

Notes

On atom-bond connectivity index and its chemical applicability

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A critical re-examination confirms that the atom-bond connectivity index (ABC) is well reproducing the heats of formation of alkanes (ΔH_f°). Moreover, the simple empirical formula $\Delta H_f^\circ = -(a+b \cdot ABC)$, with $a = 65.98$, $b = 20.37$, reproduces the heats of formation with an accuracy comparable to that of high-level *ab initio* and DFT (MP2, B3LYP) quantum chemical calculations.

Keywords: Theoretical chemistry, Atom-bond connectivity index, Heat of formation, Alkanes

The present study is concerned with the atom-bond connectivity index, one of the several currently used molecular-graph-based structure descriptors, and the extent to which it can be used for (quantitative) prediction of physico-chemical properties of organic compounds. The atom-bond connectivity (ABC) index was put forward in 1998 by Estrada *et al.*¹ in an attempt to provide an improved version of Randić's classic connectivity index.² Herein, a seemingly excellent linear correlation between the ABC index and the standard gas phase heats of formation (ΔH_f°) of alkanes has been demonstrated, *cf.* Fig. 1, and the simple formula, Eq (1), is proposed. This work attracted little attention and has for a long time been ignored by theoretical chemists.

$$\Delta H_f^\circ = -(65.98 + 20.37 \cdot ABC) \quad \dots (1)$$

Ten years later, Estrada published another paper on the ABC index,³ in which he offered its physico-chemical rationalization, a mathematical elaboration thereof. This article did attract the attention of colleagues, especially of mathematical chemists, and a long series of mathematical investigations of the ABC index appeared in the literature.⁴⁻¹³

In all mathematical studies of the ABC index,⁴⁻¹³ its applicability for modelling thermochemical data is being emphasized. In view, of the doubts explained below, we have undertaken a more detailed examination of the quality of the correlation between ABC and ΔH_f° .

Let G be a molecular graph¹⁴ and let v_1, v_2, \dots, v_n be its vertices. The number of the first neighbours of a vertex is said to be its degree denote by d_i , the degree of the vertex v_i , $i = 1, 2, \dots, n$. Then, the ABC index of the graph G is defined as¹

$$ABC = ABC(G) = \sum_{i \sim j} \sqrt{\frac{2(d_i + d_j - 2)}{d_i d_j}}$$

where the summation is over all pairs of adjacent vertices of G .

The popularity of the ABC index, and the motivation for its detailed mathematical investigation, were based on the existence of a very good linear correlation between it and the (experimental) heats of formation.^{1,3} This is shown in Fig. 1, in which the exactly same set of alkanes is used as in the original work.¹

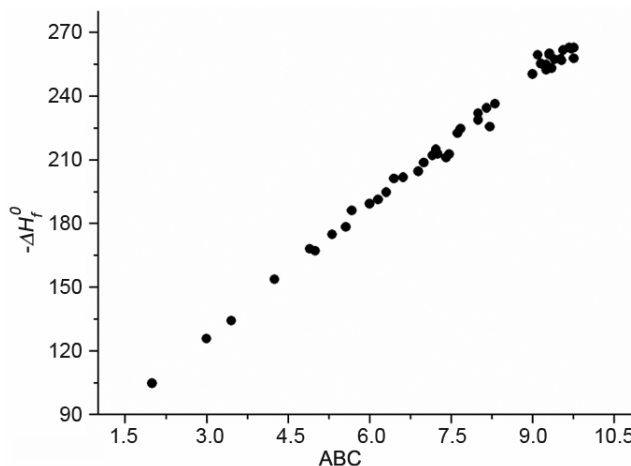


Fig. 1—Heats of formation of alkanes (in kJ mol⁻¹) versus the ABC index. The data set used is the same as in the earlier study by Estrada *et al.*¹ This data set consists of alkanes with n carbon atoms for n between 3 and 10.

