23	5.93	5.70	5.52	5.37	5.25	-0.32	0.32	0.34	5.71	0.333	5.11	0.9993	5.42
B1B95	9.24	7.93	7.13	6.59	6.20	5.91	5.68	5.51	5.37	5.25	-0.35	0.35	0.37	5.72	0.343	5.13	0.9993	5.43
B3LYP	9.26	7.95	7.14	6.60	6.21	5.92	5.70	5.52	5.38	5.26	-0.34	0.34	0.35	5.74	0.344	5.14	0.9993	5.44
HCTH/147	9.30	7.95	7.15	6.61	6.23	5.94	5.71	5.53	5.39	5.27	-0.32	0.32	0.34	5.77	0.347	5.16	0.9991	5.50
tHCTH	9.27	7.95	7.15	6.62	6.24	5.95	5.73	5.55	5.40	5.28	-0.32	0.32	0.33	5.70	0.344	5.17	0.9991	5.50
mPW1PBE	9.26	7.98	7.18	6.64	6.25	5.96	5.74	5.56	5.42	5.30	-0.31	0.31	0.32	5.67	0.339	5.17	0.9994	5.46
PBE0	9.26	7.98	7.18	6.64	6.25	5.97	5.74	5.56	5.42	5.31	-0.30	0.30	0.31	5.67	0.339	5.18	0.9994	5.47
M06	9.20	7.94	7.15	6.62	6.24	5.96	5.74	5.56	5.42	5.31	-0.33	0.33	0.34	5.58	0.340	5.18	0.9993	5.47
tHCTHhyb	9.31	7.99	7.19	6.65	6.26	5.97	5.75	5.57	5.43	5.31	-0.29	0.29	0.30	5.73	0.344	5.19	0.9992	5.50
BMK	9.31	8.04	7.22	6.67	6.28	5.99	5.76	5.58	5.44	5.33	-0.27	0.27	0.28	5.72	0.339	5.19	0.9995	5.46

B3PW91	9.29	8.00	7.19	6.65	6.27	5.98	5.75	5.58	5.44	5.32	-0.29	0.29	0.30	5.69	0.342	5.20	0.9993	5.50	0.9999
HCTH/407	9.34	8.01	7.20	6.67	6.28	5.99	5.77	5.59	5.44	5.32	-0.27	0.27	0.29	5.75	0.345	5.21	0.9991	5.53	0.9998
mPW3PBE	9.31	8.01	7.21	6.67	6.28	5.99	5.77	5.59	5.45	5.33	-0.27	0.27	0.29	5.70	0.341	5.21	0.9993	5.50	0.9998
mPW2PLYPD	9.23	7.97	7.17	6.64	6.25	5.97	5.76	5.59	5.45	5.35	-0.31	0.31	0.32	5.60	0.346	5.22	0.9995	5.47	0.9999
B2PLYPD	9.24	7.96	7.16	6.63	6.25	5.97	5.75	5.59	5.45	5.35	-0.32	0.32	0.33	5.62	0.350	5.23	0.9994	5.47	0.9999
CAM-B3LYP	9.30	8.07	7.27	6.73	6.34	6.05	5.83	5.66	5.52	5.42	-0.22	0.22	0.23	5.59	0.337	5.27	0.9996	5.50	0.99991
wB97	9.28	8.13	7.34	6.80	6.40	6.11	5.88	5.71	5.57	5.46	-0.18	0.18	0.19	5.48	0.320	5.27	0.9998	5.47	0.99997
wB97X	9.29	8.11	7.32	6.78	6.39	6.11	5.89	5.72	5.59	5.48	-0.19	0.19	0.20	5.48	0.332	5.32	0.9997	5.56	0.9999
wB97XD	9.27	8.04	7.26	6.73	6.35	6.07	5.86	5.70	5.57	5.47	-0.23	0.23	0.24	5.49	0.345	5.34	0.9996	5.53	0.99996
M052X	9.36	8.19	7.39	6.85	6.46	6.17	5.95	5.78	5.64	5.53	-0.11	0.11	0.13	5.50	0.327	5.36	0.9997	5.57	0.99997
LC-wPBE	9.39	8.26	7.46	6.92	6.52	6.23	6.00	5.82	5.69	5.58	-0.06	0.06	0.09	5.47	0.318	5.38	0.9998	5.57	0.99998
M062X	9.46	8.25	7.44	6.90	6.51	6.22	6.00	5.82	5.68	5.57	-0.06	0.06	0.09	5.58	0.331	5.41	0.9996	5.66	0.99994
M06HF	9.66	8.56	7.76	7.22	6.82	6.52	6.30	6.12	5.98	5.86	0.24	0.24	0.25	5.44	0.311	5.65	0.9998	5.82	0.99998
B3P86	9.86	8.56	7.76	7.22	6.83	6.54	6.32	6.14	6.00	5.89	0.28	0.28	0.29	5.70	0.343	5.76	0.9993	6.05	0.9998
AM1	9.25	8.29	7.63	7.17	6.85	6.60	6.41	6.26	6.14	6.04	0.11	0.18	0.19	4.58	0.316	5.88	0.9997	6.07	0.99997
PM3	9.43	8.45	7.78	7.32	7.00	6.75	6.56	6.40	6.29	6.19	0.27	0.28	0.31	4.63	0.320	6.04	0.9997	6.24	0.99996
PDDG	9.44	8.48	7.82	7.36	7.04	6.79	6.61	6.46	6.34	6.25	0.30	0.31	0.34	4.57	0.320	6.10	0.9997	6.26	0.99997
PM6	9.28	8.41	7.80	7.38	7.07	6.83	6.65	6.50	6.39	6.29	0.28	0.33	0.36	4.25	0.303	6.12	0.9997	6.30	0.99996
MP2	9.57	8.31	7.54	7.09	6.80	6.63	6.54	6.51	6.52	6.57	0.14	0.14	0.15	5.36	0.540	6.46	0.9993	6.37	0.999993

264 ^a not available. ^b regression statistics for the experiment values obtained using the average of multiple experimental datapoints where available. ^c calculation failed to converge, and resulting error metrics and regression statistics

265 omit this datapoint from the corresponding analysis.

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Table 2. Estimated vertical ionization energies (VIEs) for the [n]acenes (n=1-10) at the B3LYP//B3LYP/6-31G(d) level of theory. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)=VIE$ in eV; $c=VIE$ at the polymeric limit). Values are in eV.

basis set	[n]acene										regression statistics (n=1-10)			regression statistics (n=1-6)		
	1	2	3	4	5	6	7	8	9	10	a	b	c	r	c	r
6-31G(d)	9.01	7.69	6.87	6.33	5.94	5.64	5.42	5.24	5.10	4.98	5.78	0.344	4.86	0.9993	5.16	0.9998
6-311++G(d,p)	9.27	7.96	7.16	6.62	6.23	5.94	5.71	5.54	n/c ^a	5.27	5.72	0.344	5.16	0.9992	5.46	0.9998
6-311++G(2d,2p)	9.25	7.94	7.14	6.60	6.21	5.92	5.70	5.52	5.37	5.26	5.72	0.342	5.13	0.9993	5.44	0.9998
SVP	9.25	7.92	7.11	6.56	6.17	5.88	5.66	5.48	5.33	5.22	5.79	0.346	5.10	0.9993	5.40	0.9998
TZV	9.31	7.97	n/c	6.60	6.21	5.91	5.69	5.51	5.36	5.25	5.83	0.339	5.11	0.9993	5.44	0.9998
TZVP	9.26	7.95	7.14	6.60	6.21	5.92	5.70	5.52	5.38	5.26	5.74	0.344	5.14	0.9993	5.44	0.9998
cc-pVDZ	9.16	7.85	7.04	6.49	6.10	5.81	5.59	5.41	5.27	5.15	5.76	0.344	5.03	0.9993	5.32	0.9998
cc-pVTZ	9.23	7.92	7.11	6.57	6.18	n/c	5.66	5.48	5.34	5.22	5.77	0.344	5.09	0.9994	5.52	0.99991

^a calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

274 **Table 3.** Benchmark theoretical [35] and estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) well-to-well ionization energies (WWIEs) for the [n]acenes (n=1-9). Error metrics (MSD=mean signed deviation; MAD=mean absolute deviation; and RMSD=root mean squared deviation) are between WWIEs obtained at the x/TZVP//B3LYP/6-31G(d) level of theory and the benchmark theoretical [35] values for the n=1-6 [n]acenes. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)$ =WWIE in eV; c = WWIE at the polymERIC limit). Values are in eV. Note that semiempirical method WWIEs are at the x//B3LYP/6-31G(d) level of theory.

	1 ^a	[n]acene									error metrics				regression statistics (n=1-9)			
		2	3	4	5	6	7	8	9	MSD	MAD	RMSD	a	b	c	r	c	r
benchmark theoretical [35]	9.37	8.23	7.49	6.97	6.60	6.46	n/a	n/a	n/a	n/a	n/a	n/a	5.10	0.416	6.01	0.9997	6.01	0.9997
HF	7.83	6.84	6.06	5.49	5.06	4.73	4.46	4.24	4.07	-1.52	1.52	1.52	5.53	0.264	3.57	0.99994	3.71	0.99998
HFB	7.93	6.70	5.94	5.44	5.07	4.80	4.59	4.42	4.28	-1.54	1.54	1.54	5.38	0.354	4.11	0.9994	4.35	0.9998
HFS	8.08	6.79	6.01	5.48	5.11	4.83	4.62	4.44	4.30	-1.47	1.47	1.47	5.58	0.359	4.14	0.9993	4.38	0.9998
XAlpha	8.47	7.15	6.35	5.82	5.44	5.16	4.94	4.76	4.62	-1.12	1.12	1.13	5.69	0.361	4.46	0.9993	4.72	0.9998
BLYP	8.93	7.62	6.84	6.31	5.93	5.65	5.43	5.26	5.11	-0.64	0.64	0.65	5.63	0.359	4.95	0.9993	5.20	0.9998
BHandHLYP	8.95	7.77	6.98	6.44	6.05	5.75	5.53	5.35	5.21	-0.53	0.53	0.54	5.51	0.331	4.97	0.9997	5.15	0.99993
BHandH	9.03	7.82	7.02	6.47	6.08	5.78	5.55	5.37	5.23	-0.49	0.49	0.50	5.60	0.334	4.99	0.9997	5.20	0.99993
B1LYP	8.95	7.71	6.92	6.39	6.01	5.72	5.50	5.33	5.19	-0.57	0.57	0.58	5.55	0.347	4.99	0.9996	5.21	0.9999
M06L	9.05	7.76	6.96	6.42	6.03	5.74	5.52	5.34	5.19	-0.52	0.52	0.54	5.69	0.350	5.00	0.9994	5.24	0.9998
mPW1LYP	8.98	7.74	6.95	6.42	6.03	5.75	5.53	5.35	5.21	-0.54	0.54	0.55	5.56	0.346	5.01	0.9996	5.23	0.9999
B97D	8.97	7.68	6.90	6.38	6.00	5.72	5.50	5.32	5.18	-0.58	0.58	0.59	5.58	0.355	5.01	0.9993	5.27	0.9998
VSXC	9.01	7.72	6.93	6.40	6.02	5.73	5.51	5.34	5.19	-0.56	0.56	0.57	5.63	0.354	5.02	0.9994	5.26	0.9998
TPSSh	9.03	7.77	6.98	6.45	6.07	5.78	5.56	5.38	5.24	-0.51	0.51	0.52	5.58	0.348	5.05	0.9995	5.29	0.9998
O3LYP	9.04	7.76	6.97	6.43	6.05	5.76	5.54	5.37	5.23	-0.52	0.52	0.53	5.63	0.353	5.05	0.9995	5.27	0.9998
M05	8.90	7.72	6.97	6.45	6.07	5.79	5.58	5.41	5.28	-0.54	0.54	0.54	5.34	0.341	5.07	0.9997	5.26	0.9999
OPBE	9.11	7.81	7.01	6.48	6.10	5.81	5.59	5.41	5.27	-0.47	0.47	0.48	5.67	0.356	5.10	0.9994	5.35	0.9998
OTPSS	9.13	7.82	7.02	6.49	6.11	5.82	5.60	5.43	5.28	-0.45	0.45	0.47	5.68	0.358	5.11	0.9994	5.36	0.9998
X3LYP	9.09	7.83	7.05	6.51	6.13	5.84	5.62	5.45	5.31	-0.44	0.44	0.45	5.58	0.349	5.12	0.9995	5.34	0.9998
B98	9.08	7.83	7.05	6.52	6.14	5.85	5.63	5.46	5.32	-0.44	0.44	0.45	5.55	0.348	5.13	0.9995	5.35	0.9998
B1B95	9.13	7.86	7.07	6.53	6.15	5.86	5.64	5.46	5.32	-0.42	0.42	0.43	5.62	0.349	5.13	0.9995	5.36	0.9998
B3LYP	9.13	7.87	7.08	6.55	6.17	5.88	5.66	5.49	5.35	-0.40	0.40	0.42	5.58	0.351	5.16	0.9995	5.39	0.9998
PBE0	9.14	7.91	7.12	6.59	6.20	5.92	5.70	5.52	5.38	-0.38	0.38	0.39	5.54	0.344	5.18	0.9996	5.40	0.9999
mPW1PBE	9.13	7.90	7.12	6.58	6.20	5.91	5.69	5.52	5.38	-0.38	0.38	0.39	5.53	0.344	5.18	0.9996	5.38	0.9999
tHCTH	9.15	7.87	7.09	6.56	6.19	5.90	5.68	5.51	5.37	-0.39	0.39	0.40	5.58	0.355	5.19	0.9994	5.44	0.9998
M06	9.09	7.87	7.10	6.57	6.19	5.91	5.70	5.52	5.39	-0.40	0.40	0.41	5.46	0.347	5.19	0.9996	5.40	0.9999
HSE06	9.13	7.89	7.10	6.56	6.18	5.89	5.66	5.48	n/c	-0.40	0.40	0.41	5.57	0.354	5.19	0.9997	5.37	0.9999
HCTH/147	9.18	7.88	7.09	6.56	6.18	5.89	5.67	5.50	5.36	-0.39	0.39	0.41	5.65	0.357	5.19	0.9994	5.43	0.9998
BMK	9.14	7.94	7.16	6.63	6.24	5.95	5.73	5.56	5.42	-0.34	0.34	0.35	5.48	0.338	5.20	0.9997	5.39	0.9999
tHCTHhyb	9.17	7.91	7.12	6.60	6.22	5.93	5.71	5.54	5.40	-0.36	0.36	0.37	5.56	0.351	5.21	0.9995	5.45	0.9998
B3PW91	9.17	7.92	7.13	6.60	6.22	5.93	5.71	5.54	5.40	-0.36	0.36	0.37	5.57	0.349	5.21	0.9995	5.43	0.9999
mPW3PBE	9.19	7.94	7.15	6.62	6.23	5.95	5.73	5.55	5.41	-0.34	0.34	0.36	5.57	0.347	5.22	0.9995	5.44	0.9999
mPW2PLYPD	9.11	7.89	7.11	6.58	6.20	5.92	5.71	5.55	5.42	-0.38	0.38	0.39	5.48	0.352	5.23	0.9997	5.40	0.9999
HCTH/407	9.23	7.93	7.14	6.61	6.23	5.95	5.72	5.55	5.41	-0.34	0.34	0.36	5.64	0.357	5.24	0.9994	5.49	0.9998
B2PLYPD	9.10	7.88	7.10	6.57	6.20	5.92	5.71	5.55	5.42	-0.39	0.39	0.40	5.46	0.354	5.24	0.9997	5.42	0.99991
wB97	9.12	8.03	7.27	6.75	6.37	6.08	5.86	5.69	5.56	-0.25	0.25	0.26	5.25	0.322	5.30	0.9998	5.45	0.99996
wB97X	9.14	8.02	7.25	6.73	6.35	6.07	5.86	5.69	5.56	-0.26	0.26	0.27	5.29	0.333	5.33	0.9998	5.48	0.99997
CAM-B3LYP	9.18	7.99	7.21	6.68	6.30	6.01	5.80	5.63	n/c	-0.29	0.29	0.30	5.44	0.352	5.34	0.9998	5.46	0.99992
wB97XD	9.14	7.96	7.19	6.67	6.30	6.03	5.82	5.66	5.54	-0.30	0.30	0.31	5.35	0.351	5.35	0.9997	5.52	0.99994
M052X	9.23	8.10	7.32	6.79	6.41	6.13	5.91	5.74	5.60	-0.19	0.19	0.20	5.35	0.331	5.37	0.9998	5.53	0.99998

LC-wPBE	9.27	8.17	7.40	6.87	6.48	6.19	5.97	5.80	5.66	-0.12	0.12	0.14	5.32	0.321	5.39	0.9999	5.54	0.99997
M062X	9.28	8.16	7.38	6.85	6.47	6.18	5.96	5.79	5.65	-0.13	0.13	0.15	5.35	0.327	5.40	0.9998	5.56	0.99997
M06HF	9.46	8.46	7.69	7.17	6.78	6.49	6.27	6.10	5.96	0.16	0.16	0.17	5.17	0.306	5.65	0.99993	5.73	0.99996
B3P86	9.74	8.49	7.70	7.16	6.78	6.50	6.28	6.10	5.96	0.21	0.21	0.23	5.58	0.349	5.77	0.9995	5.99	0.9999
AM1	9.13	8.15	7.52	7.08	6.77	6.53	6.35	6.21	6.10	0.01	0.12	0.14	4.47	0.338	5.92	0.9997	6.08	0.9999
PM3	9.31	8.32	7.68	7.24	6.92	6.68	6.49	6.35	6.24	0.17	0.19	0.21	4.53	0.336	6.05	0.9997	6.22	0.9999
PDDG	9.32	8.34	7.70	7.26	6.94	6.71	6.53	6.38	6.28	0.19	0.21	0.23	4.50	0.339	6.10	0.9997	6.25	0.99993
PM6	9.13	8.28	7.72	7.32	7.03	6.81	6.65	6.51	6.41	0.20	0.28	0.30	4.00	0.323	6.22	0.9997	6.34	0.99991
MP2	9.33	8.24	7.49	7.04	6.76	6.59	6.50	6.47	6.49	0.05	0.07	0.09	4.88	0.493	6.37	0.9994	6.26	0.99991

279 ^a the benzene cation has a single imaginary frequency at the B3LYP/6-31G(d) level; thus, calculations were conducted at the x/TZVP//B3LYP/6-311++G(d,p) level where the benzene cation is absent imaginary frequencies.

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Table 4. Estimated well-to-well ionization energies (WWIEs) for the [n]acenes (n=1-9) at the B3LYP/6-31G(d) level of theory. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)=\text{WWIE}$ in eV; $c=\text{WWIE}$ at the polymeric limit). Values are in eV.

basis set	[n]acene									regression statistics (n=1-9)				regression statistics (n=1-6)			
	1	2	3	4	5	6	7	8	9	a	b	c	r	a	b	c	r
6-31G(d)	8.86	7.59	6.80	6.27	5.89	5.60	5.38	5.21	5.07	5.60	0.352	4.89	0.9995	5.12		5.12	0.9998
6-311++G(d,p)	9.13	7.88	7.09	6.56	6.18	5.90	5.68	5.51	n/c ^a	5.55	0.364	5.25	0.9997	5.41		5.41	0.9999
6-311++G(2d,2p)	9.12	7.86	7.08	6.55	6.17	5.88	5.66	5.49	5.35	5.56	0.350	5.16	0.9995	5.39		5.39	0.9998
SVP	9.09	7.83	7.04	6.51	6.13	5.84	5.62	5.45	5.31	5.58	0.351	5.12	0.9995	5.35		5.35	0.9998
TZV	9.16	7.88	n/c	6.55	6.16	5.88	5.66	5.48	5.34	5.63	0.347	5.14	0.9995	5.40		5.40	0.9999
TZVP	9.13	7.87	7.08	6.55	6.17	5.88	5.66	5.49	5.35	5.58	0.351	5.16	0.9995	5.39		5.39	0.9998
cc-pVDZ	9.01	7.75	6.97	6.44	6.06	5.78	5.56	5.38	5.25	5.55	0.351	5.06	0.9995	5.30		5.30	0.9998
cc-pVTZ	9.10	7.84	7.05	6.52	6.13	n/c	5.62	5.45	5.31	5.61	0.350	5.11	0.9996	5.45		5.45	0.99991

^a calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

287 **Table 5.** Estimated relaxation energies (E_{relax}) from the cationic form of the neutral geometry to the
288 optimized cationic geometry for the [n]acenes (n=1-9) at the x/TZVP//B3LYP/6-31G(d) level of theory.
289 Values are in eV. Note that semiempirical method E_{relax} are at the x//B3LYP/6-31G(d) level of theory.
290

	[n]acene								
model chemistry	1	2	3	4	5	6	7	8	9
MP2	-0.23	-0.07	-0.05	-0.05	-0.04	-0.04	-0.04	-0.04	-0.03
HFB	-0.23	-0.12	-0.07	-0.04	-0.02	0.00	0.01	0.02	0.03
M06HF	-0.20	-0.10	-0.07	-0.05	-0.04	-0.03	-0.02	-0.02	-0.02
M062X	-0.18	-0.09	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.03
BMK	-0.17	-0.09	-0.06	-0.05	-0.04	-0.03	-0.03	-0.02	-0.02
wB97	-0.16	-0.10	-0.07	-0.05	-0.04	-0.03	-0.02	-0.02	-0.01
PM6	-0.15	-0.13	-0.08	-0.05	-0.03	-0.02	0.00	0.01	0.02
B97D	-0.15	-0.09	-0.06	-0.05	-0.05	-0.04	-0.03	-0.03	-0.03
B98	-0.14	-0.09	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.03
wB97X	-0.14	-0.09	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.02
tHCTHhyb	-0.14	-0.08	-0.06	-0.05	-0.05	-0.04	-0.04	-0.03	-0.03
TPSSh	-0.14	-0.08	-0.06	-0.06	-0.05	-0.04	-0.04	-0.04	-0.03
VSXC	-0.14	-0.08	-0.07	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
M052X	-0.14	-0.09	-0.07	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
B2PLYPD	-0.14	-0.08	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
wB97XD	-0.14	-0.08	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04	-0.03
B1LYP	-0.13	-0.08	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.03
O3LYP	-0.13	-0.08	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04	-0.03
B3LYP	-0.13	-0.08	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.03
mPW1LYP	-0.13	-0.08	-0.06	-0.05	-0.04	-0.04	-0.04	-0.03	-0.03
X3LYP	-0.13	-0.08	-0.06	-0.05	-0.04	-0.04	-0.04	-0.03	-0.03
mPW2PLYPD	-0.13	-0.08	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
OTPSS	-0.13	-0.08	-0.07	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
OPBE	-0.13	-0.08	-0.07	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04
LC-wPBE	-0.13	-0.09	-0.06	-0.05	-0.04	-0.04	-0.03	-0.03	-0.03
B3PW91	-0.13	-0.08	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.04
mPW3PBE	-0.13	-0.08	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
HCTH/147	-0.12	-0.08	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04	-0.03
PBE0	-0.12	-0.08	-0.06	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04
mPW1PBE	-0.12	-0.08	-0.06	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04
HSE06	-0.12	-0.08	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	n/c ^a
CAM-B3LYP	-0.12	-0.08	-0.06	-0.05	-0.04	-0.04	-0.04	-0.03	n/c
AM1	-0.12	-0.14	-0.11	-0.09	-0.08	-0.07	-0.06	-0.05	-0.04
B3P86	-0.12	-0.07	-0.06	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04
tHCTH	-0.12	-0.07	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.04
PM3	-0.12	-0.13	-0.10	-0.09	-0.08	-0.07	-0.06	-0.06	-0.05
PDDG	-0.12	-0.14	-0.11	-0.10	-0.09	-0.09	-0.08	-0.08	-0.07
M06	-0.12	-0.07	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.04
HCTH/407	-0.11	-0.07	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
M06L	-0.11	-0.07	-0.05	-0.05	-0.05	-0.05	-0.04	-0.04	-0.04
B1B95	-0.11	-0.07	-0.06	-0.05	-0.05	-0.05	-0.05	-0.05	-0.04

BHandHLYP	-0.11	-0.08	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.04
M05	-0.10	-0.08	-0.07	-0.06	-0.05	-0.05	-0.04	-0.04	-0.04
XAlpha	-0.10	-0.06	-0.06	-0.05	-0.05	-0.05	-0.05	-0.05	-0.04
HF	-0.08	-0.11	-0.08	-0.05	-0.04	-0.03	-0.03	-0.02	-0.02
BHandH	-0.08	-0.06	-0.06	-0.06	-0.06	-0.06	-0.06	-0.06	-0.06
HFS	n/c	-0.09	-0.07	-0.05	-0.04	-0.03	-0.02	-0.02	-0.01
BLYP	n/c	-0.09	-0.06	-0.05	-0.04	-0.03	-0.02	-0.02	-0.01

^a calculation failed to converge.

291
292

293 **Table 6.** Experimental, benchmark theoretical [35], and estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) adiabatic ionization energies (AIEs) for the [n]acenes (n=1-9). Error metrics (MSD=mean signed deviation; MAD=mean absolute deviation; and RMSD=root mean squared deviation) are between AIEs obtained at the x/TZVP//B3LYP/6-31G(d) level of theory and the benchmark theoretical [35] values for the n=1-6 [n]acenes. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ (x=n, y(x)=AIE in eV; c=AIE at the polymERIC limit). Values are in eV. Note that semiempirical method WWIEs are at the x//B3LYP/6-31G(d) level of theory.

297

expt.	[n]acene										error metrics			regression statistics (n=1-9)						regression statistics (n=1-6)		
	1 ^a	2	3	4	5	6	7	8	9	MSD	MAD	RMSD	a	b	c	r	c	r				
9.24±0.00 [149]	8.14±0.00 [149]	7.44±0.01 [149]	6.97±0.05 [149]	6.63±0.05 [149]	6.44±0.04 [150]	6.44 [151]	n/a ^b	n/a	n/a	n/a	n/a	n/a	n/a	4.86°	0.403	5.99	0.9999	5.99	0.9999			
benchmark theoretical [35]	9.22	8.14	7.42	6.91	6.56	6.42	n/a	n/a	n/a	n/a	n/a	n/a	n/a	4.91	0.409	5.97	0.9997	5.97	0.9997			
HF	7.78	6.84	6.08	5.52	5.10	4.76	4.50	4.28	4.11	-1.43	1.43	1.44	5.42	0.256	3.58	0.99996	3.67	0.99997				
HFB	7.88	6.70	5.96	5.46	5.10	4.83	4.62	4.46	4.32	-1.46	1.46	1.46	5.24	0.347	4.14	0.9995	4.36	0.9998				
HFS	8.03	6.79	6.02	5.51	5.14	4.87	4.65	4.48	4.34	-1.39	1.39	1.39	5.44	0.353	4.17	0.9994	4.42	0.9998				
XAlpha	8.41	7.15	6.37	5.85	5.47	5.19	4.98	4.80	4.66	-1.04	1.04	1.04	5.53	0.353	4.48	0.9994	4.72	0.9998				
BLYP	8.88	7.62	6.85	6.34	5.96	5.69	5.47	5.30	5.15	-0.55	0.55	0.57	5.49	0.353	4.98	0.9993	5.24	0.9998				
BHandHLYP	8.89	7.77	7.00	6.47	6.08	5.79	5.57	5.39	5.25	-0.45	0.45	0.46	5.35	0.322	4.99	0.9998	5.16	0.99996				
BHandH	8.97	7.82	7.04	6.50	6.11	5.82	5.59	5.41	5.27	-0.40	0.40	0.42	5.44	0.325	5.01	0.9998	5.20	0.99996				
B1LYP	8.90	7.71	6.94	6.42	6.04	5.76	5.54	5.37	5.23	-0.48	0.48	0.50	5.40	0.340	5.02	0.9996	5.23	0.9999				
M06L	9.00	7.76	6.98	6.45	6.06	5.78	5.55	5.38	5.23	-0.44	0.44	0.46	5.54	0.343	5.03	0.9995	5.27	0.9999				
mPW1LYP	8.93	7.73	6.97	6.44	6.06	5.78	5.56	5.39	5.25	-0.46	0.46	0.47	5.42	0.340	5.04	0.9996	5.25	0.9999				
B97D	8.92	7.68	6.92	6.40	6.03	5.75	5.54	5.36	5.22	-0.50	0.50	0.51	5.44	0.349	5.04	0.9994	5.28	0.9998				
VSXC	8.95	7.71	6.94	6.42	6.05	5.77	5.55	5.38	5.23	-0.47	0.47	0.49	5.47	0.349	5.05	0.9994	5.30	0.9998				
TPSSh	8.97	7.77	6.99	6.47	6.10	5.82	5.60	5.42	5.28	-0.43	0.43	0.44	5.43	0.342	5.08	0.9995	5.31	0.99991				
O3LYP	8.99	7.76	6.98	6.46	6.08	5.80	5.58	5.41	5.27	-0.43	0.43	0.45	5.49	0.348	5.08	0.9995	5.30	0.9999				
M05	8.85	7.72	6.98	6.47	6.10	5.83	5.62	5.45	5.32	-0.45	0.45	0.46	5.20	0.336	5.10	0.9997	5.29	0.99993				
OPBE	9.06	7.80	7.02	6.50	6.13	5.85	5.63	5.45	5.31	-0.39	0.39	0.40	5.52	0.352	5.13	0.9994	5.39	0.9998				
X3LYP	9.04	7.83	7.06	6.54	6.16	5.88	5.66	5.49	5.35	-0.36	0.36	0.38	5.44	0.343	5.15	0.9996	5.37	0.9999				
OTPSS	9.08	7.82	7.04	6.51	6.14	5.86	5.64	5.47	5.32	-0.37	0.37	0.39	5.54	0.352	5.15	0.9994	5.39	0.9999				
B1B95	9.07	7.86	7.09	6.56	6.18	5.89	5.67	5.50	5.36	-0.34	0.34	0.36	5.46	0.341	5.15	0.9996	5.36	0.9999				
B98	9.03	7.83	7.06	6.54	6.17	5.89	5.67	5.50	5.36	-0.36	0.36	0.37	5.41	0.343	5.16	0.9996	5.39	0.9999				
B3LYP	9.08	7.87	7.10	6.58	6.20	5.92	5.70	5.53	5.39	-0.32	0.32	0.34	5.44	0.343	5.19	0.9996	5.41	0.9999				
PBE0	9.08	7.91	7.13	6.61	6.23	5.95	5.73	5.56	5.42	-0.29	0.29	0.31	5.39	0.338	5.20	0.9997	5.40	0.99994				
mPW1PBE	9.08	7.90	7.13	6.61	6.23	5.95	5.73	5.56	5.42	-0.30	0.30	0.31	5.39	0.339	5.21	0.9996	5.41	0.99991				
M06	9.03	7.87	7.11	6.60	6.23	5.95	5.73	5.56	5.43	-0.31	0.31	0.33	5.30	0.338	5.21	0.9996	5.42	0.99991				
HSE06	9.07	7.89	7.12	6.59	6.21	5.92	5.70	5.52	n/c	-0.31	0.31	0.33	5.41	0.344	5.21	0.9997	5.36	0.99991				
tHCTH	9.10	7.87	7.11	6.59	6.22	5.94	5.72	5.55	5.41	-0.31	0.31	0.33	5.43	0.347	5.22	0.9994	5.46	0.9998				
HCTH/147	9.12	7.87	7.10	6.58	6.21	5.93	5.71	5.54	5.40	-0.31	0.31	0.33	5.48	0.352	5.22	0.9994	5.47	0.9998				
BMK	9.08	7.94	7.18	6.65	6.27	5.99	5.77	5.60	5.46	-0.26	0.26	0.27	5.33	0.331	5.23	0.9998	5.40	0.99995				
tHCTHhyb	9.11	7.91	7.14	6.62	6.25	5.97	5.75	5.58	5.44	-0.28	0.28	0.30	5.41	0.343	5.24	0.9996	5.47	0.9999				
B3PW91	9.11	7.92	7.15	6.62	6.25	5.97	5.75	5.58	5.44	-0.28	0.28	0.29	5.41	0.341	5.24	0.9996	5.45	0.99992				
mPW3PBE	9.13	7.94	7.16	6.64	6.26	5.98	5.77	5.59	5.45	-0.26	0.26	0.28	5.42	0.342	5.25	0.9996	5.45	0.99992				
mPW2PLYPD	9.05	7.89	7.12	6.61	6.23	5.96	5.75	5.59	5.46	-0.30	0.30	0.31	5.32	0.345	5.26	0.9997	5.43	0.99993				
HCTH/407	9.17	7.93	7.16	6.64	6.26	5.98	5.76	5.59	5.45	-0.26	0.26	0.28	5.48	0.348	5.26	0.9995	5.49	0.9998				
B2PLYPD	9.05	7.88	7.11	6.60	6.23	5.96	5.75	5.59	5.46	-0.31	0.31	0.32	5.32	0.348	5.27	0.9997	5.45	0.99993				
wB97	9.07	8.03	7.29	6.77	6.40	6.12	5.90	5.73	5.60	-0.17	0.17	0.18	5.11	0.315	5.33	0.9999	5.46	0.999991				

CAM-B3LYP	9.13	7.99	7.23	6.71	6.33	6.05	5.83	5.67	n/c ^d	-0.21	0.21	0.22	5.30	0.343	5.35	0.9998	5.48	0.99994
wB97X	9.09	8.02	7.27	6.75	6.38	6.11	5.90	5.73	5.60	-0.17	0.17	0.19	5.15	0.327	5.36	0.9998	5.50	0.999994
wB97XD	9.08	7.96	7.21	6.70	6.33	6.06	5.86	5.70	5.58	-0.22	0.22	0.23	5.19	0.342	5.37	0.9998	5.51	0.99995
M052X	9.17	8.10	7.34	6.82	6.44	6.16	5.95	5.78	5.64	-0.11	0.11	0.13	5.20	0.322	5.39	0.9999	5.52	0.99999
M062X	9.22	8.16	7.40	6.88	6.50	6.22	6.00	5.83	5.69	-0.05	0.06	0.09	5.20	0.318	5.42	0.9999	5.57	0.99999
LC-wPBE	9.21	8.17	7.42	6.89	6.51	6.23	6.01	5.84	5.70	-0.04	0.05	0.08	5.17	0.313	5.42	0.9999	5.54	0.999998
M06HF	9.41	8.46	7.70	7.19	6.81	6.53	6.31	6.14	6.00	0.24	0.24	0.25	5.03	0.300	5.68	0.99991	5.76	0.99992
B3P86	9.68	8.48	7.71	7.19	6.81	6.53	6.31	6.14	6.00	0.29	0.29	0.31	5.42	0.342	5.80	0.9996	6.01	0.9999
AM1	9.08	8.15	7.53	7.11	6.80	6.57	6.39	6.25	6.14	0.09	0.14	0.16	4.33	0.331	5.95	0.9997	6.11	0.99993
PM3	9.26	8.32	7.69	7.26	6.95	6.71	6.53	6.39	6.28	0.25	0.25	0.28	4.39	0.331	6.08	0.9997	6.23	0.99993
PDDG	9.26	8.34	7.72	7.29	6.97	6.74	6.56	6.42	6.32	0.28	0.28	0.30	4.34	0.328	6.11	0.9998	6.24	0.99995
PM6	9.07	8.28	7.73	7.35	7.07	6.85	6.68	6.55	6.45	0.28	0.33	0.36	3.85	0.310	6.23	0.9998	6.37	0.99994
MP2	9.28	8.24	7.51	7.07	6.79	6.63	6.54	6.51	6.53	0.14	0.14	0.15	4.71	0.487	6.41	0.9993	6.29	0.9999

298 ^a the benzene cation has a single imaginary frequency at the B3LYP/6-31G(d) level; thus, calculations were conducted at the x/TZVP//B3LYP/6-311++G(d,p) level where the benzene cation is absent imaginary frequencies. ^b Not
299 available. ^c Regression statistics for the experiment values obtained using the average of multiple experimental datapoints where available. ^d calculation failed to converge, and resulting error metrics and regression statistics omit
300 this datapoint from the corresponding analysis.
301

302 **Table 7.** Benchmark theoretical [36] and estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) vertical electron affinities (VEAs) for the [n]acenes (n=1-10). Error metrics (MSD=mean signed deviation; MAD=mean absolute deviation; and RMSD=root mean squared deviation) are between VEAs obtained at the x/TZVP//B3LYP/6-31G(d) level of theory and the benchmark theoretical [36] values for the n=1-6 [n]acenes. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{bx}+c$ ($x=n$, $y(x)=\text{VEA in eV}$; $c=\text{VEA at the polymeric limit}$). Values are in eV. Note that semiempirical method WWIEs are at the x//B3LYP/6-31G(d) level of theory.

306

	[n]acene										error metrics		regression statistics (n=1-10)					regression statistics (n=1-6)	
	1	2	3	4	5	6	7	8	9	10	MSD	MAD	RMSD	a	b	c	r	c	r
benchmark theoretical [36]	-1.53	-0.48	0.28	0.82	1.21	1.47	1.47	n/a ^a	n/a	n/a	n/a	n/a	n/a	-5.17	0.338	2.16	0.99999	2.16	0.99999
MP2	-2.17	-1.05	-0.23	0.28	0.62	0.83	0.95	1.01	1.02	0.98	-0.58	0.58	0.58	-5.25	0.457	1.12	0.9991	1.30	0.9999
HFB	-2.48	-1.27	n/c ^b	0.10	0.50	0.81	1.04	1.23	1.39	1.51	-0.77	0.77	0.77	-5.68	0.311	1.72	0.9996	1.44	0.99993
HFS	-2.53	-1.29	-0.45	0.13	0.54	0.85	1.10	1.29	1.45	1.58	-0.75	0.75	0.76	-5.85	0.316	1.77	0.9996	1.49	0.99997
XAlpha	-2.22	-0.96	-0.12	0.46	0.88	1.19	1.43	1.63	1.79	1.92	-0.42	0.42	0.44	-5.89	0.318	2.11	0.9996	1.83	0.99995
HF	-2.53	-1.43	-0.57	0.07	0.55	0.92	1.22	1.47	1.66	1.83	-0.80	0.80	0.81	-6.19	0.256	2.28	0.99991	2.08	0.99999
B2PLYPD	-1.86	-0.65	0.19	0.77	1.18	1.49	1.72	1.90	2.05	2.17	-0.11	0.12	0.16	-5.78	0.322	2.36	0.9998	2.16	0.99998
mPW2PLYPD	-1.85	-0.64	0.20	0.78	1.19	1.50	1.74	1.93	2.07	2.19	-0.10	0.11	0.15	-5.79	0.320	2.39	0.9998	2.17	0.99998
wB97XD	-1.70	-0.49	0.34	0.92	1.33	1.64	1.87	2.06	2.20	2.31	0.04	0.11	0.12	-5.77	0.322	2.50	0.9998	2.31	0.99998
B1LYP	-1.79	-0.57	0.27	0.85	1.27	1.58	1.83	2.02	2.17	2.30	-0.03	0.09	0.12	-5.84	0.315	2.50	0.9997	2.26	0.99998
mPW1LYP	-1.77	-0.55	0.29	0.87	1.29	1.61	1.85	2.04	2.20	2.32	0.00	0.10	0.12	-5.84	0.314	2.53	0.9997	2.30	0.99996
BLYP	-1.75	-0.49	n/c	0.91	1.32	1.63	1.87	2.06	2.22	2.35	0.03	0.12	0.14	-5.83	0.315	2.55	0.9996	2.24	0.99992
O3LYP	-1.76	-0.50	0.35	0.93	1.34	1.66	1.90	2.09	2.25	2.38	0.04	0.12	0.14	-5.90	0.320	2.56	0.9996	2.29	0.99994
BHandHLYP	-1.81	-0.63	0.22	0.81	1.25	1.57	1.83	2.03	2.18	2.31	-0.06	0.11	0.14	-5.88	0.303	2.56	0.9998	2.36	0.99999
BHandH	-1.85	-0.65	0.21	0.81	1.25	1.58	1.83	2.04	2.19	2.32	-0.07	0.12	0.16	-5.96	0.304	2.57	0.9998	2.37	0.99999
wB97X	-1.68	-0.50	0.34	0.93	1.35	1.67	1.91	2.10	2.25	2.37	0.06	0.11	0.13	-5.80	0.311	2.59	0.9998	2.42	0.99999
B1B95	-1.77	-0.52	0.33	0.92	1.34	1.66	1.91	2.10	2.26	2.39	0.03	0.13	0.15	-5.93	0.316	2.59	0.9997	2.33	0.99996
BMK	-1.80	-0.56	0.30	0.89	1.33	1.65	1.90	2.10	2.26	2.38	0.01	0.12	0.15	-5.98	0.312	2.60	0.9998	2.37	0.99997
CAM-B3LYP	-1.63	-0.44	0.40	0.98	1.40	1.71	1.95	2.14	2.29	2.41	0.11	0.14	0.15	-5.79	0.314	2.62	0.9998	2.42	0.99999
X3LYP	-1.67	-0.44	0.40	0.98	1.40	1.71	1.95	2.15	2.30	2.43	0.10	0.15	0.16	-5.85	0.316	2.63	0.9997	2.38	0.99997
M06L	-1.73	-0.44	0.41	0.99	1.41	1.72	1.97	2.16	2.32	2.46	0.10	0.16	0.18	-5.96	0.322	2.63	0.9995	2.33	0.99993
B98	-1.71	-0.47	0.38	0.97	1.39	1.71	1.95	2.15	2.30	2.43	0.08	0.14	0.16	-5.91	0.316	2.63	0.9997	2.39	0.99997
TPSSH	-1.71	-0.45	0.40	0.98	1.41	1.72	1.97	2.16	2.32	2.45	0.10	0.16	0.17	-5.93	0.318	2.64	0.9996	2.38	0.99995
B97D	-1.68	-0.41	n/c	1.00	1.41	1.72	1.96	2.16	2.31	2.44	0.11	0.17	0.18	-5.87	0.316	2.64	0.9996	2.33	0.99993
wB97	-1.69	-0.52	0.33	0.92	1.35	1.68	1.93	2.12	2.28	2.40	0.05	0.12	0.13	-5.85	0.304	2.65	0.9999	2.47	0.99998
M05	-1.67	-0.41	0.43	1.01	1.43	1.74	1.98	2.18	2.33	2.46	0.13	0.17	0.18	-5.89	0.320	2.65	0.9996	2.38	0.99995
VSXC	-1.79	-0.47	0.40	1.00	1.43	1.75	2.00	2.20	2.36	2.50	0.09	0.18	0.20	-6.11	0.322	2.68	0.9995	2.39	0.99994
B3LYP	-1.62	-0.39	0.44	1.02	1.44	1.68	2.00	2.19	2.35	2.47	0.13	0.16	0.17	-5.81	0.311	2.68	0.9994	2.28	0.99996
OTPSS	-1.69	-0.38	0.47	1.05	1.47	1.79	2.03	2.23	2.38	2.52	0.16	0.21	0.22	-5.99	0.324	2.69	0.9995	2.39	0.9999
OPBE	-1.70	-0.39	n/c	1.04	1.46	1.78	2.02	2.22	2.38	2.51	0.14	0.21	0.22	-5.99	0.317	2.71	0.9995	2.38	0.9999
M06	-1.59	-0.35	0.48	1.06	1.48	1.79	2.03	2.23	2.38	2.51	0.18	0.20	0.22	-5.84	0.316	2.71	0.9996	2.45	0.99995
PBE0	-1.63	-0.39	0.45	1.04	1.47	1.79	2.03	2.23	2.38	2.51	0.16	0.19	0.21	-5.91	0.314	2.72	0.9997	2.49	0.99996
mPW1PBE	-1.63	-0.39	0.45	1.04	1.47	1.79	2.03	2.23	2.38	2.51	0.16	0.19	0.21	-5.91	0.314	2.72	0.9997	2.49	0.99996
M062X	-1.67	-0.44	0.42	1.02	1.45	1.78	2.03	2.23	2.38	2.51	0.13	0.18	0.20	-5.97	0.311	2.73	0.9998	2.52	0.99998
B3PW91	-1.60	-0.35	0.49	1.08	1.50	1.81	2.06	2.25	2.41	2.54	0.19	0.22	0.24	-5.90	0.317	2.74	0.9996	2.47	0.99997
tHCTHhyb	-1.59	-0.33	0.52	1.10	1.52	1.84	2.08	2.28	2.43	2.56	0.21	0.23	0.25	-5.92	0.319	2.75	0.9996	2.49	0.99994
mPW3PBE	-1.58	-0.34	0.51	1.09	1.51	1.83	2.08	2.27	2.43	2.56	0.21	0.23	0.25	-5.90	0.315	2.76	0.9997	2.50	0.99996
M052X	-1.68	-0.44	0.43	1.03	1.47	1.80	2.05	2.25	2.41	2.53	0.14	0.19	0.21	-6.03	0.312	2.76	0.9998	2.55	0.99997
HSE06	-1.63	-0.38	0.47	1.06	1.49	1.81	2.06	2.26	2.42	2.56	0.17	0.21	0.22	-5.96	0.312	2.77	0.9996	2.50	0.99996
LC-wPBE	-1.55	-0.37	0.47	1.06	1.50	1.82	2.07	2.27	2.42	2.55	0.19	0.20	0.23	-5.86	0.304	2.79	0.9998	2.61	0.99999

HCTH/147	-1.54	-0.26	0.58	1.16	1.57	1.88	2.13	2.32	2.48	2.61	0.27	0.27	0.30	-5.91	0.322	2.79	0.9995	2.48	0.99993
tHCTH	-1.49	-0.22	0.62	1.20	1.61	1.92	2.16	2.36	2.51	2.64	0.31	0.31	0.34	-5.89	0.322	2.82	0.9995	2.53	0.99994
HCTH/407	-1.50	-0.21	n/c	1.21	1.62	1.93	2.17	2.37	2.53	2.66	0.31	0.31	0.35	-5.92	0.317	2.86	0.9995	2.52	0.99992
M06HF	-1.66	-0.46	0.43	1.05	1.50	1.85	2.11	2.31	2.48	2.61	0.16	0.20	0.23	-6.11	0.300	2.88	0.9999	2.72	0.99998
B3P86	-1.03	0.21	1.06	1.64	2.06	2.38	2.63	2.82	2.98	3.11	0.76	0.76	0.77	-5.90	0.315	3.31	0.9997	3.05	0.99996
AM1	-0.11	0.74	1.39	1.86	2.21	2.47	2.68	2.85	2.98	3.09	1.13	1.13	1.14	-4.56	0.277	3.35	0.9999	3.22	0.999991
PM3	-0.07	0.81	1.47	1.93	2.27	2.53	2.74	2.90	3.03	3.13	1.20	1.20	1.20	-4.56	0.288	3.36	0.9999	3.20	0.99998
PDDG	-0.08	0.83	1.49	1.95	2.30	2.57	2.77	2.94	3.07	3.18	1.21	1.21	1.22	-4.63	0.288	3.41	0.9998	3.24	0.99997
PM6	0.01	0.92	1.57	2.03	2.38	2.65	2.86	3.04	3.18	3.29	1.30	1.30	1.31	-4.64	0.280	3.54	0.9997	3.32	0.99996

307 ^a not available. ^b calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

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Table 8. Estimated vertical electron affinities (VEAs) for the [n]acenes (n=1-10) at the B3LYP/y//B3LYP/6-31G(d) level of theory. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)=\text{VEA}$ in eV; $c=\text{VEA}$ at the polymeric limit). Values are in eV.

basis set	1	2	3	4	5	6	7	8	9	10	a	b	c	r	regression statistics (n=1-10)	regression statistics (n=1-6)
6-31G(d)	-2.30	-0.90	0.01	0.62	1.06	1.38	1.64	1.84	2.00	2.13	-6.35	0.334	2.29	0.9995	1.98	0.99993
6-311++G(d,p)	-0.60	-0.31	0.51	1.07	1.49	1.80	2.04	2.23	n/c ^a	2.51	-4.90	0.194	3.27	0.994	6.21	0.992
6-311++G(2d,2p)	-0.59	-0.29	0.51	1.08	1.49	1.80	2.04	2.24	2.39	2.52	-4.86	0.194	3.26	0.995	6.11	0.992
SVP	-1.93	-0.58	0.30	0.90	1.33	1.66	1.91	2.11	2.26	2.39	-6.18	0.328	2.57	0.9996	2.28	0.9999
TZV	-1.75	-0.49	n/c	0.94	1.37	1.68	1.92	2.12	2.27	2.40	-5.92	0.314	2.61	0.9997	2.34	0.99995
TZVP	-1.62	-0.39	0.44	1.02	1.44	1.68	2.00	2.19	2.35	2.47	-5.81	0.311	2.68	0.9994	2.28	0.99996
cc-pVDZ	-1.99	-0.64	0.24	0.85	1.28	1.60	1.85	2.05	2.21	2.35	-6.19	0.327	2.52	0.9995	2.23	0.99994
cc-pVTZ	-1.71	-0.44	0.41	1.00	1.42	n/c	1.98	2.18	2.33	2.46	-5.97	0.322	2.65	0.9997	2.31	0.99998

^a calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

315 **Table 9.** Estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) well-to-well electron affinities (WWEAs) for the [n]acenes (n=1-10). Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ (x=n, y(x)=WWEA in eV; c=WWEA at the polymERIC limit). Values are in eV. Note that semiempirical method WWEAs are at the x//B3LYP/6-31G(d) level of theory.

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	[n]acene										error metrics		regression statistics (n=1-10)				regression statistics (n=1-6)	
	1	2	3	4	5	6	7	8	9	10	MSD	MAD	RMSD	a	b	c	r	r
MP2	-2.12	-0.98	-0.19	0.32	0.64	0.84	0.95	0.99	0.99	0.95	-0.80	0.80	0.81	-5.22	0.478	1.08	0.999	0.99994
HFS	-2.30	-1.11	n/c	0.26	0.66	0.96	1.19	1.37	1.53	n/c	-0.87	0.87	0.89	-5.63	0.322	1.80	0.9998	0.99997
HFB	-2.14	-1.01	n/c ^b	0.28	0.66	0.95	1.17	1.35	1.50	1.62	-0.81	0.81	0.82	-5.35	0.308	1.82	0.9997	0.99995
XAlpha	-2.09	-0.87	n/c	0.52	0.93	1.24	1.47	1.66	1.81	1.94	-0.61	0.61	0.65	-5.75	0.314	2.14	0.9997	0.99995
HF	-2.36	-1.34	-0.53	0.07	0.53	0.89	1.18	1.42	1.62	1.78	-1.01	1.01	1.02	-5.89	0.246	2.26	0.99991	0.99999
B2PLYPD	-1.72	-0.55	0.26	0.82	1.22	1.52	1.74	1.92	2.06	2.17	-0.30	0.30	0.34	-5.59	0.323	2.35	0.9998	0.99998
mPW2PLYPD	-1.72	-0.55	0.26	0.82	1.23	1.53	1.75	1.93	2.08	2.19	-0.29	0.29	0.34	-5.61	0.320	2.38	0.9998	0.99998
wB97XD	-1.56	-0.41	0.39	0.95	1.35	1.65	1.88	2.06	2.19	2.30	-0.16	0.16	0.23	-5.55	0.318	2.50	0.9998	0.99998
BHandH	-1.80	-0.63	0.21	0.80	1.22	1.55	1.80	1.99	2.15	2.28	-0.33	0.33	0.39	-5.82	0.303	2.52	0.9998	0.99998
BHandHLYP	-1.71	-0.58	0.24	0.82	1.24	1.56	1.80	2.00	2.15	2.28	-0.29	0.29	0.34	-5.69	0.299	2.53	0.9998	0.999991
mPW1LYP	-1.62	-0.45	0.36	0.92	1.33	1.63	1.87	2.06	2.21	2.33	-0.19	0.19	0.26	-5.64	0.311	2.54	0.9997	0.99998
B1LYP	-1.64	-0.47	n/c	0.90	1.31	1.61	1.85	2.04	2.19	2.31	-0.22	0.22	0.29	-5.64	0.307	2.54	0.9998	0.99998
wB97X	-1.54	-0.41	0.40	0.96	1.37	1.68	1.91	2.09	2.24	2.35	-0.14	0.16	0.22	-5.58	0.310	2.57	0.9999	0.99998
BMK	-1.62	-0.44	0.38	0.95	1.37	1.68	1.92	2.11	2.26	2.39	-0.17	0.18	0.26	-5.72	0.310	2.60	0.9998	0.99997
BLYP	-1.54	-0.34	n/c	1.01	1.41	1.71	1.94	2.12	2.28	2.40	-0.11	0.15	0.22	-5.61	0.313	2.60	0.9996	0.99993
B1B95	-1.66	-0.46	n/c	0.95	1.36	1.67	1.91	2.10	2.25	2.38	-0.19	0.20	0.29	-5.77	0.310	2.60	0.9998	0.99998
O3LYP	-1.61	-0.40	n/c	0.99	1.40	1.70	1.94	2.13	2.28	2.40	-0.14	0.17	0.26	-5.73	0.313	2.61	0.9997	0.99997
wB97	-1.53	-0.41	0.39	0.96	1.37	1.68	1.92	2.11	2.26	2.38	-0.14	0.16	0.22	-5.58	0.302	2.62	0.9998	0.999992
TPSSH	-1.55	-0.35	0.48	1.05	1.46	1.76	2.00	2.19	2.35	n/c	-0.08	0.15	0.21	-5.73	0.324	2.62	0.9998	0.99998
CAM-B3LYP	-1.50	-0.36	0.44	1.01	1.41	1.72	1.95	2.14	2.28	2.40	-0.10	0.14	0.20	-5.58	0.310	2.62	0.9998	0.99998
X3LYP	-1.52	-0.35	0.47	1.03	1.44	1.74	1.98	2.17	2.32	2.44	-0.08	0.14	0.20	-5.65	0.312	2.65	0.9997	0.99998
M05	-1.52	-0.32	0.49	1.06	1.47	1.77	2.01	2.19	2.34	2.46	-0.06	0.14	0.20	-5.69	0.318	2.65	0.9997	0.99997
M06L	-1.60	-0.37	0.46	1.03	1.45	1.75	1.99	2.18	2.34	2.47	-0.10	0.16	0.24	-5.80	0.317	2.66	0.9996	0.99996
B98	-1.54	-0.35	n/c	1.03	1.44	1.75	1.98	2.17	2.32	2.45	-0.09	0.16	0.23	-5.69	0.309	2.67	0.9997	0.99996
B97D	-1.49	-0.28	n/c	1.08	1.48	1.78	2.01	2.20	2.35	2.48	-0.04	0.16	0.21	-5.65	0.313	2.68	0.9996	0.99994
B3LYP	-1.47	-0.29	0.52	1.08	1.49	1.79	2.03	2.21	2.37	2.49	-0.04	0.14	0.19	-5.64	0.313	2.69	0.9997	0.99997
VSXC	-1.60	-0.35	0.49	1.07	1.48	1.80	2.04	2.23	2.39	2.52	-0.07	0.17	0.24	-5.87	0.318	2.71	0.9996	0.99994
M062X	-1.54	-0.36	0.47	1.05	1.47	1.78	2.03	2.22	2.37	2.49	-0.07	0.16	0.22	-5.76	0.310	2.71	0.9998	0.99999
mPW1PBE	-1.50	-0.31	0.51	1.08	1.50	1.81	2.05	2.24	2.39	2.51	-0.04	0.15	0.20	-5.73	0.312	2.72	0.9998	0.99997
M06	-1.46	-0.28	n/c	1.09	1.50	1.81	2.04	2.23	2.38	2.50	-0.03	0.17	0.20	-5.65	0.309	2.72	0.9998	0.99996
PBE0	-1.50	-0.31	n/c	1.09	1.50	1.81	2.05	2.24	2.39	2.52	-0.04	0.18	0.22	-5.73	0.308	2.74	0.9998	0.99998
OPBE	-1.54	-0.28	n/c	1.12	1.53	1.84	2.08	2.26	2.42	2.55	-0.02	0.20	0.24	-5.83	0.317	2.74	0.9996	0.99992
M052X	-1.55	-0.36	n/c	1.06	1.48	1.80	2.04	2.24	2.39	2.51	-0.07	0.19	0.25	-5.81	0.306	2.75	0.9998	0.99998
LC-wPBE	-1.42	-0.30	0.51	1.08	1.50	1.81	2.05	2.24	2.39	2.51	-0.03	0.14	0.17	-5.62	0.302	2.75	0.9999	0.999994
OTPSS	-1.52	-0.27	n/c	1.14	1.54	1.85	2.09	2.28	2.43	2.56	-0.01	0.20	0.24	-5.82	0.317	2.76	0.9996	0.99995
mPW3PBE	-1.45	-0.25	0.57	1.14	1.55	1.86	2.10	2.29	2.44	2.56	0.02	0.16	0.20	-5.73	0.315	2.76	0.9997	0.99996
B3PW91	-1.46	-0.27	n/c	1.13	1.54	1.84	2.08	n/c	2.42	2.55	0.00	0.18	0.22	-5.73	0.309	2.77	0.9997	0.99999
HSE06	-1.49	-0.30	0.53	1.10	1.52	1.83	2.08	2.27	2.43	2.56	-0.02	0.16	0.21	-5.76	0.308	2.78	0.9997	0.99997
tHCTHhyb	-1.42	-0.22	n/c	1.17	1.58	1.88	2.12	2.31	2.46	2.58	0.04	0.19	0.22	-5.71	0.312	2.79	0.9997	0.99998
M06HF	-1.53	-0.38	0.46	1.06	1.49	1.82	2.07	2.27	2.42	2.55	-0.07	0.17	0.22	-5.83	0.299	2.81	0.9999	0.999993
HCTH/147	-1.39	-0.16	0.67	1.23	1.63	1.94	2.17	2.36	2.51	2.64	0.10	0.21	0.23	-5.75	0.322	2.81	0.9996	0.99994
tHCTH	-1.34	-0.12	0.70	1.26	1.67	1.97	2.20	2.39	2.54	2.67	0.14	0.23	0.24	-5.72	0.320	2.85	0.9996	0.99995

HCTH/407	-1.36	-0.12	0.71	1.27	1.68	1.98	2.22	2.40	2.56	2.69	0.14	0.23	0.25	-5.77	0.322	2.86	0.9995	2.59	0.99995
PM3	-0.09	0.85	1.49	1.94	2.27	2.52	2.71	2.87	2.99	3.09	0.94	0.94	0.94	-4.52	0.306	3.27	0.9997	3.07	0.99995
AM1	-0.14	0.80	1.44	1.90	2.24	2.49	2.69	2.85	2.98	3.08	0.90	0.90	0.90	-4.57	0.300	3.28	0.9997	3.07	0.99996
PDDG	-0.10	0.86	1.50	1.95	2.28	2.54	2.73	2.89	3.01	3.11	0.95	0.95	0.95	-4.56	0.307	3.29	0.9997	3.08	0.9999
B3P86	-0.90	0.29	1.12	1.69	2.10	2.41	2.64	2.83	2.99	3.11	0.56	0.56	0.60	-5.73	0.315	3.31	0.9997	3.09	0.99998
PM6	0.02	0.99	1.62	2.07	2.40	2.66	2.86	3.03	3.16	3.28	1.07	1.07	1.07	-4.58	0.297	3.47	0.9994	3.19	0.9998

^a not available. ^b calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

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Table 10. Estimated vertical electron affinities (VEAs) for the [n]acenes (n=1-10) at the B3LYP/y//B3LYP/6-31G(d) level of theory. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ ($x=n$, $y(x)=\text{VEA}$ in eV; $c=\text{VEA}$ at the polymeric limit). Values are in eV.

basis set	[n]acene										regression statistics (n=1-10)			regression statistics (n=1-6)		
	1	2	3	4	5	6	7	8	9	10	a	b	c	r	c	r
6-31G(d)	-2.10	-0.77	0.11	0.70	1.12	1.44	1.68	1.88	2.03	2.16	-6.10	0.331	2.32	0.9995	2.04	0.99993
6-311++G(d,p)	-1.29	-0.20	0.59	1.14	1.54	1.84	2.07	2.26	n/c ^a	2.53	-5.44	0.303	2.75	0.9998	2.57	0.999991
6-311++G(2d,2p)	-1.29	-0.20	0.58	1.13	1.53	1.83	2.07	2.26	2.41	n/c	-5.43	0.305	2.73	0.9999	2.56	0.999991
SVP	-1.72	-0.43	0.42	1.00	1.42	1.73	1.97	2.16	2.31	2.44	-5.95	0.327	2.61	0.9996	2.34	0.99993
TZV	-1.56	-0.37	n/c	1.02	1.42	1.73	1.96	2.15	n/c	2.43	-5.69	0.311	2.63	0.9997	2.40	0.99997
TZVP	-1.47	-0.29	0.52	1.08	1.49	1.79	2.03	2.21	2.37	2.49	-5.64	0.313	2.69	0.9997	2.45	0.99997
cc-pVDZ	-1.78	-0.49	0.36	0.94	1.36	1.67	1.91	2.10	2.26	2.39	-5.95	0.325	2.56	0.9995	2.28	0.99993
cc-pVTZ	-1.56	-0.35	0.48	1.05	1.46	n/c	2.00	2.19	2.35	2.47	-5.77	0.319	2.66	0.9997	2.35	0.999993

^a calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the corresponding analysis.

326 **Table 11.** Estimated relaxation energies (E_{relax}) from the anionic form of the neutral geometry to the
 optimized anionic geometry for the [n]acenes (n=1-10) at the x/TZVP//B3LYP/6-31G(d) level of
 theory. Values are in eV. Note that semiempirical method E_{relax} are at the x//B3LYP/6-31G(d) level of
 theory.

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model chemistry	[n]acene									
	1	2	3	4	5	6	7	8	9	10
AM1	-0.03	0.06	0.05	0.04	0.03	0.02	0.01	0.00	-0.01	-0.01
PM3	-0.03	0.04	0.02	0.01	0.00	-0.01	-0.02	-0.03	-0.04	-0.05
PDDG	-0.02	0.03	0.01	0.00	-0.02	-0.03	-0.04	-0.05	-0.06	-0.07
HFS	n/c ^a	0.18	n/c	0.13	0.12	0.10	0.09	0.08	0.08	n/c
BLYP	n/c	0.15	n/c	0.10	0.09	0.08	0.07	0.06	0.06	0.05
PM6	0.01	0.07	0.05	0.03	0.02	0.01	0.00	0.00	-0.01	-0.02
MP2	0.05	0.07	0.05	0.03	0.02	0.00	-0.01	-0.02	-0.03	-0.04
BHandH	0.05	0.01	0.00	-0.02	-0.03	-0.03	-0.04	-0.04	-0.05	-0.05
BHandHLYP	0.10	0.05	0.02	0.01	-0.01	-0.01	-0.02	-0.03	-0.03	-0.03
B1B95	0.11	0.06	n/c	0.03	0.02	0.01	0.00	0.00	-0.01	-0.01
M06	0.13	0.07	n/c	0.04	0.02	0.02	0.01	0.00	0.00	0.00
XAlpha	0.13	0.08	n/c	0.06	0.05	0.05	0.04	0.03	0.03	0.03
LC-wPBE	0.13	0.07	0.04	0.01	0.00	-0.01	-0.02	-0.03	-0.03	-0.03
M06L	0.13	0.08	0.06	0.05	0.04	0.03	0.03	0.02	0.02	0.01
B3P86	0.13	0.08	0.06	0.04	0.03	0.02	0.02	0.01	0.01	0.00
CAM-B3LYP	0.13	0.08	0.05	0.03	0.02	0.01	0.00	-0.01	n/c	-0.01
M052X	0.13	0.08	n/c	0.03	0.01	0.00	-0.01	-0.02	-0.02	-0.02
mPW1PBE	0.13	0.08	0.06	0.04	0.03	0.02	0.02	0.01	0.01	0.00
HSE06	0.13	0.08	0.06	0.04	0.03	0.02	0.02	0.01	n/c	0.00
PBE0	0.13	0.08	n/c	0.04	0.03	0.02	0.02	0.01	0.01	0.00
mPW2PLYPD	0.13	0.09	0.06	0.04	0.03	0.02	0.01	0.01	0.00	0.00
M062X	0.13	0.08	0.05	0.03	0.02	0.01	0.00	-0.01	-0.01	-0.02
HCTH/407	0.14	0.09	n/c	0.06	0.06	0.05	0.04	0.04	0.03	0.03
M06HF	0.14	0.08	0.04	0.01	-0.01	-0.03	-0.04	-0.05	-0.05	-0.05
mPW3PBE	0.14	0.09	0.06	0.05	0.04	0.03	0.02	0.02	0.01	0.01
wB97XD	0.14	0.08	0.05	0.04	0.02	0.01	0.00	0.00	-0.01	-0.01
B3PW91	0.14	0.09	n/c	0.05	0.04	0.03	0.02	n/c	0.01	0.01
wB97X	0.14	0.09	0.06	0.03	0.02	0.01	0.00	-0.01	-0.01	-0.02
B2PLYPD	0.14	0.10	0.07	0.05	0.04	0.03	0.02	0.02	0.01	0.01
tHCTH	0.15	0.10	0.08	0.07	0.06	0.05	0.04	0.04	0.03	0.03
mPW1LYP	0.15	0.09	0.07	0.05	0.04	0.03	0.02	0.02	0.01	0.01
X3LYP	0.15	0.10	0.07	0.05	0.04	0.03	0.02	0.02	0.01	0.01
O3LYP	0.15	0.10	n/c	0.06	0.05	0.04	0.04	0.03	0.03	0.02
M05	0.15	0.09	0.06	0.05	0.04	0.03	0.02	0.02	0.01	0.01
B1LYP	0.15	0.10	n/c	0.05	0.04	0.03	0.02	0.02	0.01	0.01
B3LYP	0.15	0.10	0.07	0.06	0.04	0.11	0.03	0.02	0.02	0.01
HCTH/147	0.16	0.11	0.09	0.07	0.06	0.05	0.05	0.04	0.04	0.03
OPBE	0.16	0.11	n/c	0.08	0.07	0.06	0.06	0.05	0.04	0.04
OTPSS	0.16	0.11	n/c	0.08	0.07	0.06	0.06	0.05	0.04	0.04
TPSSh	0.16	0.11	0.08	0.06	0.05	0.04	0.03	0.03	0.02	n/c

wB97	0.16	0.11	0.07	0.04	0.02	0.01	0.00	-0.01	-0.01	-0.02
tHCTHhyb	0.17	0.11	n/c	0.07	0.06	0.05	0.04	0.03	0.03	0.02
B98	0.17	0.11	n/c	0.06	0.05	0.04	0.03	0.03	0.02	0.02
HF	0.18	0.09	0.04	0.01	-0.01	-0.03	-0.04	-0.04	-0.05	-0.05
BMK	0.18	0.12	0.08	0.06	0.04	0.03	0.02	0.01	0.01	0.00
VSXC	0.19	0.12	0.09	0.07	0.06	0.05	0.04	0.03	0.03	0.02
B97D	0.20	0.13	n/c	0.08	0.07	0.06	0.05	0.04	0.04	0.03
HFB	0.34	0.26	n/c	0.18	0.16	0.14	0.13	0.12	0.11	0.11

^a calculation failed to converge.

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333 **Table 12.** Experimental, benchmark theoretical [36], and estimated (at the x/TZVP//B3LYP/6-31G(d) level of theory) adiabatic electron affinities (AEAs) for the [n]acenes (n=1-10). Error metrics (MSD=mean signed deviation; MAD=mean absolute deviation; and RMSD=root mean squared deviation) are between AEAs obtained at the x/TZVP//B3LYP/6-31G(d) level of theory and the benchmark theoretical [36] values for the n=1-6 [n]acenes. Regression analysis parameters employ a single exponential decay function having a y-axis offset of the general form $y=ae^{-bx}+c$ (x=n, y(x)=AEA in eV; c=AEA at the polymERIC limit). Values are in eV. Note that semiempirical method AEAs are at the x//B3LYP/6-31G(d) level of theory.

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expt.	1 ^a	[n]acene										error metrics			regression statistics (n=1-10)				regression statistics (n=1-6)		
		2	3	4	5	6	7	8	9	10	MSD	MAD	RMSD	a	b	c	r	n/a			
benchmark theoretical [36]	-1.12±0.03	0.1480±0.0060 [153]	0.41998 [161] <0.481±0.039 [154, 155] 0.5560±0.0080 [153]	0.880±0.040 [162] 1.0580±0.0050 [167] 1.067±0.043 [168]	1.392±0.043 [168]	n/a ^a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a ^b	n/a	n/a	n/a	n/a		
	<0.134±0.043 [154, 155]	0.140±0.050 [156] -0.1908 [157] -0.200±0.050 [158] -0.18 [159] 0.2 [160]	0.570±0.020 [162] 0.660±0.060 [163] [153] 0.60±0.10 [164] 0.5300±0.0050 [165] 0.530±0.020 [166]																		
		-0.19	0.53	1.03	1.39	1.63	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	-4.72	0.311	2.38	0.9998	2.38	0.9998	
	-1.89	-0.82	-0.06	0.43	0.74	0.93	1.05	1.09	1.09	1.05	-0.66	0.66	0.67	0.67	-4.96	0.468	1.18	0.999	1.35	0.9999	
	-2.06	-0.95	n/c	0.37	0.76	1.05	1.29	1.47	1.63	n/c	-0.72	0.72	0.74	0.74	-5.40	0.308	1.93	0.9998	1.72	0.99999	
	-1.91	-0.86	n/c	0.39	0.77	1.05	1.27	1.45	1.60	1.72	-0.67	0.67	0.68	0.68	-5.15	0.296	1.95	0.9997	1.71	0.99998	
	-1.85	-0.72	n/c	0.64	1.03	1.33	1.57	1.76	1.91	2.04	-0.47	0.47	0.50	0.50	-5.53	0.301	2.27	0.9997	2.02	0.99999	
	-2.12	-1.19	-0.40	0.19	0.64	0.99	1.28	1.52	1.72	1.88	-0.87	0.87	0.88	0.88	-5.72	0.235	2.41	0.99992	2.28	0.99992	
	-1.48	-0.40	0.39	0.93	1.32	1.61	1.84	2.02	2.16	2.27	-0.16	0.16	0.20	0.20	-5.37	0.309	2.48	0.9998	2.30	0.99999	
	-1.48	-0.40	0.39	0.93	1.33	1.62	1.85	2.03	2.18	2.29	-0.15	0.15	0.20	0.20	-5.39	0.306	2.51	0.9998	2.33	0.99999	
	-1.33	-0.25	0.52	1.07	1.46	1.75	1.98	2.16	2.29	2.40	-0.02	0.09	0.12	0.12	-5.35	0.309	2.62	0.9999	2.46	0.999997	
	-1.47	-0.42	0.37	0.93	1.35	1.66	1.90	2.10	2.25	2.38	-0.15	0.16	0.21	0.21	-5.49	0.288	2.66	0.9999	2.51	0.999993	
	-1.56	-0.48	0.33	0.91	1.33	1.65	1.90	2.09	2.25	2.38	-0.19	0.20	0.25	0.25	-5.62	0.290	2.66	0.9999	2.50	0.999992	
	-1.38	-0.30	0.49	1.03	1.43	1.73	1.97	2.16	2.31	2.43	-0.05	0.10	0.14	0.14	-5.43	0.298	2.67	0.9998	2.45	0.99998	
	-1.40	-0.32	n/c	1.01	1.41	1.71	1.95	2.14	2.29	2.41	-0.07	0.12	0.16	0.16	-5.43	0.293	2.67	0.9999	2.46	0.999996	
	-1.30	-0.25	0.52	1.07	1.47	1.77	2.01	2.19	2.34	2.45	0.00	0.10	0.12	0.12	-5.36	0.296	2.70	0.9999	2.54	0.999997	
	-1.42	-0.30	n/c ^b	1.06	1.47	1.77	2.01	2.20	2.35	2.48	-0.04	0.14	0.18	0.18	-5.56	0.298	2.72	0.9998	2.51	0.999995	
	-1.39	-0.29	0.51	1.07	1.47	1.78	2.02	2.21	2.36	2.49	-0.03	0.12	0.15	0.15	-5.52	0.299	2.73	0.9998	2.52	0.99999	
	-1.30	-0.19	n/c	1.12	1.51	1.81	2.04	2.22	2.38	2.50	0.03	0.13	0.15	0.15	-5.40	0.299	2.73	0.9997	2.49	0.99997	
	-1.37	-0.24	n/c	1.10	1.50	1.80	2.04	2.23	2.38	2.50	0.00	0.14	0.17	0.17	-5.51	0.300	2.74	0.9998	2.49	0.99998	
-1.26	-0.21	0.57	1.12	1.52	1.82	2.05	2.24	n/c	2.50	0.04	0.11	0.13	0.13	-5.37	0.298	2.74	0.9999	2.59	0.999992		
-1.29	-0.26	0.52	1.07	1.48	1.78	2.02	2.21	2.36	2.48	0.00	0.10	0.12	0.12	-5.38	0.290	2.75	0.9999	2.60	0.99999		
-1.31	-0.19	0.61	1.16	1.56	1.86	2.10	2.29	2.45	n/c	0.06	0.14	0.17	0.17	-5.51	0.311	2.75	0.9998	2.55	0.99998		
-1.28	-0.19	0.60	1.14	1.54	1.84	2.08	2.27	2.42	2.54	0.05	0.13	0.15	0.15	-5.44	0.300	2.78	0.9998	2.55	0.99998		
-1.36	-0.21	0.59	1.15	1.55	1.85	2.09	2.28	2.44	2.57	0.04	0.15	0.17	0.17	-5.58	0.306	2.78	0.9996	2.52	0.99998		
-1.29	-0.17	0.62	1.17	1.57	1.87	2.11	2.29	2.44	2.56	0.08	0.15	0.17	0.17	-5.49	0.306	2.78	0.9998	2.56	0.99998		
-1.30	-0.20	n/c	1.14	1.54	1.85	2.08	2.27	2.42	2.55	0.05	0.14	0.17	0.17	-5.48	0.296	2.80	0.9998	2.60	0.99998		
-1.25	-0.13	n/c	1.19	1.58	1.88	2.11	2.30	2.45	2.58	0.10	0.17	0.18	0.18	-5.44	0.299	2.81	0.9997	2.55	0.99997		
-1.23	-0.14	0.65	1.19	1.59	1.89	2.13	2.31	2.47	2.59	0.10	0.16	0.17	0.17	-5.44	0.300	2.82	0.9998	2.60	0.99998		
-1.36	-0.20	0.62	1.18	1.59	1.90	2.14	2.33	2.49	2.62	0.07	0.17	0.19	0.19	-5.66	0.306	2.84	0.9997	2.59	0.99997		

M062X	-1.30	-0.20	0.60	1.17	1.57	1.88	2.13	2.32	2.47	2.59	0.07	0.15	0.17	-5.55	0.298	2.84	0.9998	2.64	0.999991
mPW1PBE	-1.27	-0.16	0.64	1.20	1.60	1.91	2.15	2.34	2.49	2.61	0.10	0.17	0.18	-5.53	0.302	2.85	0.9998	2.64	0.99999
M06	-1.23	-0.13	n/c	1.21	1.60	1.91	2.14	2.33	2.48	2.60	0.11	0.18	0.19	-5.46	0.298	2.85	0.9998	2.63	0.99998
PBE0	-1.27	-0.16	n/c	1.20	1.61	1.91	2.15	2.34	2.49	2.62	0.10	0.18	0.20	-5.54	0.297	2.87	0.9998	2.66	0.999998
OPBE	-1.30	-0.13	n/c	1.24	1.64	1.94	2.18	2.36	2.52	2.65	0.12	0.21	0.23	-5.61	0.306	2.87	0.9997	2.60	0.99998
OTPSS	-1.29	-0.12	n/c	1.25	1.65	1.95	2.19	2.38	2.53	2.66	0.13	0.22	0.23	-5.62	0.306	2.88	0.9997	2.61	0.99998
M052X	-1.32	-0.21	n/c	1.17	1.59	1.90	2.14	2.34	2.49	2.61	0.07	0.17	0.20	-5.62	0.295	2.88	0.9999	2.70	0.999999
mPW3PBE	-1.21	-0.10	0.70	1.25	1.66	1.96	2.20	2.39	2.54	2.66	0.16	0.20	0.22	-5.52	0.302	2.89	0.9998	2.68	0.99999
LC-wPBE	-1.19	-0.15	0.63	1.19	1.60	1.91	2.15	2.34	2.49	2.61	0.11	0.15	0.17	-5.43	0.289	2.89	0.99992	2.75	0.999994
HSE06	-1.26	-0.15	0.65	1.22	1.62	1.93	2.18	2.37	n/c	2.66	0.12	0.18	0.20	-5.57	0.298	2.90	0.9997	2.67	0.999991
B3PW91	-1.22	-0.11	n/c	1.24	1.64	1.94	2.18	n/c	2.52	2.65	0.14	0.20	0.22	-5.51	0.297	2.90	0.9998	2.66	0.999995
tHCTHhyb	-1.18	-0.06	n/c	1.28	1.68	1.98	2.22	2.41	2.56	2.68	0.18	0.23	0.24	-5.50	0.299	2.92	0.9998	2.68	0.99999
M06HF	-1.29	-0.22	0.59	1.17	1.60	1.92	2.17	2.37	2.52	2.65	0.07	0.16	0.18	-5.63	0.288	2.94	0.99992	2.81	0.999992
HCTH/147	-1.15	0.00	0.80	1.34	1.74	2.04	2.27	2.46	2.61	2.74	0.24	0.27	0.29	-5.53	0.310	2.94	0.9996	2.69	0.99996
tHCTH	-1.11	0.03	0.83	1.38	1.77	2.07	2.30	2.49	2.64	2.77	0.27	0.29	0.32	-5.52	0.310	2.97	0.9996	2.72	0.99998
HCTH/407	-1.12	0.03	0.83	1.38	1.78	2.08	2.32	2.50	2.66	2.79	0.28	0.30	0.32	-5.55	0.308	2.99	0.9996	2.74	0.99997
PM3	0.14	1.01	1.61	2.05	2.37	2.62	2.81	2.97	3.09	3.19	1.08	1.08	1.08	-4.33	0.290	3.40	0.9998	3.22	0.99995
AM1	0.09	0.96	1.57	2.01	2.34	2.59	2.79	2.95	3.08	3.18	1.04	1.04	1.04	-4.38	0.286	3.40	0.9998	3.21	0.99996
PDDG	0.14	1.02	1.63	2.06	2.39	2.64	2.83	2.99	3.11	3.21	1.09	1.09	1.10	-4.35	0.292	3.42	0.9998	3.23	0.99993
B3P86	-0.67	0.45	1.24	1.80	2.20	2.51	2.74	2.93	3.09	3.21	0.70	0.70	0.72	-5.52	0.302	3.44	0.9998	3.23	0.99998
PM6	0.25	1.15	1.75	2.18	2.51	2.76	2.96	3.13	3.26	3.38	1.21	1.21	1.21	-4.39	0.283	3.60	0.9995	3.33	0.9999

338 ^a not available. ^b excessive scatter in the experimental AEA dataset precludes reliable regression analysis. ^c calculation failed to converge, and resulting error metrics and regression statistics omit this datapoint from the

339 corresponding analysis.

340

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Electronic supplementary material

Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short-through long-chain [n]acenes

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B3LYP/6-31G(d) optimized geometries of neutral [n]acenes

benzene

C,-2.1024350367,2.7684261838,0.
C,-3.2924054082,2.0370655744,0.
C,-0.8739208597,2.1035389105,0.
C,-3.2540363572,0.640695652,0.
C,-0.8355687627,0.7073184931,0.
C,-2.0256614591,-0.0241308599,0.
H,0.0521743901,2.6728213411,0.
H,0.1204183816,0.1897932184,0.
H,-2.1322366388,3.8550982588,0.
H,-4.2484678658,2.5544456156,0.
H,-4.1802209909,0.0715527558,0.
H,-1.9956893926,-1.1107951435,0.

naphthalene

C,-2.118444498,2.8046440598,0.
C,-3.3350004959,2.0782362577,0.
C,-0.9130799056,2.1397370861,0.
C,-3.3214231547,0.7017114086,0.
C,-0.8635627452,0.7195342525,0.
C,-2.0946548086,-0.0155528505,0.
H,0.0222439927,2.6949382531,0.
C,0.3632054109,0.0022694752,0.
H,-2.1415996453,3.8911134667,0.
H,-4.2804757979,2.61398684,0.
H,-4.2538571832,0.1416706881,0.
C,-2.0451380094,-1.4357562499,0.
C,0.3767829621,-1.3742551286,0.
C,-0.8397735662,-2.1006628323,0.
H,1.2956396265,0.5623102048,0.
H,1.3222578928,-1.9100060884,0.
H,-0.8166178288,-3.1871322971,0.
H,-2.9804622461,-1.9909565458,0.

anthracene

C,-2.1095172445,2.8570582802,0.
C,-3.3503654272,2.1538123923,0.
C,-0.923447811,2.1716002049,0.
C,-3.3716663706,0.7840825822,0.
C,-0.8997651337,0.7418352051,0.
C,-2.1572029122,0.0291874076,0.
H,0.0241068891,2.7054160654,0.
C,0.2959389143,0.0127317045,0.
H,-2.1120632797,3.9437088024,0.
H,-4.2813228596,2.7142895895,0.

H,-4.3164700801,0.245411981,0.
 C,-2.1460087031,-1.3712325117,0.
 C,0.3071337172,-1.3876878351,0.
 C,-0.9503040037,-2.1003358148,0.
 H,1.2428489703,0.5493892071,0.
 C,1.5215979915,-2.1425819399,0.
 C,-0.9266200346,-3.5301005073,0.
 H,-3.0929184699,-1.9078899403,0.
 C,1.5002982309,-3.5123118016,0.
 C,0.2594500135,-4.2155575869,0.
 H,2.4664012954,-1.6039113795,0.
 H,2.4312553238,-4.0727889657,0.
 H,-1.8741749174,-4.0639167659,0.
 H,0.2619959017,-5.3022083734,0.

tetracene

C,0.0073635402,0.0001051461,-0.00692426
 C,1.4381786905,0.0008042616,-0.0044840198
 C,2.1315286296,1.1788541899,0.0014621079
 C,1.4475080983,2.439061893,0.0052814931
 C,-0.004358779,2.4383605246,0.0028181871
 C,-0.687135969,1.1774883881,-0.0033806289
 C,2.1273321664,3.6545474242,0.0113634795
 C,1.4465900206,4.8895800395,0.0151652544
 C,-0.0058309297,4.888879381,0.0126616339
 C,-0.6853677281,3.6531912365,0.0065490623
 C,2.1261229876,6.1252523329,0.0214027455
 C,1.4451158731,7.3401009682,0.0250883126
 C,-0.006747761,7.3393983322,0.0225513185
 C,-0.6865730637,6.1238976504,0.0165065466
 C,2.1278848101,8.6009664328,0.0313911983
 C,1.433397871,9.7783634581,0.0349841507
 C,0.0025900868,9.7776666172,0.032502474
 C,-0.690755122,8.5996050152,0.0265181037
 H,-0.5238967256,-0.9477831507,-0.0116055668
 H,1.9703679612,-0.9465720565,-0.0073531891
 H,3.2190464795,1.1819219425,0.0033593608
 H,-1.7746583172,1.1795007104,-0.005224357
 H,3.2155550452,3.6552456396,0.0132636542
 H,-1.7735903111,3.6528446848,0.00469389
 H,3.214346267,6.1256097794,0.02328875
 H,-1.7747948032,6.1232122841,0.014637125
 H,3.2154084589,8.5989539433,0.0333232918
 H,1.9646539206,10.7262517544,0.0398327793
 H,-0.5296076193,10.7250370986,0.0354658962
 H,-1.7782737778,8.5965540787,0.0246612059

pentacene

C,0.0087471113,0.0000720191,-0.0154149664
C,1.4419064271,0.0016772875,-0.0111454518
C,2.1344914571,1.1784685053,0.0003642767
C,1.4502410988,2.4406998149,0.0083298224
C,-0.0051191363,2.4390829079,0.0039544408
C,-0.6864971958,1.1753263176,-0.0081059471
C,2.1290426494,3.6524911607,0.0200104939
C,1.4483788437,4.8928400954,0.027859108
C,-0.0088051485,4.8912237726,0.0234667109
C,-0.686658353,3.6493665951,0.0115425275
C,2.1269929178,6.1200174774,0.0396539247
C,1.4456085229,7.3456926318,0.0473428465
C,-0.0115751974,7.3440809869,0.0429182194
C,-0.6901891203,6.1169013832,0.0311319788
C,2.1234672313,8.5875430083,0.0592478337
C,1.4419298838,9.7978309332,0.0667591521
C,-0.0134287046,9.796221341,0.062323645
C,-0.6922346271,8.5844341813,0.0506689801
C,2.1233231874,11.0615733797,0.0788125578
C,1.4280832731,12.2368314574,0.0860117813
C,-0.0050768669,12.2352480173,0.0816321547
C,-0.697668214,11.058460363,0.0702108193
H,-0.5210313611,-0.9485911565,-0.0245640635
H,1.9738388731,-0.9458070619,-0.017130445
H,3.2219932925,1.182065812,0.00361377
H,-1.7740061255,1.1765097067,-0.0113865567
H,3.21723734,3.6537638506,0.0232445207
H,-1.7748536703,3.6482268553,0.0082240209
H,3.2150471533,6.1212179001,0.0428800731
H,-1.7782431613,6.1156987493,0.0277724305
H,3.2116625406,8.5886756698,0.0625073887
H,-1.7804291593,8.5831681724,0.0473113671
H,3.2108314628,11.0603834595,0.0821124207
H,1.9578654219,13.1854928406,0.0951608209
H,-0.537001393,13.1827361917,0.0875136018
H,-1.7851712535,11.0548753737,0.0668657426

hexacene

C,0.0098292826,0.0007885093,-0.0261574231
C,1.4442132264,0.0030739825,-0.037543105
C,2.1364301593,1.179144404,-0.0210665881
C,1.4521629912,2.4421954173,0.007693015
C,-0.0051054837,2.4398889248,0.0190763058
C,-0.6857474949,1.1746761908,0.0010008882
C,2.1304514576,3.652014671,0.0247151074
C,1.4499242664,4.8948694667,0.053065796

C,-0.0098917313,4.8925660538,0.0644928588
 C,-0.6868550587,3.6475638188,0.046769688
 C,2.128015726,6.1178397866,0.0702176537
 C,1.446999517,7.3488966203,0.0982674903
 C,-0.0139920272,7.3465950523,0.1097668719
 C,-0.6914787228,6.1133954456,0.0923508352
 C,2.1244929313,8.5820886995,0.1154875111
 C,1.4429075873,9.8029262627,0.1432974142
 C,-0.0169075621,9.8006312983,0.1548124953
 C,-0.6950003681,8.5776561036,0.1377139834
 C,2.119877781,11.0479227397,0.1606721626
 C,1.4381356744,12.2556135492,0.1881188876
 C,-0.0191280872,12.2533280647,0.1996508314
 C,-0.6974199517,11.0435019408,0.1829178702
 C,2.1187946323,13.5208181811,0.2057920623
 C,1.4232250463,14.6947194046,0.2327282137
 C,-0.011153513,14.6924692045,0.2440601089
 C,-0.7033826031,13.5163964446,0.2281075877
 H,-0.5191972599,-0.9482291196,-0.0396175571
 H,1.9759630392,-0.9442688373,-0.0592279542
 H,3.2238977987,1.1831493099,-0.0295421826
 H,-1.7732234108,1.1752526487,0.0094465403
 H,3.218612016,3.6537601793,0.0160563422
 H,-1.7750181448,3.645879111,0.055192312
 H,3.2160054695,6.1194915478,0.0615116132
 H,-1.7794713016,6.1116215604,0.1007453129
 H,3.2124820893,8.5838681546,0.1067861484
 H,-1.7829930646,8.5760182059,0.1461526435
 H,3.2080374303,11.0496058093,0.1519931808
 H,-1.7855828433,11.0417715559,0.191413049
 H,3.2062669608,13.5202319315,0.1971351101
 H,1.952260798,15.6437371692,0.2458403702
 H,-0.542888252,15.6398254496,0.2655650941
 H,-1.7908490003,13.5124050866,0.2366414544

heptacene

C,0.0111932331,0.0021987414,-0.0519823282
 C,1.4461830611,0.0044339974,-0.0450050621
 C,2.1382174607,1.17999544,-0.0167512201
 C,1.4537553159,2.4436704969,0.0067508306
 C,-0.00447991,2.441398333,-0.000321257
 C,-0.684741843,1.1755976752,-0.0304382146
 C,2.1318758648,3.6522089039,0.0356566367
 C,1.4511881126,4.8965687518,0.0587526124
 C,-0.0100602666,4.8942923928,0.0516808289
 C,-0.686611492,3.6478182821,0.0219965645
 C,2.1290228848,6.1170736068,0.0879262899

C,1.4480740611,7.3511719782,0.1108348403
 C,-0.0150965087,7.3488928362,0.1037588473
 C,-0.6919444392,6.1126797284,0.0742816105
 C,2.1252771814,8.579834547,0.1401998514
 C,1.4439981726,9.8063905143,0.1629676704
 C,-0.0191717957,9.8041115568,0.1559010532
 C,-0.6963754102,8.5754400417,0.1265641866
 C,2.1208463405,11.042594269,0.1925105742
 C,1.4389615548,12.2609888699,0.2151314122
 C,-0.0222839243,12.2587129193,0.2080790828
 C,-0.7001202678,11.0382008142,0.1788899856
 C,2.1155148706,13.5074538084,0.2449049697
 C,1.433382834,14.713878415,0.2673024453
 C,-0.0248478462,14.7116070578,0.260268382
 C,-0.7029714098,13.5030643839,0.2313052183
 C,2.1136470826,15.9796720115,0.2975224529
 C,1.4177120006,17.1530724979,0.3191668151
 C,-0.0172740425,17.150837579,0.3122473789
 C,-0.7093104354,15.9752757678,0.2839077147
 H,-0.5175710321,-0.9468005376,-0.074633153
 H,1.9780962615,-0.9429122346,-0.0625166769
 H,3.2256822367,1.1836104734,-0.0114189982
 H,-1.7722133213,1.1758268221,-0.0356422791
 H,3.2200239143,3.6536940532,0.0409469107
 H,-1.7747592513,3.6459141618,0.0167413425
 H,3.2170242159,6.1184730868,0.0932197259
 H,-1.7799453261,6.1106909625,0.0690457612
 H,3.2132544965,8.5815299052,0.1454941649
 H,-1.7843531313,8.5737467154,0.1213440055
 H,3.2088466544,11.0445863808,0.1978050425
 H,-1.7881218845,11.0368041867,0.1736775771
 H,3.2036621755,13.5093611352,0.2501884159
 H,-1.7911196208,13.5015830685,0.2260876337
 H,3.2011182704,15.9794451579,0.3027345623
 H,1.9464798416,18.1020673602,0.3419082179
 H,-0.5491896317,18.0981807058,0.3298743976
 H,-1.7967753074,15.9716623791,0.2786331767

octacene

C,-0.0072860705,-0.0169583489,-0.0625153006
 C,1.4280199934,-0.0194948945,-0.0546566053
 C,2.123910337,1.1535245851,-0.0238997038
 C,1.4438449788,2.4197715255,0.0014204932
 C,-0.0151001754,2.4223499281,-0.0065619174
 C,-0.699319105,1.1585147921,-0.0393537967
 C,2.1258127561,3.625466586,0.0328270622
 C,1.4495943146,4.8727985919,0.0576956393

C,-0.0127825332,4.8753873634,0.0497088411
 C,-0.6931015003,3.6304533351,0.0174141733
 C,2.1312045616,6.0898880933,0.0893029055
 C,1.4548800178,7.3278100891,0.1139187729
 C,-0.0099802486,7.3304064351,0.1059409077
 C,-0.690384906,6.09488643,0.0739117163
 C,2.1358457348,8.5519105984,0.1456179334
 C,1.459303203,9.7838189057,0.1700522946
 C,-0.0062975796,9.786421971,0.1620969376
 C,-0.6869105131,8.556919411,0.1302690999
 C,2.1399138253,11.0133142035,0.2018093478
 C,1.4629987891,12.2398295109,0.2260841033
 C,-0.0018612278,12.2424413531,0.218159297
 C,-0.6828424461,11.0183381353,0.1865132479
 C,2.1434162644,13.4753375533,0.257927171
 C,1.4658396866,14.694847156,0.2820174568
 C,0.003464723,14.6974647501,0.2741285265
 C,-0.6781742273,13.4803788458,0.2426864927
 C,2.1461837404,15.9397691975,0.3140455261
 C,1.4682125851,17.1478903507,0.3378632016
 C,0.0092676206,17.1505054802,0.3300068551
 C,-0.6727304493,15.9448162375,0.2988554279
 H,-0.5391317696,-0.9641656388,-0.0871942049
 H,1.9567544953,-0.9685765536,-0.0735284299
 H,3.2114057344,1.1536112314,-0.017902728
 H,-1.7868070876,1.1624515907,-0.0452636706
 H,3.2140217755,3.6231841452,0.0387751043
 H,-1.781310199,3.6320329885,0.0114591012
 H,3.219266668,6.0874000303,0.0952414451
 H,-1.7784475377,6.0962672598,0.0679780754
 H,3.2238764833,8.54978884,0.1515431165
 H,-1.7749398501,8.5586662041,0.1243603151
 H,3.2279455722,11.0115649779,0.2077095302
 H,-1.7708705872,11.020460474,0.180620392
 H,3.2314815608,13.4739534681,0.2638021833
 H,-1.7662344601,13.4828725006,0.2368071202
 H,3.2343934419,15.9381808654,0.3198952064
 C,2.15246339,18.4117151353,0.3703216296
 C,-0.6707670326,18.4167736557,0.3551254521
 H,-1.760938786,15.9471099156,0.2929796153
 C,0.0251530867,19.5897829702,0.3855994096
 C,1.4604588468,19.5872086881,0.3933229731
 H,3.2399534781,18.4077624788,0.3761176431
 H,1.9923340083,20.5344081595,0.4177601103
 H,-1.7582621382,18.4167051563,0.3492152406
 H,-0.5035512429,20.5388832855,0.4043292631

nonacene

C,0.0713604665,-0.0607770196,-0.0703840184
C,1.5068745201,-0.0462267034,-0.0615709206
C,2.1887483317,1.1347539602,-0.0292838725
C,1.4935420552,2.393010133,-0.0032805588
C,0.0345342856,2.3782217675,-0.0122359311
C,-0.6346548564,1.1061358494,-0.0466168813
C,2.1612146506,3.6062466,0.0296987212
C,1.4700294006,4.8460000751,0.0553100457
C,0.0076004488,4.8311766062,0.0463374439
C,-0.6579482786,3.5776710297,0.0123975262
C,2.1373150073,6.0702055328,0.0885729953
C,1.4460940204,7.300961823,0.1139939808
C,-0.0189576024,7.2861094855,0.1050106189
C,-0.6847240184,6.0415983786,0.0712628666
C,2.112691272,8.5316122218,0.1474353356
C,1.4213908865,9.7570316393,0.1727651643
C,-0.0447834499,9.7421631923,0.163780618
C,-0.7107323786,8.5029841682,0.1301275418
C,2.0875902521,10.9921081294,0.206345225
C,1.3961134464,12.2134121861,0.2316163745
C,-0.0700608242,12.1985367892,0.2226364118
C,-0.7362606222,10.9634637482,0.1890449838
C,2.0620507038,13.452599698,0.2653314834
C,1.3702656647,14.6694690054,0.2905366479
C,-0.0947856622,14.6545965267,0.2815663257
C,-0.7613722907,13.4239442214,0.2480411797
C,2.036010519,15.9139911789,0.3244164918
C,1.3436667589,17.1244001335,0.3495005078
C,-0.1187618532,17.1095464753,0.3405475082
C,-0.7860275387,15.8853348722,0.3071387278
H,-0.4488942576,-1.0143769506,-0.0962748991
H,2.0466287157,-0.9890834735,-0.0809515773
H,3.2761274793,1.1477186718,-0.0225523946
H,-1.7220740233,1.0970548899,-0.0532380129
H,3.2492937281,3.6170890571,0.0363916585
H,-1.7460236548,3.5664502356,0.0057341844
H,3.225252731,6.0808642765,0.0952627906
H,-1.7726544444,6.0301904915,0.0646048331
H,3.2005905699,8.5424735972,0.1541298257
H,-1.7986287007,8.4917732943,0.1234829402
H,3.1754780271,11.003145538,0.2130397346
H,-1.8241491109,10.9524248355,0.1824080911
H,3.1499463676,13.4638127199,0.2720238306
H,-1.8492722175,13.4130781351,0.2414074474
H,3.123940466,15.9254065524,0.3311063702
C,2.0091865215,18.3779166308,0.3836251376

C,-0.8099755256,18.3492794581,0.3663668575
 H,-1.87396564,15.8746667827,0.3005055645
 C,-0.1423291588,19.562524716,0.3995412787
 C,1.3166782816,19.577347736,0.4084727607
 H,3.0972617242,18.3891515802,0.3903050311
 C,1.9858343511,20.8494434237,0.4430923491
 H,-1.8980546104,18.3384214757,0.3597242689
 C,-0.8375681744,20.8207586292,0.4258087722
 C,1.2797882583,22.0163354837,0.4670852312
 C,-0.1557254664,22.0017498064,0.4582977408
 H,3.0732536298,20.8585435693,0.4497078163
 H,1.8000151502,22.9699465895,0.4931420575
 H,-1.9249470017,20.8077741223,0.4191115804
 H,-0.6955073299,22.9445864215,0.4778661879

decacene

C,0.1915347495,0.0327675993,-0.0782905439
 C,1.6266710473,0.0720417521,-0.0650050162
 C,2.2880023566,1.2644546501,-0.0289800124
 C,1.5711602738,2.5106532195,-0.0033780698
 C,0.1124531562,2.4707334951,-0.0168813126
 C,-0.5345691719,1.1872114452,-0.0551090935
 C,2.2177259478,3.7349735886,0.0333318482
 C,1.5052192911,4.9628901022,0.0584969792
 C,0.0430315908,4.922873526,0.0449620874
 C,-0.6006688085,3.6578425891,0.0072425189
 C,2.1512350227,6.1979717494,0.0954684747
 C,1.4388445728,7.4171567086,0.1204066527
 C,-0.0260757615,7.3770626862,0.1068470949
 C,-0.6701383587,6.1207553488,0.069352803
 C,2.0840850774,8.6583347997,0.1575173318
 C,1.3717367581,9.872620787,0.182320825
 C,-0.0945278178,9.8324862535,0.1687497264
 C,-0.7388134776,8.5810705004,0.1313890774
 C,2.016535067,11.1176349548,0.2195129631
 C,1.3041416821,12.3285606838,0.2442190931
 C,-0.1625338087,12.2884102994,0.2306454001
 C,-0.8070428898,11.0403433513,0.1933805307
 C,1.9486456049,13.5766330246,0.2814729
 C,1.2361270096,14.7844900759,0.3060875338
 C,-0.2301373212,14.7443455385,0.2925192522
 C,-0.8749321292,13.4993306702,0.2553431873
 C,1.8803993464,16.0359166618,0.3434109515
 C,1.1676498081,17.2399194805,0.3679138228
 C,-0.2972701576,17.1998058463,0.3543599462
 C,-0.9424985953,15.9586214894,0.3172909773
 H,-0.3121358581,-0.9296111774,-0.1071082682

H,2.182663704,-0.8613383873,-0.0840123113
 H,3.3749672907,1.2960769609,-0.0188711284
 H,-1.6216375837,1.1593379882,-0.0651259943
 H,3.3054214591,3.7645084881,0.0433899265
 H,-1.6883511957,3.6278423924,-0.0028364944
 H,3.2387816588,6.2273583522,0.1055198296
 H,-1.757663582,6.0906108503,0.0592710679
 H,3.171586062,8.6879103504,0.1675705964
 H,-1.826303184,8.5511118387,0.1213116107
 H,3.1040176458,11.1473430443,0.2295673364
 H,-1.8945212002,11.0105126221,0.1833065185
 H,3.0361248174,13.6064667735,0.2915286311
 H,-1.9624137302,13.469620311,0.24527295
 H,2.9678897857,16.06588391,0.3534689994
 C,1.8116918581,18.4962414727,0.4053468426
 C,-1.0096806092,18.418977702,0.3792449483
 H,-2.0299985753,15.9290380358,0.3072254858
 C,-0.3636843848,19.654070074,0.4161541637
 C,1.0985027693,19.6941143104,0.4296806717
 H,2.8992174956,18.5264006776,0.4154099526
 C,1.7421768223,20.9591620244,0.4673233957
 H,-2.0972262691,18.3895771242,0.369186632
 C,-1.076216741,20.8819717456,0.4412528443
 C,1.0290303744,22.1462591391,0.4913763945
 C,-0.4296759966,22.1063062447,0.4778839911
 H,2.829859222,20.9891828271,0.4773844671
 H,-2.1639113506,20.8524169521,0.4311924315
 C,-1.1465468349,23.3524893785,0.5034022109
 C,1.6760232397,23.4297993514,0.5295074278
 C,-0.4852426076,24.5449195168,0.5393466322
 C,0.9498928821,24.5842279835,0.5526191465
 H,2.7630911042,23.4576972919,0.5395111755
 H,1.4535404439,25.546620959,0.5813703854
 H,-2.2335111947,23.3208428672,0.4932997312
 H,-1.041257802,25.4782871277,0.5582998706

B3LYP/6-311++G(d,p) optimized geometries of neutral [n]acenes

benzene

C,-2.1023616046,2.7660722355,0.
C,-3.2902839551,2.0359162058,0.
C,-0.8760364082,2.102274208,0.
C,-3.2519500354,0.6419968065,0.
C,-0.8377061855,0.7084245618,0.
C,-2.0256876039,-0.0217693242,0.
H,0.0477531659,2.6700865366,0.
H,0.1158948631,0.1922359318,0.
H,-2.1321305413,3.8500042066,0.
H,-4.2439279887,2.5520235436,0.
H,-4.1757887428,0.0742629249,0.
H,-1.9958249635,-1.105697837,0.

B3LYP/6-31G(d) optimized geometries of cationic [n]acenes

naphthalene

C,-2.1386052488,2.8144518028,0.
C,-3.3340714284,2.100637122,0.
C,-0.9085628831,2.1323663006,0.
C,-3.3170769565,0.6942388705,0.
C,-0.8642238159,0.7191393622,0.
C,-2.0939939504,-0.0151582624,0.
H,0.0208252355,2.6952915671,0.
C,0.3588591902,0.0097422293,0.
H,-2.1506782547,3.8996060947,0.
H,-4.283645513,2.6260080886,0.
H,-4.2534956202,0.143088059,0.
C,-2.0496548831,-1.4283852008,0.
C,0.3758536621,-1.3966560222,0.
C,-0.8196125174,-2.110470703,0.
H,1.295277854,0.5608930408,0.
H,1.3254277467,-1.9220269889,0.
H,-0.8075395115,-3.1956249949,0.
H,-2.9790430017,-1.9913104673,0.

anthracene

C,-2.122200271,2.8586625532,0.
C,-3.3452267278,2.1655171045,0.
C,-0.9175812073,2.1627517692,0.
C,-3.3670891362,0.7745027456,0.
C,-0.9060979187,0.7482188634,0.
C,-2.1594250682,0.0379006149,0.
H,0.0252149552,2.7023299548,0.
C,0.2977755202,0.0137725933,0.
H,-2.1186700913,3.9440167165,0.
H,-4.2781934723,2.72011531,0.
H,-4.3143912555,0.2428751419,0.
C,-2.1478438286,-1.3722725761,0.
C,0.3093567508,-1.3964006073,0.
C,-0.9439704025,-2.1067188489,0.
H,1.2437982422,0.5499272588,0.
C,1.5170208122,-2.1330027541,0.
C,-0.9324871311,-3.5212517522,0.
H,-3.0938665514,-1.908427242,0.
C,1.4951583832,-3.5240171113,0.
C,0.2721319235,-4.2171625547,0.
H,2.4643229368,-1.6013751521,0.
H,2.4281251319,-4.0786153152,0.
H,-1.8752832924,-4.0608299323,0.
H,0.2686017472,-5.3025167153,0.

tetracene

C,0.015657587,-0.000559999,-0.0069574158
C,1.4298850349,0.0001216821,-0.0045165431
C,2.1321004206,1.1908186653,0.0014991471
C,1.4440499372,2.4315988381,0.0053226147
C,-0.0008856001,2.4309022339,0.0028276967
C,-0.6877222238,1.1894592594,-0.0033671252
C,2.1294018214,3.6607237937,0.0114662087
C,1.4458157068,4.8895798306,0.0152456467
C,-0.0050557115,4.888880343,0.0127417497
C,-0.6874394834,3.6593657627,0.0066028106
C,2.1281995479,6.1190942363,0.0213820497
C,1.441645517,7.3475578972,0.0251582164
C,-0.003289885,7.3468613331,0.0226657868
C,-0.6886418468,6.1177361708,0.0165228525
C,2.1284823261,8.5890004696,0.0313541801
C,1.4251022078,9.7790199065,0.0349440726
C,0.0108750871,9.7783382167,0.0325032899
C,-0.6913405549,8.5876410593,0.0264873832
H,-0.5185340878,-0.9454820402,-0.0116926196
H,1.9650007066,-0.9442848103,-0.0074056353
H,3.2183501951,1.1887079961,0.003363535
H,-1.7739693868,1.1863012561,-0.0052523546
H,3.2166907388,3.659485556,0.0133345915
H,-1.77472668,3.6570791325,0.0047189576
H,3.2154867247,6.1213812115,0.0232665547
H,-1.7759307728,6.1189747217,0.0146537633
H,3.2147294596,8.5921588644,0.0332386012
H,1.95929453,10.7239416038,0.0396772569
H,-0.5242410073,10.7227444781,0.0353919894
H,-1.7775903085,8.5897520201,0.0246227369

pentacene

C,0.0154198931,0.0045805648,-0.0153369313
C,1.4352142487,0.0061507572,-0.011038989
C,2.1351140193,1.1919100261,0.0004844584
C,1.4464827594,2.4368311529,0.0082909439
C,-0.001342464,2.4352297423,0.0039091923
C,-0.6871583447,1.1887884903,-0.0080570488
C,2.1306813945,3.6623266341,0.0200850643
C,1.4473008408,4.8902863909,0.0277708137
C,-0.0077060891,4.8886770016,0.0233677278
C,-0.6883094345,3.6592085508,0.0115538915
C,2.1294305051,6.1200190571,0.0395915995
C,1.4445229352,7.3482395615,0.047276907
C,-0.0104839981,7.3466300978,0.0428743918

C,-0.6926136665,6.1168974572,0.0310521174
 C,2.1251261904,8.5777080896,0.0590920322
 C,1.4381592043,9.8016868607,0.0667388685
 C,-0.0096660165,9.8000853487,0.0623587145
 C,-0.6938646008,8.5745897726,0.0505631958
 C,2.1239748502,11.0481283185,0.0787067184
 C,1.4213965695,12.2323362057,0.085990079
 C,0.0016022633,12.2307656852,0.0816945053
 C,-0.6982974281,11.0450063617,0.0701676943
 H,-0.5161922021,-0.9418760726,-0.0244531087
 H,1.968964177,-0.9391274678,-0.0169307925
 H,3.2214107371,1.191781917,0.0037628524
 H,-1.7734520243,1.1862572767,-0.0113534888
 H,3.2179262824,3.6615935303,0.0233602349
 H,-1.7755499374,3.6560702345,0.0082485023
 H,3.2167529636,6.1212218651,0.0428831728
 H,-1.7799361278,6.1156947128,0.027763365
 H,3.2123666896,8.5808465808,0.0623983667
 H,-1.781109486,8.5753228126,0.047290082
 H,3.2102685383,11.0506596171,0.0820038673
 H,1.9530086505,13.1787928227,0.0951088399
 H,-0.5321477693,13.1760438481,0.0875905056
 H,-1.784594121,11.0451343009,0.0668916396

hexacene

C,0.0151648842,0.0090002993,-0.0257871242
 C,1.4388357333,0.011240623,-0.0370140461
 C,2.1371066448,1.1935990075,-0.0207566358
 C,1.4484832711,2.4419621611,0.0076610878
 C,-0.0014275459,2.4396805711,0.0190665773
 C,-0.6864813529,1.1891555845,0.0014662612
 C,2.1316510659,3.663864073,0.0247484232
 C,1.448165775,4.8928092969,0.0527579684
 C,-0.0081129123,4.8905179667,0.0642088344
 C,-0.6880837713,3.6594272306,0.046928997
 C,2.1302244894,6.1224149421,0.0699900643
 C,1.4460874042,7.3489013855,0.0979365218
 C,-0.0130526776,7.3466056757,0.1094113442
 C,-0.6936822483,6.1179718893,0.0921946371
 C,2.1267165202,8.5775351618,0.1151443102
 C,1.4411472943,9.8049898234,0.1431126236
 C,-0.0151313103,9.8026985761,0.1545634973
 C,-0.6971900704,8.5730920198,0.1373516309
 C,2.1211175555,11.0360810636,0.1603615442
 C,1.4344609614,12.2558289695,0.1881817782
 C,-0.0154496284,12.2535474741,0.1995833355
 C,-0.6986173108,11.0316443184,0.182532702

C,2.1195136745,13.5063548771,0.2057354382
 C,1.4178671895,14.6865116357,0.2329430886
 C,-0.0058037757,14.6842716533,0.2441337061
 C,-0.7040737549,13.5019118521,0.2279332578
 H,-0.5141032584,-0.9388019913,-0.03906357
 H,1.970809353,-0.9348916127,-0.0586302
 H,3.2234137812,1.1956883841,-0.0292985529
 H,-1.7727895184,1.1878257233,0.0100101844
 H,3.2188109327,3.6650246839,0.0161776755
 H,-1.7752421073,3.657166165,0.0554653014
 H,3.2174733996,6.1238662742,0.0614229336
 H,-1.780930528,6.1160015951,0.1007299656
 H,3.2139647019,8.5795059728,0.1065914293
 H,-1.7844390521,8.5716414451,0.1458965615
 H,3.2082758222,11.038342763,0.1518148171
 H,-1.7857771949,11.0304847128,0.1910814847
 H,3.2058218438,13.5076850099,0.197183695
 H,1.9471349555,15.6343146962,0.2461658209
 H,-0.5377783168,15.630404692,0.2657003939
 H,-1.7903809184,13.4998233399,0.2364622364

heptacene

C,0.0155455817,0.0134019207,-0.0518202676
 C,1.4417903788,0.0156232653,-0.0449263187
 C,2.1390680771,1.1959162712,-0.0164993841
 C,1.4505267384,2.4469447368,0.0067764491
 C,-0.0012634244,2.444683632,-0.0002415861
 C,-0.6856474245,1.1915168735,-0.0301547814
 C,2.132901232,3.6660975854,0.0359558976
 C,1.4495154432,4.8965623334,0.0588196397
 C,-0.0083855105,4.8942917215,0.0517712679
 C,-0.6876823077,3.6617046317,0.0223205851
 C,2.1309162128,6.1252094472,0.0881955002
 C,1.4473435795,7.3508028925,0.1109523502
 C,-0.0143623615,7.348526358,0.1038857845
 C,-0.6938621957,6.1208099896,0.0745388857
 C,2.1274404004,8.5798380799,0.1403285556
 C,1.4432663947,9.8067485971,0.1631092558
 C,-0.01843951,9.8044720723,0.1560424735
 C,-0.6985363678,8.5754367668,0.1266663242
 C,2.1227662201,11.0344647948,0.1924531053
 C,1.4372895772,12.260983225,0.2152176506
 C,-0.0206112995,12.2587126389,0.2081691585
 C,-0.7020121183,11.030065376,0.1787962731
 C,2.1165864004,13.493570143,0.2446626249
 C,1.4301675552,14.7105913867,0.2672195273
 C,-0.0216224927,14.708330331,0.2602005277

C,-0.7039970544,13.4891772704,0.2310259674
 C,2.1145516241,15.9637581019,0.2971242909
 C,1.413358663,17.1418733288,0.318783134
 C,-0.0128859827,17.1396520587,0.3118875938
 C,-0.7101637623,15.9593588036,0.2834675393
 H,-0.5136178587,-0.9343909453,-0.07450098
 H,1.9740980367,-0.9305164048,-0.0624753715
 H,3.2255072737,1.1976463708,-0.0112476086
 H,-1.7720867389,1.189862745,-0.035407692
 H,3.2201578559,3.6664608034,0.041182687
 H,-1.7749345108,3.658681111,0.0170351517
 H,3.218226107,6.1260675902,0.0934327098
 H,-1.7811693109,6.118281235,0.0692631367
 H,3.2148011727,8.5815317103,0.145584049
 H,-1.7858971371,8.5737433816,0.121407862
 H,3.2100733154,11.0369937994,0.1977261494
 H,-1.7893219842,11.0292075284,0.1735558659
 H,3.2038385807,13.4965938957,0.2499459634
 H,-1.7912536458,13.4888143446,0.2257962251
 H,3.2009909285,15.965412389,0.3023753969
 H,1.942522332,18.0896662479,0.3414563065
 H,-0.5451937468,18.0857918093,0.3294288264
 H,-1.796602938,15.9576289636,0.2782133291

octacene

C,-0.0037386715,-0.0032433839,-0.0617580835
 C,1.4244285966,-0.0057830143,-0.0540068883
 C,2.1249402367,1.1706473127,-0.023312144
 C,1.4409427702,2.426197201,0.0016176846
 C,-0.0122064504,2.4287813065,-0.0062692131
 C,-0.7003539907,1.1756713909,-0.0386461788
 C,2.1268290688,3.6407651625,0.0331040666
 C,1.447761938,4.875375273,0.0575847365
 C,-0.0109222788,4.8779692654,0.0496675379
 C,-0.6940703201,3.6457815105,0.0177935587
 C,2.132995057,6.1005088851,0.0893108315
 C,1.4538122169,7.3285673621,0.1136428213
 C,-0.0088557098,7.331168573,0.1057035746
 C,-0.6920978871,6.1055328751,0.0739768774
 C,2.1379203411,8.5557118711,0.1454107864
 C,1.4584509475,9.7838254605,0.1697445921
 C,-0.0053704328,9.7864288361,0.1617985477
 C,-0.688899485,8.5607391603,0.1300665115
 C,2.1419799698,11.0095149783,0.2014785917
 C,1.4619363075,12.239085545,0.2258443385
 C,-0.0007316266,12.2416869055,0.2179040163
 C,-0.6848398603,11.0145424462,0.1861332926

C,2.1451785134,13.4647209047,0.2575777546
 C,1.4640031241,14.6922845187,0.2818927197
 C,0.0053188732,14.6948788279,0.2739735905
 C,-0.6799143982,13.4697454166,0.2422408673
 C,2.1471513537,15.9244717538,0.3137767583
 C,1.4652878312,17.1414719819,0.3378476226
 C,0.0121386369,17.1440565544,0.3299582859
 C,-0.6737480272,15.9294890016,0.2984619408
 H,-0.5355433807,-0.9495921487,-0.0862757627
 H,1.9530991231,-0.9540175861,-0.0727689567
 H,3.2114513628,1.1691147179,-0.0174057063
 H,-1.7868638487,1.1780029356,-0.0445336078
 H,3.2141130008,3.6377739191,0.0389817698
 H,-1.7813578747,3.6466571222,0.0118687424
 H,3.2202971541,6.0977953105,0.0951949771
 H,-1.779402746,6.1066862809,0.0680577338
 H,3.2252859105,8.5535673684,0.1513088224
 H,-1.7762659711,8.5624621229,0.1241598694
 H,3.2293462367,11.0077919292,0.2073868473
 H,-1.772205651,11.0166871168,0.1802361219
 H,3.2324831793,13.4635671339,0.2634991964
 H,-1.7672166884,13.472459361,0.2363568243
 H,3.2344387782,15.9235956104,0.3197049391
 C,2.1534357338,18.3945812561,0.3702384913
 C,-0.6718584356,18.3996064764,0.35489949
 H,-1.7610320805,15.9324807293,0.2925842354
 C,0.028653633,19.5760363039,0.3856051256
 C,1.4568208724,19.5734961243,0.3933589489
 H,3.2399455186,18.3922491368,0.3761288052
 H,1.9886258572,20.5198444639,0.4178864726
 H,-1.758369613,18.4011396111,0.3489920981
 H,-0.500016715,20.5242708218,0.4043751246

nonacene

C,11.0204486581,-0.71613061,0.0022636051
 C,11.0200935477,0.7134244749,0.0040201994
 C,9.842882535,1.4110832017,0.0048113355
 C,8.586623061,0.7251258658,0.0038974685
 C,8.5869905023,-0.7291200757,0.0021111593
 C,9.8435959656,-1.414408471,0.0013399148
 C,7.3720619249,1.4081873786,0.0046654045
 C,6.1367549952,0.7270630399,0.0037541964
 C,6.1371248157,-0.7323930583,0.0019627555
 C,7.3727714666,-1.4128339113,0.0012013018
 C,4.9110775534,1.4095269503,0.0045132966
 C,3.6833213048,0.7284171992,0.0035941669
 C,3.6836777565,-0.7350570731,0.001799803

C,4.911765213,-1.4154991796,0.0010477302
 C,2.4544360047,1.4098723128,0.0043393828
 C,1.2278934506,0.7286375313,0.0034101516
 C,1.2282190817,-0.7364755219,0.001615409
 C,2.4550810245,-1.4170991544,0.0008751596
 C,-0.0002905141,1.4096032069,0.0041461512
 C,-1.228189013,0.7281235989,0.003162235
 C,-1.2279012822,-0.7369894456,0.0013689777
 C,0.0003016172,-1.4179438119,0.0006846162
 C,-2.4550168335,1.4088449525,0.0038434649
 C,-3.6836166607,0.7268757629,0.0028542023
 C,-3.6833602774,-0.7365985609,0.0010644272
 C,-2.4544780101,-1.418126582,0.0003847568
 C,-4.911657939,1.4074717994,0.0035276157
 C,-6.1370495349,0.724495059,0.0025312864
 C,-6.1368082682,-0.7349610986,0.0007471735
 C,-4.9111627727,-1.4175544141,0.0000734803
 H,11.9682492566,-1.2460373518,0.0016648725
 H,11.9676272478,1.2438052451,0.0047247213
 H,9.8420832442,2.4976952646,0.0061462485
 H,9.8433883936,-2.5010205566,0.0000046063
 H,7.3728788695,2.4955553784,0.006000451
 H,7.3742068726,-2.5002011609,-0.0001340342
 H,4.911760981,2.4968886092,0.0058478129
 H,4.9130569502,-2.5028598021,-0.0002853787
 H,2.4545491658,2.4972962865,0.0056758987
 H,2.4557413248,-2.5045220977,-0.0004528167
 H,-0.0005182447,2.4970391012,0.0054516034
 H,0.0005293062,-2.5053773151,-0.0006677904
 H,-2.4555853482,2.4962688544,0.0051760243
 H,-2.4546829928,-2.5055496297,-0.0009429454
 H,-4.9127964763,2.4948330491,0.004855456
 C,-7.3726416575,1.405102391,0.0031990132
 C,-7.3721697969,-1.415918989,-0.000249185
 H,-4.9119993638,-2.5049155473,-0.0012578372
 C,-8.586675153,-0.7327134387,0.0004239513
 C,-8.5869165239,0.7215325769,0.0022012891
 H,-7.3739138518,2.4924699089,0.0045261053
 C,-9.8434631786,1.406963958,0.0028702648
 H,-7.3731499026,-2.5032867975,-0.0015802883
 C,-9.8429935077,-1.4185277926,-0.0005827938
 C,-11.0203820364,0.7088127975,0.0018592404
 C,-11.0201383833,-0.7207423269,0.000112224
 H,-9.8431188501,2.4935763669,0.0041974705
 H,-11.9681376535,1.2387969781,0.0023795625
 H,-9.8423309757,-2.5051396214,-0.0019114769
 H,-11.9677170881,-1.2510457038,-0.0006630969

B3LYP/6-311++G(d,p) optimized geometries of cationic [n]acenes

benzene

C,-2.0719540776,2.7948980264,0.
C,-3.2796245851,2.0300172484,0.
C,-0.8683462229,2.1434938107,0.
C,-3.2596618281,0.6008073233,0.
C,-0.8483813596,0.7142920124,0.
C,-2.0560576285,-0.0505947811,0.
H,0.067469586,2.6887618425,0.
H,0.1059554146,0.1976603121,0.
H,-2.1272549799,3.8765728333,0.
H,-4.2339669319,2.5466387915,0.
H,-4.1954844332,0.0555513169,0.
H,-2.0007429539,-1.1322687362,0.

B3LYP/6-31G(d,p) optimized geometries of anionic [n]acenes

benzene

C,-2.1024683209,2.7697236496,0.
C,-3.3122685281,2.0698248861,0.
C,-0.8558980792,2.1373804967,0.
C,-3.2721096222,0.6069181487,0.
C,-0.8157394498,0.6744864522,0.
C,-2.0255410453,-0.0254186369,0.
H,0.0647820118,2.7212400457,0.
H,0.1356343207,0.142081061,0.
H,-2.1326311393,3.8657883608,0.
H,-4.2636499511,2.6022159989,0.
H,-4.1927980502,0.0230724806,0.
H,-1.9953621463,-1.1214829434,0.

naphthalene

C,-2.1492980456,2.8301853713,0.
C,-3.3428501374,2.1175135953,0.
C,-0.9163101256,2.1449681404,0.
C,-3.3244959134,0.7070367302,0.
C,-0.8550528448,0.7246153631,0.
C,-2.1031649215,-0.0206342633,0.
H,0.0198754663,2.7042296666,0.
C,0.3662781471,-0.0030556304,0.
H,-2.1608734715,3.9210373657,0.
H,-4.2976761443,2.6451492278,0.
H,-4.2609136325,0.1481639607,0.
C,-2.0419076407,-1.4409870406,0.
C,0.3846323711,-1.4135324955,0.
C,-0.8089197207,-2.1262042715,0.
H,1.3026958663,0.5558171391,0.
H,1.339458378,-1.941168128,0.
H,-0.7973442948,-3.2170562659,0.
H,-2.9780932326,-2.0002485668,0.

anthracene

C,-2.1392303214,2.886194507,0.
C,-3.3600974928,2.1942728264,0.
C,-0.9377137713,2.177770206,0.
C,-3.3696302519,0.7994910682,0.
C,-0.9053066266,0.7585942722,0.
C,-2.1687329415,0.0425523597,0.
H,0.0116507368,2.7138514683,0.
C,0.2953574766,0.0124021766,0.
H,-2.1280629806,3.9757787476,0.
H,-4.3006170977,2.7444922271,0.

H,-4.3173069163,0.2604316838,0.
 C,-2.1454257864,-1.3709021601,0.
 C,0.3186646242,-1.4010523537,0.
 C,-0.944761696,-2.1170942568,0.
 H,1.2442080814,0.5501595335,0.
 C,1.5195619229,-2.1579910779,0.
 C,-0.9123545708,-3.5362701927,0.
 H,-3.0942763979,-1.9086595209,0.
 C,1.5100291505,-3.5527728303,0.
 C,0.2891619775,-4.2446945081,0.
 H,2.4672385935,-1.6189316962,0.
 H,2.4505487658,-4.102992223,0.
 H,-1.8617190781,-4.0723514483,0.
 H,0.277994649,-5.3342787438,0.

tetracene

C,0.0165903781,-0.0395288938,-0.0071105121
 C,1.428990313,-0.0388480686,-0.0046731052
 C,2.1205484991,1.1617166379,0.0013632756
 C,1.4469094381,2.4140370705,0.0052536785
 C,-0.0037278634,2.4133376478,0.0027505969
 C,-0.6761418899,1.1603683344,-0.0034635873
 C,2.123606567,3.6501251074,0.011408991
 C,1.4515203405,4.8895824708,0.0152514283
 C,-0.0107603533,4.8888774314,0.0127277916
 C,-0.6816338278,3.6487726696,0.0065673888
 C,2.1223938674,6.129687177,0.021413227
 C,1.4444877447,7.3651223125,0.0252322334
 C,-0.0061493685,7.3644229724,0.022728315
 C,-0.682846544,6.1283347504,0.0165722101
 C,2.1169019781,8.6180914845,0.031450857
 C,1.4241693572,9.8179888777,0.0351020149
 C,0.0117698269,9.8173080744,0.0326643256
 C,-0.6797886253,8.6167432356,0.0266244134
 H,-0.5266575963,-0.9832811112,-0.0118545355
 H,1.9731611054,-0.9820759494,-0.0075405593
 H,3.210461312,1.1648043386,0.0032554532
 H,-1.766057136,1.1624050715,-0.0053338005
 H,3.2138499471,3.6497645245,0.0132884843
 H,-1.7718763493,3.6473607418,0.0046834166
 H,3.2126363295,6.1310994875,0.0233001164
 H,-1.7730899205,6.1286956702,0.0146960091
 H,3.2068171156,8.6160551502,0.0333220244
 H,1.967417929,10.7617407794,0.0398498363
 H,-0.5324012239,10.7605358504,0.0355358502
 H,-1.7697013505,8.6136558351,0.0247341607

pentacene

C,0.0161195479,-0.0385411965,-0.0156804492
C,1.4346120815,-0.0369722977,-0.0113876935
C,2.1241245708,1.1580651805,0.0001833984
C,1.4479340722,2.4123492327,0.00810187
C,-0.0027384106,2.4107445023,0.0037112463
C,-0.6760924813,1.1549677847,-0.0082919917
C,2.1238126938,3.6439652594,0.019920568
C,1.4515048402,4.8818174416,0.0277204434
C,-0.0118910111,4.8801987143,0.0232918328
C,-0.6813992855,3.6408623048,0.0114305889
C,2.1232682955,6.1200122518,0.0395775961
C,1.4487077616,7.3567178523,0.0473612321
C,-0.0146881054,7.3550991069,0.0429333066
C,-0.686451567,6.1169043023,0.0310752732
C,2.1182160132,8.5960542502,0.0592196889
C,1.4395551567,9.8261719902,0.0669386436
C,-0.0111173517,9.8245673784,0.0625497743
C,-0.6869959988,8.592951283,0.0507325388
C,2.112909044,11.0819488159,0.0789387052
C,1.4206970296,12.2754578416,0.0863261684
C,0.0022045142,12.2738887997,0.0820347578
C,-0.6873080162,11.07885135,0.0704674174
H,-0.5238240258,-0.9836416852,-0.0248157601
H,1.9766904328,-0.9808758117,-0.0172483591
H,3.2136933067,1.1621642719,0.0035043665
H,-1.7656676512,1.1566561726,-0.0115667645
H,3.2138406637,3.6442135579,0.0232128958
H,-1.7714250661,3.6386990574,0.0081250694
H,3.2130396515,6.1212178361,0.0428759466
H,-1.776222911,6.1156988345,0.0277782914
H,3.2082418123,8.598217597,0.0625255749
H,-1.7770239671,8.5927030354,0.0474425027
H,3.2024842734,11.0802602532,0.0822119795
H,1.960640711,13.2205582303,0.0954577456
H,-0.5398739161,13.2177923621,0.0878932417
H,-1.7768767056,11.0747522491,0.067148339

hexacene

C,0.0157605236,-0.0367698055,-0.02660204
C,1.438371639,-0.0345314442,-0.0377963144
C,2.1271578859,1.1564948513,-0.0213335806
C,1.449284634,2.4124383341,0.0071117454
C,-0.0021446663,2.4101545323,0.0185278652
C,-0.6764261186,1.1520833859,0.0007207685
C,2.1248292397,3.6400007242,0.024347773
C,1.4514409423,4.8774176538,0.0524148111

C,-0.01134469,4.8751159963,0.0639192623
 C,-0.6811940445,3.6355855808,0.0464181126
 C,2.1238033949,6.1141469642,0.0698422819
 C,1.4501644325,7.3489089434,0.0978600012
 C,-0.0171305625,7.3466002285,0.1093994696
 C,-0.6872381983,6.1097239685,0.0919505693
 C,2.1202718542,8.5857852482,0.1153069138
 C,1.4443783598,9.8203933062,0.1433366472
 C,-0.0184072433,9.8180916609,0.1548400009
 C,-0.6907697045,8.581362159,0.137413195
 C,2.1142275564,11.059923821,0.1608324394
 C,1.4351780093,12.2853550391,0.1887159822
 C,-0.0162512534,12.2830711397,0.2001298848
 C,-0.691795879,11.0555085411,0.1828983996
 C,2.1094590695,13.543426334,0.2065171376
 C,1.4172723505,14.7322797967,0.2338312746
 C,-0.0053388102,14.7300413241,0.2450178432
 C,-0.6941247509,13.5390147336,0.2285633895
 H,-0.521856765,-0.9827853132,-0.0397505979
 H,1.9786896916,-0.9788505789,-0.0594295984
 H,3.2164100172,1.1611784797,-0.0298469665
 H,-1.7656866499,1.1533387057,0.0093440528
 H,3.2146325171,3.6409248988,0.0157625124
 H,-1.7709950014,3.6330798958,0.0549763414
 H,3.2133463284,6.1153736744,0.0612650476
 H,-1.776779661,6.1075217959,0.1005114193
 H,3.2098133987,8.5879874801,0.1067479279
 H,-1.7803125563,8.580135537,0.1459909124
 H,3.2040285805,11.0624295502,0.1522774427
 H,-1.7815990728,11.0545846203,0.1914832119
 H,3.1987196924,13.5421710073,0.1978970192
 H,1.9548896818,15.6782952482,0.2469754908
 H,-0.5456572859,15.6743605738,0.2666379356
 H,-1.7833768856,13.5343313922,0.2370740255

heptacene

C,0.0159704689,-0.0346864219,-0.0528284378
 C,1.4415248852,-0.0324662104,-0.0459368472
 C,2.1300602918,1.1554685787,-0.0173953635
 C,1.4509119034,2.4130886155,0.0060605597
 C,-0.0015362325,2.4108265301,-0.0009607651
 C,-0.6765055493,1.1510975149,-0.0309625686
 C,2.1263061155,3.6371299706,0.035306749
 C,1.4517339187,4.8752037742,0.0583696947
 C,-0.0105329351,4.8729263784,0.0513007428
 C,-0.6809910052,3.6327577741,0.0217358791
 C,2.1245582193,6.1100102224,0.0878329886

C,1.4505058457,7.3435074116,0.1108017838
 C,-0.017500178,7.3412210743,0.1037047568
 C,-0.687453584,6.1056306734,0.0742386787
 C,2.1211513343,8.5798283821,0.140287418
 C,1.4464044357,9.8140541248,0.1632688253
 C,-0.021601585,9.8117677776,0.1561715353
 C,-0.6922470724,8.5754466645,0.1266858312
 C,2.1163578357,11.0496443526,0.1927363083
 C,1.4394371582,12.2823487983,0.215675328
 C,-0.0228296895,12.2800713848,0.2086056548
 C,-0.6956539853,11.0452647881,0.1791410785
 C,2.1098951929,13.5225172031,0.2452431899
 C,1.4304403383,14.744448556,0.2679415338
 C,-0.0220077359,14.7421864391,0.2609191739
 C,-0.6974019428,13.5181449689,0.2316704494
 C,2.1054096092,16.0041773858,0.2979470064
 C,1.4129335118,17.1899613575,0.3198149892
 C,-0.0126207696,17.1877411228,0.3129225831
 C,-0.7011561618,15.9998062834,0.2843776003
 H,-0.5199104996,-0.9812343835,-0.0755091768
 H,1.980545808,-0.9773400832,-0.0634209429
 H,3.2190976372,1.1601143348,-0.0120681583
 H,-1.7655526876,1.1523509603,-0.036164302
 H,3.2159524837,3.6381982162,0.0405609132
 H,-1.7706352799,3.6304318709,0.0164550734
 H,3.213971564,6.1110959014,0.0930866489
 H,-1.7768648938,6.1033229167,0.068959112
 H,3.2105228779,8.5815251614,0.1455539987
 H,-1.781618609,8.5737501576,0.121419135
 H,3.2057691482,11.0519523738,0.1980162565
 H,-1.7850673188,11.0441793784,0.1738870339
 H,3.1995394647,13.5248433035,0.2505248472
 H,-1.7870482983,13.517076903,0.2264156221
 H,3.1944567407,16.0029240452,0.3031499855
 H,1.948814604,18.1365091821,0.3424986839
 H,-0.5516418828,18.1326148361,0.3304092277
 H,-1.790193499,15.9951606588,0.2790497108

octacene

C,-0.0035594505,-0.0528880102,-0.0629011067
 C,1.4240803949,-0.0554277221,-0.0551538107
 C,2.1167033429,1.127928438,-0.0243412729
 C,1.4409991302,2.3891178678,0.0007678528
 C,-0.0123869363,2.3917033344,-0.0071193373
 C,-0.6922614743,1.1329254703,-0.0395846434
 C,2.1206086016,3.6081004253,0.0323234574
 C,1.4493449549,4.8493107276,0.0570011539

C,-0.0125904117,4.8519111421,0.0490671084
 C,-0.6879577632,3.6130965003,0.0170817535
 C,2.1268499314,6.0799101967,0.0888115869
 C,1.456352049,7.3150900401,0.1133564242
 C,-0.0114374771,7.3177006396,0.1053898244
 C,-0.6860185613,6.0849134989,0.0735453176
 C,2.1318084719,8.5486645176,0.1452249058
 C,1.4613711561,9.7838200752,0.1697698913
 C,-0.0082875272,9.7864337998,0.1617921714
 C,-0.6828075538,8.5536704158,0.1299473476
 C,2.1358914152,11.0165836838,0.2016160087
 C,1.4645206634,12.2525534108,0.226174551
 C,-0.0032688638,12.2551635634,0.2182059936
 C,-0.6787246068,11.0215890333,0.1863364718
 C,2.1391014734,13.4853410755,0.2580224693
 C,1.465672266,14.718343089,0.2825016912
 C,0.0037368718,14.7209425567,0.2745641207
 C,-0.6737669623,13.49034277,0.2427506016
 C,2.1410388874,15.9571583404,0.3144918085
 C,1.4654668122,17.1785509539,0.3386936172
 C,0.0120807864,17.1811351012,0.3308020065
 C,-0.6675274414,15.9621520879,0.2992420797
 H,-0.5414208247,-0.9980553726,-0.0874274274
 H,1.9588101574,-1.0025031799,-0.0738596285
 H,3.2055509941,1.1288593872,-0.0183670677
 H,-1.7810995394,1.1377302285,-0.0454279203
 H,3.2100863182,3.6056396429,0.0382231104
 H,-1.7774370445,3.6145113687,0.0111566086
 H,3.216121019,6.0773503699,0.0947078575
 H,-1.7752914874,6.0862282267,0.0676180151
 H,3.2210415563,8.5465078786,0.1511308724
 H,-1.7720411351,8.5553880396,0.1240287634
 H,3.2251252175,11.0148662598,0.2075333686
 H,-1.7679574689,11.0237457404,0.1804277444
 H,3.2283745789,13.4840266208,0.2639505897
 H,-1.7630378583,13.4929024511,0.2368507892
 H,3.2305183025,15.955743927,0.3204194948
 C,2.1453402324,18.437329429,0.3711639607
 C,-0.663624496,18.4423237923,0.3559115836
 H,-1.757004997,15.9646124448,0.2933385487
 C,0.0289972057,19.6256805537,0.3867288945
 C,1.4566370153,19.6231422358,0.3944808832
 H,3.2341783547,18.4325253909,0.3770108683
 H,1.9944974031,20.5683100406,0.4190112155
 H,-1.7524720481,18.4413921093,0.3499337649
 H,-0.5057336348,20.5727553975,0.4054350666

nonacene

C,0.075058564,-0.0963748222,-0.0717649072
C,1.5040982659,-0.0818747157,-0.0624672113
C,2.1828460142,1.1079071314,-0.0296477834
C,1.4914421141,2.3619861957,-0.00387291
C,0.0373528452,2.3472321308,-0.0133339237
C,-0.6280641359,1.079382849,-0.0479363829
C,2.1566879941,3.5867368886,0.0296994765
C,1.4698829056,4.8207792953,0.0550285584
C,0.0082437009,4.8059508257,0.0455174593
C,-0.6529874847,3.5582275635,0.0114174303
C,2.1332043524,6.0575034393,0.0888820989
C,1.4473165527,7.2845475454,0.1140514732
C,-0.0199478138,7.2696647022,0.1045021216
C,-0.6804107826,6.0289602746,0.0705718182
C,2.1086735316,8.5253140639,0.1479964002
C,1.4232077812,9.7513502168,0.1731490108
C,-0.0466404554,9.7364460136,0.1635810812
C,-0.7067104455,8.4967629468,0.1296710043
C,2.0835082102,10.9920519432,0.2070950842
C,1.3978079461,12.2191110306,0.232277093
C,-0.0720403689,12.2042137541,0.2227078146
C,-0.7323342081,10.9635089245,0.1887632815
C,2.057895166,13.4587842842,0.2662064463
C,1.3711376416,14.6858858588,0.2913909828
C,-0.0961270058,14.6710213683,0.2818376403
C,-0.7574892941,13.4302595869,0.2478754042
C,2.0316267727,15.9265747865,0.3253556525
C,1.342989393,17.149594714,0.3504371532
C,-0.1186502377,17.1347922307,0.3409199018
C,-0.7819890383,15.8980801923,0.3070349625
H,-0.4506672974,-1.0481528525,-0.0979126628
H,2.0493262808,-1.0227843777,-0.0816477318
H,3.2714061179,1.1214764409,-0.0225058531
H,-1.7166761644,1.0708581333,-0.0549594478
H,3.2459435518,3.5970231292,0.0367708895
H,-1.742227954,3.5464097618,0.0043139025
H,3.2222790392,6.0676515398,0.095950262
H,-1.7694681388,6.0170153005,0.0634652986
H,3.1977170013,8.5358730242,0.155077149
H,-1.7957456974,8.4852369082,0.1225744394
H,3.1725466784,11.0030908836,0.2141902742
H,-1.8213747311,10.9524698592,0.1816783801
H,3.1469286997,13.4703031316,0.2733151262
H,-1.8465346346,13.4197072515,0.2408021242
H,3.1206830172,15.938504862,0.3324741263
C,2.004252765,18.3972989998,0.3845793214

C,-0.8054233807,18.3688526469,0.366284109
 H,-1.871065136,15.8879460699,0.299970393
 C,-0.1401506999,19.5935869903,0.3999007321
 C,1.3139390147,19.6083090338,0.4093690767
 H,3.0934926605,18.4090942322,0.3916955185
 C,1.9793888659,20.8761385494,0.4440296951
 H,-1.8946799328,18.3585881247,0.3592146479
 C,-0.8315218978,20.8476840931,0.4257260887
 C,1.2762967563,22.0519140368,0.4678903567
 C,-0.1527432687,22.0374470484,0.4585848332
 H,3.0680011456,20.8846368999,0.451058759
 H,1.8020476463,23.0036770897,0.4940674353
 H,-1.9200822214,20.8341410353,0.4185783047
 H,-0.6979465667,22.9783709356,0.477788221

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C,0.1952695833,-0.002064957,-0.0787801245
 C,1.6249388456,0.0370649298,-0.0652948884
 C,2.2832529878,1.2370328844,-0.029105843
 C,1.5698033421,2.4797207284,-0.0038243618
 C,0.1155500817,2.4399175057,-0.0175404769
 C,-0.5282577872,1.1600788818,-0.0556245478
 C,2.2139811671,3.7139919426,0.0331140065
 C,1.5053931998,4.9367789683,0.0579454864
 C,0.0442918607,4.8967905593,0.0441665913
 C,-0.5957564951,3.6370842162,0.0066143415
 C,2.1476556398,6.1831408738,0.095189086
 C,1.4401051628,7.3983225324,0.1198528074
 C,-0.0263407586,7.3581910544,0.1060268898
 C,-0.6657690876,6.1061297167,0.0686587012
 C,2.0804342493,8.6494292989,0.1572210496
 C,1.3734746266,9.8627950126,0.1818689968
 C,-0.0957926234,9.8225894327,0.1680214292
 C,-0.7347287118,8.572368733,0.1306816809
 C,2.0126688055,11.1145966489,0.2192724114
 C,1.3058264109,12.3286084946,0.2439691493
 C,-0.1642947641,12.2883795206,0.2301192146
 C,-0.8030786223,11.0375196587,0.1927374021
 C,1.944621268,13.57946722,0.2813741965
 C,1.2373269955,14.7943995493,0.3061244541
 C,-0.2319399166,14.7541889221,0.2922884566
 C,-0.8711259748,13.5023902788,0.2548504844
 C,1.8762725508,16.0446163357,0.3435404926
 C,1.1678798477,17.2587960471,0.3682944236
 C,-0.2985657165,17.2186543548,0.3544910215
 C,-0.9388900272,15.967553668,0.3170348704
 H,-0.3131201332,-0.9630027682,-0.1075963684

H,2.1855780729,-0.8946128561,-0.0840265005
 H,3.3712634062,1.2693098173,-0.0187766759
 H,-1.616405894,1.1327899436,-0.0658216464
 H,3.3027535634,3.7431278014,0.0433737407
 H,-1.6844924486,3.6066139511,-0.0036631286
 H,3.2362705483,6.2120478842,0.1054437214
 H,-1.7543357977,6.0754346884,0.0583826645
 H,3.1690204633,8.6786445158,0.1674847777
 H,-1.8232849231,8.5419830005,0.1204207323
 H,3.1012523031,11.1441890884,0.2295442906
 H,-1.891654128,11.0075180324,0.1824917147
 H,3.0331935126,13.6094631995,0.2916514104
 H,-1.9597130906,13.4728019176,0.2446186121
 H,2.9648265285,16.0749902581,0.3538192242
 C,1.8073110241,18.5108531442,0.4057817983
 C,-1.0061133491,18.4338332226,0.3793052882
 H,-2.027479326,15.9383488634,0.3068142378
 C,-0.3638552951,19.6801890657,0.4166771166
 C,1.0972457989,19.7201916895,0.4304248008
 H,2.8958766657,18.5415381251,0.4160594658
 C,1.7372888558,20.9798952323,0.468126315
 H,-2.0947302094,18.4049352882,0.369093289
 C,-1.072448532,20.9029702663,0.4416939711
 C,1.0259757564,22.1770561361,0.4924676002
 C,-0.4282773924,22.13723875,0.4787882223
 H,2.8260245863,21.0103628002,0.4783926271
 H,-2.1612217628,20.8738363651,0.4314760299
 C,-1.141738099,23.3799170364,0.5042834009
 C,1.6697725843,23.4568941179,0.5307264533
 C,-0.4834341336,24.5798845438,0.5406285766
 C,0.9462350951,24.6190293335,0.5540746209
 H,2.7579210974,23.4841854982,0.5408988432
 H,1.4546125207,25.5799691722,0.5830150534
 H,-2.2297485279,23.3476372151,0.4939900565
 H,-1.0440854806,25.5115526476,0.5595182629

Table S1. Molecular energies (298.15 K and 1 atm) of the neutral compounds at the optimized neutral geometries for the n=1-10 [n]acenes at the x¹/TZVP//B3LYP/6-31G(d) level of theory (note that semiempirical method energies are at the x//B3LYP/6-31G(d) level of theory).

model chemistry	1	2	3	4	5	6	7	8	9	10]
AM1	0.035586	0.065669	0.101919	0.140960	0.181525	0.223000	0.265037	0.307569	0.350160	0.393046
B1B95	-232.204127	-385.824919	-539.439235	-693.050901	-846.661290	-1000.271015	-1153.880393	-1307.489545	-1461.098626	-1614.707599
B1LYP	-232.192414	-385.799895	-539.401061	-692.999625	-846.596935	-1000.193591	-1153.789893	-1307.385983	-1460.981978	-1614.577888
B2PLYPD	-232.075557	-385.611632	-539.141776	-692.669499	-846.196107	-999.722177	-1153.247999	-1306.773683	-1460.299344	-1613.824969
B3LYP	-232.328219	-386.016675	-539.698972	-693.378770	-847.057382	-1000.735385	-1154.413064	-1308.090554	-1461.767954	-1615.445282
B3P86	-233.078858	-387.234311	-541.383523	-695.530226	-849.675745	-1003.820661	-1157.965265	-1312.109678	-1466.254017	-1620.398274
B3PW91	-232.232519	-385.859989	-539.481220	-693.099942	-846.717479	-1000.334413	-1153.951033	-1307.567463	-1461.183817	-1614.800092
B97D	-232.144714	-385.713611	-539.277313	-692.838973	-846.399713	-999.960009	-1153.520080	-1307.080046	-1460.639929	-1614.199793
B98	-232.226083	-385.850890	-539.469479	-693.085537	-846.700389	-1000.314620	-1153.928520	-1307.542224	-1461.155837	-1614.769380
BHandH	-230.504574	-383.034238	-535.556621	-688.075866	-840.593513	-993.110280	-1145.626568	-1298.142509	-1450.658357	-1603.174010
BHandHLYP	-232.174622	-385.768374	-539.354965	-692.938418	-846.520255	-1000.101197	-1153.681630	-1307.261708	-1460.841677	-1614.421464
BLYP	-232.216826	-385.842633	-539.463034	-693.081363	-846.698771	-1000.315734	-1153.932464	-1307.549099	-1461.165633	-1614.782164
BMK	-232.149211	-385.730226	-539.304488	-692.875869	-846.445809	-1000.014968	-1153.583687	-1307.152123	-1460.720449	-1614.288660
CAM-B3LYP	-232.184085	-385.783711	-539.376316	-692.965882	-846.553903	-1000.141072	-1153.727760	-1307.314122	-1460.900373	-1614.486467
HCTH/147	-232.303740	-385.968752	-539.628177	-693.285479	-846.941841	-1000.597755	-1154.253450	-1307.909037	-1461.564552	-1615.220039
HCTH/407	-232.296215	-385.953611	-539.605365	-693.254979	-846.903648	-1000.551866	-1154.199868	-1307.847761	-1461.495586	-1615.143377
HF	-230.771827	-383.462402	-536.144585	-688.822642	-841.498342	-994.172594	-1146.845918	-1299.518535	-1452.190899	-1604.862878
HFB	-230.827827	-383.562567	-536.292124	-689.019649	-841.746268	-994.472445	-1147.198363	-1299.924208	-1452.649897	-1605.375637
HFS	-227.496763	-378.109455	-528.716731	-679.321954	-829.926284	-980.530186	-1131.133871	-1281.737485	-1432.340976	-1582.944478
HSE06	-232.056009	-385.576746	-539.091201	-692.603109	-846.113807	-999.623881	-1153.133631	-1306.643179	-1460.152648	-1613.662029
LC-wPBE	-232.141943	-385.707292	-539.264903	-692.818983	-846.371165	-999.922241	-1153.472654	-1307.022576	-1460.572349	-1614.121863
M05	-232.115115	-385.674109	-539.226714	-692.776691	-846.325403	-999.873457	-1153.421160	-1306.968640	-1460.516041	-1614.063344
M052X	-232.295147	-385.973979	-539.645706	-693.314367	-846.981469	-1000.647713	-1154.313479	-1307.978905	-1461.644242	-1615.309413
M06	-232.129570	-385.697831	-539.259829	-692.819237	-846.377386	-999.934871	-1153.492003	-1307.048907	-1460.605729	-1614.162444
M062X	-232.215251	-385.842856	-539.463519	-693.081163	-846.697266	-1000.312518	-1153.927287	-1307.541727	-1461.156055	-1614.770228
M06HF	-232.262534	-385.921684	-539.572944	-693.220521	-846.866082	-1000.510452	-1154.154094	-1307.797189	-1461.440118	-1615.082768
M06L	-232.284453	-385.952488	-539.614703	-693.274653	-846.933573	-1000.591988	-1154.250153	-1307.908182	-1461.566138	-1615.224041
MP2	-231.593266	-384.820162	-538.041058	-691.259572	-844.477092	-997.694237	-1150.911324	-1304.128466	-1457.345734	-1610.563135
mPW1LYP	-232.189531	-385.797107	-539.398366	-692.997023	-846.594425	-1000.191173	-1153.787569	-1307.383752	-1460.979840	-1614.575842
mPW1PBE	-232.172643	-385.766493	-539.353918	-692.938725	-846.522282	-1000.105193	-1153.687765	-1307.270124	-1460.852406	-1614.434593
mPW2PLYPD	-232.076658	-385.613505	-539.144205	-692.672365	-846.199330	-999.725702	-1153.251789	-1306.777706	-1460.303591	-1613.829418
mPW3PBE	-232.154861	-385.734478	-539.307849	-692.878710	-846.448387	-1000.017462	-1153.586225	-1307.154798	-1460.723295	-1614.291713
O3LYP	-232.237739	-385.868940	-539.494137	-693.116970	-846.738719	-1000.359930	-1153.980868	-1307.601652	-1461.222363	-1614.843020
OPBE	-232.218556	-385.839204	-539.454145	-693.066948	-846.678818	-1000.290251	-1153.901479	-1307.512600	-1461.123666	-1614.734704
OTPSS	-232.221465	-385.844250	-539.461331	-693.076277	-846.690292	-1000.303871	-1153.917246	-1307.530516	-1461.143728	-1614.756914
PBE0	-232.035930	-385.543306	-539.044267	-692.542613	-846.039711	-999.536164	-1153.032280	-1306.528183	-1460.024009	-1613.519740
PDDG	0.037631	0.067126	0.102977	0.141659	0.181893	0.223047	0.264726	0.306987	0.349151	0.391679

PM3	0.037767	0.065978	0.100368	0.137552	0.176269	0.215902	0.256083	0.296795	0.337497	0.378521
PM6	0.038923	0.065059	0.096847	0.131310	0.167323	0.204317	0.241978	0.280198	0.318569	0.357265
tHCTH	-232.257416	-385.890745	-539.518476	-693.144076	-846.768733	-1000.392938	-1154.016924	-1307.640798	-1461.264603	-1614.888376
tHCTHhyb	-232.286136	-385.946018	-539.599892	-693.251374	-846.901742	-1000.551547	-1154.201060	-1307.850407	-1461.499671	-1615.148880
TPSSh	-232.340656	-386.040664	-539.734682	-693.426327	-847.116875	-1000.806874	-1154.496591	-1308.186148	-1461.875630	-1615.565056
VSXC	-232.426229	-386.186876	-539.941857	-693.694675	-847.446517	-1001.197885	-1154.949015	-1308.700028	-1462.450964	-1616.201867
wB97	-232.264696	-385.918683	-539.565100	-693.208028	-846.849070	-1000.489008	-1154.128270	-1307.767047	-1461.405653	-1615.044018
wB97X	-232.251458	-385.894969	-539.531048	-693.163801	-846.794803	-1000.424808	-1154.054223	-1307.683220	-1461.312082	-1614.940738
wB97XD	-232.237640	-385.870035	-539.495496	-693.117937	-846.738846	-1000.358916	-1153.978518	-1307.597795	-1461.216978	-1614.836007
X3LYP	-232.210614	-385.826753	-539.436670	-693.044051	-846.650221	-1000.255767	-1153.860980	-1307.465996	-1461.070921	-1614.675768
XAlpha	-228.986406	-380.564538	-532.137055	-683.707467	-835.276959	-986.846014	-1138.414867	-1289.983626	-1441.552305	-1593.120950

Table S2. Molecular energies (298.15 K and 1 atm) of the cationic compounds at the optimized neutral geometries for the n=1-10[n]acenes at the x/TZVP//B3LYP/6-31G(d) level of theory (note that semiempirical method energies are at the x//B3LYP/6-31G(d) level of theory).

model chemistry	1	2	3	4	5	6	7	8	9	10]
AM1	0.375606	0.370309	0.382194	0.404606	0.433195	0.465660	0.500698	0.537629	0.575809	0.615067
B1B95	-231.864723	-385.533339	-539.177258	-692.808857	-846.433520	-1000.053908	-1153.671518	-1307.287160	-1460.901454	-1614.514685
B1LYP	-231.858569	-385.513551	-539.144316	-692.762844	-846.374473	-999.981841	-1153.586421	-1307.189045	-1460.790293	-1614.390498
B2PLYPD	-231.736048	-385.319101	-538.878492	-692.425871	-845.966442	-999.502836	-1153.036533	-1306.568345	-1460.098880	-1613.628439
B3LYP	-231.987818	-385.724466	-539.436393	-693.136116	-846.829005	-1000.517692	-1154.203638	-1307.887667	-1461.570342	-1615.251999
B3P86	-232.716567	-386.919718	-541.098400	-695.264915	-849.424625	-1003.580154	-1157.732968	-1311.883868	-1466.033441	-1620.181988
B3PW91	-231.891034	-385.566145	-539.216871	-692.855424	-846.487168	-1000.114727	-1153.739564	-1307.362488	-1460.984079	-1614.604647
B97D	-231.809671	-385.428058	-539.021317	-692.602691	-846.177542	-999.748432	-1153.316753	-1306.883297	-1460.448561	-1614.012895
B98	-231.886932	-385.559849	-539.208092	-692.844091	-846.473225	-1000.098135	-1153.720290	-1307.340515	-1460.959384	-1614.577231
BHandH	-230.170043	-382.744572	-535.296469	-687.835877	-840.368051	-992.895689	-1145.420349	-1297.942862	-1450.463925	-1602.983786
BHandHLYP	-231.841968	-385.479922	-539.096034	-692.699708	-846.296148	-999.888031	-1153.476899	-1307.063601	-1460.648821	-1614.232843
BLYP	n/c ^a	-385.559248	-539.209483	-692.847680	-846.479300	-1000.106934	-1153.731977	-1307.355244	-1460.977206	-1614.598248
BMK	-231.807148	-385.434849	-539.038995	-692.630581	-846.215011	-999.794982	-1153.372020	-1306.946987	-1460.520517	-1614.092944
CAM-B3LYP	-231.842163	-385.487080	-539.109065	-692.718538	-846.320822	-999.918604	-1153.513418	-1307.106120	-1460.697360	-1614.287450
HCTH/147	-231.961979	-385.676498	-539.365503	-693.042538	-846.713024	-1000.379543	-1154.043497	-1307.705671	-1461.366575	-1615.026540
HCTH/407	-231.952872	-385.659407	-539.340692	-693.010021	-846.672807	-1000.331628	-1153.987889	-1307.642370	-1461.295585	-1614.947855
HF	-230.480893	-383.206952	-535.918995	-688.618724	-841.310680	-993.997583	-1146.680999	-1299.361838	-1452.040851	-1604.718357
HFB	-230.527880	-383.311861	-536.071023	-688.818330	-841.559122	-994.295946	-1147.030157	-1299.762614	-1452.493712	-1605.223943
HFS	n/c	-377.856691	-528.493609	-679.118554	-829.736983	-980.351468	-1130.963395	-1281.573583	-1432.182455	-1582.790430
HSE06	-231.716100	-385.283904	-538.827925	-692.359831	-845.884927	-999.405824	-1152.923989	-1306.440226	-1459.955124	-1613.468987
LC-wPBE	-231.796720	-385.403797	-538.990685	-692.564800	-846.131473	-999.693379	-1153.252098	-1306.808511	-1460.363351	-1613.916905
M05	-231.784121	-385.387182	-538.968247	-692.537600	-846.100226	-999.658690	-1153.214423	-1306.768222	-1460.320674	-1613.872082
M052X	-231.950998	-385.673108	-539.374138	-693.062575	-846.743925	-1000.420805	-1154.094741	-1307.766563	-1461.436960	-1615.106206
M06	-231.791390	-385.406112	-538.996922	-692.575823	-846.147969	-999.715927	-1153.281150	-1306.844438	-1460.406382	-1613.967278
M062X	-231.867763	-385.539839	-539.189966	-692.827516	-846.457966	-1000.083930	-1153.706939	-1307.327843	-1460.947302	-1614.565621
M06HF	-231.907436	-385.606987	-539.287846	-692.955365	-846.615470	-1000.270707	-1153.922711	-1307.572365	-1461.220450	-1614.867242
M06L	-231.947798	-385.664736	-539.356828	-693.036803	-846.710087	-1000.379289	-1154.045846	-1307.710559	-1461.373968	-1615.036392
MP2	-231.241737	-384.514750	-537.763836	-690.999019	-844.227089	-997.450524	-1150.670919	-1303.889112	-1457.105950	-1610.321661
mPW1LYP	-231.854693	-385.509839	-539.140710	-692.759338	-846.371064	-999.978529	-1153.583206	-1307.185926	-1460.787271	-1614.387571
mPW1PBE	-231.832477	-385.473216	-539.090101	-692.694769	-846.292564	-999.886118	-1153.476910	-1307.065750	-1460.653240	-1614.239680
mPW2PLYPD	-231.737284	-385.320605	-538.880581	-692.428468	-845.969473	-999.506239	-1153.040257	-1306.572346	-1460.103129	-1613.632903
mPW3PBE	-231.812661	-385.439982	-539.042865	-692.633567	-846.217456	-999.797160	-1153.374143	-1306.949213	-1460.522949	-1614.095662
O3LYP	-231.900572	-385.580835	-539.235792	-692.878564	-846.514586	-1000.146489	-1153.775719	-1307.403082	-1461.029133	-1614.654194
OPBE	-231.879036	-385.549388	-539.194099	-692.826740	-846.452797	-1000.074874	-1153.694386	-1307.312112	-1460.928581	-1614.544106
OTPSS	-231.881245	-385.553898	-539.200793	-692.835603	-846.463822	-1000.088057	-1153.709725	-1307.329606	-1460.948225	-1614.565904
PBE0	-231.695533	-385.249879	-538.780303	-692.298512	-845.809849	-999.316947	-1152.821284	-1306.323672	-1459.824709	-1613.324698
PDDG	0.384371	0.378831	0.390188	0.412217	0.440494	0.472710	0.507512	0.544336	0.582285	0.621405

PM3	0.384297	0.376651	0.386367	0.406742	0.433355	0.463901	0.497053	0.532170	0.568500	0.605956
PM6	0.379941	0.374246	0.383631	0.402435	0.427045	0.455410	0.486348	0.519189	0.553328	0.588560
tHCTH	-231.916565	-385.598616	-539.255669	-692.900855	-846.539539	-1000.174277	-1153.806466	-1307.436880	-1461.066034	-1614.694248
tHCTHhyb	-231.943987	-385.652329	-539.335745	-693.007035	-846.671581	-1000.331998	-1153.989729	-1307.645584	-1461.300117	-1614.953660
TPSSh	-232.003768	-385.752188	-539.475821	-693.187339	-846.892125	-1000.592796	-1154.290794	-1307.986921	-1461.681736	-1615.375560
VSXC	-232.090174	-385.900304	-539.684927	-693.457541	-847.223549	-1000.985542	-1154.744937	-1308.502529	-1462.258838	-1616.014194
wB97	-231.923755	-385.619790	-539.295403	-692.958289	-846.613771	-1000.264497	-1153.912041	-1307.557291	-1461.200959	-1614.843364
wB97X	-231.910165	-385.596966	-539.262180	-692.914671	-846.559846	-1000.200378	-1153.837828	-1307.473069	-1461.106793	-1614.739308
wB97XD	-231.896823	-385.574411	-539.228869	-692.870741	-846.505476	-1000.135750	-1153.763092	-1307.388349	-1461.012176	-1614.634875
X3LYP	-231.871807	-385.535942	-539.175482	-692.802802	-846.423264	-1000.039502	-1153.652985	-1307.264537	-1460.874730	-1614.483894
XAlpha	-228.671556	-380.299474	-531.901458	-683.491483	-835.074998	-986.654576	-1138.231624	-1289.806919	-1441.380946	-1592.954036

^a calculation failed to converge.

Table S3. Molecular energies (298.15 K and 1 atm) of the anionic compounds at the optimized neutral geometries for the n=1-10[n]acenes at the x/TZVP//B3LYP/6-31G(d) level of theory (note that semiempirical method energies are at the x//B3LYP/6-31G(d) level of theory).

model chemistry	1	2	3	4	5	6	7	8	9	10
	[n]acene									
AM1	0.039530	0.038397	0.050721	0.072682	0.100470	0.132137	0.166474	0.202803	0.240515	0.279398
B1B95	-232.139091	-385.805750	-539.451373	-693.084666	-846.710686	-1000.332133	-1153.950554	-1307.566895	-1461.181688	-1614.795363
B1LYP	-232.126701	-385.778947	-539.410855	-693.030730	-846.643474	-1000.251723	-1153.856979	-1307.460195	-1461.061859	-1614.662442
B2PLYPD	-232.007100	-385.587816	-539.148722	-692.697620	-846.239426	-999.776783	-1153.311213	-1306.843656	-1460.374629	-1613.904577
B3LYP	-232.268556	-386.002221	-539.715294	-693.416356	-847.110350	-1000.797180	-1154.486519	-1308.171130	-1461.854212	-1615.536238
B3P86	-233.040910	-387.242089	-541.422398	-695.590572	-849.751616	-1003.908187	-1158.061800	-1312.213390	-1466.363456	-1620.512445
B3PW91	-232.173836	-385.847008	-539.499309	-693.139477	-846.772519	-1000.401092	-1154.026706	-1307.650300	-1461.272369	-1614.893365
B97D	-232.082837	-385.698378	n/c ^a	-692.875599	-846.451519	-1000.023237	-1153.592186	-1307.159274	-1460.724916	-1614.289593
B98	-232.163228	-385.833796	-539.483509	-693.121049	-846.751428	-1000.377312	-1154.000212	-1307.621082	-1461.240408	-1614.858667
BHandH	-230.436492	-383.010432	-535.564326	-688.105694	-840.639453	-993.168339	-1145.693968	-1298.217315	-1450.738988	-1603.259393
BHandHLYP	-232.108060	-385.745338	-539.362990	-692.968302	-846.566082	-1000.159025	-1153.748715	-1307.336136	-1460.921875	-1614.506369
BLYP	-232.152673	-385.824591	n/c	-693.114787	-846.747283	-1000.375605	-1154.001170	-1307.624897	-1461.247169	-1614.868497
BMK	-232.082916	-385.709486	-539.315400	-692.908756	-846.494603	-1000.075684	-1153.653575	-1307.229277	-1460.803335	-1614.376233
CAM-B3LYP	-232.124297	-385.767645	-539.390880	-693.001793	-846.605277	-1000.204019	-1153.799580	-1307.392940	-1460.984655	-1614.575176
HCTH/147	-232.247103	-385.959141	-539.649546	-693.327988	-846.999589	-1000.666965	-1154.331566	-1307.994299	-1461.655591	-1615.315905
HCTH/407	-232.241242	-385.945770	n/c	-693.299281	-846.963185	-1000.622861	-1154.279764	-1307.934798	-1461.588394	-1615.241008
HF	-230.678771	-383.409894	-536.123558	-688.825033	-841.518419	-994.206447	-1146.890754	-1299.572399	-1452.252034	-1604.930141
HFB	-230.736740	-383.515896	n/c	-689.023317	-841.764760	-994.502105	-1147.236708	-1299.969525	-1452.700851	-1605.431300
HFS	-227.403681	-378.062156	-528.700224	-679.326550	-829.946123	-980.561507	-1131.174121	-1281.784903	-1432.394193	-1583.002542
HSE06	-231.996280	-385.562630	-539.108377	-692.641998	-846.168459	-999.690419	-1153.209394	-1306.726328	-1460.241723	-1613.756029
LC-wPBE	-232.084992	-385.693521	-539.282145	-692.858060	-846.426155	-999.989189	-1153.548793	-1307.105981	-1460.661394	-1614.215468
M05	-232.053702	-385.658975	-539.242427	-692.813716	-846.377840	-999.937457	-1153.494080	-1307.048647	-1460.601669	-1614.153590
M052X	-232.233286	-385.957817	-539.661458	-693.352342	-847.035544	-1000.713849	-1154.388881	-1308.061631	-1461.732714	-1615.402561
M06	-232.071166	-385.684813	-539.277463	-692.858094	-846.431611	-1000.000642	-1153.566694	-1307.130700	-1460.693170	-1614.254539
M062X	-232.153762	-385.826617	-539.478958	-693.118619	-846.750667	-1000.377864	-1154.001814	-1307.623517	-1461.243551	-1614.862376
M06HF	-232.201349	-385.904814	-539.588608	-693.259104	-846.921366	-1000.578273	-1154.231544	-1307.882246	-1461.531089	-1615.178523
M06L	-232.220968	-385.936212	-539.629601	-693.310923	-846.985275	-1000.655302	-1154.322486	-1307.987746	-1461.651539	-1615.314313
MP2	-231.513388	-384.781465	-538.032507	-691.270024	-844.499883	-997.724826	-1150.946414	-1304.165618	-1457.383128	-1610.599328
mPW1LYP	-232.124615	-385.776997	-539.409015	-693.028991	-846.641833	-1000.250178	-1153.855531	-1307.458843	-1461.060603	-1614.661280
mPW1PBE	-232.112653	-385.752024	-539.370624	-692.977010	-846.576180	-1000.170807	-1153.762422	-1307.351971	-1460.939971	-1614.526867
mPW2PLYPD	-232.008708	-385.589994	-539.151522	-692.700967	-846.243239	-999.780994	-1153.315767	-1306.848506	-1460.379743	-1613.909921
mPW3PBE	-232.096629	-385.722021	-539.326501	-692.918832	-846.504029	-1000.084754	-1153.662518	-1307.238262	-1460.812480	-1614.385623
O3LYP	-232.173031	-385.850636	-539.506868	-693.150999	-846.788112	-1000.420859	-1154.050727	-1307.678642	-1461.305074	-1614.930479
OPBE	-232.156207	-385.824731	n/c	-693.105277	-846.732542	-1000.355542	-1153.975749	-1307.594070	-1461.210953	-1614.826849
OTPSS	-232.159462	-385.830209	-539.478686	-693.114999	-846.744389	-1000.369518	-1153.991859	-1307.612317	-1461.231338	-1614.849376
PBE0	-231.975893	-385.528828	-539.060985	-692.580924	-846.093644	-999.601821	-1153.106986	-1306.610085	-1460.111634	-1613.612079
PDDG	0.040505	0.036639	0.048298	0.069854	0.097356	0.128755	0.162783	0.198878	0.236192	0.274730

PM3	0.040172	0.036074	0.046523	0.066753	0.092867	0.122866	0.155514	0.190183	0.226154	0.263311
PM6	0.038545	0.031250	0.039203	0.056571	0.079847	0.107005	0.136846	0.168643	0.201858	0.236204
tHCTH	-232.202591	-385.882698	-539.541303	-693.187994	-846.827860	-1000.463507	-1154.096384	-1307.727392	-1461.356962	-1614.985550
tHCTHhyb	-232.227777	-385.933858	-539.618874	-693.291772	-846.957602	-1000.619017	-1154.277511	-1307.934024	-1461.589027	-1615.242989
TPSSh	-232.277821	-386.024083	-539.749307	-693.462437	-847.168510	-1000.870177	-1154.568933	-1308.265711	-1461.960987	-1615.655223
VSXC	-232.360608	-386.169609	-539.956623	-693.731318	-847.498932	-1001.262163	-1155.022509	-1308.780913	-1462.537822	-1616.293711
wB97	-232.202438	-385.899607	-539.577046	-693.241806	-846.898750	-1000.550634	-1154.199080	-1307.845119	-1461.489367	-1615.132296
wB97X	-232.189591	-385.876627	-539.543577	-693.197882	-846.844496	-1000.486169	-1154.124509	-1307.760526	-1461.394819	-1615.027848
wB97XD	-232.175163	-385.851865	-539.507998	-693.151630	-846.787779	-1000.419170	-1154.047381	-1307.673393	-1461.297771	-1614.920967
X3LYP	-232.149308	-385.810551	-539.451260	-693.079938	-846.701521	-1000.318643	-1153.932802	-1307.544945	-1461.155552	-1614.765091
XAlpha	-228.904934	-380.529314	-532.132758	-683.724343	-835.309124	-986.889691	-1138.467495	-1290.043438	-1441.617931	-1593.191432

^a calculation failed to converge.

Table S4. Molecular energies (298.15 K and 1 atm) of the cationic compounds at the optimized cationic geometries for the n=1-10 [n]acenes at the x/TZVP//B3LYP/6-31G(d) level of theory (note that semiempirical method energies are at the x//B3LYP/6-31G(d) level of theory).

model chemistry	1	2	3	4	5	6	7	8	9	10
AM1	0.371488	0.365247	0.378195	0.401258	0.430297	0.463096	0.498514	0.535690	0.574206	n/c ^a
B1B95	-231.869138	-385.535928	-539.179421	-692.810840	-846.435404	-1000.055723	-1153.673241	-1307.288829	-1460.903031	n/c
B1LYP	-231.863642	-385.516553	-539.146572	-692.764706	-846.376084	-999.983267	-1153.587684	-1307.190186	-1460.791318	n/c
B2PLYPD	-231.741175	-385.322152	-538.880877	-692.427932	-845.968299	-999.504548	-1153.038110	-1306.569837	-1460.100260	n/c
B3LYP	-231.992816	-385.727402	-539.438624	-693.137978	-846.830629	-1000.519135	-1154.204921	-1307.888825	-1461.571385	n/c
B3P86	-232.721224	-386.922465	-541.100666	-695.266954	-849.426523	-1003.581940	-1157.734634	-1311.885446	-1466.034913	n/c
B3PW91	-231.895876	-385.568994	-539.219162	-692.857440	-846.489007	-1000.116427	-1153.741127	-1307.363946	-1460.985422	n/c
B97D	-231.814914	-385.431231	-539.023694	-692.604646	-846.179215	-999.749872	-1153.318010	-1306.884386	-1460.449516	n/c
B98	-231.892270	-385.562977	-539.210409	-692.845976	-846.474830	-1000.099532	-1153.721506	-1307.341593	-1460.960332	n/c
BHandH	-230.173488	-382.746846	-535.298581	-687.837969	-840.370178	-992.897857	-1145.422505	-1297.945046	-1450.466056	n/c
BHandHLYP	-231.846467	-385.482774	-539.098280	-692.701650	-846.297930	-999.889722	-1153.478483	-1307.065143	-1460.650272	n/c
BLYP	-231.888237	-385.562480	-539.211786	-692.849456	-846.480707	-1000.108041	-1153.732848	-1307.355900	-1460.977713	n/c
BMK	-231.813429	-385.438301	-539.041350	-692.632349	-846.216419	-999.796147	-1153.372982	-1306.947821	-1460.521213	n/c
CAM-B3LYP	-231.846938	-385.489987	-539.111248	-692.720354	-846.322421	-999.920061	-1153.514735	-1307.107358	n/c	n/c
HCTH/147	-231.966564	-385.679314	-539.367780	-693.044532	-846.714817	-1000.381156	-1154.044947	-1307.706972	-1461.367750	n/c
HCTH/407	-231.957199	-385.662065	-539.342931	-693.012050	-846.674684	-1000.333361	-1153.989480	-1307.643828	-1461.296927	n/c
HF	-230.484592	-383.211104	-535.921817	-688.620712	-841.312206	-993.998820	-1146.681971	-1299.362666	-1452.041498	n/c
HFB	-230.535261	-383.316316	-536.073652	-688.819850	-841.559857	-994.296071	-1147.029842	-1299.761902	-1452.492762	n/c
HFS	-227.198872	-377.860018	-528.496005	-679.120411	-829.738447	-980.352590	-1130.964267	-1281.574196	-1432.182906	n/c
HSE06	-231.720853	-385.286741	-538.830238	-692.361884	-845.886813	-999.407579	-1152.925612	-1306.441751	n/c	n/c
LC-wPBE	-231.801796	-385.406959	-538.992960	-692.566603	-846.132999	-999.694730	-1153.253266	-1306.809594	-1460.364294	n/c
M05	-231.788120	-385.390245	-538.970724	-692.539774	-846.102196	-999.660495	-1153.216061	-1306.769734	-1460.322048	n/c
M052X	-231.956338	-385.676378	-539.376672	-693.064730	-846.745855	-1000.422592	-1154.096379	-1307.768133	-1461.438400	n/c
M06	-231.795923	-385.408696	-538.999029	-692.577710	-846.149726	-999.717589	-1153.282700	-1306.845913	-1460.407760	n/c
M062X	-231.874597	-385.543063	-539.192290	-692.829362	-846.459529	-1000.085314	-1153.708160	-1307.328978	-1460.948320	n/c
M06HF	-231.915116	-385.610836	-539.290359	-692.957146	-846.616823	-1000.271815	-1153.923605	-1307.573189	-1461.221128	n/c
M06L	-231.952141	-385.667138	-539.358845	-693.038665	-846.711855	-1000.380968	-1154.047425	-1307.712049	-1461.375372	n/c
MP2	-231.250485	-384.517477	-537.765737	-691.000805	-844.228701	-997.452034	-1150.672292	-1303.890508	-1457.107222	n/c
mPW1LYP	-231.859694	-385.512802	-539.142954	-692.761204	-846.372691	-999.979979	-1153.584499	-1307.187102	-1460.788334	n/c
mPW1PBE	-231.837257	-385.476069	-539.092431	-692.696846	-846.294485	-999.887917	-1153.478582	-1307.067332	-1460.654709	n/c
mPW2PLYPD	-231.742260	-385.323593	-538.882938	-692.430523	-845.971343	-999.507981	-1153.041874	-1306.573891	-1460.104569	n/c
mPW3PBE	-231.817443	-385.442810	-539.045158	-692.635598	-846.219319	-999.798889	-1153.375739	-1306.950707	-1460.524330	n/c
O3LYP	-231.905542	-385.583745	-539.238101	-692.880561	-846.516373	-1000.148102	-1153.777168	-1307.404397	-1461.030320	n/c
OPBE	-231.883682	-385.552328	-539.196552	-692.828941	-846.454807	-1000.076706	-1153.696044	-1307.313614	-1460.929933	n/c
OTPSS	-231.885892	-385.556835	-539.203233	-692.837783	-846.465805	-1000.089857	-1153.711347	-1307.331069	-1460.949539	n/c
PBE0	-231.700303	-385.252743	-538.782644	-692.300597	-845.811774	-999.318747	-1152.822955	-1306.325249	-1459.826172	n/c
PDDG	0.380205	0.373788	0.386023	0.408507	0.437075	0.469476	0.504610	0.541535	0.579888	n/c

PM3	0.380013	0.371842	0.382552	0.403487	0.430475	0.461275	0.494770	0.530052	0.566720	n/c
PM6	0.374473	0.369356	0.380521	0.400468	0.425849	0.454765	0.486241	0.519435	0.553971	n/c
tHCTH	-231.921054	-385.601351	-539.257929	-692.902875	-846.541387	-1000.175969	-1153.808011	-1307.438291	-1461.067326	n/c
tHCTHhyb	-231.949223	-385.655396	-539.338086	-693.008991	-846.673281	-1000.333497	-1153.991052	-1307.646766	-1461.301168	n/c
TPSSh	-232.008999	-385.755221	-539.478196	-693.189374	-846.893937	-1000.594430	-1154.292262	-1307.988258	-1461.682942	n/c
VSXC	-232.095261	-385.903333	-539.687338	-693.459643	-847.225445	-1000.987268	-1154.746504	-1308.503956	-1462.260133	n/c
wB97	-231.929650	-385.623410	-539.297834	-692.960046	-846.615099	-1000.265543	-1153.912832	-1307.557940	-1461.201434	n/c
wB97X	-231.915640	-385.600233	-539.264505	-692.916494	-846.561360	-1000.201692	-1153.838948	-1307.474085	-1461.107667	n/c
wB97XD	-231.902046	-385.577417	-539.231143	-692.872664	-846.507194	-1000.137334	-1153.764538	-1307.389717	-1461.013427	n/c
X3LYP	-231.876747	-385.538857	-539.177711	-692.804674	-846.424907	-1000.040974	-1153.654303	-1307.265737	-1460.875817	n/c
XAlpha	-228.675173	-380.301790	-531.903543	-683.493488	-835.076942	-986.656431	-1138.233395	-1289.808581	-1441.382524	n/c

^a calculation failed to converge.

Table S5. Molecular energies (298.15 K and 1 atm) of the anionic compounds at the optimized anionic geometries for the n=1-10[n]acenes at the x/TZVP//B3LYP/6-31G(d) level of theory (note that semiempirical method energies are at the x//B3LYP/6-31G(d) level of theory).

model chemistry	1	2	3	4	5	6	7	8	9	10]
	[n]acene									
AM1	0.040773	0.036239	0.048913	0.071207	0.099353	0.131388	0.166106	0.202746	0.240802	0.279941
B1B95	-232.143160	-385.808012	n/c ^a	-693.085691	-846.711337	-1000.332499	-1153.950691	-1307.566825	-1461.181481	-1614.795055
B1LYP	-232.132319	-385.782528	n/c	-693.032679	-846.644953	-1000.252853	-1153.857846	-1307.460822	-1461.062348	-1614.662805
B2PLYPD	-232.012420	-385.591359	-539.151297	-692.699542	-846.240864	-999.777859	-1153.312009	-1306.844208	-1460.375027	-1613.904838
B3LYP	-232.274206	-386.005854	-539.718000	-693.418442	-847.111985	-1000.801202	-1154.487555	-1308.171923	-1461.854868	-1615.536764
B3P86	-233.045654	-387.244981	-541.424534	-695.592181	-849.752827	-1003.909090	-1158.062454	-1312.213813	-1466.363732	-1620.512598
B3PW91	-232.178998	-385.850234	n/c	-693.141335	-846.773959	-1000.402209	-1154.027565	n/c	-1461.272840	-1614.893706
B97D	-232.090088	-385.703270	n/c	-692.878690	-846.454085	-1000.025401	-1153.594038	-1307.160829	-1460.726302	-1614.290800
B98	-232.169573	-385.837940	n/c	-693.123420	-846.753289	-1000.378792	-1154.001403	-1307.622011	-1461.241184	-1614.859294
BHandH	-230.438434	-383.010952	-535.564199	-688.105108	-840.638523	-993.167150	-1145.692567	-1298.215737	-1450.737275	-1603.257627
BHandHLYP	-232.111827	-385.747227	-539.363885	-692.968546	-846.565871	-1000.158488	-1153.747937	-1307.335162	-1460.920774	-1614.505192
BLYP	-232.160382	-385.830038	n/c	-693.118533	-846.750520	-1000.378450	-1154.003716	-1307.627146	-1461.249264	-1614.870410
BMK	-232.089608	-385.713878	-539.318416	-692.910874	-846.496092	-1000.076720	-1153.654284	-1307.229714	-1460.803610	-1614.376359
CAM-B3LYP	-232.129049	-385.770447	-539.392637	-693.002874	-846.605877	-1000.204270	-1153.799573	-1307.392714	-1460.984293	-1614.574717
HCTH/147	-232.252840	-385.963024	-539.652730	-693.330686	-847.001910	-1000.668981	-1154.333332	-1307.995813	-1461.656958	-1615.317122
HCTH/407	-232.246259	-385.949093	-539.631289	-693.301652	-846.965240	-1000.624653	-1154.281333	-1307.936135	-1461.589595	-1615.242075
HF	-230.685276	-383.413120	-536.125011	-688.825329	-841.517963	-994.205478	-1146.889435	-1299.570823	-1452.250300	-1604.928315
HFB	-230.749126	-383.525279	n/c	-689.029916	-841.770563	-994.507310	-1147.241486	-1299.973886	-1452.705021	-1605.435192
HFS	-227.412321	-378.068686	n/c	-679.331370	-829.950372	-980.565296	-1131.177544	-1281.787951	-1432.397035	n/c
HSE06	-232.001138	-385.565604	-539.110556	-692.643620	-846.169661	-999.691295	-1153.210009	-1306.726702	-1460.241945	-1613.756125
LC-wPBE	-232.089676	-385.696136	-539.283505	-692.858609	-846.426130	-999.988751	-1153.548049	-1307.105003	-1460.660248	-1614.214220
M05	-232.059250	-385.662181	-539.244810	-692.815553	-846.379270	-999.938570	-1153.494939	-1307.049272	-1460.602141	-1614.153932
M052X	-232.238094	-385.960618	n/c	-693.353279	-847.035932	-1000.713835	-1154.388562	-1308.061072	-1461.731984	-1615.401708
M06	-232.075801	-385.687469	n/c	-692.859398	-846.432517	-1000.001246	-1153.567059	-1307.130846	-1460.693174	-1614.254435
M062X	-232.158672	-385.829720	-539.480923	-693.119806	-846.751299	-1000.378094	-1154.001748	-1307.623211	-1461.243094	-1614.861804
M06HF	-232.206372	-385.907864	-539.590028	-693.259410	-846.920894	-1000.577254	-1154.230139	-1307.880571	-1461.529225	-1615.176534
M06L	-232.225711	-385.939021	-539.631772	-693.312665	-846.986688	-1000.656452	-1154.323419	-1307.988460	-1461.652124	-1615.314783
MP2	-231.515288	-384.784207	-538.034188	-691.271183	-844.500486	-997.724928	-1150.946073	-1304.164900	-1457.382053	-1610.597919
mPW1LYP	-232.130105	-385.780472	-539.411525	-693.030859	-846.643239	-1000.251240	-1153.856333	-1307.459408	-1461.061032	-1614.661586
mPW1PBE	-232.117506	-385.754968	-539.372759	-692.978587	-846.577337	-1000.171642	-1153.762999	-1307.352314	-1460.940161	-1614.526933
mPW2PLYPD	-232.013610	-385.593164	-539.153743	-692.702552	-846.244353	-999.781758	-1153.316261	-1306.848768	-1460.379858	-1613.909911
mPW3PBE	-232.101719	-385.725194	-539.328877	-692.920658	-846.505441	-1000.085845	-1153.663352	-1307.238856	-1460.812924	-1614.385937
O3LYP	-232.178576	-385.854262	n/c	-693.153349	-846.790069	-1000.422505	-1154.052123	-1307.679798	-1461.306085	-1614.931351
OPBE	-232.162100	-385.828743	n/c	-693.108243	-846.735143	-1000.357832	-1153.977772	-1307.595826	-1461.212537	-1614.828261
OTPSS	-232.165447	-385.834278	n/c	-693.118016	-846.747041	-1000.371861	-1153.993936	-1307.614128	-1461.232979	-1614.850845
PBE0	-231.980778	-385.531831	n/c	-692.582563	-846.094860	-999.602711	-1153.107613	-1306.610474	-1460.111867	-1613.612185
PDDG	0.041147	0.035394	0.047841	0.069970	0.097965	0.129811	0.164302	0.200677	0.238415	0.277225

PM3	0.041181	0.034636	0.045719	0.066409	0.092940	0.123327	0.156367	0.191303	0.227623	0.265014
PM6	0.038350	0.028561	0.037342	0.055365	0.079103	0.106635	0.136789	0.168827	0.202259	0.236777
tHCTH	-232.208015	-385.886280	-539.544210	-693.190437	-846.829943	-1000.465299	-1154.097935	-1307.728699	-1461.358126	-1614.986572
tHCTHhyb	-232.234018	-385.938021	n/c	-693.294288	-846.959632	-1000.620676	-1154.278883	-1307.935129	-1461.589973	-1615.243780
TPSSh	-232.283829	-386.027944	-539.752275	-693.464794	-847.170411	-1000.871725	-1154.570202	-1308.266720	-1461.961836	n/c
VSXC	-232.367523	-386.173863	-539.959928	-693.733967	-847.501084	-1001.263926	-1155.023964	-1308.782071	-1462.538797	-1616.294510
wB97	-232.208481	-385.903591	-539.579521	-693.243291	-846.899537	-1000.550918	-1154.199001	-1307.844756	-1461.488816	-1615.131605
wB97X	-232.194909	-385.879976	-539.545636	-693.199113	-846.845141	-1000.486391	-1154.124421	-1307.760190	-1461.394321	-1615.027232
wB97XD	-232.180270	-385.854962	-539.509987	-693.152918	-846.788571	-1000.419601	-1154.047540	-1307.673325	-1461.297555	-1614.920637
X3LYP	-232.154799	-385.814048	-539.453836	-693.081896	-846.703030	-1000.319814	-1153.933716	-1307.545620	-1461.156090	-1614.765503
XAlpha	-228.909604	-380.532433	n/c	-683.726642	-835.311108	-986.891404	-1138.468968	-1290.044654	-1441.618989	-1593.192355

^a calculation failed to converge.

Table S6. Molecular energies (298.15 K and 1 atm) of the neutral compounds at the optimized neutral geometries for the n=1-10[n]acenes at the B3LYP/y//B3LYP/6-31G(d) level of theory.

basis set	1	2	3	4	5	[n]acene					8	9	10]
6-31G(d)	-232.248659	-385.892730	-539.530524	-693.165812	-846.799944	-1000.433489	-1154.066724	-1307.699787	-1461.332757	-1614.965672			
6-311++G(d,p)	-232.311251	-385.988898	-539.660288	-693.329253	-846.996945	-1000.664088	-1154.330850	-1307.997475	n/c ^a	-1615.330385			
6-311++G(2d,2p)	-232.320440	-386.003624	-539.680623	-693.355124	-847.028415	-1000.701094	-1154.373439	-1308.045594	-1461.717646	-1615.389643			
SVP	-232.084562	-385.619041	-539.147373	-692.673251	-846.197987	-999.722142	-1153.245987	-1306.769666	-1460.293243	-1613.816774			
TZV	-232.261006	-385.906810	n/c	-693.183462	-846.819346	-1000.454631	-1154.089595	-1307.724383	-1461.359079	-1614.993718			
TZVP	-232.328219	-386.016675	-539.698972	-693.378770	-847.057382	-1000.735385	-1154.413064	-1308.090554	-1461.767954	-1615.445282			
cc-pVDZ	-232.262815	-385.915685	-539.562359	-693.206530	-846.849535	-1000.491950	-1154.134049	-1307.775974	-1461.417799	-1615.059573			
cc-pVTZ	-232.333067	-386.025123	-539.711016	-693.394406	-847.076603	n/c	-1154.439440	-1308.120500	-1461.801470	-1615.482363			

^a calculation failed to converge.

Table S7. Molecular energies (298.15 K and 1 atm) of the cationic compounds at the optimized neutral geometries for the n=1-10[n]acenes at the B3LYP/y//B3LYP/6-31G(d) level of theory.

basis set	1	2	3	4	5	[n]acene					8	9	10
6-31G(d)	-231.917531	-385.610215	-539.277934	-692.933321	-846.581828	-1000.226111	-1153.867639	-1307.507246	-1461.145489	-1614.782723			
6-311++G(d,p)	-231.970591	-385.696265	-539.397220	-693.086087	-846.768032	-1000.445851	-1154.120873	-1307.794037	n/c ^a	-1615.136548			
6-311++G(2d,2p)	-231.980611	-385.711651	-539.418193	-693.112585	-846.800135	-1000.483492	-1154.164103	-1307.842799	-1461.520129	-1615.196459			
SVP	-231.744669	-385.327878	-538.886092	-692.432033	-845.971126	-999.506015	-1153.038157	-1306.568391	-1460.097253	-1613.625116			
TZV	-231.918701	-385.613852	-539.283617	-692.940914	-846.591252	-1000.237324	-1153.880614	-1307.521972	-1461.161960	-1614.800936			
TZVP	-231.987818	-385.724466	-539.436393	-693.136116	-846.829005	-1000.517692	-1154.203638	-1307.887667	-1461.570342	-1615.251999			
cc-pVDZ	-231.926091	-385.627292	-539.303716	-692.967884	-846.625207	-1000.278327	-1153.928702	-1307.577166	-1461.224263	-1614.870357			
cc-pVTZ	-231.993999	-385.734181	-539.449731	-693.153080	-846.849582	n/c	-1154.231411	-1307.919024	-1461.605282	-1615.290512			

^a calculation failed to converge.

Table S8. Molecular energies (298.15 K and 1 atm) of the anionic compounds at the optimized neutral geometries for the n=1-10[n]acenes at the B3LYP/y//B3LYP/6-31G(d) level of theory.

basis set	1	2	3	4	5	6	7	8	9	10]
6-31G(d)	-232.164070	-385.859739	-539.530746	-693.188520	-846.838767	-1000.484356	-1154.126874	-1307.767321	-1461.406178	-1615.043956
6-311++G(d,p)	-232.289282	-385.977676	-539.678854	-693.368664	-847.051549	-1000.730141	-1154.405784	-1308.079495	-1461.751659	-1615.422759
6-311++G(2d,2p)	-232.298861	-385.992869	-539.699521	-693.394809	-847.083253	-1000.767363	-1154.448573	-1308.127809	-1461.805523	-1615.482205
SVP	-232.013682	-385.597780	-539.158511	-692.706447	-846.247039	-999.783066	-1153.316072	-1306.847043	-1460.376438	-1613.904776
TZV	-232.196855	-385.888917	-539.559673	-693.218182	-846.869528	-1000.516396	-1154.160294	-1307.802191	-1461.442551	-1615.081867
TZVP	-232.268556	-386.002221	-539.715294	-693.416356	-847.110350	-1000.797180	-1154.486519	-1308.171130	-1461.854212	-1615.536238
cc-pVDZ	-232.189687	-385.892197	-539.571342	-693.237645	-846.896571	-1000.550911	-1154.202217	-1307.851476	-1461.499155	-1615.145768
cc-pVTZ	-232.270315	-386.008871	-539.726053	-693.430974	-847.128726	-1000.821990	-1154.512277	-1308.200540	-1461.887264	-1615.572914

^a calculation failed to converge.

Table S9. Molecular energies (298.15 K and 1 atm) of the cationic compounds at the optimized cationic geometries for the n=1-10 [n]acenes at the B3LYP//B3LYP/6-31G(d) level of theory.

basis set	1	2	3	4	5	6	7	8	9	10
6-31G(d)	-231.923065	-385.613632	-539.280491	-692.935395	-846.583570	-1000.227593	-1153.868899	-1307.508326	-1461.146414	n/a ^a
6-311++G(d,p)	-231.975768	-385.699432	-539.399570	-693.088027	-846.769684	-1000.447259	-1154.122054	-1307.795090	n/a	n/a
6-311++G(2d,2p)	-231.985547	-385.714608	-539.420433	-693.114467	-846.801778	-1000.484957	-1154.165385	-1307.843985	-1461.521197	n/a
SVP	-231.750117	-385.331376	-538.888692	-692.434106	-845.972824	-999.507410	-1153.039301	-1306.569321	-1460.098011	n/a
TZV	-231.924392	-385.617177	-539.286000	-692.942787	-846.592792	-1000.238617	-1153.881698	-1307.522892	-1461.162743	n/a
TZVP	-231.992816	-385.727402	-539.438624	-693.137978	-846.830629	-1000.519135	-1154.204921	-1307.888825	-1461.571385	n/a
cc-pVDZ	-231.931571	-385.630786	-539.306296	-692.969935	-846.626887	-1000.279711	-1153.929839	-1307.578097	-1461.225024	n/a
cc-pVTZ	-231.998898	-385.737066	-539.451954	-693.154959	-846.851242	-1000.543367	-1154.232756	-1307.920255	-1461.606402	n/a

^a calculation failed to converge.

Table S10. Molecular energies (298.15 K and 1 atm) of the anionic compounds at the optimized anionic geometries for the n=1-10[n]acenes at the B3LYP/y//B3LYP/6-31G(d) level of theory.

basis set	1	2	3	4	5	6	7	8	9	10
6-31G(d)	-232.171361	-385.864558	-539.534441	-693.191493	-846.841217	-1000.486408	-1154.128620	-1307.768779	-1461.407470	-1615.045079
6-311++G(d,p)	-232.263724	-385.981561	-539.681912	-693.371053	-847.053529	-1000.731732	-1154.407058	-1308.080557	-1461.752536	-1615.423516
6-311++G(2d,2p)	-232.273017	-385.996104	-539.702004	-693.396720	-847.084742	-1000.768517	-1154.449453	-1308.128471	-1461.806048	n/a ^a
SVP	-232.021525	-385.603268	-539.162864	-692.710050	-846.250085	-999.785680	-1153.318350	-1306.849003	-1460.378213	-1613.906357
TZV	-232.203567	-385.893315	-539.562982	-693.220798	-846.871657	-1000.518165	-1154.161797	-1307.803443	n/a	-1615.082841
TZVP	-232.274206	-386.005854	-539.718000	-693.418442	-847.111985	-1000.801202	-1154.487555	-1308.171923	-1461.854868	-1615.536764
cc-pVDZ	-232.197563	-385.897622	-539.575597	-693.241134	-846.899497	-1000.553404	-1154.204376	-1307.853321	-1461.500815	-1615.147238
cc-pVTZ	-232.275834	-386.012270	-539.728507	-693.432821	-847.130139	-1000.823079	-1154.513119	-1308.201152	-1461.887744	-1615.573274

^a calculation failed to converge.

Table S11. Molecular enthalpies (298.15 K and 1 atm) of the neutral, cationic, and anionic n=1-10 [n]acenes at the B3LYP/y//B3LYP/6-31G(d) level of theory.

n	neutral	cationic	anionic
1	-232.205860	-231.872304	-232.073935
2	-385.737156	-385.458104	-385.714692
3	-539.325605	-539.075005	-539.334223
4	-692.911636	-692.680307	-692.941488
5	-846.496563	-846.279051	-846.541681
6	-1000.080942	-999.873751	-1000.137498
7	-1153.665034	-1153.465829	c/e ^a
8	-1307.248984	c/e	c/e
9	-1460.832841	c/e	c/e
10	-1614.416672	c/e	c/e

^a calculation not completed due to computational expense.