The Correlated Electronic States of a few Polycyclic Aromatic Hydrocarbons: A Computational study

Geetanjali Giri, Y. Anusooya Pati, and S. Ramasesha*

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India

E-mail: ramasesh@sscu.iisc.ernet.in

*To whom correspondence should be addressed

Table 1: Electronic excitation gap and singlet-triplet gaps in eV for PAH molecules. Numbers in the bracket are experimental gaps obtained from references shown as superscript.

Molecule	Optical gap (Expt gap)	singlet-triplet gap
Naphthalene	6.01 (5.63)[1]	2.52
Anthracene	3.70 (3.31)[2]	1.71
Phenanthrene	4.28 (3.60)[2]	2.54

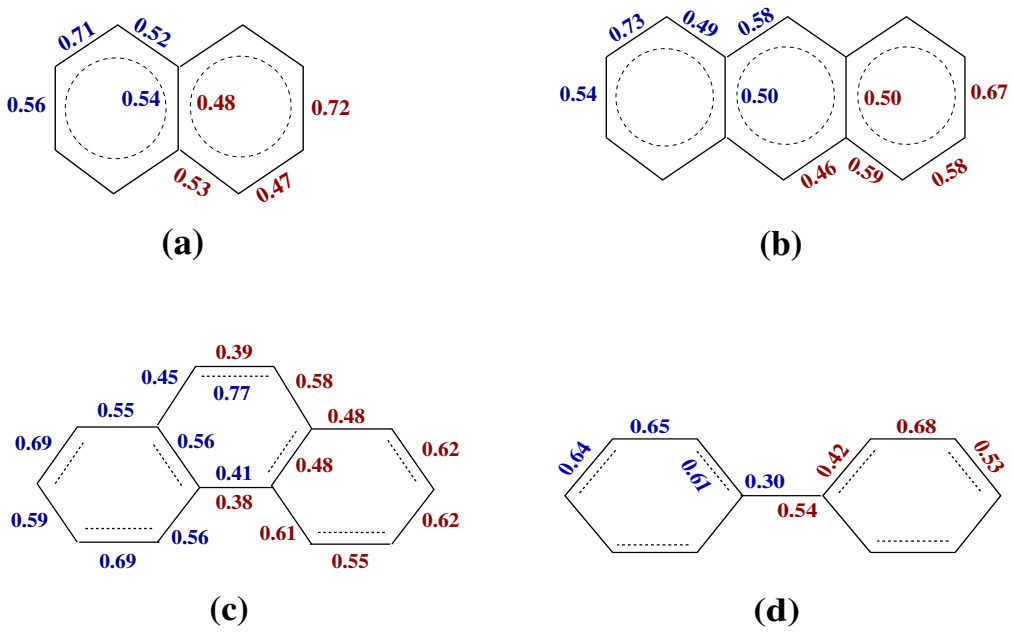

Figure 1: Bond orders for the lowest singlet (blue in colour) and triplet states for (a) naphthalene, (b) anthracene, (c) phenanthrene and (d) biphenyl (red in colour).

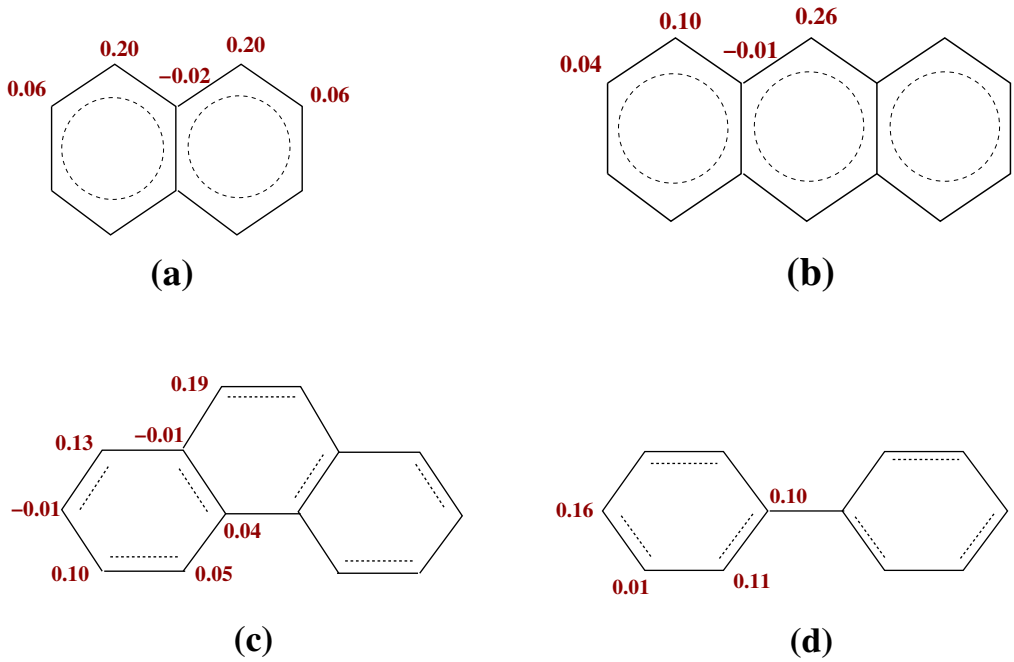

Figure 2: Spin densities of the lowest triplet states for (a) naphthalene, (b) anthracene, (c) phenanthrene and (d) biphenyl.

References

1. Birks, J. B.; Christophorou, L. G.; Huebner, R. H.; Excited Electronic States of Benzene and Naphthalene, *Nature*, **1968**, *217*, 809-812.

2. Clarence K. Jr. The Longest Wavelength Band in the Electronic Spectra of Polycyclic Aromatic Hydrocarbons for Analytical Use, *Appl. Spectr.*, **1959**, *13*, 15-25.