

# Temperature effects on the retention of *n*-alkanes and arenes in helium–squalane gas–liquid chromatography: Experiment and molecular simulation

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## Abstract

Experiments and molecular simulations were carried out to study temperature effects (in the range of 323 to 383 K) on the absolute and relative retention of *n*-hexane, *n*-heptane, *n*-octane, benzene, toluene, and the three xylene isomers in gas–liquid chromatography. Helium and squalane were used as the carrier gas and retentive phase, respectively. Both the experiments and the simulations show a markedly different temperature dependence of the retention for the *n*-alkanes compared to the arenes. For example, over the 60 K temperature range studied, the Kovats retention index of benzene is found to increase by about 14 or  $18 \pm 10$  retention index units determined from the experiments or simulations, respectively. For toluene and the xylenes the experimentally measured increases are similar in magnitude and range from 11 to 16 retention index units for *m*-xylene to *p*-xylene. The molecular simulation data provide an independent method of obtaining the transfer enthalpies and entropies. The change in retention indices is shown to be the result of the larger entropic penalty for the transfer of the flexible alkane molecules.

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