O-atom exchange in O(3P) + H2O(1A1) collisions

Matthew Braunstein *, Patrick F. Conforti

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

**Abstract**

Global potential energy surfaces for the three lowest electronic triplet states of O(3P) + H2O(1A1) are used to explore two unusual reaction pathways, not previously identified. Both pathways go through a D2h rhombus geometry, with zero potential gradient and two imaginary frequencies. Motion along one imaginary frequency leads to O + H2O, 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.

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