

研究通讯

## $\text{CH}_2\text{XH} \rightarrow \text{CH}_3\text{X}$ ( $\text{X} = \text{O}, \text{S}, \text{Se}$ ) 异构化的量子拓扑研究

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**摘要** 利用从头算和量子拓扑方法讨论了 $\text{CH}_2\text{XH} \rightarrow \text{CH}_3\text{X}$  ( $\text{X} = \text{O}, \text{S}, \text{Se}$ ) 异构化过程的反应机理。

着重从电子密度拓扑分析计算了反应进程中的各点, 讨论了反应进程中键的断裂和生成,

上述反应都经历了三元环过渡结构, 找到了这类反应的“能量过渡态”和“结构过渡态”,

且结构过渡态均在能量过渡态之后出现. 三元结构过渡态结构出现的范围与反应热成正比.

**关键词** [异构化反应](#) [电子密度拓扑分析](#) [反应机理](#) [结构过渡态](#)

分类号

## Quantum Topological Study of $\text{CH}_2\text{XH} \rightarrow \text{CH}_3\text{X}$ ( $\text{X} = \text{O}, \text{S}, \text{Se}$ ) Isomerization Reactions

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**Abstract** The isomerization reaction of  $\text{CH}_2\text{XH} \rightarrow \text{CH}_3\text{X}$  ( $\text{X} = \text{O}, \text{S}, \text{Se}$ ) has been studied by the *ab initio* and quantum topological analysis method. The breakage and formation of the chemical bonds in the reactions have been discussed by the topological analysis method of electronic density, and the calculated results show that there is a transitional structure of three-membered ring on the isomerization reaction paths. The “energy transition state” and the “structure transition state” in all of the studied reactions have been found. And in all these reactions, the structure transition state appeared after the energy transition state. The more the reaction energy is, the wider scope the three-membered ring appears in.

**Key words** [isomerization reaction](#) [topological analysis of electronic density](#) [reaction mechanism](#) [structure transition state](#)

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