Energy barrier of the reaction of ground-state ozone with atomic oxygen

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The atmospheric reaction of ozone with atomic oxygen

$$O(^3P) + O_3(^1A_1) \longrightarrow 2O_2\left(X^3\Sigma_g^-\right)$$

plays an important role in atmospheric chemistry and is also of interest for re-entry chemistry in aerospace applications. There are a many experimental studies of this reaction in the literature, but theoretical work is scarce. Due to the highly multi-reference characters of the reactant and the transition state of this reaction, its study is very challenging from the theoretical point of view. The reaction is believed to occur on the triplet potential energy surface of O_4, since spin-orbit coupling is small for oxygen. The study of this reaction is part of the development of a global triplet potential energy surface of O_4. A global potential energy surface describes all kinds of collisions of two diatomic molecules, as well as a triatomic molecule interacting with an atom and a triatomic surface as a sub-surface of the four-body PES. In this study we have compared the energy barrier of this reaction using single- and multi-reference wave function methods and Kohn-sham density functional theory

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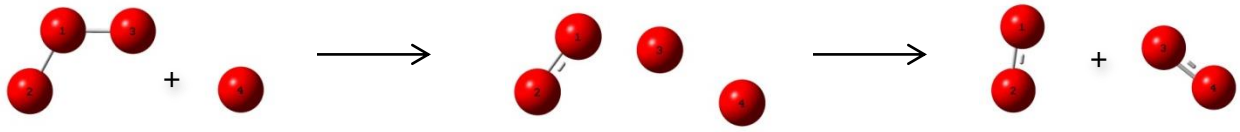

Figure 1. Geometries of the reactants, transition state, and products for the reaction of ozone with atomic oxygen.