Chemical Physics Letters 523 (2012) 34–38

Contents lists available at SciVerse ScienceDirect

Chemical Physics Letters

journal homepage: www.elsevier.com/locate/cplett

O-atom exchange in $O(^3P) + H_2O(^1A_1)$ collisions

Matthew Braunstein *, Patrick F. Conforti

Spectral Sciences Inc., 4 Fourth Avenue, Burlington, MA 01803, United States

ARTICLE INFO

Article history:
Received 15 November 2011
In final form 8 December 2011
Available online 16 December 2011

ABSTRACT

Global potential energy surfaces for the three lowest electronic triplet states of $O(^3P) + H_2O(^1A_1)$ are used to explore two unusual reaction pathways, not previously identified. Both pathways go through a D_{2h} rhombus geometry, with zero potential gradient and two imaginary frequencies. Motion along one imaginary frequency leads to $O + H_2O$, while motion along the other leads to OH + OH. In each case, an O-atom is exchanged. Classical trajectory methods are used to compute exchange cross sections up to 11 km s^{-1}. Transition state theory rate constants for O-atom exchange processes are also computed.