Bond Phase Determination of HOMO/LUMO and 'Ethylene' in Benzenoid Hydrocarbons

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Classical valence theory suggests the existence of strongly localized bonds (double bonds), *i.e.*, of ethylene-like molecules, in benzenoid hydrocarbons (molecular graphs Bs); such an 'ethylene' is an edge in a hexagon that contacts with three hexagon faces in B. The phase of a bond is defined as the sign either plus for bonding or minus for antibonding. By use of perturbation molecular orbital theory we conclude that the phase of each bond that meets at the ethylene has necessarily the minus sign in HOMO of B; the bond phase alters in HOMO and LUMO of B.

Key words: Bond Phase; HOMO and LUMO; Ethylene; Benzenoid Hydrocarbon; Pauling Bond Order.