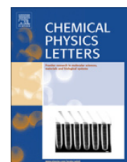




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O-atom exchange in $O(^3P) + H_2O(^1A_1)$ collisions

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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.

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