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一个新的拓扑指数用于有机化合物的**QSPR/QSAR**研究

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摘要 在分子图的邻接矩阵和距离矩阵的基础上提出了一个新的拓扑指数Xu,该拓扑指数易于计算,对C~2-C~1~6饱和烷烃有较高的结构区分能力,通过适当的处理可方便地推广到含多重键杂原子体系。该指数与饱和烷烃的正常沸点等理化性质,
不饱和链烃类化合物的热容以及某些脂肪醇的毒性和疏水性参数均具有较好的性质相关性。绝大多数理化性质与Xu指数均能建立简单线性模型,且相关系数均大于0.99,表明该指数有望在QSPR/QSAR研究中作为一个新的参数而获得推广应用。

关键词 拓扑指数 有机化合物 图论 烷烃

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A novel topological index for QSPR/QSAR study of organic compounds

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Abstract A novel topological index Xu based on the adjacency matrix A and distance matrix D was derived in this paper. The index, which was very easy to calculate and also had good discrimination between isomeric alkanes, was highly correlated with the selected physicochemical properties of alkanes, and most properties were well modeled (r>0.99). Moreover, it was also convenient to extend the Xu index to the multipolybonds, heteroatom-containing compounds using the relative ratio of bond length to C-C bond in place of the adjacent topological distance and the valence δ~i instead of the degree of vertex v~i. The index also produced a fair regression for the heat capacity of olefins and the toxicity and hydrophobicity parameters of alkanols (r>0.99). The calculated values were in good agreement with experimental data. The results suggested that the proposed index with fairly high correlation ability and structural selectivity promised to be a useful parameter in QSPR/QSAR research.

Key words ORGANIC COMPOUNDS GRAPH THEORY ALKANE

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