

*Supplementary Materials to the article:*

**Structural Descriptors of Benzenoid Hydrocarbons: a Mismatch between the Estimates and Parity Effects in Helicenes**

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Section SA. Numerical data associated with Figure 11.

Helicene	$\alpha$ (Å <sup>3</sup> )*	$E_{\text{HOMO}}$ (kJ/mol)		$E_{\text{LUMO}}$ (kJ/mol)	
		PBE/3 $\zeta$	$\omega$ B97X-D3/6-311G(d,p)	PBE/3 $\zeta$	$\omega$ B97X-D3/6-311G(d,p)
[4]	41.81	-509.3	-767.8	-228.5	41.8
[5]	48.92	-505.9	-762.6	-228.5	41.5
[6]	55.26	-499.8	-756.8	-241.8	21.8
[7]	61.31	-493.1	-747.1	-244.2	19.4
[8]	67.59	-487.1	-736.8	-245.6	14.4
[9]	73.91	-482.3	-734.2	-247.7	11.8
[10]	80.13	-476.6	-725.5	-247.5	9.5
[11]	86.29	-472.3	-717.7	-248.8	8.7
[12]	92.42	-469.1	-715.6	-247.6	8.4
[13]	41.81	-463.7	-708.7	-248.3	9.2

\* Calculated with the PBE/3 $\zeta$  method.

## Section SB. Optimized geometries of the helicene molecules.

Helicene	DFT method	
	PBE/3 $\zeta$	$\omega$ B97X-D3/6-311G(d,p)
<b>[4]</b>	6 -1.98728108 -3.13174248 -0.55193478	6 -1.7413287103 -3.1981176067 -0.8157149837
	6 -0.97609669 -3.82882690 -1.18475318	6 -0.6615612917 -3.7966726191 -1.4092263352
	6 -1.81521559 -1.78017724 -0.16183007	6 -1.6752712291 -1.8639954834 -0.3524797608
	6 -0.54434258 -1.13596082 -0.35185438	6 -0.4549146466 -1.1476144447 -0.4303594884
	6 0.43935344 -1.85954928 -1.07880628	6 0.6156481206 -1.7701046176 -1.1225681539
	6 0.23162027 -3.16794991 -1.48316836	6 0.5184791054 -3.0549840217 -1.5958365753
	6 -2.91985464 -1.03573120 0.35052642	6 -2.8566145339 -1.2088055364 0.1179772651
	6 -2.79795671 0.30459869 0.58389431	6 -2.8337812009 0.1106674451 0.4077706823
	6 -1.53787792 0.96696603 0.45505217	6 -1.6079146289 0.8501668671 0.3847318763
	6 -0.36972323 0.23260251 0.10891674	6 -0.3974911860 0.2090043726 0.0949584346
	6 -1.46706021 2.37698364 0.67859036	6 -1.6382528017 2.2543693138 0.6640092562
	6 -0.27984178 3.04755497 0.59703439	6 -0.5022669472 2.9853439888 0.6852872942
	6 0.94113779 2.32988691 0.42071694	6 0.7699690587 2.3422659611 0.5658598817
	6 0.91384655 0.90392798 0.24149790	6 0.8352029752 0.9451561814 0.3382329403
	6 2.16061211 0.22500940 0.30750880	6 2.1062295524 0.3295775131 0.4747188715
	6 2.18298936 3.00869417 0.49518436	6 1.9579939727 3.0839706054 0.7584306074
	6 3.37926030 2.31776977 0.47446826	6 3.1794969863 2.4655978934 0.8037480246
	6 3.35906649 0.91027325 0.41990811	6 3.2437504748 1.0652411449 0.6979263989
	1 -2.95481420 -3.60370994 -0.37035537	1 -2.6821585052 -3.7323226285 -0.7156936840
	1 -1.12531161 -4.86528540 -1.48865151	1 -0.7253564390 -4.8176470001 -1.7710403104
	1 1.35765409 -1.36130857 -1.37729645	1 1.5129179958 -1.2059091199 -1.3369096338
	1 1.00590050 -3.68215132 -2.05385470	1 1.3543855515 -3.4935737878 -2.1314242813
	1 -3.87468386 -1.54476082 0.49267921	1 -3.7805972900 -1.7766438009 0.1773923865
	1 -3.66022515 0.89515495 0.89863080	1 -3.7433621830 0.6320573629 0.6919368357
	1 -2.39413476 2.91133785 0.89381886	1 -2.6039238330 2.7237698831 0.8285194934
	1 -0.23789434 4.13045454 0.72582996	1 -0.5302817159 4.0581197072 0.8528380036
	1 2.17339301 4.09494925 0.60384589	1 1.8797738027 4.1587658529 0.8974827588
	1 4.32743359 2.85176206 0.54293096	1 4.0840667884 3.0435029822 0.9628600932
	1 2.17717409 -0.86123496 0.32684270	1 2.1808175502 -0.7491157462 0.4636739389
	1 4.29287338 0.35046318 0.48462814	1 4.1963452167 0.5579298275 0.8128983730
<b>[5]</b>	6 -3.50223446 -0.44986784 -0.34164453	C -3.4606845457 -0.7066947180 -0.1472159515

	6 -2.48780274 0.40742511 0.18966389	6 -2.4883341103 0.2939367800 0.1865770579
	6 -3.20021653 -1.68872821 -0.83099002	6 -3.0929446622 -1.9800824791 -0.4039075449
	6 -1.11509860 0.02193965 0.12840161	6 -1.1169870680 -0.0117005990 0.1559338116
	6 -0.83691037 -1.38070953 -0.15651786	6 -0.7527527082 -1.4255623150 0.1299454182
	6 -1.87819505 -2.21087289 -0.68960708	6 -1.7336655276 -2.3878829362 -0.2047885245
	6 -2.86185217 1.63000774 0.81707835	6 -2.9251502307 1.5891562598 0.5826762183
	6 -1.91406357 2.42608452 1.40183234	6 -2.0239456842 2.5259295603 0.9698651619
	6 -0.52895927 2.15457582 1.21200335	6 -0.6303650194 2.2980520167 0.7928547813
	6 -0.11704406 1.02444863 0.44401273	6 -0.1747758486 1.0836381528 0.2518350828
	6 0.44472006 3.04638314 1.76240385	6 0.3026022791 3.3310930606 1.1399913613
	6 1.77552688 2.89850616 1.49311101	6 1.6188971845 3.2047084438 0.8687067281
	6 2.20842052 1.93032587 0.53623247	6 2.0880986289 2.0931635544 0.0954536623
	6 1.25854492 1.02260399 -0.03946286	6 1.1912477666 1.0606250633 -0.2645780382
	1 -3.92146468 1.88430965 0.87534648	1 -3.9920154502 1.7877069499 0.6276256441
	1 -2.19935942 3.31402016 1.96841884	1 -2.3502388624 3.4860637350 1.3587216638
	1 0.09390511 3.85331059 2.40829015	1 -0.0812050306 4.2190955872 1.6340273732
	1 2.51532459 3.56685805 1.93682551	1 2.3271470286 3.9765592362 1.1553688605
	6 3.55299139 1.92100215 0.08570753	6 3.4146530705 2.0767716400 -0.3940654293
	6 1.68615413 0.25661844 -1.15470743	6 1.6296625917 0.1265405092 -1.2355491242
	6 0.38366634 -2.01434660 0.19286264	6 0.5076159835 -1.9030756058 0.5661229152
	6 -1.61022937 -3.57099032 -0.98827541	6 -1.3903036565 -3.7590096609 -0.2417412649
	6 0.60504508 -3.35571313 -0.06560561	6 0.8080202732 -3.2417271510 0.5624735100
	6 -0.38482705 -4.13783979 -0.69549948	6 -0.1394102740 -4.1836951273 0.1215081211
	1 1.15845335 -1.43459749 0.68824744	1 1.2454054786 -1.1982110688 0.9276522475
	1 -2.41031337 -4.17439938 -1.42130256	1 -2.1527392581 -4.4769343441 -0.5310732107
	1 1.55143332 -3.81044436 0.22917317	1 1.7791905003 -3.5751635288 0.9136794243
	1 -0.19591855 -5.18894482 -0.91574621	1 0.1103211219 -5.2396725553 0.1044843350
	6 2.99349022 0.29975653 -1.60649431	6 2.9086671945 0.1522788218 -1.7305385089
	6 3.94934297 1.11067355 -0.96067530	6 3.8279595057 1.1184279344 -1.2819307608
	1 -4.53100443 -0.08519762 -0.34643698	1 -4.5036857579 -0.4069899885 -0.1946335735
	1 -3.97505784 -2.32736182 -1.25832963	1 -3.8285641279 -2.7295134203 -0.6809453626
	1 4.26384163 2.60011983 0.56030095	1 4.0947335423 2.8632096925 -0.0785113581
	1 0.96542025 -0.36891887 -1.67535639	1 0.9331802173 -0.6123893130 -1.6104924747
	1 3.28150439 -0.29374436 -2.47490215	1 3.2068732292 -0.5723276217 -2.4813722980
	1 4.98276567 1.12370896 -1.30835760	1 4.8434895822 1.1236820128 -1.6641609910
[6]	6 -1.41199255 -3.33523393 0.20796651	C -1.2392630825 -3.2064629777 0.6133211983
	6 -0.17571746 -3.87943983 0.66164684	6 0.0247115846 -3.6178906121 1.1267207867

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6	0.97666669	-3.14905858	0.55471277	6	1.1228277024	-2.8511337709	0.9236235786
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6	2.14112449	-1.03325593	0.06272218	6	2.1666048808	-0.7551349130	0.1548610837
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6	-2.57719707	-4.16517782	0.18170404	6	-2.3631596415	-4.0918136809	0.7188131602
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6	-2.65482903	-0.49945822	-1.93204701	6	-2.6272624965	-0.7876487788	-1.8802727976
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1	-4.63000727	-4.36789989	-0.39374879	1	-4.3946122991	-4.4624739270	0.2244603042
6	-3.76432562	-0.19469628	-2.70146227	6	-3.7546539745	-0.6301896685	-2.6459505855
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	1 -5.78477478 -2.79623938 -1.83463335 1 -3.73833942 0.67281473 -3.36174750 1 -5.79802561 -0.74109203 -3.23684502	1 -5.6502104597 -3.1374597415 -1.3744834398 1 -3.7749336970 0.1308798740 -3.4192097575 1 -5.7730981521 -1.3095242104 -3.0364725923
[7]	6 0.44187248 -3.12708688 0.66314864 6 1.70231771 -3.68017507 1.03393364 6 0.35331333 -1.76358080 0.23757812 6 1.47420311 -0.89350784 0.56448227 6 2.75124002 -1.51510143 0.74004638 6 2.83818746 -2.92058086 0.96182638 6 1.40479767 0.54455137 0.74658710 6 2.60744739 1.29483092 0.59928143 6 3.86731458 0.62907821 0.54208058 6 3.93867183 -0.72704631 0.70939785 6 0.21038929 1.27140915 1.14904070 6 0.20184033 2.70368576 1.07394099 6 1.39236581 3.40339565 0.70930153 6 2.56537938 2.72306538 0.54441959 6 -0.92024475 0.64450645 1.73118508 6 -2.03179359 1.37133980 2.12118578 6 -2.07362151 2.76906228 1.94468081 6 -0.96397161 3.42110395 1.44226444 6 -0.72860461 -3.93972850 0.70235890 1 1.74661779 -4.73372746 1.31451261 6 -0.83524126 -1.37326455 -0.49775273 1 3.82168317 -3.36095977 1.13347507 1 4.77223825 1.23042476 0.44072455 1 4.90172052 -1.23394489 0.78900063 1 1.36144662 4.49204493 0.63912988 1 3.49946094 3.25822234 0.36427578 1 -0.90500957 -0.42867121 1.89979029 1 -2.87696815 0.85550964 2.57823896 1 -2.96016359 3.33282065 2.23666787 1 -0.95396668 4.50904799 1.35267735 6 -2.00938869 -2.16509175 -0.33771437 6 -1.93737960 -3.43501282 0.30682704 1 -0.64238310 -4.95799017 1.08505964 6 -0.89551258 -0.27600259 -1.45136702	6 0.4728960736 -3.0076040827 1.1221146473 6 1.7323239035 -3.4897831297 1.5912509761 6 0.3839219137 -1.7371708203 0.5204584107 6 1.4964465937 -0.8202727836 0.7252743649 6 2.7555248104 -1.3821529025 1.0128140498 6 2.8500273121 -2.7406098511 1.4420930275 6 1.4083771549 0.6249499893 0.6564475435 6 2.5832578284 1.3461155556 0.3982815066 6 3.8530786397 0.7034872611 0.4898596140 6 3.9352826824 -0.5921613236 0.8799237365 6 0.1876742848 1.3859475859 0.8849943706 6 0.1414451724 2.7445053019 0.4990394239 6 1.3301424523 3.3878871016 0.0231632754 6 2.5127307432 2.7349993908 0.0471840197 6 -0.9342525309 0.8580981834 1.5672332137 6 -2.0746979294 1.5999294644 1.7485422870 6 -2.1522637611 2.9159251020 1.2584356275 6 -1.0547172758 3.4796289859 0.6621113927 6 -0.6943680234 -3.8150743724 1.2594624535 1 1.7794292872 -4.4910116062 2.0091260027 6 -0.8057615571 -1.4475552935 -0.2562351701 1 3.8272715666 -3.1339884478 1.7062971011 1 4.7489786742 1.2904694520 0.3093704443 1 4.8979196678 -1.0641834843 1.0536099059 1 1.2744553583 4.4277065689 -0.2858024721 1 3.4347122233 3.2428859408 -0.2214413170 1 -0.8888997014 -0.1426764233 1.9770006501 1 -2.9182329002 1.1673972832 2.2769157857 1 -3.0636578105 3.4910883723 1.3869093829 1 -1.0775392102 4.5121499424 0.3248688601 6 -1.9654249141 -2.1914575754 0.0070484831 6 -1.8912044538 -3.3733920090 0.8014825103 1 -0.6090647339 -4.7679581138 1.7735124122 6 -0.8650096439 -0.4644501673 -1.3291970500

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