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N-4-戊烯基硝酮的分子内环加成反应的区域选择性的理论研究

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摘要 用MINDO/3方法求出了N-4-戊烯基硝酮分子内环加成反应的过渡态和反应途径.
两个环加成区域异构体是由N-4-戊烯基硝酮的两个不同的构象经过各自的过渡态得到的.
理论分析满意地解释了实验结果.

关键词 量子化学 选择性 环加成反应 过渡态理论 构型 微分重叠间忽略近似 硝基酮 戊烯基

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A theoretical study on the regiochemistry of intramolecular N-4-pentenylnitron addition

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Abstract The geometries of three conformers of N-4-pentenylnitrone (Ra, Rb, and Rc) were optimized with the aid of the energy gradient technique. The geometries of two transition states (Ta and Tb) were obtained by Komornicki's method. The reaction paths were also determine The conformers Ra, Rb and Rc are all stable, but only the first two are active in the intramol. cycloaddn., generating regioisomers Pa and Pb via transition states Ta and Tb, resp. Actually, intramol. cycloaddn. of N-4-pentenylnitrone consists of two parallel reactions. Because the activation barrier of the reaction from Rb to Pb is lower than that from Ra to Pa, the higher yield of the former is predicted. This is consistent with experiments The mechanism of the two reactions are similar. All the calcns. were performed on semiempirical MINDO/3 MO method.

Key words QUANTUM CHEMISTRY SELECTIVITY CYCLOADDITION REACTION TRANSITION STATE THEORY CONFIGURATION INTERMEDIATE NEGLECT OF DIFFERENTIAL OVERLAP APPROXIMATION (IND NITROKETONE PENTENYL GROUP

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