Turkish Journal of Chemistry

Turkish Journal

On the Türker Angles in the Theory of Total π -Electron Energy

of

Chemistry

Ivan GUTMAN
Faculty of Science, University of Kragujevac
P.O. Box 60, YU-34000 Kragujevac, YUGOSLAVIA



Abstract: The Türker angles θ , α and β are quantities invented by Lemi Türker, and are used in the theory of total π -electron energy (E) of unsaturated conjugated hydrocarbons. We report here expressions for θ , α and β in terms of E and the parameters n (= half the number of carbon atoms) and e (= the number of carbon-carbon bonds). The forms of these expressions are remarkably similar. Numerical calculation performed on a representative set of benzenoid hydrocarbons reveals that the dependence of the angles α and β on molecular structure is very similar, and that their ratio is almost constant (α / β \approx 1.564 \pm 0.015).



Turk. J. Chem., 22, (1998), 399-402.

Full text: pdf

Other articles published in the same issue: Turk. J. Chem., vol.22, iss.4.

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