Dependence of GCRT of polychlorinated dioxins on their connectivity indices
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A quantitative structure and property relationships(QSPR) analysis on gas chromatograph relative retention times(GCRT) of dioxin related compounds(Dioxins), such as polychlorinated dibenzo-p-dioxin and polychlorinated dibenzofuran, and their molecular geometrical and topological parameters was carried out. It was found that there was a different change in GCRT depending on solvent accessible surface area(SAS) between the congeners and the isomers. To elucidate the retention characteristics of the isomers, the GCRT were classified in terms of the number of the pair of proximitive hydrogen substituents bonding to the dibenzo-p-dioxin skeleton(Nad-H). The correlation coefficients were markedly improved between SAS and GCRT ranging in the same Nad-H category. Next an analysis on the basis of the connectivity indices, which had been derived by Randic, Kier, and Hall, was performed to clarify the topological characteristics for the proximitive positions. It was found that there was a close correlation between the third-order connectivity descriptor, $3\sigma$, and GCRT for the isomers. On the other hand, from analyses on the correlation between $3\sigma$ and some electrical descriptors, it was revealed that there was a significant correlation between $3\sigma$ and sum of net charge at hydrogen substituents.