A SEMI-EMPIRICAL MOLECULAR ORBITAL METHOD FOR THE CALCULATION OF TRANSITION ENERGIES AND IONISATION POTENTIALS OF π ETECTRON SYSTEMS.

by

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Based on the Zero Differential Overlap approximation, a semi-empirical molecular orbital method is developed for the calculation of transition energies and Ionisation Potentials of planar π electron systems. The method is simple and has been applied to Ethylene, cis and trans Butadiene and Benzene. The calculated values are all within 1 eV of the experimental values for these compounds.