

Relation between Pauling and Coulson Bond Orders in Benzenoid Hydrocarbons

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The relation between Pauling and Coulson bond orders in benzenoid hydrocarbons is examined. The carbon–carbon bonds of benzenoid hydrocarbons have to be classified into three classes, depending on the number of attached hydrogen atoms. Within each class the correlation between the bond orders is linear. The results can be used to rationalize the recently discovered correlation between the energy and electron contents of rings. An approximate expression for the total π -electron energy is also deduced.

Key words: Pauling Bond Order; Coulson Bond Order; Benzenoid Hydrocarbons;
Electron Content of Ring; Energy Content of Ring.