Letter to the Editor

CHROM. 4505

Dear Sir,

the paper by DIMOV AND SHOPOV (*J. Chromatog.*, 44 (1969) 170–172) mentions the method for predicting I^S values by means of structural increments described by myself in several papers[1–7].

The authors compare the differences between calculated and experimental values given in my paper found in *J. Chromatog.*, 23 (1966) 1–17, page 4, Table II with differences determined by their own method of index calculation. The authors overlooked that this table was only given to point out the existence of increments of the second order for the calculation of I^S values of double- and multiple-branched hydrocarbons where the branches are close together within the molecule. This is to be seen from the sentence: "Durch zusätzliche Inkremente für die 2,3- und 2,2-Dimethylalkane werden auch die Indexwerte der Dimethylalkane vorausberechenbar". In other papers published during the years 1964, 1966, 1967 and 1968, I defined these increments of second order which are to compensate for interactions between functional groups, in more detail in refs. 5 and 6. Using these additional increments for the calculation of the $I_{\text{theor.}} - I_{\text{exp.}}$ in the Table of DIMOV AND SHOPOV, the differences become small or vanish completely.

The greatest accuracy of prediction of I^S values is of course not obtained with smaller molecules, for example below C_8. Because the I^S values of hydrocarbons with carbon numbers up to C_{10} have been measured by several authors (MATUKUMA[8], HIVELY AND HINTON[9] and LOEWENGUTH AND TOURRES[10]) with high accuracy, the calculation of I^S values for practical applications is especially useful for greater molecules, although the rules of calculation are valid approximately even for smaller molecules.

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