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用**TG/DTG/DTA**研究硅沸石与有机分子的主体/客体相互作用

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摘要 用TG/DTA/DTA法研究无阳离子与Si-OH缺陷、结构完美的硅沸石上烃类、烷基醇、烷基胺的热脱附行为。有机分子从硅沸石上脱附的温度低于300℃。其亲和性值AT=Td-Tb, 式中Td为有机分子在DTG上的失重峰温, Tb为该有机物在标准压力下的沸点。饱和烷烃的AT值为60~90, 而苯、甲苯、对二甲苯等的AT值为6~13。电负性较强的羟基使烷基醇与硅沸石的亲和性明显下降。多羟基醇的AT值为负值。对二甲苯、烷基醇、烷基胺在脱附时有明显吸热效应。AT值及脱附热效应的不同是硅沸石骨架O^2^-微孔表面与有机分子C-H基团, 其它极性基团之间相互作用不同, 以及受到硅沸石骨架空间限制的被吸附分子间缔合情况下同所致, 反应了不同类型的主体/客体超分子相互作用。

关键词 硅 催化剂 沸石 载体 热重量分析 差热分析 相互作用

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The host/guest interaction of organic molecules on silicalite-1 studied by TG/DTA/DTA

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Abstract The thermal desorption behaviour of hydrocarbons, alcohols and alkyl-amines from zeolite silicalite-1, which possesses perfect framework without cations and Si-OH defect, was studied by TG/DTG/DTA. The temperatures of desorption of these organics from silicalite-1 are lower than 300℃. AT a new concept on affinity of silicalite framework to the guest molecule has been defined as difference between Td and Tb, where Td is the temperature of weight loss peak at DTG curve and Tb the boiling temperature at standard pressure. The AT values for saturated hydrocarbons are 60~90, while 6~13 for benzene, toluene, ethyl-benzene and p-xylene. The AT value evidently decreases for alkyl -alcohol since stronger electronegativety of its hydroxy group. The AT values are negative for alcohols with muti-hydroxy groups. For methylamine and ethylamine, the AT values are 160 and 127 respectively, much higher than that for other alkylamines. The endothermal effect of desorption from silicalite-1 in DTA curves is obvious for p-xylene, alkyl-alcohols and alkylamines. The difference in AT value as well as thermal effect of desorption is from the different interaction between the framework micropore surface constructed by O^2^- and C-H groups and other polar groups of organics, and from the different situation of associate for the molecules adsorbed, which is limited by the void space in framework of silicalite-1. These facts reflect a different type of supermolecular interaction for host/guest system.

Key words SILICON CATALYST ZEOLITE CARRIERS THERMOGRAVIMETRY DIFFERENTIAL THERMAL ANALYSIS INTERACTIONS

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