Supporting Information

Theoretical study of electronically excited radical cations of naphthalene and anthracene as archetypical models for astrophysical observations. I. Static aspects

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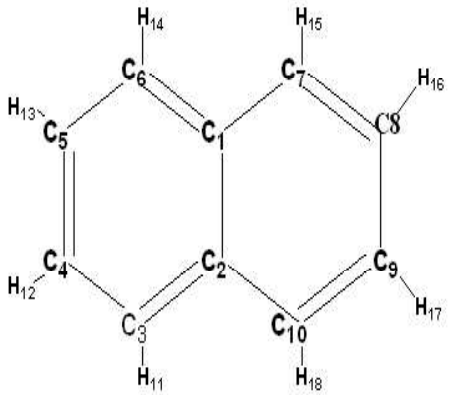
This PDF file includes

Table S1, Table S2 and FIG. S1

TABLE S1: *Ab initio* calculated equilibrium geometry parameters of the electronic ground state of neutral naphthalene along with the experimental data. The atom numbering in the table is illustrated in the schematic drawing below the table.

Np (MP2/cc-pVDZ)	our data	Expt data[a]
Bond lenght ($\AA$)		
C_1 - C_2	1.4415	1.412
C_2 - C_3	1.4270	–
C_3 - C_4	1.3892	–
C_4 - C_5	1.4231	1.417
C_5 - C_6	1.3892	–
C_3 - H_{11}	1.0965	1.092
C_4 - H_{12}	1.0953	1.092
Bond Angle (deg)		
C_1 - C_2 - C_3	118.981	–
C_2 - C_3 - C_4	120.7356	–
C_3 - C_4 - C_5	120.2834	–
C_6 - C_1 - C_7	122.0380	–
C_2 - C_3 - H_{11}	118.8773	–
C_3 - C_4 - H_{11}	120.3871	–
C_3 - C_4 - H_{12}	119.9362	–
C_4 - C_5 - H_{12}	119.7804	–

[a] N. Ketkar *et al.* , *J. Mol. Struc.* 1981, **77**, 139.

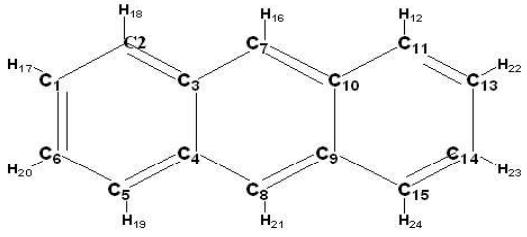


Np

TABLE S2: Same as in Table S1 for the electronic ground state of neutral anthracene.

An (MP2/cc-pVDZ)	our data	Expt data[b]
Bond lenght (Å)		
C_1 - C_2	1.3844	1.397
C_1 - C_6	1.4299	1.422
C_2 - C_3	1.4337	1.437
C_3 - C_4	1.4511	1.437
C_3- C_7	1.4103	1.392
C_1 - H_{17}	1.0954	–
C_2 - H_{18}	1.0966	–
C_7 - H_{16}	1.0979	–
Bond Angle (deg)		
C_1 - C_2 - C_3	120.815	–
C_2 - C_3 - C_4	118.775	–
C_2 - C_3 - C_7	121.990	122.3
C_2 - C_1 - C_6	120.416	120.4
C_5 - C_6 - C_1	120.410	–
C_3 - C_7 - C_{10}	121.529	121.0
C_7 - C_{10} - C_9	119.236	–
C_7 - C_3 - C_4	119.236	118.4
H_{17} - C_1 - C_2	119.938	–
H_{17} - C_1 - C_6	119.652	–
H_{18} - C_2 - C_3	118.697	–
H_{18} - C_2 - C_1	120.488	–
H_{16} - C_7 - C_3	119.236	–

[b] N. Ketkar *et al.* , *J. Mol. Struc.* 1981, **77**, 127.



An

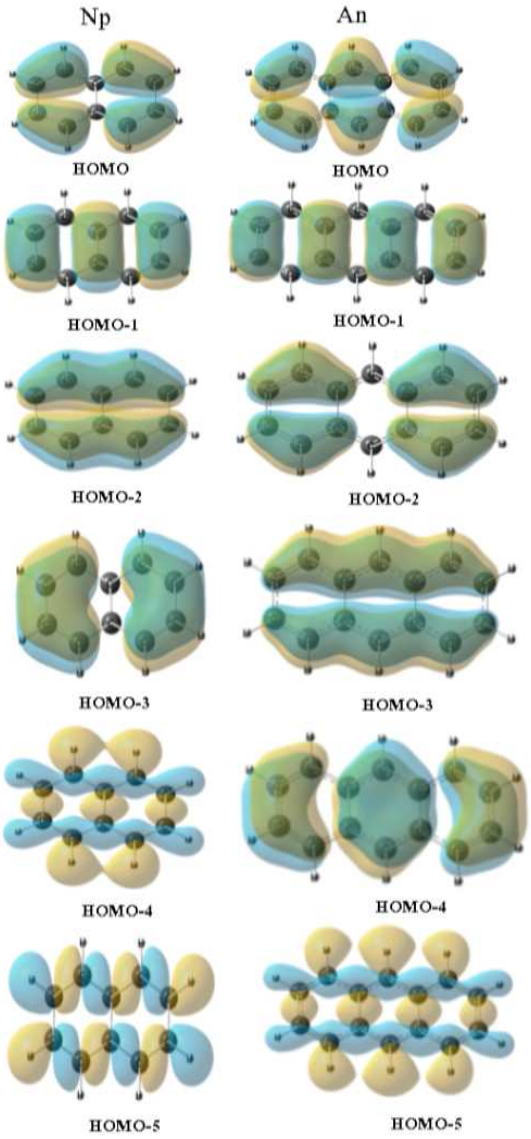


FIG. S1: The first six highest occupied molecular orbitals of the electronic ground state of neutral naphthalene and anthracene.