化学学报 2006 64 (20): 2046～2050 ISSN: 0567-7351 CN: 31-1320/06

研究论文

二元硅氧环与CF_n (n＝1～3)自由基反应的理论研究

郭冠伦, 朱荣秀, 张冬菊*, 刘成卜

(山东大学化学与化工学院 济南 250100)

收稿日期 2006-2-14 修回日期 2006-4-20 网络版发布日期 2006-10-27 接受日期 2006-6-5

摘要 用密度泛函理论在UB3LYP/6-31G(d)水平上研究了二元硅氧环与CF_n (n＝1～3)自由基的反应, 弄清了微观反应机理, 计算了反应的活化能和反应热. 计算结果表明反应按两类相互竞争的机理进行: 一类是不涉及C—F键断裂的反应, 另一类是Si—O和C—F键同时断裂的反应. CF_2 自由基与二元硅氧环反应所需活化能最小、驱动力最大, 是Si—O键最有效的刻蚀剂, 与实验结果一致.

关键词 二氧化硅 CF_n (n＝1～3) 反应机理 密度泛函

分类号

Theoretical Study on the Reactions of Two-membered Si-O Rings with CF_n (n＝1～3) Radicals

GUO Guan-Lun, ZHU Rong-Xiu, ZHANG Dong-Ju*, LIU Cheng-Bu

(*School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100*)

Abstract The reactions of the two-membered Si-O ring with CF_n (n＝1～3) radicals have been studied by using density functional theory calculations at the UB3LYP/6-31G(d) level. Calculated results show that these reactions proceed via either the mechanism without C—F bond breakage or the mechanism with the C—F and Si—O bond breakages. The activation energies, reaction heats, and details of the potential energy surfaces for these reactions have been obtained. CF_2 radical was found to be the most effective etchant to Si—O bonds. This result is in good agreement with the corresponding experimental finding.

Key words silicon dioxide CF_n (n＝1～3) reaction mechanism density functional theory

DOI:

通讯作者 张冬菊 zhangdj@sdu.edu.cn