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Stabilizing cyclacene molecules

Stabilizing cyclacene molecules
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Abstract: It is shown that introducing a single methylene group into each trannulene ring of a cyclacene molecule compels the formation of a non-bonded molecular orbital, NBMO, in the ring. The union of both trannulenes conforms to a first order perturbation change in the total energy according to Dewar's PMO theory. The NBMO coefficients can be calculated then according to Coulson's pairing theorem. The PMO calculated new HOMO-LUMO energies of the cyclacene indicate the relative stabilization of the singlet over the triplet state of the cyclacene. The results are confirmed by the DFT calculation of differently substituted bis, methylene cyclacenes. The same arguments apply to