改进的分子连接性方法

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摘要　　通过用Mulliken键级来加权分子连接性指数中的点价,使分子轨道理论与分子连接性指数有机地结合起来,将分子连接性指数改进成为一种量子拓扑指数。对比发现,分子连接性指数的点价与Mulliken键级具有相近的物理意义,而Mulliken键级更具有独特的优越性。利用改进的分子连接性指数对几种具有代表性的烃类与其体积、疏水常数以及热力学性质进行了关联,得到了满意的结果。
关键词　　分子连接性　拓扑　疏水常数　分子轨道理论
分类号　0641

A novel molecular connectivity method

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Abstract　In this paper, the value of delta in molecular connectivity method was weighted by Mulliken bond order, it connected the molecular orbital theory with the topological theory effectively and converted the molecular connectivity method to a novel quantum-topology method. Comparing the value of delta of molecular connectivity with the Mulliken bond order could find that they have similar physical meanings, but the Mulliken bond order had its own advantage. Some typical hydrocarbons were calculated by the novel molecular connectivity index, the result showed that they have good correlationship with their volume, hydrophobic parameter and thermodynamic properties.

Key words　TOPOLOGY　MOLECULAR ORBITAL THEORY

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扩展功能

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