

# Isomerization effect on the dynamics of the H + O<sub>2</sub> collision

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The reaction of H atom with dioxygen has been termed the “single most important” elementary step in combustion. It is important to explore the factors that play crucial role in the dynamics of the reaction. We have employed the quasiclassical trajectory (QCT) method and the first excited potential energy surfaces of Guo and coworkers [1]. Most reactive trajectories in the HO<sub>2</sub> system undergo isomerization (1,2-H-atom shift) through the barrier at the C<sub>2v</sub> arrangement on both PES. Furthermore, in reactive collisions the O-O breakage occurs right after the isomerization, if the isomerization takes place in the appropriate O-O vibrational phase (when the O-O distance increases). The products of trajectories that isomerized before the bond breaking are rotationally hot and vibrationally cold. We found that if no isomerization happens in reactive collisions the picture the final state distribution is the opposite: the products are rotationally cold and vibrationally hot. This means the dynamics of isomerization involves a torque that is missing if there is no isomerization. The sharp difference of the behavior of different kinds of trajectories indicates that the internal phase space of electronically excited HO<sub>2</sub> is far from ergodic.

[1] Anyang Li, Daiqian Xie, Richard Dawes, Ahren W. Jasper, Jianyi Ma, and

Hua Guo  
, *J. Chem. Phys.*, 133, 144306, 2010