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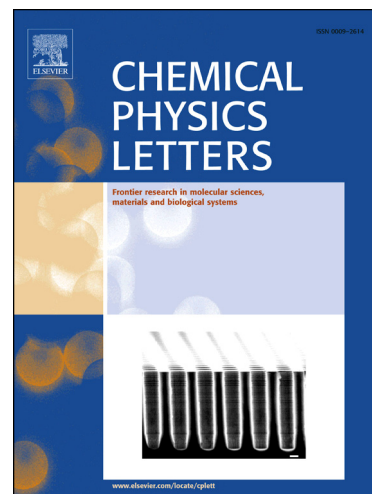
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Observation of H displacement and H₂ elimination channels in the reaction of O(³P) with 1-butene from crossed beams and theoretical studies

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ABSTRACT

We report preliminary combined experimental/theoretical results on O(³P)+1-butene reaction dynamics with focus on atomic hydrogen displacement and molecular hydrogen elimination channels. Dynamics and relative yield of the ethylvinoxy+H and ethylketene+H₂ product channels are characterized in crossed beam experiments. Stationary points and energetics of triplet/singlet C₄H₈O potential energy surfaces (PESs) are calculated at CCSD(T)/CBS and CASPT2 level. O(³P) attack occurs on both unsaturated C-atoms with preference for the less substituted one leading, among other products, to C₂H₅CHCHO+H via an exit barrier on the triplet PES, and to C₂H₅CHCO+H₂ via a very high exit barrier on the singlet PES following intersystem crossing.

KEYWORDS:

Reaction dynamics of O-atoms with 1-butene, Crossed molecular beams, Intersystem crossing, CASPT2, C₄H₈O potential energy surface.

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