

π Electron Delocalisation and Magnetic Properties of Cyclopenta-fused Pyrene Congeners

Utrecht University

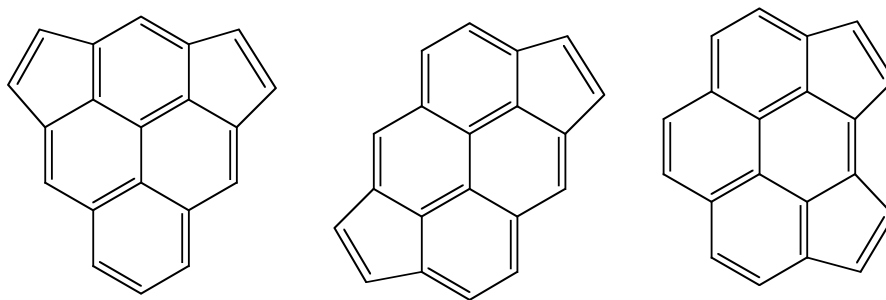
Remco Havenith,**, Fokke Dijkstra, Leo Jenneskens

University of Exeter

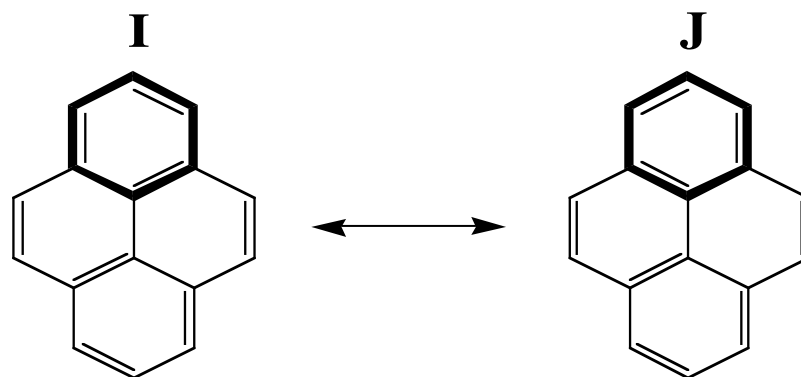
Patrick W. Fowler, Erich Steiner

Questions

- Are (CP-)PAH aromatic?
- Why do the magnetic properties of the dicyclopentapyrenes differ?
 - Influence of resonance?



Partitioning of the resonance energy in contributions of different conjugated circuits

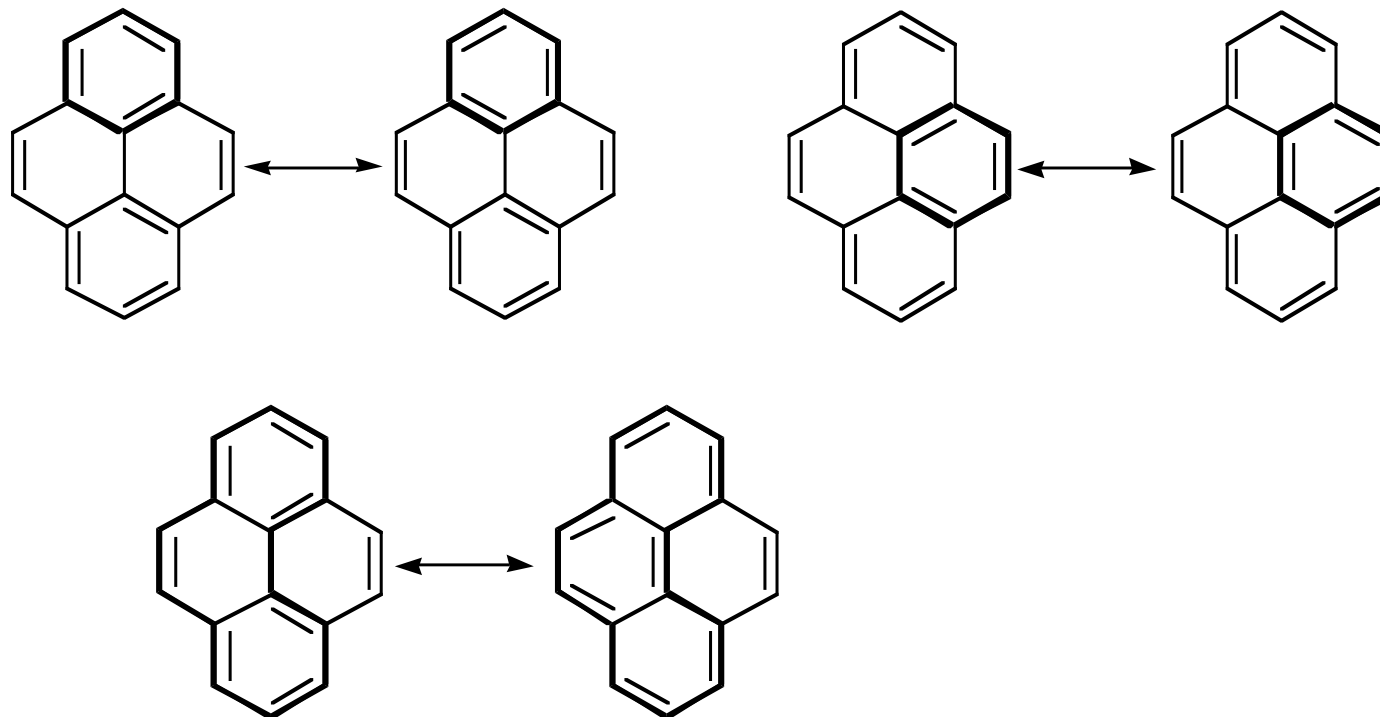


Löwdin orthogonalised structures

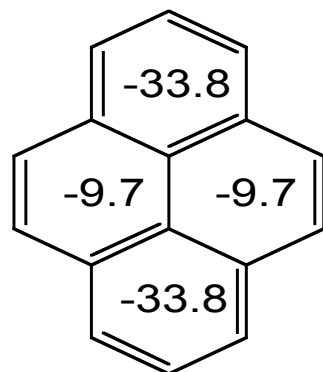
$$E = \sum_i c_i c_i H_{ii}^\perp + \sum_i \sum_{j>i} 2c_i c_j H_{ij}^\perp$$

$$2c_i c_j H_{IJ} : \Delta E_{\text{res}} \text{ for top - ring}$$

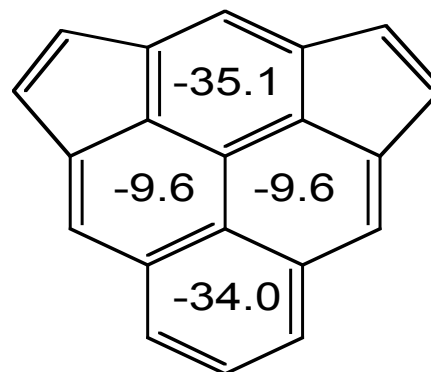
Resonance between the structures leading to benzene-like resonance in the top six π electron, central six π electron and 14 π electron conjugated circuits, respectively.



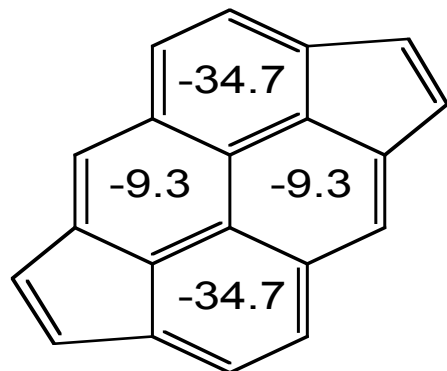
Partial Resonance Energies



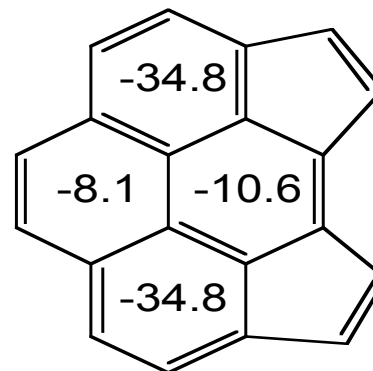
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87%



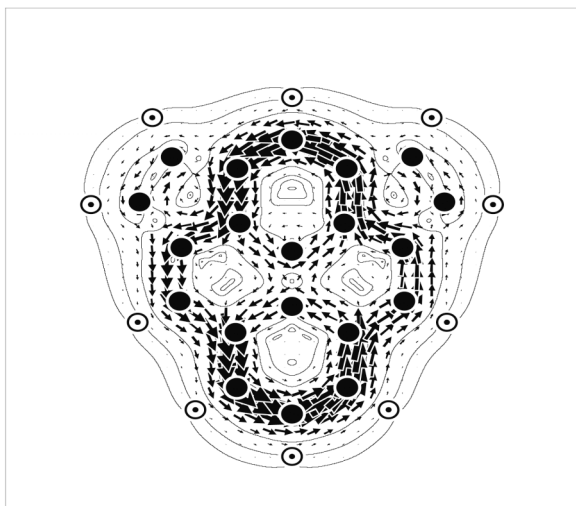
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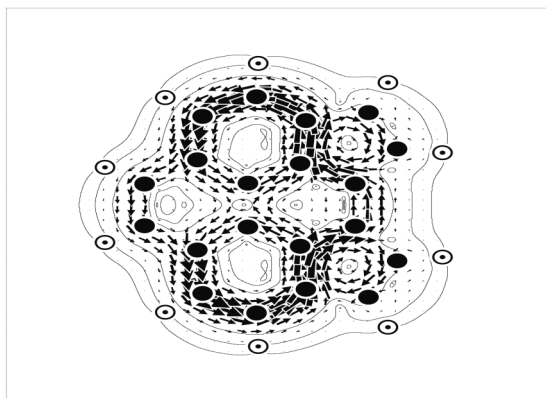
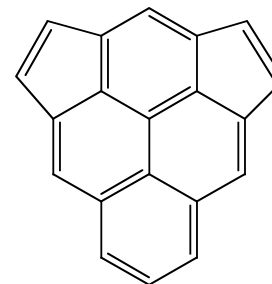
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Resonance in benzene-like rings most important
Remainder is 10/12/14/..-rings

Induced ring currents



1



3

