# CORRELATION OF GAS CHROMATOGRAPHIC RETENTION PARAMETERS WITH MOLECULAR CONNECTIVITY

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Following the observations on molecular branching and its relation to physicochemical properties by Randic(1975), Kier and others(1975a) have described a parameter, molecular connectivity($\chi$), which quantifies the degree of molecular branching. Successful correlation of $\chi$ with various physical and biological parameters has been reported(Kier and others, 1975a, 1975b). In this study $\chi$ has been correlated with GC retention parameters for several molecular series, including drug molecules.

Csicery and Pines(1962) have reported retention times for straight and branched chain hydrocarbons. Correlation with $\chi$ gave equation 1.

$$\log RT = 0.800\chi - 0.340 \qquad \text{Equation 1.}$$
$$n = 18, \quad r = 0.996, \quad s = 0.061$$

The retention times of a series of alcohols determined in this laboratory correlated with $\chi$ according to equation 2.

$$\log RT = 2.370\chi - 2.109\chi_v - 1.086 \qquad \text{Equation 2.}$$
$$n = 10, \quad r = 0.991, \quad s = 0.029$$

In this case introduction of the parameter $\chi_v$(Kier and Hall, 1976), the valence connectivity, significantly improved the correlation.

The technique has been applied to drug molecules. Amphetamine derivatives (GC data of Beckett and others, 1967) yielded equation 3.

$$\log RT = 0.503\chi - 1.673 \qquad \text{Equation 3.}$$
$$n = 9, \quad r = 0.998, \quad s = 0.093$$

A series of barbiturates(GC data of Parker and Kirk, 1961) resulted in correlation according to equation 4.

$$\log RT = 0.243\chi - 0.483 \qquad \text{Equation 4.}$$
$$n = 13, \quad r = 0.916, \quad s = 0.057$$

In equations 3 and 4 introduction of $\chi_v$ yielded no significant improvement in correlation. Equations 1 to 4 gave good agreement between observed and predicted retention values. On the basis of these results, the use of molecular connectivity as an aid to structure determination is envisaged.

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