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FULL PAPERS

HNCX→HXCN(X=O, S, Se)反应的量子拓扑研究

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摘要 采用MP2/6-311++G(2df,pd)//B3LYP/6-311++G(2df,pd)对HNCO→HOCN, HNCS→HSCN和HNCSe→HSeCN异构化反应进行了量子拓扑研究。优化得到了反应物、过渡态和产物的构型，解释了实验中HNCO和HNCS比HOCN和HSCN更容易探测的原因，预测了HNCSe比HSeCN也将更容易得到。采用电子密度拓扑分析方法对反应过程中化学键的断裂和生成进行了讨论，结果表明：所研究的异构化过程中存在两类结构过渡态。

关键词 异氰酸,异硫氰酸,异硒氰酸,电子密度拓扑分析,结构过渡态

分类号

AIM Study on Reaction HNCX → HXCN (X＝O, S and Se)

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Abstract The reactions of HNCO to HOCN, HNCS to HSCN and HNCSe to HSeCN have been studied at MP2/6-311＋＋G(2df,pd)//B3LYP/6-311＋＋G(2df,pd) level. Geometries of the reactants, transition states and products have been optimized and geometries of the transition states are reported for the first time. The reasons why HNCO and HNCS instead of HOCN and HSCN were easily detected have been explained. It was predicted that HNCSe will be more easily detected than HSeCN. The breakage and formation of the chemical bonds in the reactions have been discussed by the topological analysis method of electronic density. The calculated results show that there are two kinds of structure transition states (STS) in reactions studied.

Key words topological analysis of electronic density structure transition state isocyanic acid isothiocyanic acid isoselenocyanic acid

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