

SUPPORTING INFORMATION

Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?

Ricardo Pino-Rios^{*a}, Rodrigo Báez-Grez^b, Miquel Solà^{*c}

^aLaboratorio de Química teórica, Facultad de Química y Biología, Universidad de Santiago de Chile (USACH), Región Metropolitana, Chile; ricardo.pino@usach.cl

^bComputational and Theoretical Chemistry Group, Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, República 498, Santiago, Chile.

^cInstitute of Computational Chemistry and Catalysis, University of Girona, 17003 Girona, Catalonia, Spain; miquel.sola@udg.edu

Figures and table	Pages
Figures S1 – S9. Bond lengths for studied Acenes and Phenacenes for both singlet and triplet state at the UB3LYP/6-311G** level.	S2 – S8
Table S1. $\langle S^2 \rangle$ Values for all PAHS studied in this work in triplet state obtained at the UB3LYP/6-311G** level.	S9
Table S2. Correlation factors between Mulliken spin densities at DFT and CCSD(T) levels at the triplet state for systems $n = 3 - 5$	S9
Table S3. T_1 test computed at the CCSD(T) level for the triplet state for systems $n = 3 - 5$.	S9
Figure S10. Linear and quadratic adjustment between the number of rings and computed energy differences between acenes and phenacenes in singlet and triplet states.	S10
Table S4. ZPE-corrected singlet-triplet energy gaps (in kcal.mol ⁻¹) of acenes for closed and open shell states at the (U)B3LYP/6-311G(d,p) level.	S10
Figures S11 and S12. NICS _{zz} , delocalization indexes and HOMA computed descriptors for anthracene and phenanthrene in both singlet and triplet states.	S11 – S12
Figure S13. Spin density isosurfaces for [n]acenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.	S12
Figure S14. MCI values in both singlet and triplet states for [n]acenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.	S13
Figures S15 – S17. PDI, FLU and HOMA values in both singlet and triplet states for [n]acenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.	S13 -S14
Figure S18. MICD vector maps in both singlet and triplet states for [n]acenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.	S15
Figures S19 and S20. NICS _{zz} (0) and NICS _{zz} (1) values in both singlet and triplet states for [n]acenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.	S15 – S16
Figure S21. Spin density isosurfaces for [n]acenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.	S16
Figure S22. MCI values in both singlet and triplet states for [n]acenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.	S17
Figures S23 – S25. PDI, FLU and HOMA values in both singlet and triplet states for [n]phenacenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.	S17 – S18
Figure S26. MICD vector maps for vertical triplet state for [n]phenacenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.	S19
Figure S27. MCI values for both vertical and adiabatic triplet states of [n]phenacenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.	S19
Approximations done for the calculation of the weights of the antiaromatic Baird π -doublets, π -sextets, π -dectets,... in acenes	S20
Cartesian Coordinates	S21

Figure S1. Bond lengths (in Å) for Benzene and anthracene for both singlet and triplet state at the UB3LYP/6-311G** level.

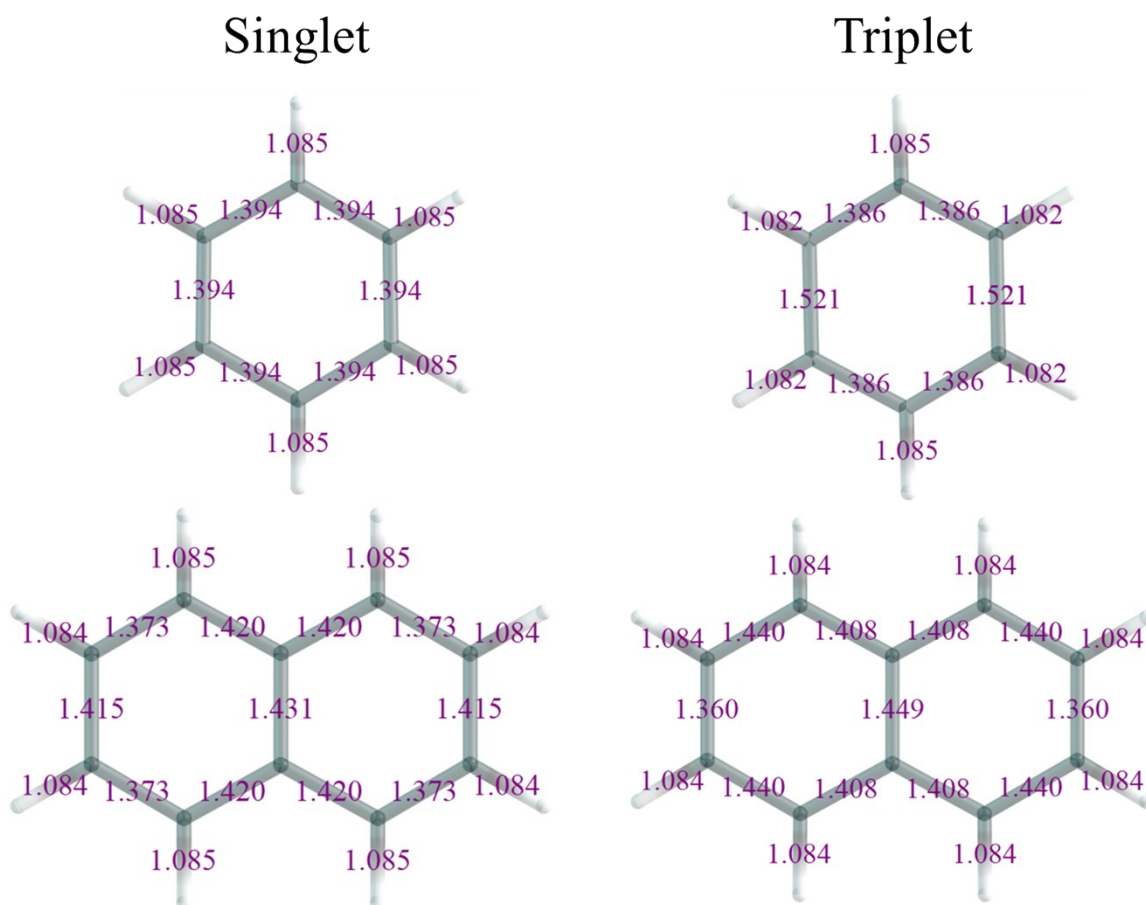


Figure S2. Bond lengths (in Å) for [3]acene and [3]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

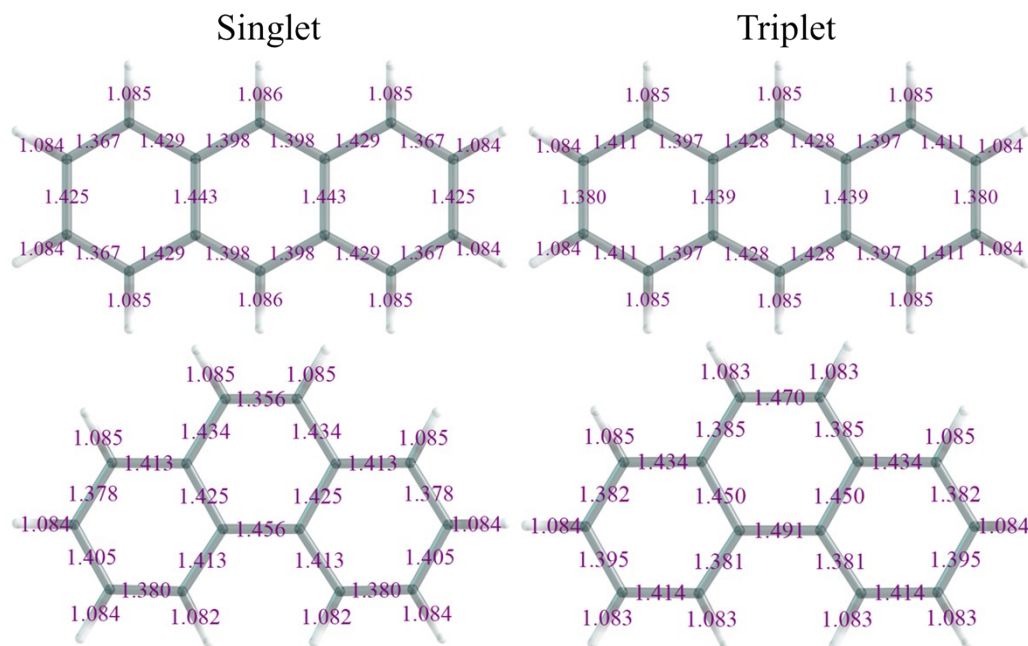


Figure S3. Bond lengths (in Å) for [4]acene and [4]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

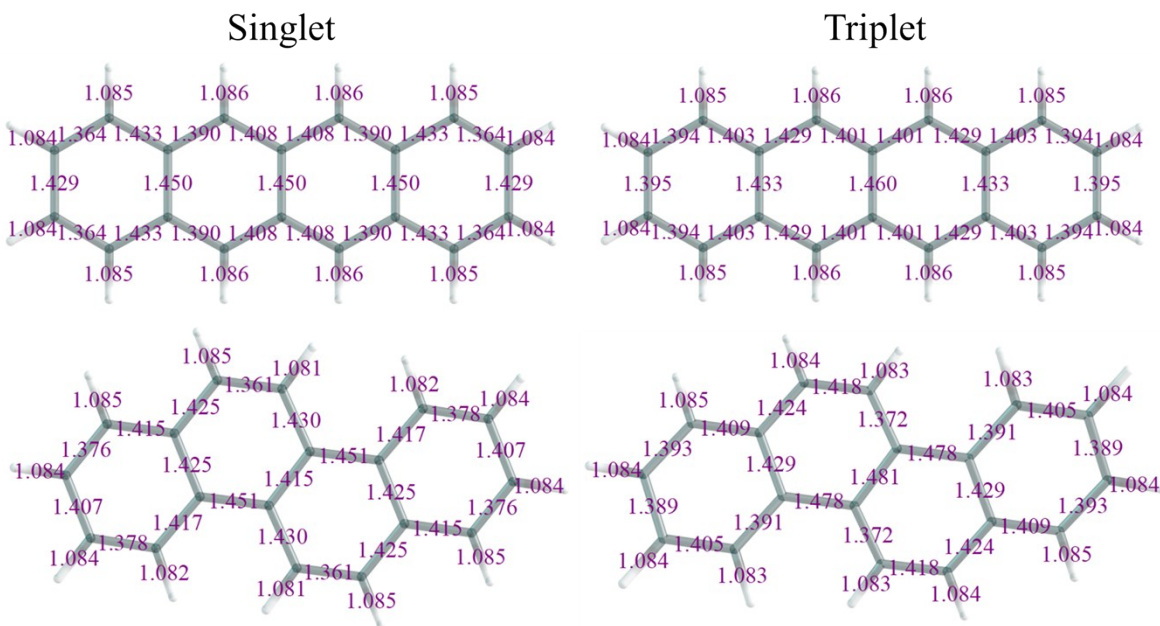


Figure S4. Bond lengths (in Å) for [5]acene and [5]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

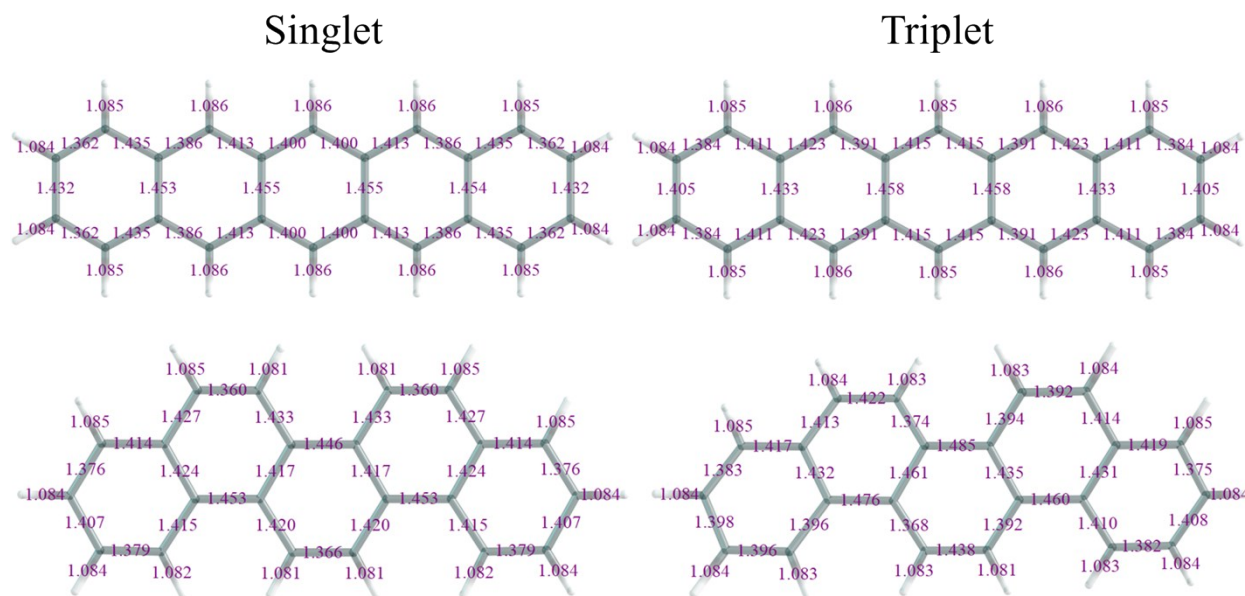


Figure S5. Bond lengths (in Å) for [6]acene and [6]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

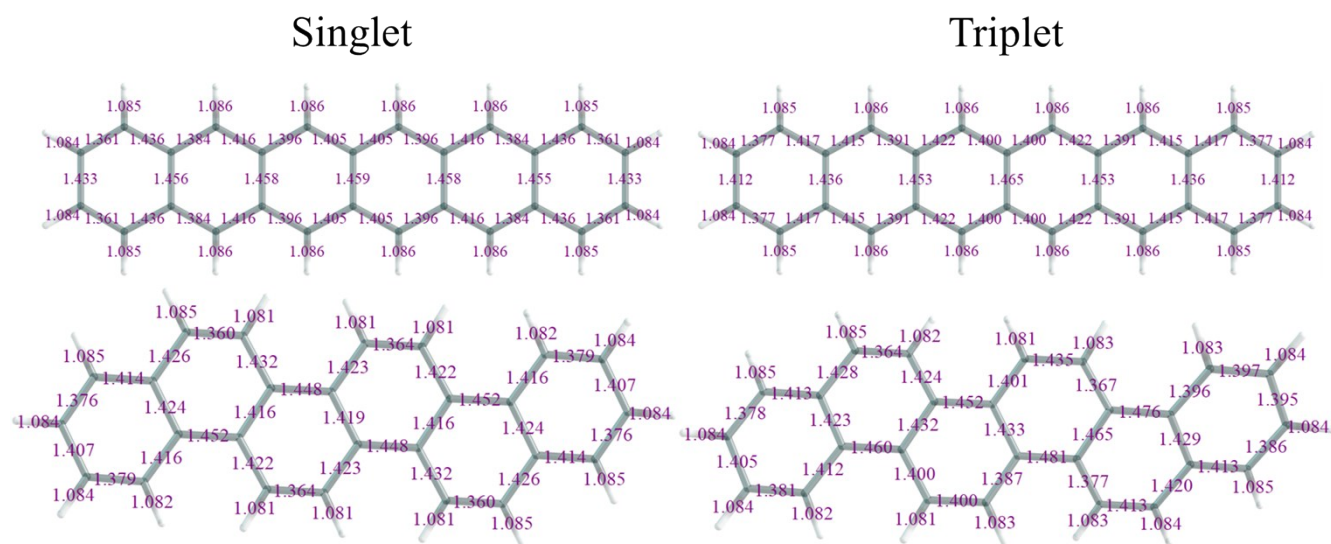


Figure S6. Bond lengths (in Å) for [7]acene and [7]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

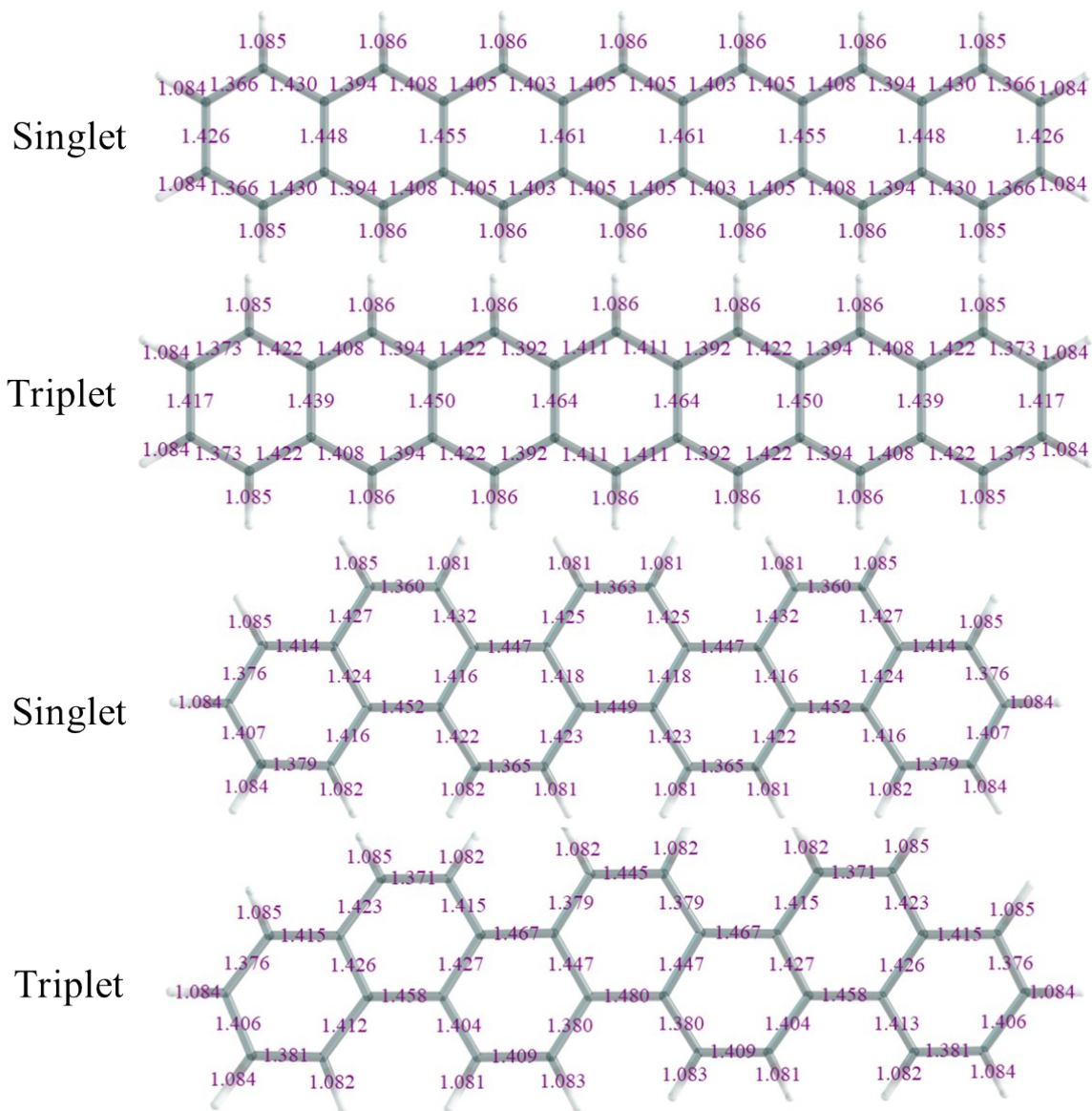


Figure S7. Bond lengths (in Å) for [8]acene and [8]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

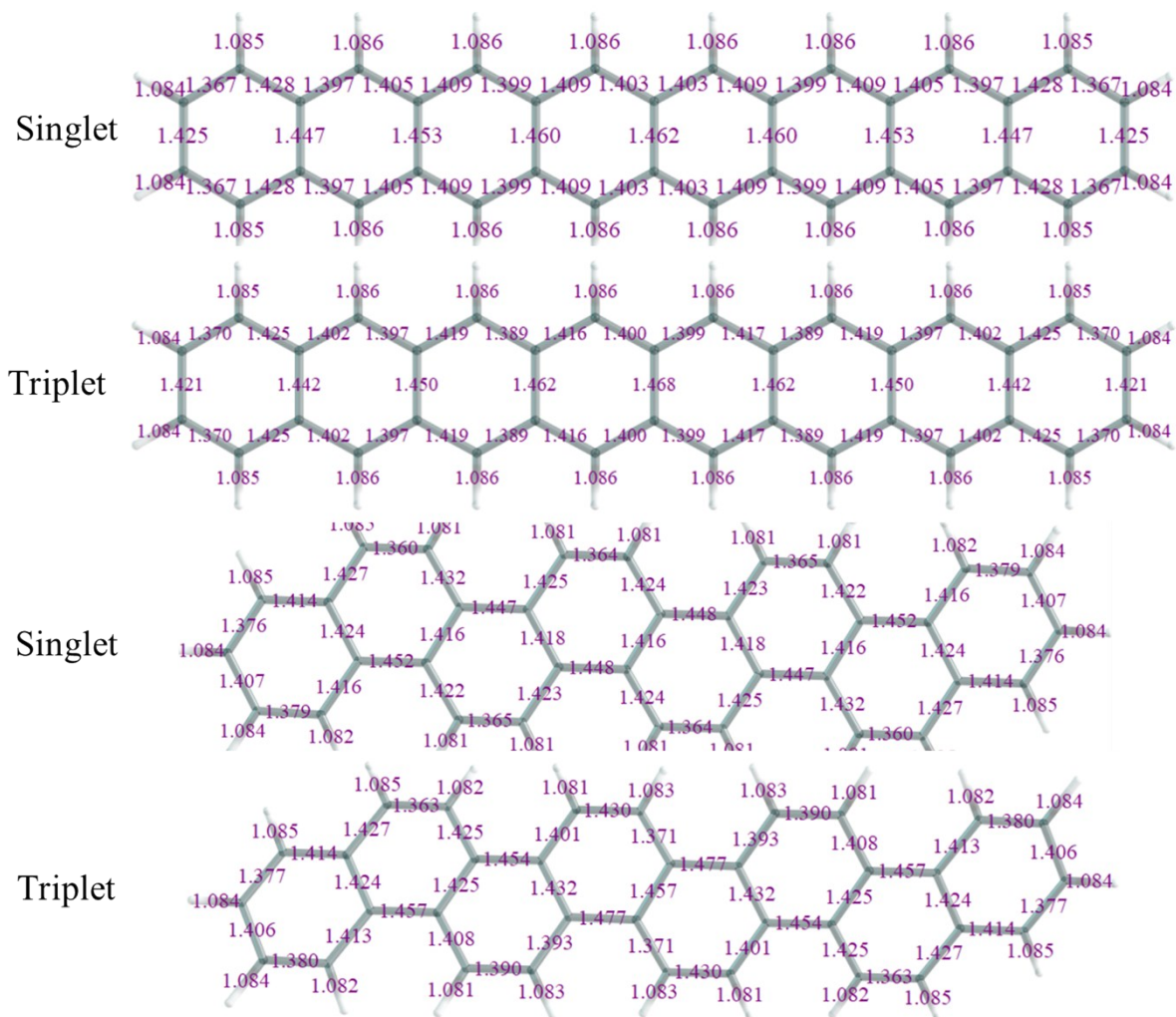


Figure S8. Bond lengths (in Å) for [9]acene and [9]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

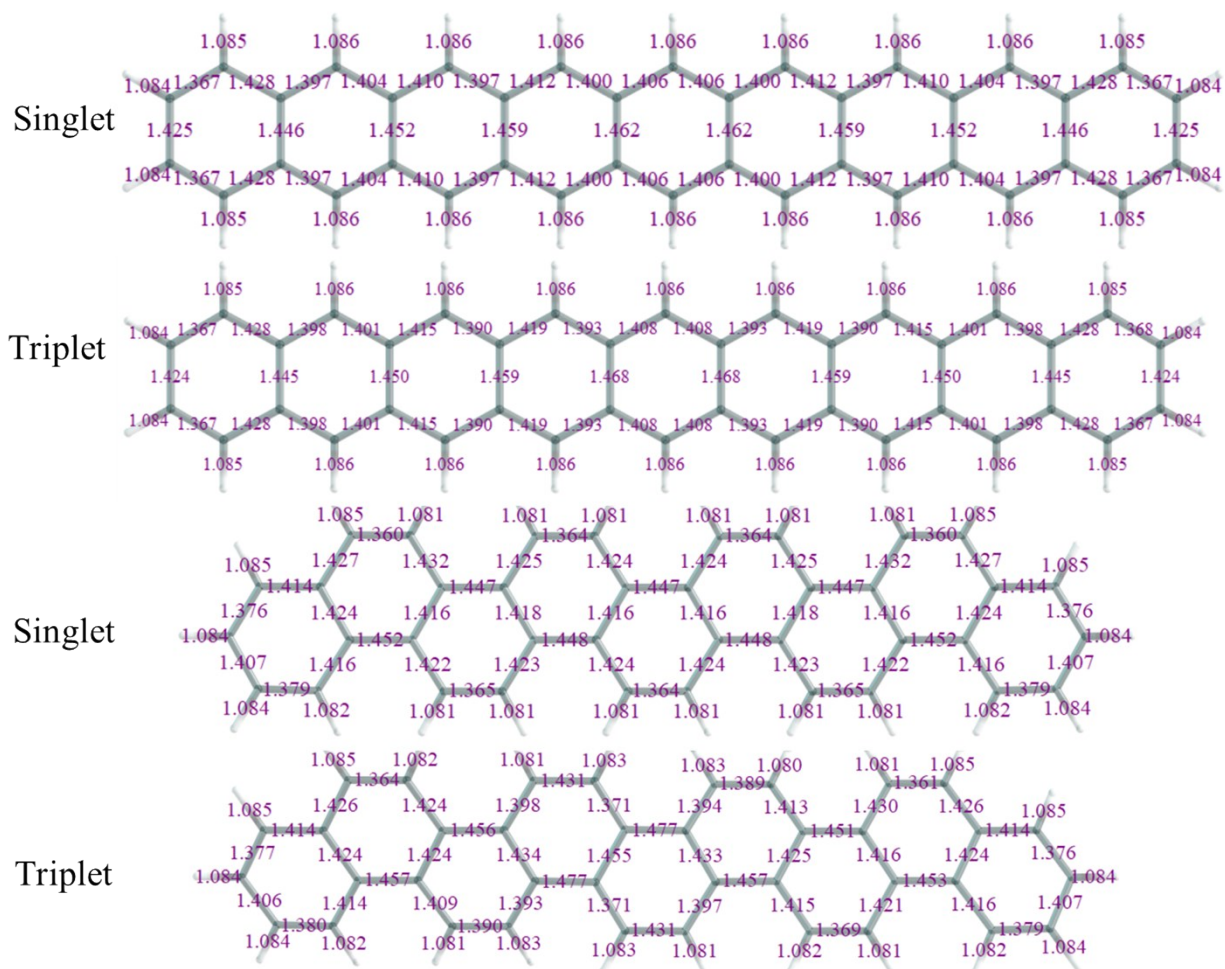


Figure S9. Bond lengths (in Å) for [10]acene and [10]phenacene for both singlet and triplet state at the UB3LYP/6-311G** level.

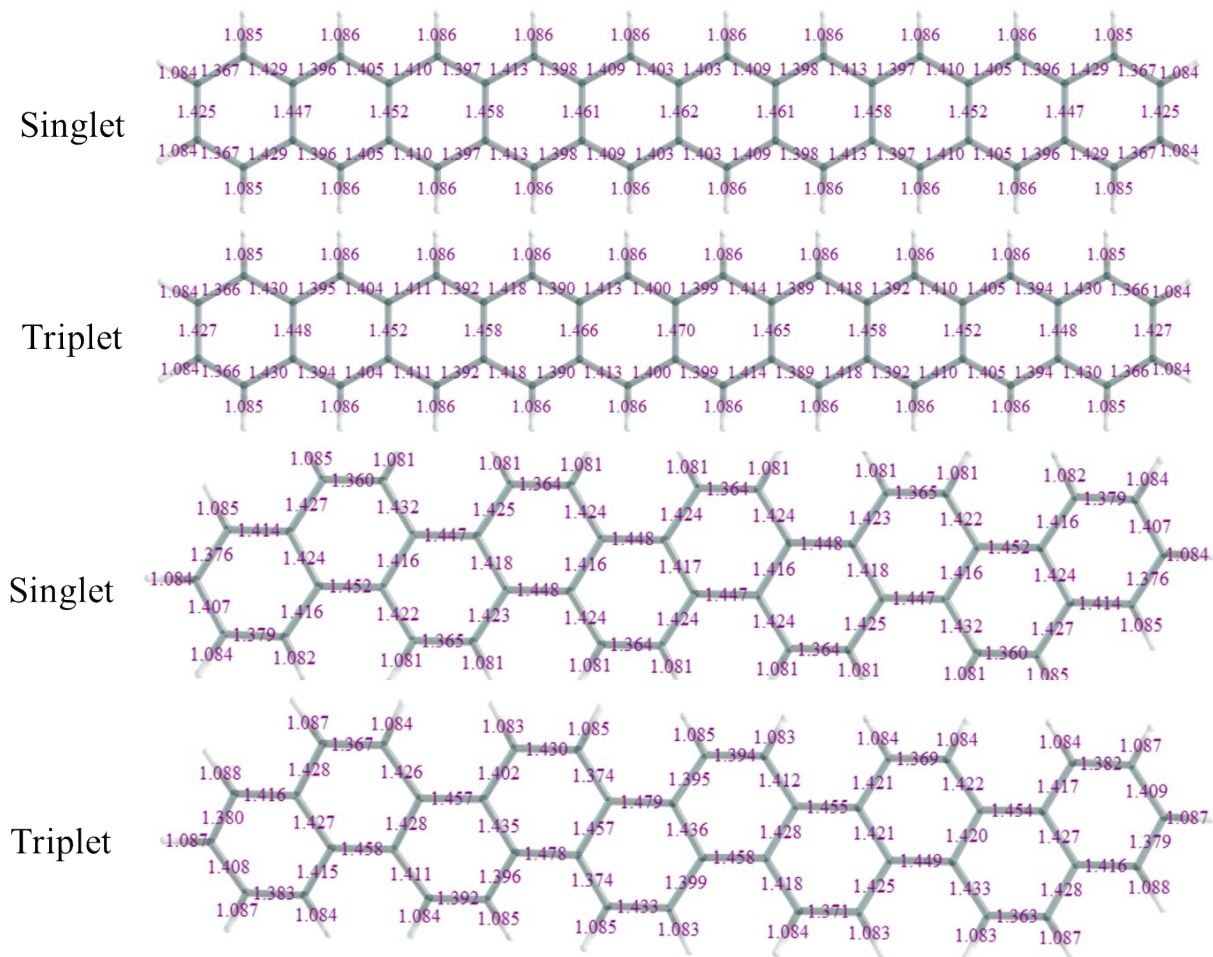


Table S1. $\langle S^2 \rangle$ Values for all PAHS studied in this work in triplet state obtained at the UB3LYP/6-311G** level.

Acenes		Phenacenes	
n	$\langle S^2 \rangle$	n	$\langle S^2 \rangle$
1	2.0011	-	2.0011
2	2.0003	-	2.0004
3	2.0003	3	2.0009
4	2.0004	4	2.0007
5	2.0005	5	2.0011
6	2.0007	6	2.0008
7	2.0008	7	2.0009
8	2.0010	8	2.0008
9	2.0011	9	2.0011
10	2.0012	10	2.0004

Table S2. Correlation factors between Mulliken spin densities at DFT and CCSD(T) levels at the triplet state for systems $n = 3 - 5$.

System	r^2
Acene[3]	0.99
Acene[4]	0.98
Acene[5]	0.97
Phenacene[3]	0.86
Phenacene[4]	0.63
Phenacene[5]	0.70

Table S3. T_1 test computed at the CCSD(T) level for the triplet state for systems $n = 3 - 5$.

System	T_1 [a]
Acene[3]	0.018
Acene[4]	0.021
Acene[5]	0.022
Phenacene[3]	0.041
Phenacene[4]	0.040
Phenacene[5]	0.046

^[a] Except for phenacene[5], the T_1 test is below the recommended threshold of 0.044 for open-shell species (see ref. J. C. Rienstra-Kiracofe, W. D. Allen, H. F. Schaefer III, *J. Phys. Chem. A* 2000, **104**, 9823–9840).

Figure S10. Linear and quadratic adjustment between the number of rings and computed energy differences between acenes and phenacenes in singlet and triplet states.

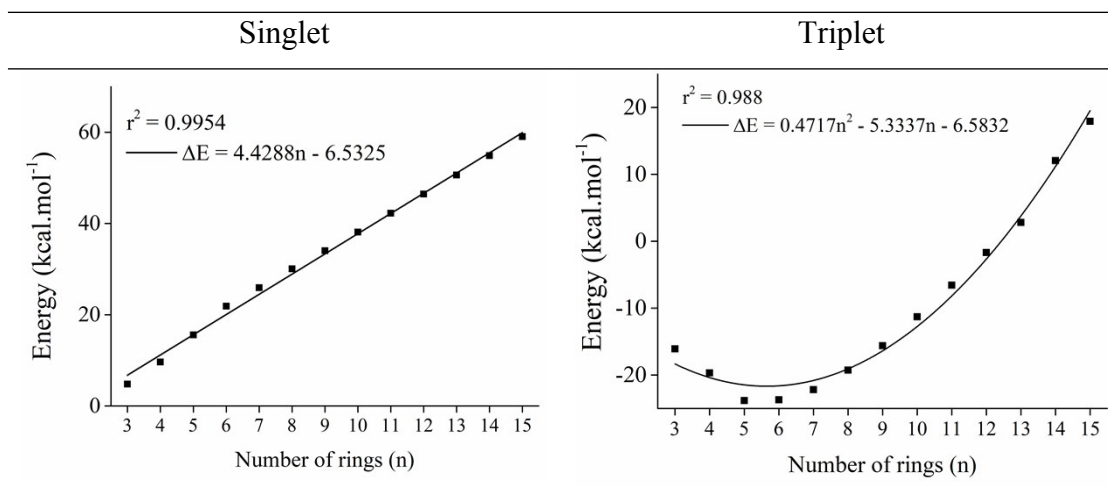


Table S4. ZPE-corrected singlet-triplet energy gaps (in kcal.mol⁻¹) of acenes for closed- and open-shell states at the (U)B3LYP/6-311G(d,p) level.

Acenes N° rings	ΔE_{S-T}	
	Open Shell	Closed Shell
1	84.0	84.0
2	59.2	59.2
3	39.6	39.6
4	26.0	26.0
5	16.5	16.5
6	9.5	9.5
7	6.8	4.4
8	5.4	0.5
9	5.0	-2.5
10	5.3	-4.9
11	5.8	-11.4
12	6.5	-10.3
13	6.8	-10.1
14	11.8	-5.7
15	13.5	-4.9

Figure S11. NICS_{zz}, delocalization indexes and HOMA computed descriptors for anthracene in both singlet (black) and triplet (blue) states.

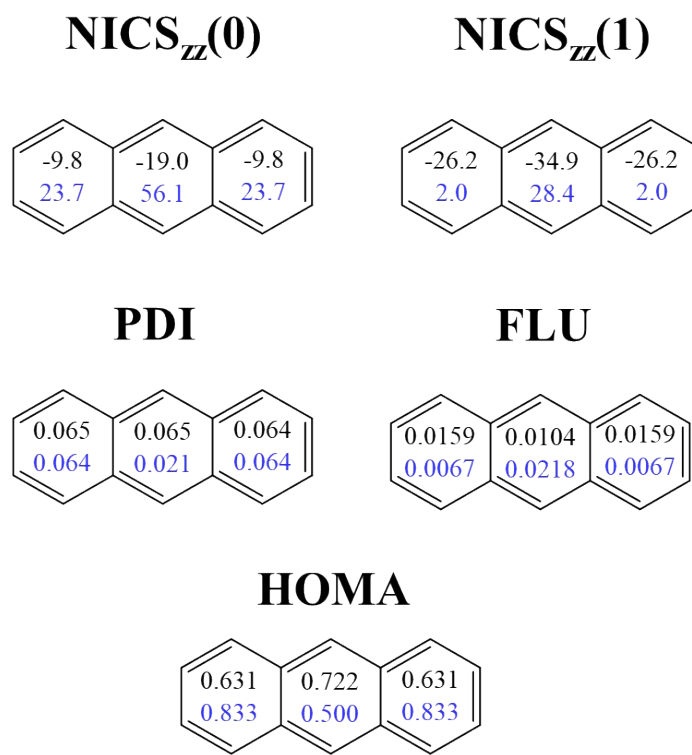


Figure S12. NICS_{zz} , delocalization indexes and HOMA computed descriptors for phenanthrene in both singlet (black) and triplet (blue) states.

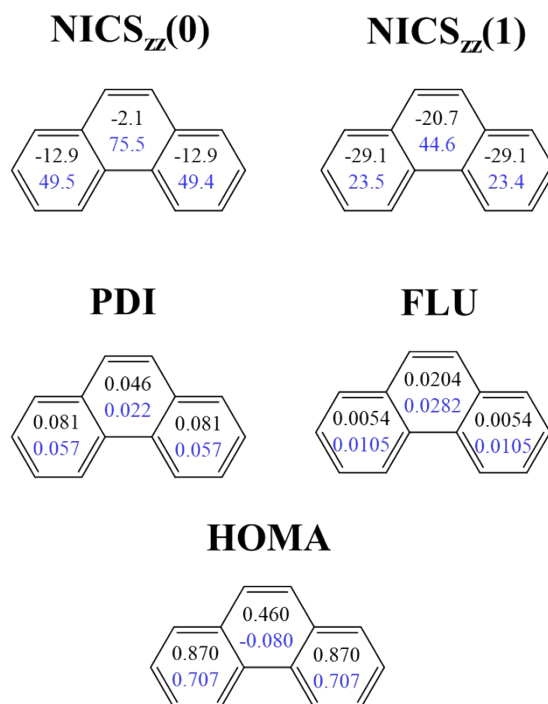


Figure S13. Spin density isosurfaces for $[n]$ acenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.

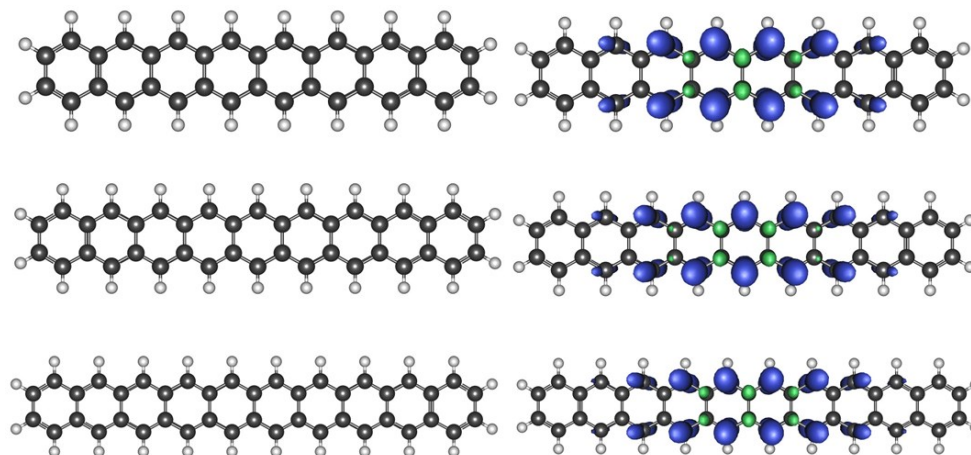


Figure S14. MCI values in both singlet (black) and triplet states (blue) for [n]acenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.

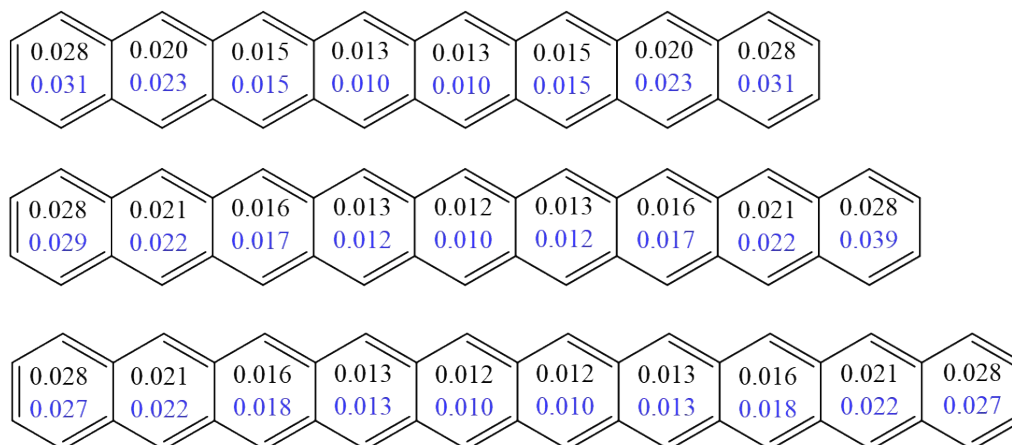


Figure S15. PDI values in both singlet (black) and triplet (blue) states for [n]acenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.

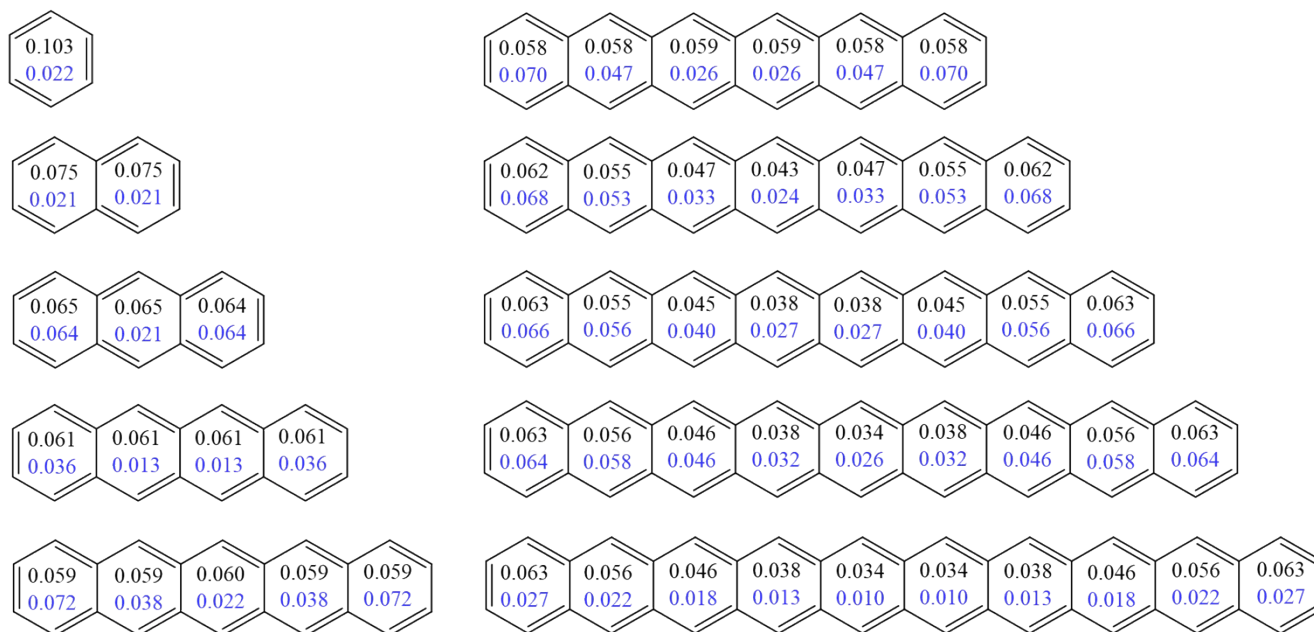


Figure S16. FLU values in both singlet (black) and triplet states (blue) for [n]acenes (n = 3 – 10) at the UB3LYP/6-311G**.

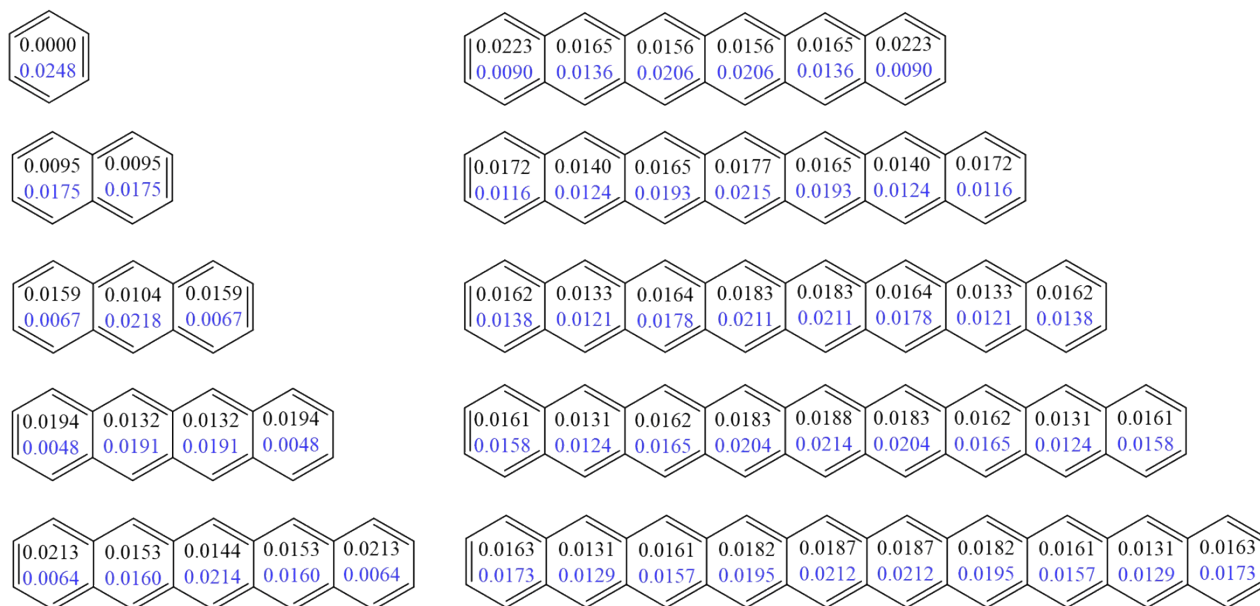


Figure S17. HOMA values in both singlet (black) and triplet (blue) states for Acenes at the UB3LYP/6-311G** level.

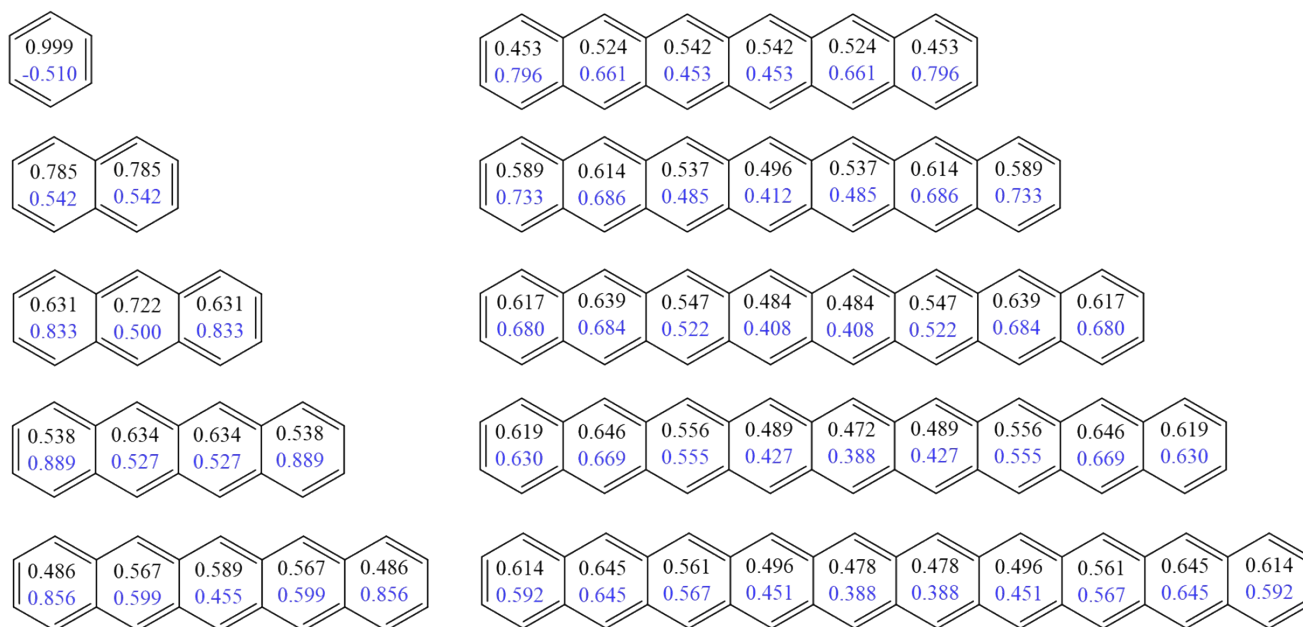


Figure S18. MICD vector maps for triplet states for [n]acenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.

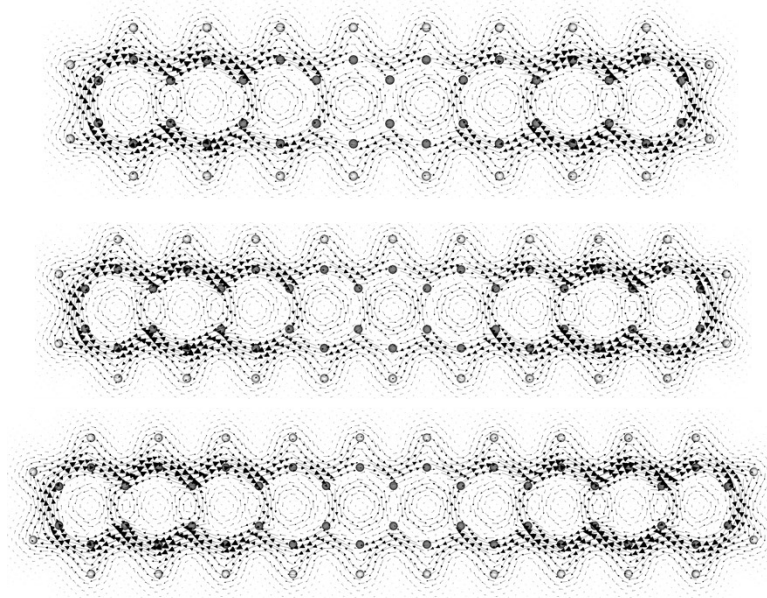


Figure S19. NICS_{zz}(0) values in both singlet (black) and triplet (blue) states for [n]acenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.

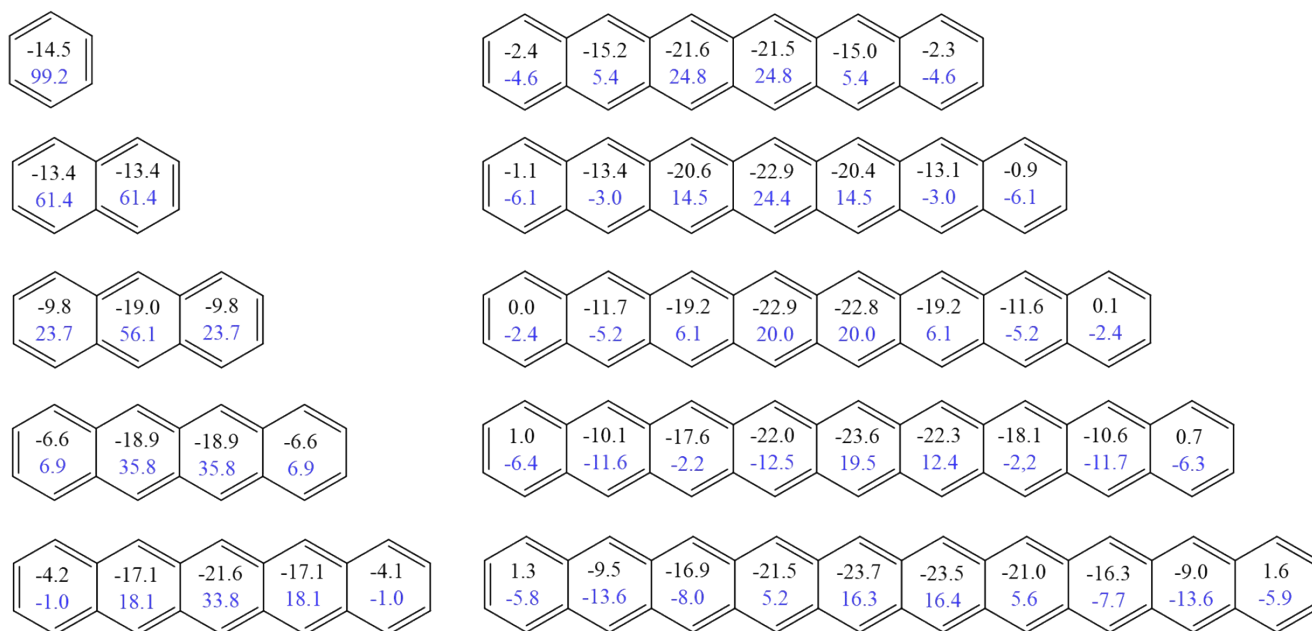


Figure S20. NICS_{zz}(1) values in both singlet (black) and triplet (blue) states for [n]cenes (n – 3 – 10) at the UB3LYP/6-311G** level.

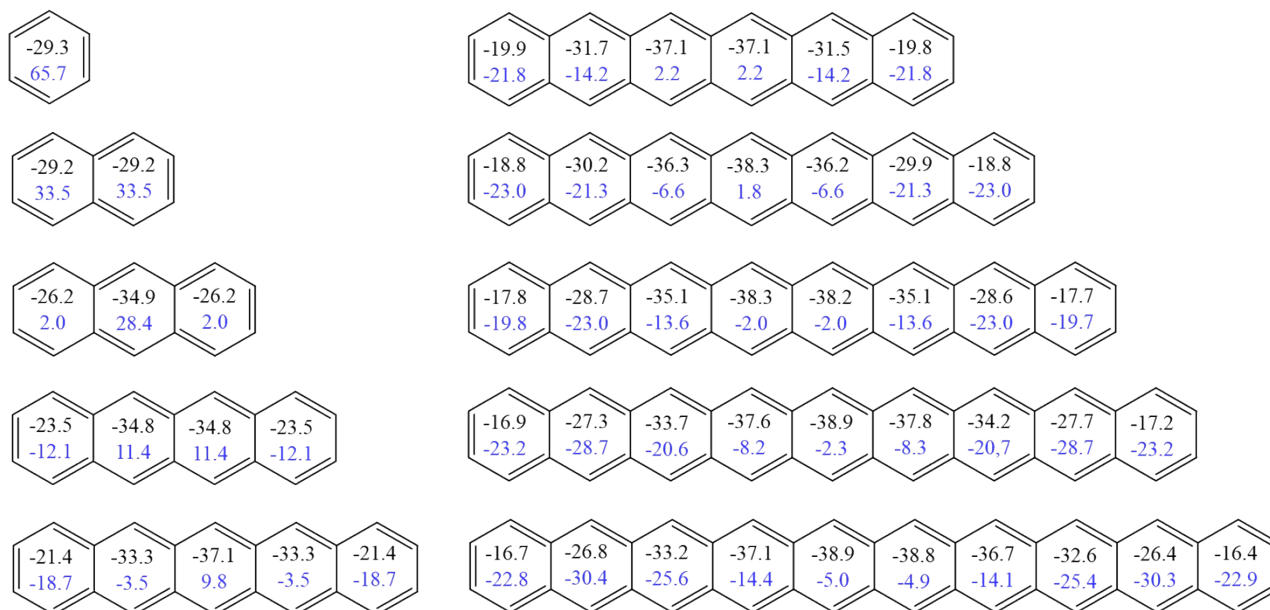


Figure S21. Spin density isosurfaces for [n]acenes, n = 8 – 10 at the UB3LYP/6-311G** level.

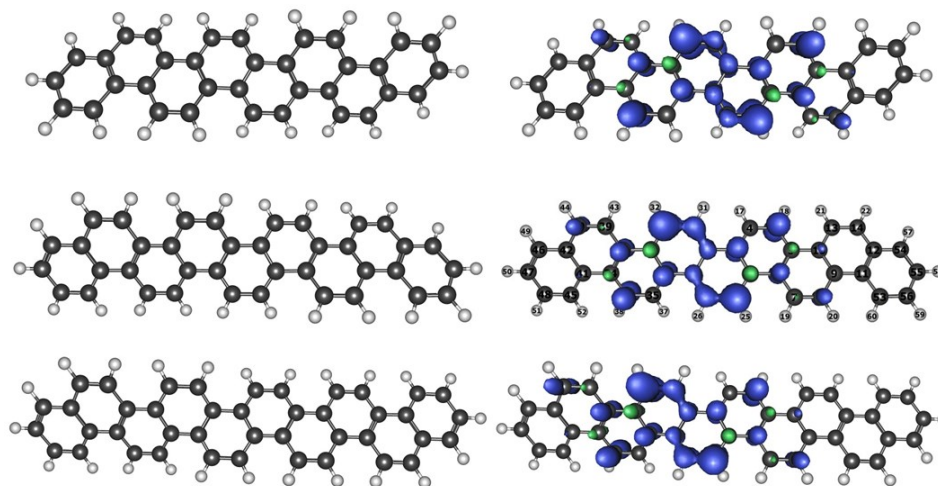


Figure S22. MCI values in both singlet (black) and triplet (blue) states for [n]acenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.

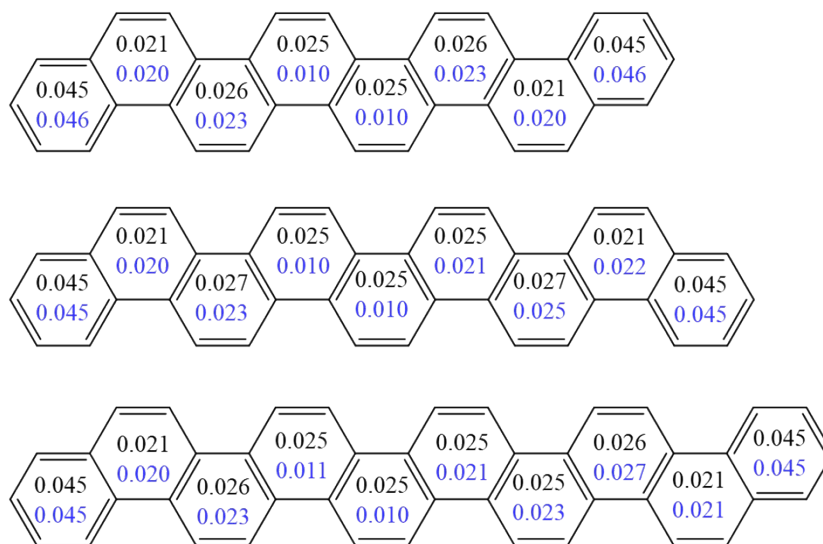


Figure S23. PDI values in both singlet (black) and triplet (blue) states for [n]phenacenes ($n = 3 - 10$) at the UB3LYP/6-311G** level.

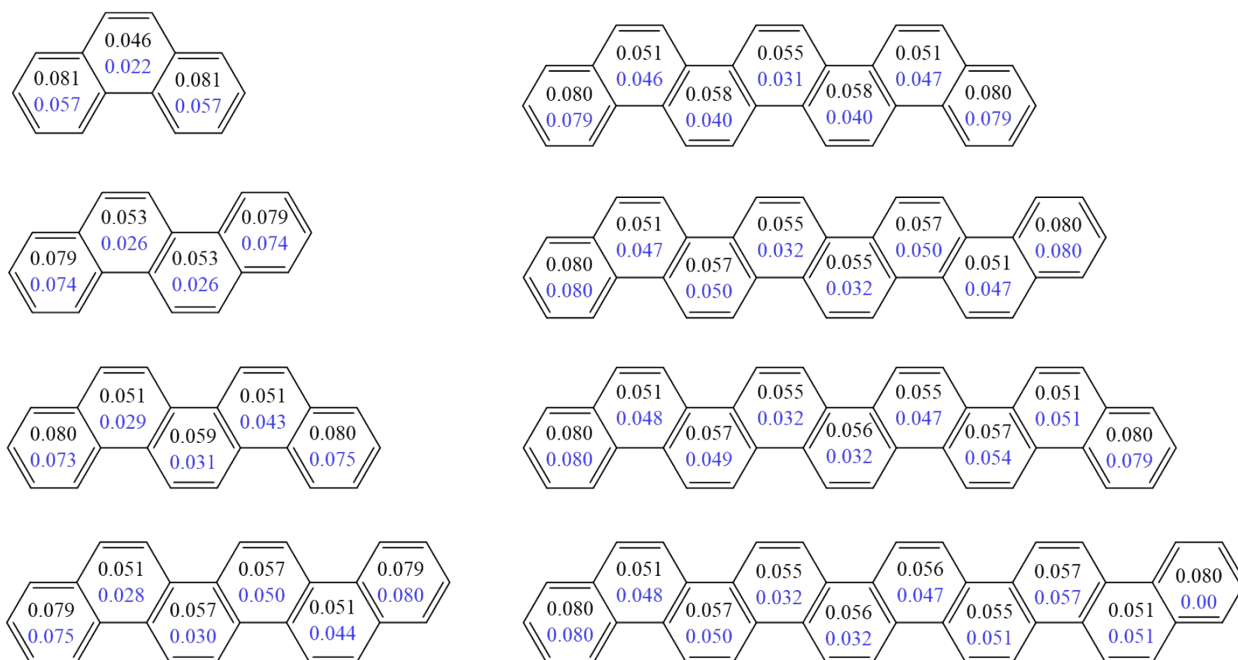


Figure S24. FLU values in both singlet (black) and triplet (blue) states for [n]phenacenes (n = 3 – 10) at the UB3LYP/6-311G** level.

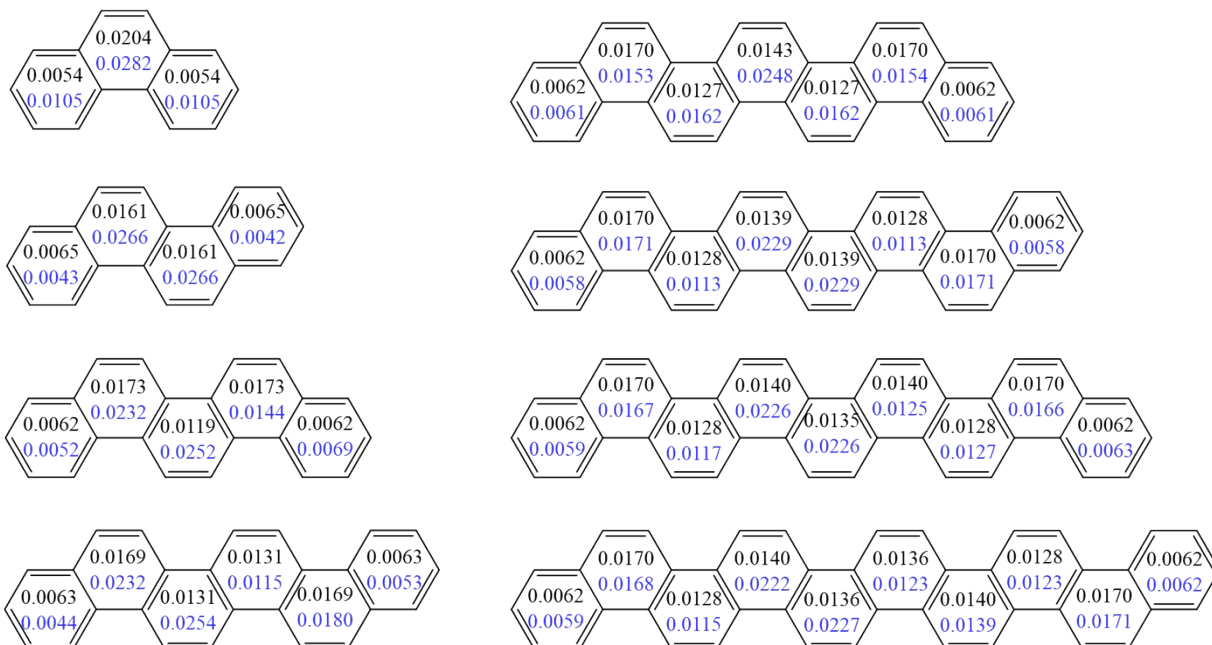


Figure S25. HOMA values in both singlet (black) and triplet (blue) states for [n]phenacenes (n = 3 – 10) at the UB3LYP/6-311G** level.

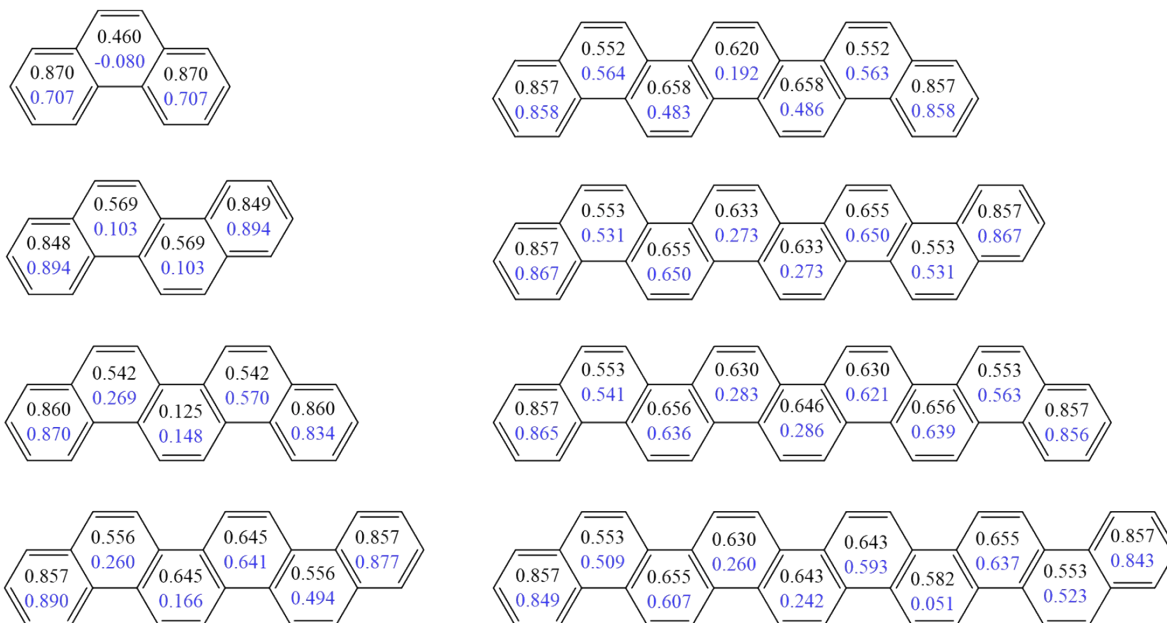


Figure S26. MICD vector maps for vertical triplet state of [n]phenacenes, $n = 8 - 10$ at the UB3LYP/6-311G** level.

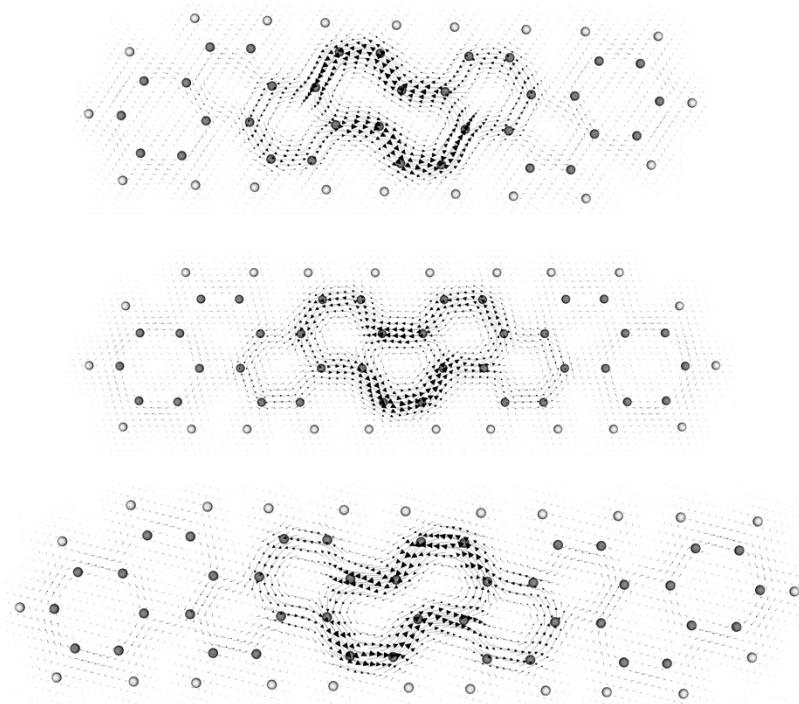
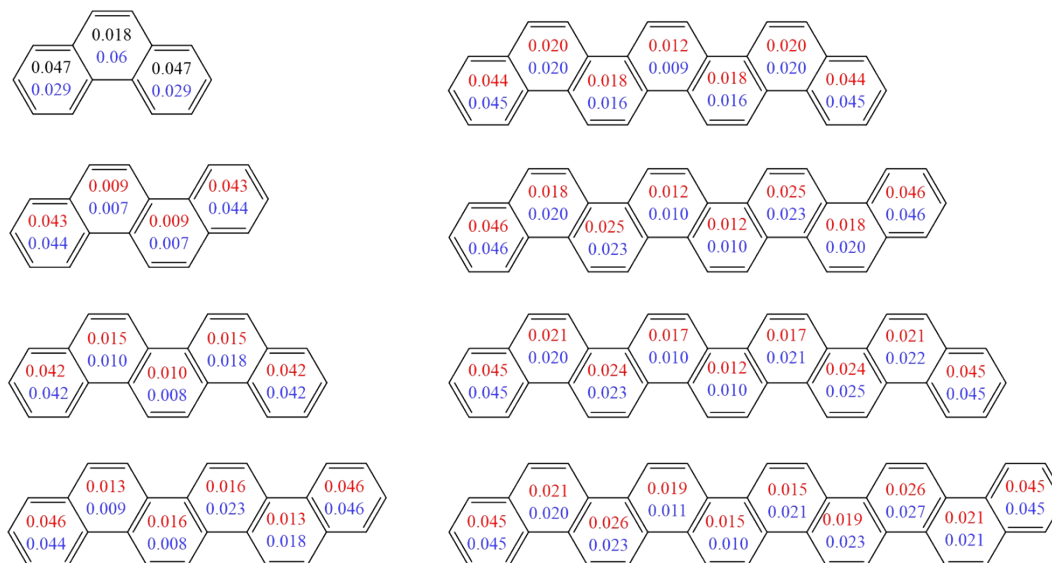


Figure S27. MCI values for both vertical (red) and adiabatic (blue) triplet states of [n]phenacenes ($n = 8 - 10$) at the UB3LYP/6-311G** level.



Approximations done for the calculation of the weights of the antiaromatic Baird π -doublet, π -sextet, π -dectet,... in acenes

To calculate the weights of the antiaromatic Baird π -doublets, π -sextets, π -dectets,... in acenes, we have performed the following assumptions:

- 1.- The spin density for the lowest-lying triplet state of acenes is well-represented at the unrestricted UB3LYP level.
- 2.- We have computed the spin densities of individual rings by summing the spin density values of each carbon atom of the ring obtained from the NBO analysis (in the case of shared C atoms, 50% of the spin density of these C atoms has been assigned to each ring).
- 3.- We have assumed that the outer rings comprise aromatic Clar π -sextets as indicated by calculated aromaticity indices, and, therefore, we have not considered the spin density in these outer rings.
- 4.- We have renormalized the spin density in the central rings (all rings except outer rings), so the total sum is 2.
- 5.- We assume that the main contributions to the exact valence bond wave function comes from resonant structures having aromatic Clar π -sextets in the outer rings and diradical antiaromatic Baird π -doublets, π -sextets, π -dectets, π -tetradectets, π -octadectets,... in the center rings. To not consider the involvement of ionic structures is another assumption done.
- 6.- We assume that a diradical antiaromatic Baird π -doublet places the total spin density in a single ring, a diradical antiaromatic Baird π -sextet places the total spin density in two rings with the same distribution (1 electron of spin density in each ring), a diradical antiaromatic Baird π -dectet places the total spin density in four rings with the same distribution (0.5 electron of spin density in each ring), and so on.
- 7.- We calculate the weights of the diradical antiaromatic Baird π -doublets, π -sextets, π -dectets, π -tetradectets, π -octadectets,... so that the sum of all contributions gives the normalized calculated spin density of our acene.

Of course, the values we obtain of the weights depend on the validity of these seven assumptions. We think that they are reasonable, so we consider that our estimation of the weights of the diradical antiaromatic Baird π -doublets, π -sextets, π -dectets,... in acenes is a good representation of the real electronic structure of these molecules in their T_1 states.

Cartesian Coordinates

[3]Acene							
SINGLET				TRIPLET			
6	1.404886262	2.476479356	0.000000000	6	1.393612453	2.476571825	0.000000000
6	0.721477716	1.221741524	0.000000000	6	0.719547769	1.252773875	0.000000000
6	1.401686629	0.000000000	0.000000000	6	1.405029288	0.000000000	0.000000000
6	-0.721477716	1.221741524	0.000000000	6	-0.719547769	1.252773875	0.000000000
6	-1.401686629	0.000000000	0.000000000	6	-1.405029288	0.000000000	0.000000000
6	-0.721477716	-1.221741524	0.000000000	6	-0.719547769	-1.252773875	0.000000000
6	0.721477716	-1.221741524	0.000000000	6	0.719547769	-1.252773875	0.000000000
6	0.712258078	3.654500156	0.000000000	6	0.690242727	3.699563610	0.000000000
6	-1.404886262	2.476479356	0.000000000	6	-1.393612453	2.476571825	0.000000000
1	-2.487560455	0.000000000	0.000000000	1	-2.490132701	0.000000000	0.000000000
6	-1.404886262	-2.476479356	0.000000000	6	-1.393612453	-2.476571825	0.000000000
6	1.404886262	-2.476479356	0.000000000	6	1.393612453	-2.476571825	0.000000000
6	0.712258078	-3.654500156	0.000000000	6	0.690242727	-3.699563610	0.000000000
6	-0.712258078	-3.654500156	0.000000000	6	-0.690242727	-3.699563610	0.000000000
1	-2.489942028	-2.475548798	0.000000000	1	-2.478578772	-2.480965028	0.000000000
1	2.489942028	-2.475548798	0.000000000	1	2.478578772	-2.480965028	0.000000000
1	1.244288635	-4.599170267	0.000000000	1	1.239459575	-4.633909759	0.000000000
1	-1.244288635	-4.599170267	0.000000000	1	-1.239459575	-4.633909759	0.000000000
6	-0.712258078	3.654500156	0.000000000	6	-0.690242727	3.699563610	0.000000000
1	2.489942028	2.475548798	0.000000000	1	2.478578772	2.480965028	0.000000000
1	2.487560455	0.000000000	0.000000000	1	2.490132701	0.000000000	0.000000000
1	1.244288635	4.599170267	0.000000000	1	1.239459575	4.633909759	0.000000000
1	-2.489942028	2.475548798	0.000000000	1	-2.478578772	2.480965028	0.000000000
1	-1.244288635	4.599170267	0.000000000	1	-1.239459575	4.633909759	0.000000000
[4]Acene							
SINGLET				TRIPLET			
6	1.404556500	1.233693855	0.000000000	6	1.403204425	1.229117022	0.000000000
6	0.725067930	0.000000000	0.000000000	6	0.730085191	0.000000000	0.000000000
6	1.404556500	-1.233693855	0.000000000	6	1.403204425	-1.229117022	0.000000000
6	-0.725067930	0.000000000	0.000000000	6	-0.730085191	0.000000000	0.000000000
6	-1.404556500	-1.233693855	0.000000000	6	-1.403204425	-1.229117022	0.000000000
6	-0.724894508	-2.446420877	-0.000000011	6	-0.716383332	-2.482735718	0.000000012
6	0.724894508	-2.446420877	-0.000000011	6	0.716383332	-2.482735718	0.000000012
6	0.724894508	2.446420877	0.000000011	6	0.716383332	2.482735718	-0.000000012
6	-1.404556500	1.233693855	0.000000000	6	-1.403204425	1.229117022	0.000000000
1	-2.490305054	-1.234045816	0.000000000	1	-2.488704351	-1.233648970	0.000000018
6	-1.407223654	-3.706391976	-0.000000016	6	-1.395126778	-3.710869207	0.000000014
6	1.407223654	-3.706391976	-0.000000016	6	1.395126778	-3.710869207	0.000000014
6	0.714630676	-4.880903811	0.000000000	6	0.697341164	-4.917936651	0.000000000
6	-0.714630676	-4.880903811	0.000000000	6	-0.697341164	-4.917936651	0.000000000
1	-2.492248410	-3.705900682	-0.000000017	1	-2.480215390	-3.712254339	0.000000023
1	2.492248410	-3.705900682	-0.000000017	1	2.480215390	-3.712254339	0.000000023

1	1.245031763	-5.826465565	0.000000000	1	1.240991516	-5.855681282	0.000000010
1	-1.245031763	-5.826465565	0.000000000	1	-1.240991516	-5.855681282	0.000000010
6	-0.724894508	2.446420877	0.000000011	6	-0.716383332	2.482735718	-0.000000012
1	2.490305054	1.234045816	0.000000000	1	2.488704351	1.233648970	-0.000000018
1	2.490305054	-1.234045816	0.000000000	1	2.488704351	-1.233648970	0.000000018
6	1.407223654	3.706391976	0.000000016	6	1.395126778	3.710869207	-0.000000014
1	-2.490305054	1.234045816	0.000000000	1	-2.488704351	1.233648970	-0.000000018
6	-1.407223654	3.706391976	0.000000016	6	-1.395126778	3.710869207	-0.000000014
6	0.714630676	4.880903811	0.000000000	6	0.697341164	4.917936651	0.000000000
6	-0.714630676	4.880903811	0.000000000	6	-0.697341164	4.917936651	0.000000000
1	2.492248410	3.705900682	0.000000017	1	2.480215390	3.712254339	-0.000000023
1	-2.492248410	3.705900682	0.000000017	1	-2.480215390	3.712254339	-0.000000023
1	1.245031763	5.826465565	0.000000000	1	1.240991516	5.855681282	-0.000000010
1	-1.245031763	5.826465565	0.000000000	1	-1.240991516	5.855681282	-0.000000010
[5]Acene							
SINGLET				TRIPLET			
6	-1.406177978	-2.464123851	0.000000030	6	-1.401368535	2.460076624	0.000000000
6	-0.727492551	-1.224510608	0.000000000	6	-0.728898750	1.242271136	0.000000000
6	-1.406701335	0.000046627	-0.000000032	6	-1.406733053	-0.000007252	0.000000000
6	0.727489577	-1.224509539	0.000000000	6	0.728896575	1.242270257	0.000000000
6	1.406697202	0.000048805	-0.000000046	6	1.406729042	-0.000008824	0.000000000
6	0.727511570	1.224408578	-0.000000050	6	0.728918033	-1.242239031	0.000000000
6	-0.727517893	1.224407514	-0.000000042	6	-0.728925193	-1.242238014	0.000000000
6	-0.726703796	-3.672576083	0.000000031	6	-0.716454337	3.707101766	0.000000000
6	1.406176878	-2.464121824	0.000000022	6	1.401367948	2.460075375	0.000000000
1	2.492306439	-0.000035775	-0.000000027	1	2.492201551	0.000014875	-0.000000012
6	1.406185265	2.464205011	-0.000000011	6	1.401366778	-2.460066395	0.000000000
6	-1.406186980	2.464204799	-0.000000013	6	-1.401367678	-2.460068411	0.000000000
6	-0.726769478	3.672523563	-0.000000011	6	-0.716468672	-3.707127521	0.000000000
6	0.726771203	3.672521790	0.000000000	6	0.716474139	-3.707126892	0.000000000
1	2.491900730	2.464749412	-0.000000088	1	2.487081259	-2.464080612	-0.000000029
1	-2.491902418	2.464759181	-0.000000095	1	-2.487082111	-2.464096191	-0.000000032
6	0.726704278	-3.672575089	0.000000023	6	0.716455231	3.707101158	0.000000000
1	-2.491887331	-2.464803013	0.000000028	1	-2.487080841	2.464088867	0.000000000
1	-2.492310498	-0.000037564	-0.000000015	1	-2.492205748	0.000019020	0.000000000
6	-1.408462923	-4.935119148	0.000000033	6	-1.397750402	4.942333289	0.000000000
1	2.491886347	-2.464799949	0.000000027	1	2.487080232	2.464085205	0.000000000
6	1.408465320	-4.935117131	0.000000022	6	1.397752370	4.942332199	0.000000000
6	-0.715854663	-6.107903775	0.000000036	6	-0.702396823	6.138913245	0.000000000
6	0.715858822	-6.107902876	0.000000034	6	0.702399850	6.138912715	0.000000000
1	-2.493470725	-4.934878160	0.000000036	1	-2.482847057	4.942371321	0.000000015
1	2.493473175	-4.934874498	0.000000000	1	2.482849021	4.942368696	0.000000014
1	-1.245422836	-7.053917489	0.000000033	1	-1.241995683	7.079090504	0.000000000
1	1.245428218	-7.053915848	0.000000030	1	1.241999144	7.079089657	0.000000000
6	-1.408497330	4.935172600	-0.000000091	6	-1.397743909	-4.942309000	-0.000000020
6	1.408498987	4.935172303	-0.000000078	6	1.397744745	-4.942308195	-0.000000020

6	-0.715884074	6.107890281	0.000000028	6	-0.702351430	-6.138948117	0.000000000
6	0.715899770	6.107884619	0.000000058	6	0.702359976	-6.138943937	0.000000015
1	-2.493505111	4.934868746	0.000000017	1	-2.482836992	-4.942382153	0.000000021
1	2.493508714	4.934869757	0.000000062	1	2.482839109	-4.942398446	0.000000044
1	-1.245446601	7.053907434	0.000000164	1	-1.242063084	-7.079062775	0.000000025
1	1.245382751	7.053948181	0.000000178	1	1.242025793	-7.079085106	0.000000028
[6]Acene							
SINGLET				TRIPLET			
6	-1.406945000	-3.693344000	0.000000000	6	-1.400754000	-3.691978000	0.000000000
6	-0.728808000	-2.450632000	0.000000000	6	-0.726259000	-2.475844000	0.000000000
6	-1.407764000	-1.230562000	0.000000000	6	-1.406505000	-1.227293000	0.000000000
6	0.728916000	-2.450650000	0.000000000	6	0.726304000	-2.475818000	0.000000000
6	1.407904000	-1.230596000	0.000000000	6	1.406505000	-1.227244000	0.000000000
6	0.729559000	-0.000165000	0.000000000	6	0.732659000	0.000015000	0.000000000
6	-0.729385000	-0.000151000	0.000000000	6	-0.732703000	-0.000011000	0.000000000
6	-0.727701000	-4.899633000	0.000000000	6	-0.717700000	-4.931063000	0.000000000
6	1.407019000	-3.693382000	0.000000000	6	1.400841000	-3.691929000	0.000000000
1	2.493476000	-1.231046000	0.000000000	1	2.492012000	-1.228691000	0.000000000
6	1.407962000	1.230676000	0.000000000	6	1.406460000	1.227293000	0.000000000
6	-1.407764000	1.230700000	0.000000000	6	-1.406547000	1.227244000	0.000000000
6	-0.728849000	2.450382000	0.000000000	6	-0.726347000	2.475819000	0.000000000
6	0.729071000	2.450374000	0.000000000	6	0.726215000	2.475845000	0.000000000
1	2.493532000	1.230726000	0.000000000	1	2.491967000	1.228773000	0.000000000
1	-2.493336000	1.230740000	0.000000000	1	-2.492055000	1.228685000	0.000000000
6	0.727740000	-4.899652000	0.000000000	6	0.717831000	-4.931038000	0.000000000
1	-2.492641000	-3.694178000	0.000000000	1	-2.486542000	-3.693658000	0.000000000
1	-2.493336000	-1.230996000	0.000000000	1	-2.492012000	-1.228779000	0.000000000
6	-1.409078000	-6.163518000	0.000000000	6	-1.399963000	-6.172967000	0.000000000
1	2.492714000	-3.694240000	0.000000000	1	2.486629000	-3.693570000	0.000000000
6	1.409082000	-6.163556000	0.000000000	6	1.400137000	-6.172918000	0.000000000
6	-0.716517000	-7.335418000	0.000000000	6	-0.705949000	-7.362458000	0.000000000
6	0.716488000	-7.335437000	0.000000000	6	0.706166000	-7.362433000	0.000000000
1	-2.494078000	-6.163445000	0.000000000	1	-2.485060000	-6.171693000	0.000000000
1	2.494082000	-6.163512000	0.000000000	1	2.485235000	-6.171606000	0.000000000
1	-1.245570000	-8.281715000	0.000000000	1	-1.241993000	-8.304725000	0.000000000
1	1.245514000	-8.281749000	0.000000000	1	1.242243000	-8.304681000	0.000000000
6	-1.406901000	3.693376000	0.000000000	6	-1.400886000	3.691932000	0.000000000
6	1.407099000	3.693387000	0.000000000	6	1.400710000	3.691982000	0.000000000
6	-0.727854000	4.899540000	0.000000000	6	-0.717874000	4.931037000	0.000000000
6	0.727980000	4.899527000	0.000000000	6	0.717654000	4.931062000	0.000000000
1	-2.492619000	3.694022000	0.000000000	1	-2.486673000	3.693563000	0.000000000
1	2.492818000	3.694112000	0.000000000	1	2.486498000	3.693653000	0.000000000
6	1.409058000	6.163870000	0.000000000	6	1.399919000	6.172968000	0.000000000
6	-1.409078000	6.163758000	0.000000000	6	-1.400190000	6.172918000	0.000000000
6	-0.717162000	7.335473000	0.000000000	6	-0.706210000	7.362430000	0.000000000
6	0.716114000	7.335638000	0.000000000	6	0.705906000	7.362456000	0.000000000

1	2.494049000	6.163884000	0.000000000	1	2.485017000	6.171688000	0.000000000
1	1.244743000	8.282216000	0.000000000	1	1.241942000	8.304727000	0.000000000
1	-1.246318000	8.281578000	0.000000000	1	-1.242281000	8.304684000	0.000000000
1	-2.494150000	6.163574000	0.000000000	1	-2.485284000	6.171601000	0.000000000
[7]Acene							
SINGLET				TRIPLET			
6	1.407451464	-4.921725068	0.000000000	6	1.401232976	-4.922941726	0.000000000
6	0.729584288	-3.677471354	0.000000000	6	0.725021304	-3.704285204	0.000000000
6	1.408542766	-2.459700633	0.000000000	6	1.405539367	-2.455964266	-0.000000001
6	-0.729661363	-3.677469100	0.000000000	6	-0.725067422	-3.704278108	-0.000000001
6	-1.408612463	-2.459697341	0.000000000	6	-1.405573478	-2.455950703	0.000000001
6	-0.730638769	-1.226206516	0.000000000	6	-0.732179596	-1.238131869	-0.000000004
6	0.730581565	-1.226212257	0.000000000	6	0.732157058	-1.238138828	0.000000003
6	0.728199839	-6.126904731	0.000000000	6	0.719439267	-6.154661930	-0.000000003
6	-1.407533836	-4.921723973	0.000000000	6	-1.401290873	-4.922928121	0.000000000
1	-2.494160163	-2.460457340	0.000000000	1	-2.491193876	-2.457348429	-0.000000002
6	-1.408982644	0.000164593	0.000000000	6	-1.408079037	-0.000015109	0.000000000
6	1.408942252	0.000156749	0.000000000	6	1.408067882	-0.000028627	0.000000000
6	0.730725168	1.225733341	0.000000000	6	0.732168779	1.238088349	0.000000004
6	-0.730735995	1.225747105	0.000000000	6	-0.732169123	1.238094588	-0.000000004
1	-2.494505409	-0.000291265	0.000000000	1	-2.493591869	-0.000014859	-0.000000004
1	2.494466377	-0.000343979	0.000000000	1	2.493580640	-0.000037370	0.000000003
6	-0.728285142	-6.126904361	0.000000000	6	-0.719509182	-6.154654892	0.000000003
1	2.493134528	-4.922770225	0.000000000	1	2.487034321	-4.923795342	-0.000000001
1	2.494090740	-2.460481339	0.000000000	1	2.491159749	-2.457372168	0.000000001
6	1.409395672	-7.391450287	0.000000000	6	1.402008548	-7.401848673	0.000000006
1	-2.493217005	-4.922759763	0.000000000	1	-2.487092244	-4.923771296	0.000000000
6	-1.409482013	-7.391450287	0.000000000	6	-1.402090597	-7.401835020	-0.000000006
6	0.716787904	-8.562891497	0.000000000	6	0.708650729	-8.586519473	0.000000000
6	-0.716874657	-8.562891550	0.000000000	6	-0.708744341	-8.586512541	0.000000001
1	2.494387503	-7.391516275	0.000000000	1	2.487081317	-7.400546579	-0.000000004
1	-2.494474008	-7.391513153	0.000000000	1	-2.487163355	-7.400522343	0.000000004
1	1.245631665	-9.509300030	0.000000000	1	1.242808579	-9.529890952	0.000000007
1	-1.245717741	-9.509300242	0.000000000	1	-1.242911356	-9.529878834	-0.000000006
6	1.408656380	2.459862831	0.000000000	6	1.405561593	2.455912909	-0.000000001
6	-1.408627450	2.459885781	0.000000000	6	-1.405551633	2.455925858	0.000000001
6	0.730078905	3.677188329	0.000000000	6	0.725047943	3.704236515	0.000000002
6	-0.729967301	3.677238754	0.000000000	6	-0.725029644	3.704241103	-0.000000002
1	2.494242657	2.459981345	0.000000000	1	2.491181832	2.457301137	0.000000002
1	-2.494214822	2.460076603	0.000000000	1	-2.491171778	2.457322008	-0.000000002
6	-1.407526142	4.922021222	0.000000000	6	-1.401247650	4.922901620	0.000000001
6	1.407448459	4.921964870	0.000000000	6	1.401284475	4.922889512	-0.000000001
6	0.728602553	6.126922353	0.000000000	6	0.719490227	6.154609224	-0.000000002
6	-0.728268558	6.126594316	0.000000000	6	-0.719454015	6.154627481	0.000000002
1	-2.493236172	4.922849713	0.000000000	1	-2.487049111	4.923747896	0.000000001
1	2.493248624	4.922849258	0.000000000	1	2.487081687	4.923724956	-0.000000001

6	-1.409298103	7.391643278	0.000000000	6	-1.402031097	7.401812953	0.000000000
6	1.409700007	7.391785732	0.000000000	6	1.402079225	7.401791839	0.000000001
6	-0.717214569	8.563069089	0.000000000	6	-0.708657921	8.586474811	0.000000008
6	0.717071035	8.562924306	0.000000000	6	0.708732921	8.586471212	-0.000000008
1	-2.494389577	7.391191201	0.000000000	1	-2.487100129	7.400511018	0.000000004
1	-1.245701601	9.509574726	0.000000000	1	-1.242808944	9.529854544	0.000000006
1	1.245384905	9.509678233	0.000000000	1	1.242897158	9.529837822	-0.000000005
1	2.494674021	7.391310213	0.000000000	1	2.487152697	7.400478844	-0.000000004
[8]Acene							
SINGLET				TRIPLET			
6	-1.407840230	-6.149981463	0.000000000	6	-1.402215986	-6.152399274	0.000000000
6	-0.730147740	-4.904448886	0.000000000	6	-0.724970016	-4.930059298	0.000000000
6	-1.409039240	-3.688408384	0.000000000	6	-1.405181516	-3.685226277	0.000000000
6	0.730147894	-4.904448886	0.000000000	6	0.724915415	-4.930058933	0.000000000
6	1.409043822	-3.688410146	0.000000000	6	1.405125741	-3.685228251	0.000000000
6	0.731285572	-2.452716319	0.000000000	6	0.730816419	-2.470905569	0.000000000
6	-0.731273665	-2.452717986	0.000000000	6	-0.730875444	-2.470906480	0.000000000
6	-0.728666658	-7.354230076	0.000000000	6	-0.721130644	-7.378262449	0.000000000
6	1.407835647	-6.149983897	0.000000000	6	1.402163968	-6.152399274	0.000000000
1	2.494586717	-3.688975472	0.000000000	1	2.490801348	-3.686988279	0.000000000
6	1.409594807	-1.229237622	0.000000000	6	1.407865731	-1.226717494	0.000000000
6	-1.409578683	-1.229237828	0.000000000	6	-1.407922596	-1.226710949	0.000000000
6	-0.731617350	-0.000063090	0.000000000	6	-0.734237434	0.000084897	0.000000000
6	0.731644767	-0.000058363	0.000000000	6	0.734179827	0.000085540	0.000000000
1	2.495104406	-1.229468100	0.000000000	1	2.493496099	-1.227693768	0.000000000
1	-2.495088218	-1.229459871	0.000000000	1	-2.493553160	-1.227689646	0.000000000
6	0.728658217	-7.354230764	0.000000000	6	0.721080309	-7.378262343	0.000000000
1	-2.493522642	-6.150895299	0.000000000	1	-2.487989221	-6.153742961	0.000000000
1	-2.494581769	-3.688967756	0.000000000	1	-2.490857208	-3.686990538	0.000000000
6	-1.409723402	-8.619387783	0.000000000	6	-1.403690967	-8.629249266	0.000000000
1	2.493518425	-6.150902073	0.000000000	1	2.487937219	-6.153739839	0.000000000
6	1.409711909	-8.619390218	0.000000000	6	1.403641939	-8.629249001	0.000000000
6	-0.717137171	-9.790419623	0.000000000	6	-0.710539384	-9.810706479	0.000000000
6	0.717122767	-9.790420311	0.000000000	6	0.710491430	-9.810706373	0.000000000
1	-2.494715461	-8.619414877	0.000000000	1	-2.488731773	-8.628720195	0.000000000
1	2.494704067	-8.619420540	0.000000000	1	2.488682718	-8.628718448	0.000000000
1	-1.245715688	-10.736971033	0.000000000	1	-1.243888132	-10.754556122	0.000000000
1	1.245700569	-10.736972250	0.000000000	1	1.243840660	-10.754555805	0.000000000
6	-1.409573899	1.229304065	0.000000000	6	-1.407923962	1.226665725	0.000000000
6	1.409605168	1.229308177	0.000000000	6	1.407877696	1.226653480	0.000000000
6	-0.731292462	2.452617960	0.000000000	6	-0.730805343	2.471006997	0.000000000
6	0.731342469	2.452628740	0.000000000	6	0.730767650	2.471005526	0.000000000
1	-2.495083726	1.229374414	0.000000000	1	-2.493550789	1.227820358	0.000000000
1	2.495115127	1.229365307	0.000000000	1	2.493504364	1.227800974	0.000000000
6	1.409110372	3.688443606	0.000000000	6	1.405176759	3.685238687	0.000000000
6	-1.409056824	3.688430959	0.000000000	6	-1.405187851	3.685259171	0.000000000

6	-0.730151534	4.904360619	0.000000000	6	-0.724924575	4.930011910	0.000000000
6	0.730245654	4.904383782	0.000000000	6	0.724947192	4.930008888	0.000000000
1	2.494653991	3.688897148	0.000000000	1	2.490849149	3.686964058	0.000000000
1	-2.494598401	3.688907499	0.000000000	1	-2.490859547	3.687014362	0.000000000
6	1.407767346	6.149993317	0.000000000	6	1.402167365	6.152436422	0.000000000
6	-1.407698611	6.149932091	0.000000000	6	-1.402113511	6.152454414	0.000000000
6	0.728824326	7.354286856	0.000000000	6	0.721238041	7.378212071	0.000000000
6	-0.728715427	7.354254365	0.000000000	6	-0.721116034	7.378206038	0.000000000
1	2.493488050	6.150998277	0.000000000	1	2.487966884	6.153736716	0.000000000
1	-2.493414568	6.150985418	0.000000000	1	-2.487912670	6.153822972	0.000000000
6	-1.409937534	8.619324758	0.000000000	6	-1.403717928	8.629156343	0.000000000
6	-0.717259173	9.790497253	0.000000000	6	-0.710461584	9.810685947	0.000000000
6	1.409704220	8.619559501	0.000000000	6	1.403766920	8.629235296	0.000000000
6	0.717065224	9.790396392	0.000000000	6	0.710740112	9.810619271	0.000000000
1	-2.494931280	8.619202518	0.000000000	1	-2.488761444	8.628497834	0.000000000
1	-1.245645731	10.737080255	0.000000000	1	-1.243666423	10.754586391	0.000000000
1	1.245832324	10.736932086	0.000000000	1	1.244235817	10.754416843	0.000000000
1	2.494590353	8.620119636	0.000000000	1	2.488769683	8.628862279	0.000000000
[9]Acene							
SINGLET				TRIPLET			
6	7.377877366	-1.408002867	0.000000000	6	1.403021124	7.382003361	0.000000000
6	6.131891274	-0.730384150	0.000000000	6	0.725166648	6.155481731	0.000000000
6	4.916513667	-1.409285143	0.000000000	6	1.405140833	4.915049762	0.000000000
6	6.131891274	0.730370307	0.000000000	6	-0.725202240	6.155481731	0.000000000
6	4.916513291	1.409270014	0.000000000	6	-1.405176209	4.915049979	0.000000000
6	3.679949671	0.731615466	0.000000000	6	-0.729563142	3.700706045	0.000000000
6	3.679949581	-0.731632426	0.000000000	6	0.729528232	3.700706114	0.000000000
6	8.581794026	-0.728828417	0.000000000	6	0.722548109	8.602896345	0.000000000
6	7.377876996	1.407989923	0.000000000	6	-1.403057002	7.382003414	0.000000000
1	4.917151336	2.494805230	0.000000000	1	-2.490851705	4.916117260	0.000000000
6	2.457694945	1.409944964	0.000000000	6	-1.407518596	2.454288864	0.000000000
6	2.457695242	-1.409963569	0.000000000	6	1.407483665	2.454288070	0.000000000
6	1.226923895	-0.732184781	0.000000000	6	0.733785648	1.235580848	0.000000000
6	1.226924080	0.732162942	0.000000000	6	-0.733820325	1.235580674	0.000000000
1	2.458069851	2.495440978	0.000000000	1	-2.493169829	2.455463262	0.000000000
1	2.458073794	-2.495459701	0.000000000	1	2.493134935	2.455462770	0.000000000
6	8.581794026	0.728816288	0.000000000	6	-0.722584146	8.602896398	0.000000000
1	7.378833219	-2.493681263	0.000000000	1	2.488785257	7.382793794	0.000000000
1	4.917154014	-2.494820560	0.000000000	1	2.490816361	4.916117335	0.000000000
6	9.847150863	-1.409836329	0.000000000	6	1.404971401	9.857248571	0.000000000
1	7.378831632	2.493668139	0.000000000	1	-2.488821114	7.382793635	0.000000000
6	9.847150652	1.409824549	0.000000000	6	-1.405007502	9.857248571	0.000000000
6	11.018040407	-0.717238673	0.000000000	6	0.712081650	11.036050955	0.000000000
6	11.018040407	0.717227248	0.000000000	6	-0.712117782	11.036051007	0.000000000
1	9.847206639	-2.494825746	0.000000000	1	2.490004508	9.856582760	0.000000000
1	9.847205845	2.494813914	0.000000000	1	-2.490040614	9.856582707	0.000000000

1	11.964628754	-1.245746428	0.000000000	1	1.244144307	11.980635043	0.000000000
1	11.964628701	1.245734992	0.000000000	1	-1.244180413	11.980635096	0.000000000
6	-0.000213875	-1.410189301	0.000000000	6	1.408716844	-0.000009624	0.000000000
6	-0.000214077	1.410165255	0.000000000	6	-1.408752415	-0.000007899	0.000000000
6	-1.226425870	-0.732207774	0.000000000	6	0.733821458	-1.235404876	0.000000000
6	-1.226425494	0.732178273	0.000000000	6	-0.733857876	-1.235404982	0.000000000
1	0.000006869	-2.495674007	0.000000000	1	2.494345317	0.000049067	0.000000000
1	0.000000764	2.495649855	0.000000000	1	-2.494380872	0.000050569	0.000000000
6	-2.458111408	1.409994764	0.000000000	6	-1.407527904	-2.454256807	0.000000000
6	-2.458111519	-1.410027774	0.000000000	6	1.407488687	-2.454259188	0.000000000
6	-3.679483434	-0.731722556	0.000000000	6	0.729590564	-3.700658398	0.000000000
6	-3.679482503	0.731680142	0.000000000	6	-0.729632687	-3.700658192	0.000000000
1	-2.458006138	2.495486726	0.000000000	1	-2.493182297	-2.455361829	0.000000000
1	-2.457996222	-2.495520080	0.000000000	1	2.493143079	-2.455364147	0.000000000
6	-4.916875952	1.409357868	0.000000000	6	-1.405212246	-4.914946572	0.000000000
6	-4.916876429	-1.409407658	0.000000000	6	1.405164731	-4.914949012	0.000000000
6	-6.131543128	0.730506401	0.000000000	6	-0.725257227	-6.155548619	0.000000000
6	-6.131543816	-0.730574839	0.000000000	6	0.725204521	-6.155549678	0.000000000
1	-4.916905279	2.494893899	0.000000000	1	-2.490888705	-4.916029438	0.000000000
1	-4.916884948	-2.494944780	0.000000000	1	2.490841179	-4.916030237	0.000000000
6	-7.378058504	-1.408183168	0.000000000	6	1.402974937	-7.381868739	0.000000000
6	-8.581811436	-0.729061514	0.000000000	6	0.722655294	-8.603023982	0.000000000
6	-7.378058504	1.408094611	0.000000000	6	-1.403027045	-7.381870803	0.000000000
6	-8.581841176	0.728936670	0.000000000	6	-0.722686214	-8.603008530	0.000000000
1	-7.378336639	-2.493828861	0.000000000	1	2.488782802	-7.382924712	0.000000000
1	-7.378396331	2.493738224	0.000000000	1	-2.488836365	-7.382933549	0.000000000
6	-9.847270881	1.409981598	0.000000000	6	-1.404913731	-9.857249470	0.000000000
6	-11.018096394	0.717443385	0.000000000	6	-0.711960236	-11.036350204	0.000000000
6	-9.847276596	-1.409841964	0.000000000	6	1.404999405	-9.857253175	0.000000000
6	-11.018248426	-0.717046624	0.000000000	6	0.712461054	-11.036315914	0.000000000
1	-9.847016294	2.494989940	0.000000000	1	-2.490007117	-9.856484862	0.000000000
1	-11.964450210	1.246500701	0.000000000	1	-1.243783958	-11.981041610	0.000000000
1	-11.964686064	-1.246028395	0.000000000	1	1.244448674	-11.980861954	0.000000000
1	-9.847326391	-2.494839632	0.000000000	1	2.490114804	-9.856358230	0.000000000
[10]Acene							
SINGLET				TRIPLET			
6	1.407429207	-8.605809254	0.000000000	6	-1.403873856	-8.611010220	0.000000000
6	0.729950114	-7.359463057	0.000000000	6	-0.725749976	-7.380533889	0.000000000
6	1.408936209	-6.144587877	0.000000000	6	-1.405427928	-6.144765098	0.000000000
6	-0.731119098	-7.359358068	0.000000000	6	0.725770968	-7.380532725	0.000000000
6	-1.409931194	-6.144385890	0.000000000	6	1.405445126	-6.144768168	0.000000000
6	-0.732267100	-4.907267718	0.000000000	6	0.728855844	-4.928236425	0.000000000
6	0.731450114	-4.907375718	0.000000000	6	-0.728846927	-4.928240055	0.000000000
6	0.728172115	-9.809450424	0.000000000	6	-0.723844779	-9.827883361	0.000000000
6	-1.408777196	-8.605608272	0.000000000	6	1.403899770	-8.611010220	0.000000000
1	-2.495462352	-6.144987882	0.000000000	1	2.491104752	-6.145321211	0.000000000

6	-1.410509193	-3.685799540	0.000000000	6	1.407177769	-3.682845329	0.000000000
6	1.409871207	-3.686005538	0.000000000	6	-1.407172990	-3.682833687	0.000000000
6	0.732308112	-2.454099360	0.000000000	6	-0.732610769	-2.468226959	0.000000000
6	-0.732764098	-2.453987360	0.000000000	6	0.732605419	-2.468218228	0.000000000
1	-2.495996350	-3.686159540	0.000000000	1	2.492832346	-3.683704967	0.000000000
1	2.495359369	-3.686534541	0.000000000	1	-2.492827049	-3.683698924	0.000000000
6	-0.729691097	-9.809347393	0.000000000	6	0.723873418	-9.827882991	0.000000000
1	2.493104365	-8.606869249	0.000000000	1	-2.489623267	-8.611528443	0.000000000
1	2.494467366	-6.145351850	0.000000000	1	-2.491087231	-6.145320787	0.000000000
6	1.409058211	-11.074991627	0.000000000	6	-1.406056850	-11.084905392	0.000000000
1	-2.494452354	-8.606511261	0.000000000	1	2.489649324	-8.611526855	0.000000000
6	-1.410756192	-11.074791598	0.000000000	6	1.406087838	-11.084904810	0.000000000
6	0.716370113	-12.245734800	0.000000000	6	-0.713319999	-12.261700553	0.000000000
6	-0.718234098	-12.245632774	0.000000000	6	0.713352549	-12.261700448	0.000000000
1	2.494045369	-11.075144612	0.000000000	1	-2.491081346	-11.084257732	0.000000000
1	-2.495743350	-11.074789587	0.000000000	1	2.491112441	-11.084255827	0.000000000
1	1.244763185	-13.192385907	0.000000000	1	-1.244444557	-13.206817894	0.000000000
1	-1.246761173	-13.192208897	0.000000000	1	1.244478196	-13.206817100	0.000000000
6	1.410407210	-1.228502187	0.000000000	6	-1.408728025	-1.226378123	0.000000000
6	-1.410678197	-1.228290188	0.000000000	6	1.408719675	-1.226404243	0.000000000
6	0.732721113	-0.000322011	0.000000000	6	-0.734773067	-0.000411906	0.000000000
6	-0.732805099	-0.000203011	0.000000000	6	0.734758604	-0.000397734	0.000000000
1	2.495879365	-1.228906187	0.000000000	1	-2.494366738	-1.227075181	0.000000000
1	-2.496149351	-1.228514189	0.000000000	1	2.494359118	-1.227088670	0.000000000
6	-1.410501192	1.228904166	0.000000000	6	1.408736100	1.226628238	0.000000000
6	1.410611208	1.228682166	0.000000000	6	-1.408746007	1.226666223	0.000000000
6	0.732756113	2.453499342	0.000000000	6	-0.732849275	2.467708884	0.000000000
6	-0.732452101	2.453629340	0.000000000	6	0.732846698	2.467724368	0.000000000
1	-2.495970352	1.228777169	0.000000000	1	2.494380370	1.226976357	0.000000000
1	2.496082368	1.228356166	0.000000000	1	-2.494389530	1.226991317	0.000000000
6	-1.409988197	3.686357521	0.000000000	6	1.407260971	3.682711812	0.000000000
6	1.410502208	3.686116517	0.000000000	6	-1.407243942	3.682746749	0.000000000
6	-0.731654096	4.907051697	0.000000000	6	0.729097715	4.928284622	0.000000000
6	0.732377111	4.906901697	0.000000000	6	-0.729055164	4.928267070	0.000000000
1	-2.495468353	3.686378518	0.000000000	1	2.492921365	3.683501413	0.000000000
1	2.495988365	3.685899518	0.000000000	1	-2.492904828	3.683498524	0.000000000
6	1.409980207	6.144517867	0.000000000	6	-1.405454260	6.144374777	0.000000000
6	0.731450114	7.359163066	0.000000000	6	-0.725913264	7.380941462	0.000000000
6	-1.409013193	6.144807856	0.000000000	6	1.405514718	6.144375042	0.000000000
6	-0.730235097	7.359361031	0.000000000	6	0.725989248	7.380990093	0.000000000
1	2.495539368	6.144749858	0.000000000	1	-2.491162628	6.145152086	0.000000000
1	-2.494563354	6.145360846	0.000000000	1	2.491218287	6.145238712	0.000000000
6	-1.407406193	8.606165232	0.000000000	6	1.403841983	8.610878031	0.000000000
6	-0.728253100	9.809347393	0.000000000	6	0.723933675	9.828294055	0.000000000
6	1.408879211	8.605752262	0.000000000	6	-1.403782837	8.610773942	0.000000000
6	0.729781110	9.809313367	0.000000000	6	-0.723724465	9.828455507	0.000000000
1	-2.493108355	8.607353234	0.000000000	1	2.489668792	8.611746411	0.000000000

1	2.494613366	8.606610270	0.000000000	1	-2.489643148	8.611509445	0.000000000
6	-1.409177196	11.075228592	0.000000000	6	1.406031280	11.084993341	0.000000000
6	-0.716308099	12.245631769	0.000000000	6	0.712825377	12.261757387	0.000000000
6	1.410611208	11.074821602	0.000000000	6	-1.405644695	11.084862687	0.000000000
6	0.718785114	12.245855769	0.000000000	6	-0.713696053	12.262422034	0.000000000
1	-2.494083353	11.074969560	0.000000000	1	2.490986618	11.084327107	0.000000000
1	-1.244235172	13.192696905	0.000000000	1	1.243890048	13.207104073	0.000000000
1	1.247083188	13.192289914	0.000000000	1	-1.244846001	13.207192128	0.000000000
1	2.495750367	11.074354603	0.000000000	1	-2.490883111	11.083780308	0.000000000
[3]Phenacene							
SINGLET				TRIPLET			
6	-2.091575000	0.678219000	0.000000000	6	-2.074890000	-0.735098000	0.000000000
6	-0.864975000	1.421060000	0.000000000	6	-0.885712000	-1.446047000	0.000000000
6	0.379670000	0.728189000	0.000000000	6	0.384240000	-0.745465000	0.000000000
6	-0.877095000	2.833833000	0.000000000	6	-0.874627000	-2.880043000	0.000000000
6	0.296503000	3.555701000	0.000000000	6	0.310296000	-3.591803000	0.000000000
6	1.527323000	2.877697000	0.000000000	6	1.527665000	-2.910167000	0.000000000
6	1.564421000	1.497959000	0.000000000	6	1.543570000	-1.496048000	0.000000000
6	-2.091584000	-0.678217000	0.000000000	6	-2.074891000	0.735099000	0.000000000
6	-0.864990000	-1.421063000	0.000000000	6	-0.885709000	1.446047000	0.000000000
6	0.379663000	-0.728201000	0.000000000	6	0.384238000	0.745466000	0.000000000
6	-0.877095000	-2.833837000	0.000000000	6	-0.874627000	2.880043000	0.000000000
6	0.296504000	-3.555696000	0.000000000	6	0.310292000	3.591802000	0.000000000
6	1.527334000	-2.877692000	0.000000000	6	1.527665000	2.910164000	0.000000000
6	1.564417000	-1.497957000	0.000000000	6	1.543572000	1.496051000	0.000000000
1	-3.026322000	1.229067000	0.000000000	1	-3.020761000	-1.263358000	0.000000000
1	2.454146000	3.440266000	0.000000000	1	2.463907000	-3.455007000	0.000000000
1	2.528192000	1.005441000	0.000000000	1	2.508149000	-1.003649000	0.000000000
1	-3.026338000	-1.229056000	0.000000000	1	-3.020760000	1.263360000	0.000000000
1	-1.834357000	-3.344805000	0.000000000	1	-1.826806000	3.399448000	0.000000000
1	0.272814000	-4.639491000	0.000000000	1	0.292266000	4.675899000	0.000000000
1	2.454153000	-3.440266000	0.000000000	1	2.463906000	3.455007000	0.000000000
1	2.528166000	-1.005407000	0.000000000	1	2.508149000	1.003650000	0.000000000
1	-1.834364000	3.344791000	0.000000000	1	-1.826804000	-3.399450000	0.000000000
1	0.272794000	4.639496000	0.000000000	1	0.292265000	-4.675900000	0.000000000
[4]Phenacene							
SINGLET				TRIPLET			
6	0.613256000	-1.804370000	0.000000000	6	0.525039000	-1.868252000	0.046568000
6	-0.630164000	-2.500926000	0.000000000	6	-0.748982000	-2.488422000	-0.142276000
6	0.613278000	-0.352886000	0.000000000	6	0.624222000	-0.398169000	-0.068992000
6	-1.843196000	-1.752244000	0.000000000	6	-1.897215000	-1.669159000	-0.335333000
6	-0.613278000	0.352886000	0.000000000	6	-0.624222000	0.398169000	-0.068992000
6	-1.833835000	-0.391541000	0.000000000	6	-1.815488000	-0.255343000	-0.258040000
6	1.833835000	0.391541000	0.000000000	6	1.815488000	0.255343000	-0.258040000
6	1.843196000	1.752244000	0.000000000	6	1.897215000	1.669159000	-0.335333000

6	0.630164000	2.500926000	0.000000000	6	0.748982000	2.488422000	-0.142276000
6	-0.613256000	1.804370000	0.000000000	6	-0.525039000	1.868252000	0.046568000
6	0.645084000	3.915490000	0.000000000	6	0.840608000	3.893645000	-0.105378000
6	-0.526508000	4.636516000	0.000000000	6	-0.280738000	4.683305000	0.140651000
6	-1.799119000	2.579110000	0.000000000	6	-1.620659000	2.678475000	0.328134000
6	-1.759022000	3.956862000	0.000000000	6	-1.509419000	4.078055000	0.368602000
6	1.799119000	-2.579110000	0.000000000	6	1.620659000	-2.678475000	0.328134000
6	-0.645084000	-3.915490000	0.000000000	6	-0.840608000	-3.893645000	-0.105378000
1	-2.785112000	-2.290713000	0.000000000	1	-2.860051000	-2.141498000	-0.491181000
1	-2.779474000	0.133059000	0.000000000	1	-2.732008000	0.312879000	-0.362946000
1	2.779474000	-0.133059000	0.000000000	1	2.732008000	-0.312879000	-0.362946000
1	2.785112000	2.290713000	0.000000000	1	2.860051000	2.141498000	-0.491181000
1	1.603572000	4.424093000	0.000000000	1	1.807606000	4.357970000	-0.267845000
1	-0.503950000	5.720313000	0.000000000	1	-0.188717000	5.763170000	0.164832000
1	-2.765328000	2.092750000	0.000000000	1	-2.584907000	2.228430000	0.531463000
1	-2.685270000	4.520403000	0.000000000	1	-2.385903000	4.678687000	0.582064000
6	1.759022000	-3.956862000	0.000000000	6	1.509419000	-4.078055000	0.368602000
6	0.526508000	-4.636516000	0.000000000	6	0.280738000	-4.683305000	0.140651000
1	2.765328000	-2.092750000	0.000000000	1	2.584907000	-2.228430000	0.531463000
1	-1.603572000	-4.424093000	0.000000000	1	-1.807606000	-4.357970000	-0.267845000
1	2.685270000	-4.520403000	0.000000000	1	2.385903000	-4.678687000	0.582064000
1	0.503950000	-5.720313000	0.000000000	1	0.188717000	-5.763170000	0.164832000
[5]Phenacene							
SINGLET				TRIPLET			
6	-0.767940000	0.723136000	0.000150000	6	-0.767194000	0.747575000	0.067925000
6	0.459151000	1.432654000	0.000145000	6	0.473933000	1.454616000	-0.065827000
6	-0.767944000	-0.723133000	0.000030000	6	-0.778294000	-0.730189000	-0.079932000
6	1.665232000	0.682830000	0.000337000	6	1.649353000	0.712058000	-0.142010000
6	0.459131000	-1.432652000	0.000148000	6	0.490396000	-1.450395000	0.001711000
6	1.665224000	-0.682858000	0.000389000	6	1.647585000	-0.723829000	-0.070407000
6	-1.987718000	-1.474652000	-0.000234000	6	-1.923459000	-1.434107000	-0.362146000
6	-1.992631000	-2.834260000	-0.000276000	6	-1.934130000	-2.853273000	-0.453096000
6	-0.778233000	-3.583222000	-0.000117000	6	-0.765011000	-3.607108000	-0.205402000
6	0.462868000	-2.885558000	0.000031000	6	0.464003000	-2.924604000	0.067282000
6	-0.791320000	-4.996992000	-0.000177000	6	-0.780569000	-5.024062000	-0.198605000
6	0.382075000	-5.716214000	-0.000121000	6	0.360272000	-5.750615000	0.091839000
6	1.650006000	-3.656457000	0.000035000	6	1.588773000	-3.685956000	0.387899000
6	1.612814000	-5.034883000	-0.000032000	6	1.549117000	-5.081591000	0.397120000
6	-1.987703000	1.474656000	0.000331000	6	-1.930627000	1.458588000	0.357957000
6	0.462881000	2.885561000	0.000009000	6	0.459081000	2.914923000	-0.059088000
1	2.617384000	1.195650000	0.000527000	1	2.608534000	1.207796000	-0.200554000
1	2.617364000	-1.195706000	0.000658000	1	2.606333000	-1.226270000	-0.101905000
1	-2.936941000	-0.957982000	-0.000483000	1	-2.853719000	-0.905822000	-0.532638000
1	-2.933708000	-3.374271000	-0.000473000	1	-2.861587000	-3.368570000	-0.673564000
1	-1.748735000	-5.507609000	-0.000279000	1	-1.712185000	-5.533918000	-0.420388000
1	0.361259000	-6.800047000	-0.000161000	1	0.329314000	-6.834307000	0.093891000

1	2.614847000	-3.167248000	0.000055000	1	2.516344000	-3.190697000	0.648601000
1	2.540055000	-5.596775000	-0.000030000	1	2.442278000	-5.642595000	0.646292000
6	-1.992608000	2.834266000	0.000328000	6	-1.946691000	2.848849000	0.426934000
6	-0.778206000	3.583219000	0.000093000	6	-0.770785000	3.600252000	0.197214000
1	-2.936933000	0.957998000	0.000587000	1	-2.850459000	0.918899000	0.547950000
1	-2.933686000	3.374273000	0.000524000	1	-2.870542000	3.369796000	0.651764000
6	1.650013000	3.656478000	-0.000259000	6	1.609572000	3.692396000	-0.301886000
6	-0.791310000	4.996990000	-0.000060000	6	-0.785597000	5.018918000	0.219676000
6	0.382053000	5.716200000	-0.000269000	6	0.359256000	5.744721000	-0.011769000
6	1.612786000	5.034890000	-0.000381000	6	1.567135000	5.073650000	-0.280026000
1	2.614853000	3.167283000	-0.000412000	1	2.550938000	3.206591000	-0.524672000
1	2.540003000	5.596817000	-0.000656000	1	2.469396000	5.642426000	-0.473845000
1	0.361234000	6.800033000	-0.000415000	1	0.333536000	6.828347000	0.006215000
1	-1.748729000	5.507591000	-0.000033000	1	-1.724903000	5.523427000	0.420672000
[6]Phenacene							
SINGLET				TRIPLET			
6	0.632675000	0.321224000	0.000380000	6	0.647440000	0.335331000	-0.096677000
6	-0.632829000	-0.321207000	0.000129000	6	-0.632659000	-0.301298000	-0.001115000
6	0.718148000	1.766356000	0.000210000	6	0.717035000	1.785910000	-0.110806000
6	-1.794068000	0.502043000	-0.000340000	6	-1.751893000	0.486020000	0.226138000
6	-0.464220000	2.544708000	-0.000098000	6	-0.469786000	2.561684000	0.086929000
6	-1.712713000	1.864028000	-0.000425000	6	-1.680738000	1.883459000	0.273437000
6	1.979814000	2.443338000	0.000283000	6	1.947435000	2.467814000	-0.329104000
6	2.064528000	3.800736000	0.000167000	6	2.028401000	3.829403000	-0.332339000
6	0.896057000	4.618859000	-0.000022000	6	0.875564000	4.644170000	-0.115127000
6	-0.383942000	3.994567000	-0.000163000	6	-0.386083000	4.019088000	0.093088000
6	0.991124000	6.029669000	-0.000084000	6	0.970062000	6.053895000	-0.111599000
6	-0.138465000	6.815639000	-0.000270000	6	-0.143591000	6.839543000	0.091648000
6	-1.524443000	4.833292000	-0.000346000	6	-1.507075000	4.852947000	0.296308000
6	-1.406988000	6.207020000	-0.000396000	6	-1.392001000	6.229585000	0.297093000
6	1.793947000	-0.501951000	0.000830000	6	1.784976000	-0.481332000	-0.122917000
6	-0.718269000	-1.766370000	0.000281000	6	-0.724422000	-1.774109000	-0.124207000
1	-2.776497000	0.051348000	-0.000761000	1	-2.714627000	0.016348000	0.386610000
1	-2.633307000	2.431591000	-0.000826000	1	-2.594422000	2.433241000	0.452002000
1	2.896549000	1.870750000	0.000366000	1	2.847257000	1.896869000	-0.514833000
1	3.035537000	4.284829000	0.000207000	1	2.981735000	4.316922000	-0.506318000
1	1.976541000	6.483888000	0.000022000	1	1.941301000	6.509978000	-0.272874000
1	-0.054770000	7.896434000	-0.000313000	1	-0.059315000	7.920275000	0.092922000
1	-2.516059000	4.400922000	-0.000422000	1	-2.484395000	4.417514000	0.457531000
1	-2.299856000	6.822062000	-0.000528000	1	-2.272476000	6.841513000	0.457423000
6	1.712641000	-1.863937000	0.000687000	6	1.697549000	-1.911031000	-0.035316000
6	0.464159000	-2.544669000	0.000227000	6	0.499687000	-2.568751000	0.007361000
1	2.776350000	-0.051182000	0.001375000	1	2.773688000	-0.045585000	-0.147506000
1	2.633239000	-2.431479000	0.001140000	1	2.626616000	-2.467358000	-0.025091000
6	-1.979885000	-2.443444000	0.000646000	6	-1.902484000	-2.418107000	-0.429287000
6	0.383956000	-3.994513000	-0.000108000	6	0.384129000	-4.037849000	0.093538000

6	-0.895984000	-4.618881000	0.000278000	6	-0.873277000	-4.649159000	-0.203807000
6	-2.064506000	-3.800851000	0.000735000	6	-1.992094000	-3.826970000	-0.499201000
1	-2.896655000	-1.870927000	0.001053000	1	-2.794569000	-1.838961000	-0.635609000
1	-3.035485000	-4.285000000	0.001176000	1	-2.939680000	-4.292968000	-0.742958000
6	-0.991027000	-6.029719000	0.000112000	6	-0.976594000	-6.058501000	-0.176838000
6	0.138641000	-6.815680000	-0.000505000	6	0.111053000	-6.850621000	0.156017000
6	1.524497000	-4.833232000	-0.000940000	6	1.452506000	-4.859762000	0.454781000
6	1.407125000	-6.207013000	-0.001092000	6	1.327976000	-6.250985000	0.482779000
1	-1.976438000	-6.483943000	0.000401000	1	-1.931121000	-6.514790000	-0.417212000
1	2.516117000	-4.400853000	-0.001475000	1	2.401286000	-4.417240000	0.733261000
1	2.300014000	-6.822022000	-0.001756000	1	2.178959000	-6.860418000	0.763959000
1	0.054886000	-7.896494000	-0.000723000	1	0.012782000	-7.930123000	0.172791000
[7]Phenacene							
SINGLET				TRIPLET			
6	-0.725108000	1.438249000	0.000258000	6	-0.593045000	0.378429000	0.059908000
6	0.499595000	0.724514000	0.000227000	6	0.653641000	-0.351680000	-0.022424000
6	-0.726909000	2.885049000	0.000050000	6	-0.552177000	1.843485000	0.121451000
6	1.707012000	1.476619000	0.000247000	6	1.816366000	0.356296000	-0.246651000
6	0.499243000	3.593424000	0.000089000	6	0.681467000	2.528542000	-0.093466000
6	1.705630000	2.841523000	0.000229000	6	1.840972000	1.764263000	-0.297542000
6	-1.947203000	3.634352000	-0.000256000	6	-1.714737000	2.598922000	0.403218000
6	-1.952641000	4.994260000	-0.000402000	6	-1.700172000	3.969309000	0.432519000
6	-0.738407000	5.743108000	-0.000261000	6	-0.504752000	4.699027000	0.178800000
6	0.503179000	5.045676000	-0.000042000	6	0.702076000	3.986448000	-0.083975000
6	-0.751480000	7.157001000	-0.000376000	6	-0.494920000	6.114060000	0.192393000
6	0.421834000	7.876159000	-0.000280000	6	0.663296000	6.817738000	-0.047790000
6	1.690375000	5.816731000	0.000036000	6	1.871634000	4.740564000	-0.325972000
6	1.652854000	7.195011000	-0.000075000	6	1.856315000	6.120939000	-0.310207000
6	-1.932855000	0.681595000	0.000589000	6	-1.768194000	-0.341838000	0.012042000
6	0.499599000	-0.724519000	0.000214000	6	0.634374000	-1.827773000	0.084105000
1	2.660928000	0.968052000	0.000310000	1	2.747402000	-0.174138000	-0.405670000
1	2.657802000	3.354366000	0.000305000	1	2.790999000	2.247927000	-0.476392000
1	-2.895675000	3.115998000	-0.000466000	1	-2.642262000	2.085785000	0.622018000
1	-2.893768000	5.534154000	-0.000657000	1	-2.608466000	4.518323000	0.656168000
1	-1.708883000	7.667620000	-0.000543000	1	-1.423323000	6.637373000	0.396124000
1	0.400949000	8.959986000	-0.000364000	1	0.658683000	7.901700000	-0.036108000
1	2.655215000	5.327504000	0.000189000	1	2.806622000	4.237456000	-0.534437000
1	2.579914000	7.757188000	-0.000004000	1	2.771063000	6.670238000	-0.502237000
6	-1.932854000	-0.681607000	0.000614000	6	-1.781884000	-1.783608000	-0.078281000
6	-0.725105000	-1.438260000	0.000279000	6	-0.622063000	-2.530012000	-0.063905000
1	-2.887323000	1.188892000	0.000947000	1	-2.724432000	0.163444000	-0.002942000
1	-2.887320000	-1.188906000	0.000988000	1	-2.748595000	-2.267409000	-0.114164000
6	1.707011000	-1.476625000	0.000176000	6	1.767931000	-2.561270000	0.368502000
6	-0.726902000	-2.885054000	0.000076000	6	-0.610696000	-3.995557000	-0.123214000
6	0.499254000	-3.593433000	0.000024000	6	0.594618000	-4.707674000	0.154904000
6	1.705634000	-2.841532000	0.000135000	6	1.758630000	-3.969144000	0.419733000

1	2.660932000	-0.968066000	0.000213000	1	2.700884000	-2.051446000	0.576303000
1	2.657817000	-3.354358000	0.000194000	1	2.686935000	-4.473657000	0.648162000
6	0.503188000	-5.045679000	-0.000127000	6	0.583482000	-6.165659000	0.145609000
6	-0.738395000	-5.743103000	-0.000150000	6	-0.623879000	-6.851551000	-0.178428000
6	-1.947192000	-3.634361000	-0.000066000	6	-1.773985000	-4.725412000	-0.463990000
6	-1.952627000	-4.994253000	-0.000121000	6	-1.788398000	-6.095700000	-0.492475000
1	-2.895673000	-3.116024000	-0.000098000	1	-2.677608000	-4.192117000	-0.729583000
1	-2.893761000	-5.534132000	-0.000179000	1	-2.696126000	-6.624694000	-0.761984000
6	1.690379000	-5.816729000	-0.000263000	6	1.722393000	-6.945316000	0.445943000
6	1.652835000	-7.194989000	-0.000323000	6	-0.644786000	-8.266442000	-0.191963000
6	-0.751484000	-7.156993000	-0.000189000	6	0.483903000	-8.995422000	0.106338000
6	0.421820000	-7.876138000	-0.000267000	6	1.677293000	-8.325008000	0.428882000
1	2.655227000	-5.327521000	-0.000295000	1	2.656696000	-6.462910000	0.701157000
1	2.579884000	-7.757176000	-0.000312000	1	2.568822000	-8.894294000	0.666496000
1	0.400949000	-8.959967000	-0.000330000	1	0.455880000	-10.079025000	0.094075000
1	-1.708889000	-7.667591000	-0.000157000	1	-1.573044000	-8.769201000	-0.442682000
[8]Phenacene							
SINGLET				TRIPLET			
6	-0.696182000	-2.496548000	-0.000072000	6	0.696820000	-2.519430000	0.154707000
6	0.551982000	-1.823748000	-0.000127000	6	-0.553862000	-1.852558000	-0.049494000
6	-0.745710000	-3.942685000	0.000027000	6	0.733042000	-3.973094000	0.159731000
6	1.733965000	-2.615560000	-0.000287000	6	-1.675475000	-2.617572000	-0.361277000
6	0.456318000	-4.691094000	-0.000106000	6	-0.448901000	-4.716920000	-0.125795000
6	1.687152000	-3.979523000	-0.000305000	6	-1.632963000	-4.006760000	-0.402668000
6	-1.990063000	-4.651153000	0.000286000	6	1.932473000	-4.684702000	0.452108000
6	-2.040482000	-6.010164000	0.000347000	6	1.980852000	-6.047226000	0.452124000
6	-0.851688000	-6.798690000	0.000168000	6	0.825993000	-6.831574000	0.157567000
6	0.412281000	-6.142639000	-0.000034000	6	-0.403013000	-6.173219000	-0.131558000
6	-0.911468000	-8.211392000	0.000219000	6	0.884468000	-8.244078000	0.154915000
6	0.237440000	-8.968900000	0.000084000	6	-0.232454000	-8.999464000	-0.124024000
6	1.573375000	-6.952522000	-0.000150000	6	-1.530131000	-6.978795000	-0.411216000
6	1.490311000	-8.328789000	-0.000097000	6	-1.449745000	-8.356689000	-0.409010000
6	-1.877812000	-1.700513000	-0.000181000	6	1.844894000	-1.730783000	0.304647000
6	0.599506000	-0.376354000	-0.000078000	6	-0.621490000	-0.380423000	0.053564000
1	2.704189000	-2.138802000	-0.000434000	1	-2.611030000	-2.124767000	-0.595824000
1	2.621705000	-4.523782000	-0.000487000	1	-2.540698000	-4.537818000	-0.653336000
1	-2.920840000	-4.101668000	0.000492000	1	2.832637000	-4.136559000	0.694943000
1	-2.998946000	-6.518635000	0.000556000	1	2.909530000	-6.558371000	0.682755000
1	-1.885211000	-8.690111000	0.000371000	1	1.831046000	-8.725172000	0.378210000
1	0.180772000	-10.051443000	0.000120000	1	-0.176459000	-10.082035000	-0.123826000
1	2.553875000	-6.495488000	-0.000275000	1	-2.483725000	-6.518649000	-0.633603000
1	2.398280000	-8.921301000	-0.000191000	1	-2.332832000	-8.946110000	-0.628467000
6	-1.831960000	-0.337611000	-0.000205000	6	1.796498000	-0.304142000	0.224509000
6	-0.599559000	0.376364000	-0.000062000	6	0.621487000	0.380421000	0.053564000
1	-2.848695000	-2.175660000	-0.000320000	1	2.814917000	-2.188733000	0.434892000
1	-2.768368000	0.202549000	-0.000344000	1	2.730645000	0.234497000	0.325444000

6	1.831912000	0.337611000	-0.000071000	6	-1.796500000	0.304140000	0.224519000
6	-0.552025000	1.823764000	0.000055000	6	0.553859000	1.852557000	-0.049484000
6	0.696145000	2.496553000	0.000095000	6	-0.696822000	2.519427000	0.154727000
6	1.877771000	1.700512000	-0.000018000	6	-1.844896000	1.730779000	0.304666000
1	2.768314000	-0.202562000	-0.000137000	1	-2.730647000	-0.234501000	0.325455000
1	2.848656000	2.175657000	-0.000061000	1	-2.814919000	2.188728000	0.434918000
6	0.745691000	3.942689000	0.000208000	6	-0.733044000	3.973092000	0.159761000
6	-0.456316000	4.691115000	0.000039000	6	0.448897000	4.716919000	-0.125766000
6	-1.733994000	2.615592000	0.000031000	6	1.675470000	2.617573000	-0.361268000
6	-1.687165000	3.979555000	-0.000031000	6	1.632958000	4.006761000	-0.402650000
1	-2.704225000	2.138846000	-0.000007000	1	2.611024000	2.124769000	-0.595823000
1	-2.621706000	4.523831000	-0.000217000	1	2.540691000	4.537820000	-0.653319000
6	1.990054000	4.651125000	0.000300000	6	-1.932474000	4.684697000	0.452150000
6	2.040509000	6.010122000	0.000320000	6	-1.980853000	6.047222000	0.452176000
6	-0.412267000	6.142646000	-0.000004000	6	0.403009000	6.173218000	-0.131519000
6	0.851722000	6.798670000	0.000285000	6	-0.825996000	6.831571000	0.157617000
1	2.920816000	4.101615000	0.000313000	1	-2.832636000	4.136553000	0.694986000
1	2.998994000	6.518572000	0.000361000	1	-2.909529000	6.558365000	0.682815000
6	-1.573356000	6.952532000	-0.000288000	6	1.530125000	6.978796000	-0.411178000
6	0.911515000	8.211344000	0.000161000	6	-0.884471000	8.244075000	0.154974000
6	-0.237363000	8.968882000	-0.000080000	6	0.232450000	8.999464000	-0.123966000
6	-1.490258000	8.328818000	-0.000244000	6	1.449739000	8.356690000	-0.408964000
1	1.885251000	8.690070000	0.000257000	1	-1.831047000	8.725168000	0.378278000
1	-0.180648000	10.051428000	-0.000124000	1	0.176455000	10.082035000	-0.123761000
1	-2.398230000	8.921324000	-0.000514000	1	2.332825000	8.946113000	-0.628422000
1	-2.553867000	6.495509000	-0.000472000	1	2.483718000	6.518652000	-0.633575000

[9]Phenacene

SINGLET				TRIPLET			
6	0.523208000	1.436304000	0.000021000	6	-0.534926000	1.455902000	-0.107110000
6	-0.700641000	0.723664000	-0.000023000	6	0.699808000	0.748833000	0.059189000
6	0.523428000	2.884659000	0.000054000	6	-0.522362000	2.912955000	-0.107338000
6	-1.908846000	1.478164000	-0.000057000	6	1.852519000	1.478524000	0.345388000
6	-0.701795000	3.598219000	0.000015000	6	0.687585000	3.621044000	0.149772000
6	-1.909317000	2.841710000	-0.000044000	6	1.857103000	2.866811000	0.394947000
6	1.730877000	3.636948000	0.000132000	6	-1.692115000	3.666623000	-0.365993000
6	1.729143000	5.001733000	0.000158000	6	-1.689722000	5.035472000	-0.358056000
6	0.522488000	5.753520000	0.000105000	6	-0.511481000	5.783016000	-0.090121000
6	-0.703610000	5.045170000	0.000038000	6	0.687787000	5.072475000	0.160044000
6	0.526416000	7.205713000	0.000125000	6	-0.514651000	7.235452000	-0.075611000
6	-0.715222000	7.903140000	0.000083000	6	0.700782000	7.929968000	0.187101000
6	-1.923898000	5.794343000	-0.000004000	6	1.880949000	5.817537000	0.416088000
6	-1.929378000	7.154279000	0.000018000	6	1.888084000	7.178487000	0.429040000
6	1.730861000	0.682060000	0.000023000	6	-1.709348000	0.708547000	-0.224149000
6	-0.700649000	-0.723657000	-0.000037000	6	0.718009000	-0.724148000	-0.050677000
1	-2.862625000	0.969255000	-0.000100000	1	2.777728000	0.955384000	0.554063000
1	-2.863833000	3.348901000	-0.000078000	1	2.789010000	3.361858000	0.627188000

1	2.684802000	3.128380000	0.000183000	1	-2.620063000	3.158424000	-0.591291000
1	2.681163000	5.514837000	0.000225000	1	-2.617140000	5.550282000	-0.568298000
1	-2.872373000	5.275992000	-0.000055000	1	2.808957000	5.296155000	0.604576000
1	-2.870539000	7.694107000	-0.000015000	1	2.809956000	7.715421000	0.626510000
6	1.730848000	-0.682091000	0.000000000	6	-1.704380000	-0.720275000	-0.154576000
6	0.523180000	-1.436305000	-0.000022000	6	-0.546706000	-1.443681000	-0.022822000
1	2.684817000	1.190611000	0.000032000	1	-2.667512000	1.198795000	-0.322562000
1	2.684790000	-1.190671000	-0.000005000	1	-2.657757000	-1.227953000	-0.232620000
6	-1.908870000	-1.478148000	-0.000065000	6	1.867313000	-1.444583000	-0.250217000
6	0.523398000	-2.884664000	-0.000032000	6	-0.523976000	-2.917313000	0.067888000
6	-0.701836000	-3.598226000	-0.000060000	6	0.701321000	-3.623445000	-0.167054000
6	-1.909352000	-2.841688000	-0.000077000	6	1.869030000	-2.872845000	-0.336310000
1	-2.862639000	-0.969224000	-0.000075000	1	2.815330000	-0.935118000	-0.370824000
1	-2.863872000	-3.348870000	-0.000101000	1	2.821233000	-3.360307000	-0.489185000
6	-0.703634000	-5.045165000	-0.000071000	6	0.689914000	-5.079064000	-0.181704000
6	0.522475000	-5.753504000	-0.000062000	6	-0.508054000	-5.785343000	0.125718000
6	1.730835000	-3.636930000	-0.000012000	6	-1.662380000	-3.648991000	0.399523000
6	1.729114000	-5.001724000	-0.000028000	6	-1.663258000	-5.038423000	0.432783000
1	2.684762000	-3.128361000	0.000020000	1	-2.576698000	-3.128655000	0.657098000
1	2.681141000	-5.514819000	-0.000010000	1	-2.581702000	-5.541873000	0.700701000
6	-1.923930000	-5.794379000	-0.000088000	6	1.858605000	-5.826550000	-0.504857000
6	-1.929394000	-7.154302000	-0.000099000	6	1.863106000	-7.190315000	-0.513217000
6	0.526408000	-7.205723000	-0.000082000	6	-0.509756000	-7.241839000	0.122616000
6	-0.715201000	-7.903144000	-0.000100000	6	0.690631000	-7.938266000	-0.197177000
1	-2.872399000	-5.276020000	-0.000088000	1	2.770271000	-5.306099000	-0.765133000
1	-2.870534000	-7.694163000	-0.000109000	1	2.769459000	-7.729562000	-0.767421000
6	1.713604000	-7.976808000	-0.000088000	6	-1.656369000	-8.012156000	0.422889000
6	-0.728313000	-9.317044000	-0.000118000	6	0.702869000	-9.352178000	-0.203134000
6	0.444985000	-10.036199000	-0.000121000	6	-0.431626000	-10.072178000	0.096493000
6	1.676030000	-9.355070000	-0.000107000	6	-1.620968000	-9.391676000	0.411683000
1	-1.685721000	-9.827643000	-0.000130000	1	1.628079000	-9.862500000	-0.449851000
1	0.424094000	-11.120022000	-0.000136000	1	-0.411210000	-11.155980000	0.089469000
1	2.603068000	-9.917276000	-0.000112000	1	-2.517748000	-9.953461000	0.647484000
1	2.678475000	-7.487650000	-0.000081000	1	-2.589350000	-7.522609000	0.668654000
6	1.713589000	7.976815000	0.000185000	6	-1.676419000	8.009374000	-0.310301000
6	-0.728338000	9.317049000	0.000106000	6	0.713982000	9.344030000	0.204307000
6	0.444945000	10.036207000	0.000133000	6	-0.434076000	10.065765000	-0.028916000
6	1.675997000	9.355074000	0.000171000	6	-1.639290000	9.387460000	-0.288006000
1	-1.685751000	9.827641000	0.000248000	1	1.651135000	9.852263000	0.406224000
1	0.424067000	11.120030000	0.000014000	1	-0.413492000	11.149478000	-0.013342000
1	2.603021000	9.917304000	0.000137000	1	-2.546668000	9.951832000	-0.471356000
1	2.678461000	7.487666000	0.000410000	1	-2.621323000	7.522612000	-0.511408000
[10]Phenacene							
SINGLET				TRIPLET			
6	-0.619643000	-0.343107000	-0.000011000	6	-0.633617000	-0.360816000	0.111125000
6	0.619741000	0.343091000	-0.000016000	6	0.622969000	0.321824000	-0.019888000

6	-0.650570000	-1.790271000	0.000004000	6	-0.651566000	-1.818908000	0.121129000
6	1.811033000	-0.437040000	-0.000026000	6	1.769821000	-0.435371000	-0.257488000
6	0.557686000	-2.528859000	-0.000012000	6	0.553596000	-2.555324000	-0.087849000
6	1.781475000	-1.800742000	-0.000029000	6	1.746619000	-1.828631000	-0.295062000
6	-1.874624000	-2.518662000	0.000038000	6	-1.846240000	-2.549626000	0.342236000
6	-1.904309000	-3.881903000	0.000043000	6	-1.875008000	-3.920728000	0.342456000
6	-0.713273000	-4.664066000	0.000015000	6	-0.702659000	-4.700778000	0.121535000
6	0.526955000	-3.976847000	-0.000008000	6	0.521686000	-4.009970000	-0.088208000
6	-0.746046000	-6.110627000	0.000012000	6	-0.734131000	-6.149246000	0.114572000
6	0.464633000	-6.845036000	-0.000012000	6	0.462732000	-6.883699000	-0.094572000
6	1.718036000	-4.754789000	-0.000031000	6	1.695388000	-4.785563000	-0.291959000
6	1.687063000	-6.119225000	-0.000033000	6	1.667167000	-6.154703000	-0.294430000
6	-1.810943000	0.437019000	-0.000028000	6	-1.795976000	0.413036000	0.188932000
6	0.650656000	1.790270000	-0.000015000	6	0.667828000	1.796776000	0.076656000
1	2.775683000	0.050959000	-0.000038000	1	2.715744000	0.065461000	-0.437675000
1	2.724152000	-2.329882000	-0.000044000	1	2.678653000	-2.345357000	-0.488154000
1	-2.817257000	-1.989403000	0.000068000	1	-2.773214000	-2.020562000	0.532380000
1	-2.869471000	-4.368542000	0.000072000	1	-2.825065000	-4.408162000	0.523898000
1	2.682660000	-4.266804000	-0.000051000	1	2.648620000	-4.295103000	-0.449551000
1	2.627878000	-6.652578000	-0.000056000	1	2.598328000	-6.685567000	-0.455207000
6	-1.781397000	1.800714000	-0.000036000	6	-1.759475000	1.843400000	0.119403000
6	-0.557610000	2.528850000	-0.000022000	6	-0.581688000	2.544733000	0.020587000
1	-2.775586000	-0.050996000	-0.000046000	1	-2.769690000	-0.056538000	0.257458000
1	-2.724078000	2.329846000	-0.000056000	1	-2.707088000	2.369560000	0.171114000
6	1.874697000	2.518667000	-0.000006000	6	1.832491000	2.497412000	0.280625000
6	-0.526890000	3.976834000	-0.000018000	6	-0.527783000	4.018501000	-0.070660000
6	0.713340000	4.664063000	-0.000011000	6	0.712532000	4.702031000	0.163914000
6	1.904374000	3.881914000	-0.000005000	6	1.864656000	3.925377000	0.349101000
1	2.817336000	1.989423000	0.000002000	1	2.770655000	1.969423000	0.418062000
1	2.869538000	4.368549000	0.000000000	1	2.828693000	4.393419000	0.505060000
6	0.746075000	6.110645000	-0.000009000	6	0.733672000	6.158621000	0.168425000
6	-0.464602000	6.845030000	-0.000021000	6	-0.452559000	6.891288000	-0.138141000
6	-1.717984000	4.754775000	-0.000020000	6	-1.653906000	4.775233000	-0.399773000
6	-1.687041000	6.119208000	-0.000023000	6	-1.625604000	6.166370000	-0.436604000
1	-2.682602000	4.266778000	-0.000017000	1	-2.582389000	4.274121000	-0.654075000
1	-2.627865000	6.652551000	-0.000023000	1	-2.537263000	6.688166000	-0.702417000
6	1.982105000	6.833569000	0.000007000	6	1.921532000	6.883845000	0.479503000
6	2.016652000	8.193065000	0.000008000	6	1.955232000	8.250386000	0.478912000
6	-0.437488000	8.296996000	-0.000028000	6	-0.423334000	8.349068000	-0.142913000
6	0.818753000	8.967701000	-0.000012000	6	0.796039000	9.022542000	0.166013000
1	2.919255000	6.295032000	0.000023000	1	2.826257000	6.345626000	0.737401000
1	2.969123000	8.712672000	0.000022000	1	2.876824000	8.772886000	0.723520000
6	-1.607935000	9.093286000	-0.000051000	6	-1.556116000	9.143762000	-0.440172000
6	0.862103000	10.380996000	-0.000016000	6	0.839756000	10.437382000	0.164192000
6	-0.295551000	11.125071000	-0.000038000	6	-0.282888000	11.182638000	-0.132590000
6	-1.540885000	10.470428000	-0.000056000	6	-1.490544000	10.525389000	-0.436698000
1	1.830206000	10.871014000	-0.000004000	1	1.780303000	10.928486000	0.402854000

1	-0.251490000	12.208198000	-0.000041000	1	-0.237989000	12.268213000	-0.131435000
1	-2.455683000	11.052335000	-0.000075000	1	-2.378977000	11.105856000	-0.670201000
1	-2.583053000	8.624881000	-0.000068000	1	-2.503580000	8.672717000	-0.677353000
6	-1.982092000	-6.833513000	0.000016000	6	-1.953502000	-6.875489000	0.313581000
6	0.437435000	-8.296996000	-0.000024000	6	0.436974000	-8.337552000	-0.100437000
6	-0.818839000	-8.967658000	0.000120000	6	-0.803545000	-9.011648000	0.104574000
6	-2.016691000	-8.192973000	0.000146000	6	-1.986393000	-8.238256000	0.308799000
1	-2.969197000	-8.712546000	0.000237000	1	-2.927475000	-8.761064000	0.462103000
1	-2.919221000	-6.294946000	-0.000092000	1	-2.881163000	-6.338672000	0.470569000
6	1.607855000	-9.093360000	-0.000035000	6	1.592421000	-9.133208000	-0.301292000
6	-0.862272000	-10.380942000	0.000264000	6	-0.846644000	-10.426496000	0.102166000
6	1.540724000	-10.470501000	-0.000084000	6	1.526632000	-10.513559000	-0.299436000
6	0.295353000	-11.125072000	0.000093000	6	0.297194000	-11.171195000	-0.096098000
1	2.582988000	-8.624989000	-0.000223000	1	2.556121000	-8.662712000	-0.460953000
1	2.455494000	-11.052459000	-0.000248000	1	2.431359000	-11.094680000	-0.456251000
1	0.251225000	-12.208199000	0.000134000	1	0.253243000	-12.256810000	-0.095994000
1	-1.830392000	-10.870917000	0.000330000	1	-1.804014000	-10.917585000	0.260519000