

Noncovalent interaction between water and (^3P) oxygen atom

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June 2022

The reaction between two OH radicals has been studied in the context of combustion chemistry, atmospheric chemistry, and astrochemistry. The global minimum on the triplet reaction surface is the van der Waals complex between water and $\text{O}(^3\text{P})$ atom. We optimized the geometry of the system using *ab initio* methods up to CCSDT/aug-cc-pVQZ. We use the focal point approach to determine an accurate dissociation energy of $1.35 \text{ kcal mol}^{-1}$ for the complex dissociating into water and $\text{O}(^3\text{P})$. We also predict the anharmonic vibrational frequencies of the complex in anticipation of future experiments aimed at detecting this system.