EVALUATION OF THE SELECTIVITY OF IONIC LIQUID-BASED GAS CHROMATOGRAPHIC COLUMNS

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Ionic liquids (ILs) have been used as stationary phases in gas chromatography (GC) due to their low vapor pressure, relative low bleeding and, in particular, because of their tailored selectivity. Up to now, a number of studies have reported on these positive features of IL-based GC phases for mixtures of compounds with different chemical structures. However, studies investigating on the selectivity of IL-based columns for complex mixtures of isomers, such as, for example, the polychlorinated biphenyls (PCBs), are still rare in the literature.

Topological or electrotopological descriptors have been frequently used in statistical studies trying to predict the GC retention of PCB congeners in specific stationary phases. However, the practical use of these approaches requires very accurate predictions due to the high number of congeners (209) and the frequent presence of co-elutions. On the contrary, the statistical estimation of the effects of simple structural PCB descriptors on the GC retention can be considered a more interesting approach, as it allows comparing the interactions of PCBs with different stationary phases and, consequently, describing the specific phase selectivity toward groups of compounds sharing a specific substructure.

In this study, the SLB-IL-60 (Sigma-Aldrich, Bellefonte, PA, EEUU) GC phase, was used as IL-based model phase. Using this column, programmed temperature retention times and retention indices of 59 PCBs representative of different groups of homologues and chemical substructures were used as dependent variables for the statistical valuation of the retention behavior of these analytes in this stationary phase. Meanwhile, the number and position of the chlorine substitutions in the ring (used as size and shape descriptors), and the number and position of the *orto*- substitutions describing interactions between the two rings, were used as independent variables. The software Statistica 7 (Statsoft, Tulsa, OK, EEUU) was used for the stepwise calculation of the regressions.

Interestingly, the proposed model provided equally valid regression values ($R>0.996$) using retention index and retention time values. It was also demonstrated to provide valid values (i.e., $R>0.99$) in both pseudo-isotherm and programmed conditions. Application of the optimized model to PCB retention data obtained using polar (SLB-IL-76 and SuplecoWax-10), semi-polar (DB-17) and non-polar (DB-5 and HT-8) stationary GC phases resulted also on satisfactory-to-acceptable regression fittings. More importantly, the statistical comparison of the PCB retention behavior in the five evaluated phases demonstrated that those based on ILs showed a completely differentiated selectivity through PCBs compared to the other more conventional stationary phases evaluated.

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