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拓扑化学行为及其对镧系元素和锕系元素的QSPR应用(英文)

Chemical Behavior of Topology and Its Application to QSPR of Lanthanide and Actinide

中文关键词：拓扑化学行为　价电子　QSPR　镧系元素　锕系元素

英文关键词：chemical behavior of topology　valence electron　QSPR　lanthanide　actinide

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作者	单位
周丛艺	南华大学化学化工学院，衡阳 421001
聂长明	南华大学化学化工学院，衡阳 421001;早稻田大学理工研究生院，东京 169-8555，日本
李珊	南华大学化学化工学院，衡阳 421001
文松年	南华大学化学化工学院，衡阳 421001
彭国文	南华大学化学化工学院，衡阳 421001
李忠海	中南林业科技大学生命科学与技术学院，长沙 410004

中文摘要：

提出拓扑化学行为概念,把对化合物性质最具影响力的因素归纳为拓扑生长力和拓扑阻滞力。根据该原理,利用价电子轨道能量对价电子距离矩阵进行修正。研究表明OET(轨道能量拓扑指数)对镧系元素和锕系元素的物理化学性质具有良好的应用，尤其是对尚未借助QSPR(定量结构性质关系)手段进行研究的光谱性质。LOO CV(留一法交叉检验)的结果验证了模型的良好稳定性和预测能力,采用的检验参数有：PRESS/SSY，SEP_{CV}，R_{CV}，S_{PRESS} 和PSE，其中PRESS/SSY比值介于0.000 6和0.114 8之间。与文献进行比较,本文方法所得结果与之接近或更好。研究显示正是基于拓扑化学行为才有本文方法良好和较广的应用。

英文摘要：

We introduce the chemical behavior of topology for the first time which consists of the topological growing power and the topological blocking power. On the basis of the principle, the OET (orbital-energy topological index) was proposed by revising the valence electron distance matrix with the orbital energy. The results demonstrate that OET has good application to the physicochemical properties of lanthanide and actinide, especially to the spectral properties which have not been reported by means of QSPR (quantitative structure-property relationships). The results of LOO CV (leave-one-out cross-validation) verify the good stability and predictive ability of the models using the cross-validation parameters: PRESS/SSY, SEP_{CV}, R_{CV}, S_{PRESS} and PSE with the PRESS/SSY ratio ranging between 0.000 6 and 0.114 8. Compared with the other methods, this work provides an easier way yielding results close to or better than the others. It is on the basis of the chemical behavior of topology that leads to the good and wide application of this method.

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服务热线：(025)83592307　　传真：(025)83592307　　邮编：210093　　Email：wjhx@netra.nju.edu.cn

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