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عنوان مقاله:

Direct Dynamics Study on the Reaction of CH3+ with O(1P) Atom

محل انتشار:

بیستمین کنگره شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Gas phase ion–atom reactions are a class of important reactions that take place in combustion or atmospheric processes where cosmic light is involved. This study focuses on the dynamics and kinetics of the reaction of CH3+ with O(1P) atoms in presence of N2 molecules as the bath gas. The mechanism of the title reaction is explored at the CCSD(T)/aug-cc-pVTZ level of theory over the lowest singlet surface. The barrier-less initiation step in this system is governed by the capture probability in the entrance channel to form an energized adduct once the centrifugal barrier is surmounted. The reaction takes place over a multiwell multichannel potential energy surface (PES) that is based on the computations at CCSD(T)/aug-cc-pVTZ level of theory. Low values of T1 diagnostic test indicates that the single determinant wave function is dominated.[1] The dynamics and kinetics of the title reaction is simulated by solving a one-dimensional chemical master equation (CME).[2] The temperature and pressure dependence of the reaction over a wide range of temperature (300–3000 K) and pressure (0.1–5000 Torr) are examined. No sign of pressure dependence was being observed for the title reaction over the stated range of pressure. The results from solving the chemical Master equation indicates that CH2O + and H are the major products in our study.Theoretical bimolecular reaction rate constants over the lowest PES are computed. The results from direct-dynamics canonical variational transition-state theory calculations depict the importance of tunneling in hydrogen transfer isomerization reactions of .+CH2O + to trans-HCOH+ and HOC+ to HCO

کلمات کلیدی:

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