

TOTAL π -ELECTRON ENERGY AND MOLECULAR TOPOLOGY

B I B L I O G R A P H Y

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The question how the total π -electron energy E of a conjugated compound (as calculated within the framework of the Hückel molecular orbital method) depends on the molecular structure was studied in a remarkably large number of publications. (1 - 65) The early impetus to study this problem came from the necessity to obtain the numerical value of E by "paper and pencil" methods, without using a computer. Later, as a consequence of the expansion of the computing facilities and the availability of extensive tables of HMO results, the emphasis was given to the finding of general regularities relating E with selected topological invariants of the molecule. The explicit or implicit use of graph theory played a significant role in many of these investigations.

The various mathematical properties of E were discussed in Refs. 4,7-11,15,16, 19, 21,25,26-32,38-41,44,45,48,54, 56,57 and 65. Using these exact results different non-empirical and semiempirical approximate expressions for E were derived. (1, 12,16,20,22-24,30,33,34,37,43,46,51,53-55,60,

61,64) Further empirical topological formulas for E (based on least squares fitting methods) were proposed in Refs. 3, 5,6,18,47,49,58 and 62. However, it is to be noted that an exact topological formula for E cannot exist at all. (21)

Different resonance energies, quantities closely related to E , were defined and analysed in Refs. 2,13,14,24,35,36,42, 50,55 and 63. The important question how E is related to the measurable thermodynamic properties of conjugated compounds was resolved in Ref. 59.

The present list of references does not include the numerous papers on E of special classes of conjugated molecules (linear polyenes, annulenes, polyacenes etc.). Benzenoid systems were studied in Refs. 3,5,6,18,43,47,49,58,60 and 61, while only two papers: 44 and 52 deal with the properties of non-alternant hydrocarbons. It was also not feasible to consider publications reporting only results of computations of E and/or resonance energy. Topological properties of E have not yet been reviewed, but some results in this field were collected and presented in Ref. 17.

The following list of references seems to be nearly complete. The author would greatly appreciate information about those publications on total π -electron energy which he failed to observe.

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