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Coulson function and Hosoya index

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Abstract

Let G be a molecular graph, n the number of its vertices and φ(G,x) its characteristic polynomial. Already in 1940 Coulson expressed the total π-electron energy of conjugated unsaturated molecules in terms of the function F(x)=n-ixφ′(G,ix)/φ(G,ix). Recently, the Coulson function F(x) found applications also in modeling the structure-dependence of physico-chemical properties of alkanes. We now analyze the Coulson function and establish some of its hitherto unnoticed features, in particular its relations with the Hosoya index. © 2002 Published by Elsevier Science B.V.

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