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单态卡宾与臭氧反应机理的量子化学研究

李来才,廖显威,王欣,田安民-

四川师范大学化学系.成都(610066);四川大学化学系.成都(610064)

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摘要 为了研究单态卡宾与臭氧反应机理，本文采用密度泛函理论Gaussian-3方法(G3B3)优化了反应物、中间体、过渡态和产物的几何构型。探讨了单态卡宾与臭氧反应可能途径，
并通过频率分析对过渡态和中间体进行了验证，研究结果表明：单态卡宾与臭氧反应有两条反应通道，分别具有亲核反应和亲电反应特征，相对而言亲核反应通道较易发生，且为强放热反应。

关键词 卡宾 碳烯 臭氧 反应机理 密度泛函理论 过渡态 几何异构

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Ab initio investigation on reaction of ozone with singlet carbene

Li Laicai,Liao Xianwei,Wang Xin,Tian Anmin

Sichuan Normal Univ, Dept Chem Eng.Chengdu(610066);Sichuan Univ, Dept Chem.Chengdu(610064)

Abstract The reaction mechanism of ozone and singlet carbene has been studied by means of the Gaussian-3 method to optimize the geometries of reactions, transition states, intermediates and products. The energies and structures of the important transition states, intermediates are reported for the first time. The results show that there are two different reaction pathways on the reaction of singlet carbene and ozone: the two reaction pathways may take place under suitable condition and nucleophilic reaction is relatively easier. Furthermore, two reactions are strong exothermic reactions.

Key words CARBENE OZONE REACTION MECHANISM TRANSITION STATE GEOMETRICAL ISOMERISM

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通讯作者