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研究论文

HCF(X~1A')+SO2反应的动力学研究

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摘要 用激光光解-激光诱导荧光方法研究了室温下(T=293 K) HCF($X^{\sim 1}A'$)自由基与SO_2分子的反应动力学. 实验中HCF($X^{\sim 1}A'$)自由基是由213 nm激光光解$HCFBr_2$产生的, 用激光诱导荧光(LIF)检测HCF($X^{\sim 1}A'$)自由基的相对浓度随着反应时间的变化, 得到此反应的二级反应速率常数为: k=(1.81±0.15)×10^{-12} cm^3•$molecule^{-1}$•s^{-1}, 体系总压为1862 Pa. 高精度理论计算表明, HCF($X^{\sim 1}A'$)和SO_2分子反应的机理是典型的加成-消除反应. 我们运用RRKM-TST理论计算了此二级反应速率常数的温度效应和压力效应, 计算结果和室温下测定的二级反应速率常数符合得较好.

关键词 X~1A')自由基')">HCF(X~1A')自由基 激光光解-激光诱导荧光 反应速率常数 压力效应 温度效应

分类号

Kinetic Study on the Reaction of HCF(&Xtilde;$^1A'$)+SO_2

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Abstract HCF($X^{\sim 1}A'$) radicals were produced by laser photolysis of $HCFBr_2$ at 213 nm, and electronically excited from the ground state to $X^{\sim 1}A''$(030) at 492.70 nm with a dye laser pumped by a Nd：YAG laser. The reaction rate constant of HCF($X^{\sim 1}A'$) with SO_2 at room temperature (T=293 K) was determined to be k=(1.81±0.15)×10^{-12} cm^3•$molecule^{-1}$•s^{-1}, when the total pressure was 1862 Pa. Based on the high level *ab initio* calculations, the mechanism of this reaction was proved to be a typical addition-elimination reaction. The temperature and pressure dependences of the total reaction rate constant were calculated by applying RRKM-TST model. The calculations could provide a well consistent description for our experimental work.

Key words X~1A') radical')">HCF(X~1A') radical laser photolysis/laser induced fluorescence reaction rate constant pressure dependence temperature dependence

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