A Theoretical Approach to Relate the Reactivity Descriptors and Mulliken Charges with Carcinogenity of Some Methylated Benzo[a]Anthracene

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Quantum chemical calculations were carried out to explain how the electronic state and reactivity indices of some methylated benzo [a] anthracenes vary with position and number of methyl substituent in molecules. The global reactivity descriptors such as ionization energy, electron affinity, molecular hardness, chemical potential and molecular philicity were estimated at ab-initio level of theory employing HF / 3-21G basis set. After that these factors were correlated with the carcinogenic activity of these compounds.

The result showed that two of these factors (The ionization potential (IP) and the total charge at K & L regions) can be correlated with carcinogenic activity of these compounds. On the other hand we found that methyl substitution leads to a great variation at the Mulliken charge of the carbon atoms at and near to the methyl substituents.