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研究论文

用量子化学参数研究烯烃聚合物定量构效关系

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摘要 以密度泛函理论(DFT)方法所得的烯烃聚合物结构单元的物性参数如总能量E_t、内能E_{in}、等容比热C_V、熵S、四极矩Q_{ii}、偶极矩 μ、平均极化率α及原子最大负电荷q^-等8个量子化学参数, 用逐步回归法分别建立了这些参数与摩尔体积$V_{298\ K}$, 摩尔等张体积P_s、摩尔吸收常数色散分量F_d、摩尔折射率R_{LL}、摩尔抗磁磁化率χ、摩尔粘度温度函数H_{vsum}、摩尔Rao函数U_R及摩尔Hartmann函数U_H的结构-性能定量关系 (QSPR) 模型, 其测试集的决定系数R^2分别是: $V_{298\ K}$ 为0.989, P_s为0.982, F_d为0.975, R_{LL}为0.997, χ为0.988, H_{vsum}为0.914, U_R为0.988及U_H为0.972. 结果表明, 用这些量子化学参数所建立的聚合物QSPR模型能用于聚合物性能的预测.

关键词 密度泛函理论 量子化学参数 结构-性能定量关系 聚合物

分类号

QSPR Studies on Vinyl Polymers Based on Quantum Chemical Descriptors

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Abstract Density functional theory calculations were carried out for repeated units of vinyl polymers, such as polyvinyls, polyacrylates, polymethylacrylates, polystyrenes and polyalkenes. The calculated results of the total energy E_t, the internal energy E_{in}, the heat capacity at constant volume C_V, the entropy S, the quadrupole moment Q_{ii}, the dipole moment μ, the average polarizability of the molecule α and the most negative net charge of atom q^- were used to predict the molar volume at room temperature $V_{298\ K}$, the molar parachor of Sugden P_s, the dispersion component F_d of the molar attractive force constant, the molar refraction of Lorentz and Lorenz R_{LL}, the molar diamagnetic susceptibility χ, the molar viscosity-temperature function estimated as a sum of the structural units in the repeated unit H_{vsum}, the molar Rao ultrasonic velocity function U_R and the molar Hartmann ultrasonic velocity function U_H. Eight quantitative structure-property relationship (QSPR) models obtained from the training sets were evaluated externally using the test sets. Data of correlation coefficient R^2 between the predicted values and experiment values are: 0.989 for $V_{298\ K}$, 0.982 for P_s, 0.975 for F_d , 0.997 for R_{LL}, 0.988 for χ, 0.914 for H_{vsum}, 0.988 for U_R and 0.972 for U_H. The results indicate that the QSPR models constructed by such quantum-chemical descriptors can be well used to predict the properties of polymers.

Key words density functional theory quantum-chemical descriptor quantitative structure-property relationship polymer

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