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几个硫-叶立德反应机理的量子拓扑研究

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摘要 采用MP2(FC)/6-311++G(d,p)对硫叶立德和类硫叶立德自由基反应机理进行了探讨。优化了中间体、过滤态和产物的几何构型。本文侧重从量子拓扑学的角度，对IRC(内禀反应坐标)反应进程中各点进行电子密度拓扑分析，讨论了反应过程中化学键的断裂、生成和化学键的变化规律。找到了这类反应的能量过渡态和结构过渡态，上述两个反应都是先经历一个没有形成三元环拓扑结构的能量过渡态，再经历一个形成了三元环拓扑结构的结构过渡态，最后到达产物。

关键词 硫叶立德 反应机理 拓扑 过渡态理论

分类号 0641

Quantum topological analysis of two S-ylide reactions

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Abstract MPS(FC)6-311+ +G(d,p) calculations were carried out for S-ylide and S-ylide-like radical reaction paths. The geometry structures of the intermediates, the transition states and the products were optimized and IRC calculations were employed. We emphasize on the investigation of the topological properties of the two reactions. The changing trends of the chemical bonds were discussed. The energy transition states (ETS) and the structure transition states (STS) of the two reactions were found. The △ type topological structure were formed in the STS, not in the ETS.

Key words REACTION MECHANISM TOPOLOGY TRANSITION STATE THEORY

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