

# Quantum chemical characterization of dimeric polyaromatic hydrocarbons

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February 3, 2006

## Abstract

Polyaromatic hydrocarbon (PAH) has been considered to be an important interstellar species for a relatively long time because of its possible linkage to lifeforms. Despite its importance, however, interactions of individual PAH molecules have not been well understood. In this study, characteristics of dimers of various PAHs are investigated using ab initio quantum chemical approach. It is found that various homo- and heterodimers can be formed with significant stability especially from cationic monomers, which may exist in abundance in the interstellar space. Such dimeric species are also found to have strong absorption features in a wide range of wavelengths. It is hypothesized that the combination of the stability and the large absorptivity can lead to chemical reactions between monomers, opening a possible route to the growth of PAH and other organic substances in space.

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