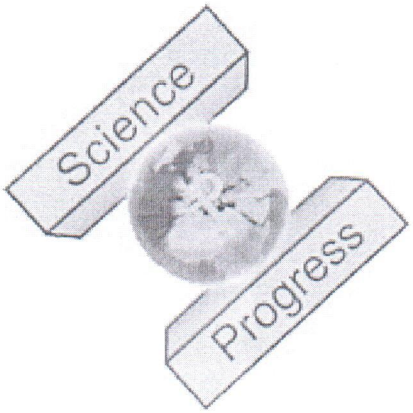

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Features of the Dependence of Retention Indices on the Content of Methanol in an Eluent in Reversed Phase HPLC

Derouiche Abdennour, Zenkevich I.G
st088750@student.spbu.ru

Saint Petersburg State University, Saint Petersburg, Russia

One of the important problems of contemporary instrumental analytical chemistry is the formation of hydrates of organic compounds in aqueous solutions (1), e.g., in conditions of reverse phase (RP) HPLC. However, the direct detecting the formation of hydrates by chromatographic or mass spectrometric methods seems to be impossible due to the instability of most of them.

$$X + nH_2O \leftrightarrows X{\times}nH_2O \quad (1)$$

In a previous study to solve this problem, an indirect approach was used to confirm the formation of hydrates; it is a recurrent approximation of retention parameters of analytes [1]. Besides that, important additional information can be obtained by using the concept of retention indices (RI) in RP HPLC measured in the scale of reference *n*-alkyl phenyl ketones $C_6H_5COC_nH_{2n+1}$:

$$RI_x = RI_n + (RI_{n+1} - RI_n)\,[\log t'_{R(x)} - \log t'_{R(n)}] / [\log t'_{R(n+1)} - \log t'_{R(n)}] \quad (2)$$

However, the RI values themselves do not provide any information indicating the formation of hydrates in an eluent, but the dependence of RIs on concentrations of organic component in an eluent (3) seems to be more informative:

$$RI = aC + b \quad (3)$$

The coefficients a and b are calculated by LSM, a = dRI/dC.

If we use methanol as the organic component of an eluent, the following regularity was revealed. The coefficients a = dRI/dC for hydrophobic analytes usually have large positive values, while these values for more hydrophylic analytes may be close to zero, or negative, as it is illustrated by table:

Table.1. Parameters of linear regression (3) for some hydrophobic and hydrophilic organic compounds.

Compound	Formation of hydrate	Mol. wt.	a = dRI/dC	b = RI at (C=0)	R
Toluene	No	92	4.0 ± 0.1	851 ± 8	0.99
o-Xylene	No	106	4.6 ± 0.3	911 ± 20	0.98
Phthalimide	Possible	137	-0.2 ± 0.0	708 ± 3	-0.95
Diethyl-*m*-toluamide	Possible	191	-2.0 ± 0.1	1050 ± 6	-0.99

The dependence of retention indices of analytes *vs* concentration of organic component of an eluent (3), we used as indirect method to confirm the forma- tion of hydrates of organic compounds in RP HPLC conditions.

References

1. T.A. Kornilova, A. Derouiche, I.G. Zenkevich // Analytics and Control., 24, p. 315-322 (2020).