CHROM. 18 640

Letter to the Editor

Correlation between retention on liquid crystalline phases and chemical structure

Reply to Lamparczyk *et al.*

Sir,

Lamparczyk *et al.*[1] state that our conclusion concerning the lack of any clear correlation between retention and the shape parameter resulted from a misunderstanding of their idea of the shape parameter. In particular, they write that "the shape parameter η must be defined unequivocally". This statement is surely correct, but one should bear in mind that there are several possibilities for choosing the reference frame for the definition of the shape parameter.

In our work[2] we have defined the shape parameter as the ratio of the shorter to the longer sides of the rectangle enveloping a molecule, relative to the natural symmetry of the naphthalene skeleton as shown in Fig. 1. On the other hand, Lamparczyk *et al.*[1] define the shape parameter as the ratio of the longer to the shorter sides of the minimum rectangle (of smallest area) enveloping a molecule, *cf.*, Fig. 1 of ref. 1. Thus, in the case, *e.g.*, of 1,2- and 1,4-dimethylnaphthalene, the shape parameter, η, defined by Lamparczyk *et al.*[1] and that, (b/l), defined by us should satisfy the condition:

$$(b/l)\eta = 1 \tag{1}$$

That this does not happen results from the differences in the values of the bond lengths and atomic radii used in the calculations. In our calculations we have used the values given in Table I, whereas the values applied by Lamparczyk *et al.* are not known.
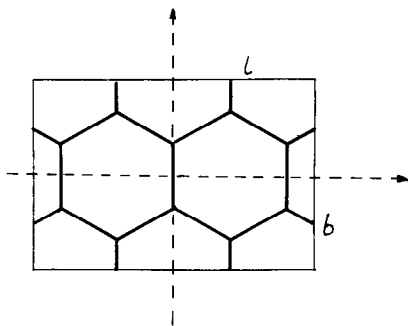

Fig. 1. The orientation of the rectangle enveloping a molecule used in the calculations of the shape parameter, b/l.

TABLE I

PARAMETERS USED IN CALCULATIONS OF THE SHAPE PARAMETERS b/l

Bond	Length ($\overset{\circ}{A}$)	Atom	Radius ($\overset{\circ}{A}$)
C–C in aromatic ring	1.39	C in aromatic ring	0.7
C–C single	1.53	C in CH_3 group	0.77
C–H in aromatic ring	1.08	H	0.30
C–H in CH_3 group	1.10		

It is interesting, however, that the shape parameter, η, defined by Lamparczyk *et al.* can be used to correlate retention data for dimethylnaphthalenes (DMNs) with η and the connectivity index, χ, *cf.* eqn. 1 of ref. 1, whereas the shape parameter, b/l, used by us does not lead to any clear correlation between retention data and b/l and χ. In fact, we have observed that for DMNs the shape parameter b/l is a linear function of χ, *cf.*, Fig. 3 of ref. 2. Our choice of the reference frame for the definition of b/l was based on the assumption that this parameter should be defined in such a way that the rectangle enveloping a molecule should be consistent with the symmetry of the aromatic skeleton (and the symmetry of distribution of π electrons). Nevertheless, it is possible that the definition proposed by Lamparczyk *et al.* is better suited for correlating retention data with the geometry of solute molecules, though, one should not forget that other authors[3] suggest that the shape-parameter considerations do not lead to any fruitful conclusions about solute retention behaviour.

In conclusion, we would emphasize that the choice of the definition of the shape parameter does not influence the conclusions presented in our previous paper[2], since those were not based on the shape parameter considerations.

Department of Chemical Physics,   Z. SUPRYNOWICZ
Institute of Chemistry,   W. M. BUDA
MCS University, 20031 Lublin   M. MARDAROWICZ
(Poland)   A. PATRYKIEJEW

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3 L. C. Chow and D. E. Martire, *J. Phys. Chem.*, 75 (1971) 2005.