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Full Paper

定量结构相关预测无机物的摩尔反磁磁化率

沐来龙*,[1]，何红梅[2]，冯长君[1]

[1]徐州师范大学化学系，江苏徐州，221116

[2]徐州工业职业技术学院，江苏徐州，221006

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摘要 为了预测无机物的摩尔反磁磁化率，基于连接矩阵和离子参数g_i提出了一种新的连接性指数^{m}G。g_i定义为：$g_i=(n_i^{0.5}\text{-}0.91)^4.x_i^{0.5}/Z_i^{0.5}$,其中$Z_i$，$n_i$和$x_i$分别代表离子$i$的电荷数，最外层主量子数和电负性。由$^{0}G$，$^{1}G$通过多元线性回归和人工神经网络方法均可以得到良好的预测摩尔反磁磁化率的模型。对144个无机物，多元线性模型和人工神经网络模型的相关系数r，标准偏差和平均绝对误差分别为0.9868，5.47.cgs,433 cgs，0.9885，5.09cgs和4.06 cgs。留一法交叉验证说明多元线性模型在统计学上具有良好的稳定性。两种模型对62个未进入模型的无机物的摩尔反磁磁化率进行预测的平均绝对偏差为4.72cgs和4.06cgs。结果表明本文的方法在预测无机物反磁磁化率方面比文献方法更有效。多元线性方法和人工神经网络方法均能得到比较理想的预测摩尔反磁磁化率的模型。而人工神经网络模型对摩尔反磁磁化率的预测结果比多元线性模型似乎更精确。

关键词 连接性指数；摩尔反磁磁化率；无机物；人工神经网络

分类号

Quantitative Structure Property Relations (QSPR) for Predicting Molar Diamagnetic Susceptibilities, χ_m, of Inorganic Compounds

MU Lai-Long*,[1], HE Hong-Mei[2], FENG Chang-Jun[1]

[1] *School of Chemistry & Chemical Engineering, Xuzhou Normal University, Xuzhou, Jiangsu 221116, China*

[2] Xuzhou College of Industrial Technology, *Xuzhou, Jiangsu 221006, China*

Abstract For predicting the molar diamagnetic susceptibilities of inorganic compounds, a novel connectivity index ^{m}G based on adjacency matrix of molecular graphs and ionic parameter g_i was proposed. The g_i is defined as $g_i=(n_i^{0.5}-0.91)^4 \cdot x_i^{0.5}/Z_i^{0.5}$, where Z_i, n_i, x_i are the valence, the outer electronic shell primary quantum number, and the electronegativity of atom i respectively. The good QSPR models for the molar diamagnetic susceptibilities can be constructed from ^{0}G and ^{1}G by using multivariate linear regression (MLR) method and artificial neural network (NN) method. The correlation coefficient r, standard error, and average absolute deviation of the MLR model and NN model are 0.9868, 5.47 cgs, 4.33 cgs, 0.9885, 5.09 cgs and 4.06 cgs, respectively, for the 144 inorganic compounds. The cross-validation by using the leave-one-out method demonstrates that the MLR model is highly reliable from the point of view of statistics. The average absolute deviations of predicted values of the molar diamagnetic susceptibility of other 62 inorganic compounds (test set) are 4.72 cgs and 4.06 cgs for the MLR model and NN model. The results show that the current method is more effective than literature methods for estimating the molar diamagnetic susceptibility of an inorganic compound. Both MLR and NN methods can provide acceptable models for the prediction of the molar diamagnetic susceptibilities. The NN model for the molar diamagnetic susceptibilities appears more reliable than the MLR model.

Key words connectivity index artificial neural network diamagnetic susceptibility inorganic compound

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通讯作者 沐来龙 mull@xznu.edu.cn