

## **C<sub>3</sub>H<sub>2</sub> oxidation by molecular oxygen: a theoretical study**

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Propynylidene is one of the commonly found in interstellar space particles. In addition, propynylidene can occur as intermediates in the hydrocarbon fuel's combustion. This particle can have several forms: singlet propynylidene may be in a cyclic and linear form, and triplet propynylidene has linear form. The low stability makes it difficult to study the transformations of propynylidene under combustion conditions by experimental methods. We have studied the interaction of triplet propynylidene with molecular oxygen in a wide range of temperatures and pressures by theoretical methods using quantum chemical calculations.

Geometries of the reactants, products, transition states, and reaction intermediates in the reactions of triplet propynylidene with molecular oxygen have been optimized using the wB97XD method with the 6-311G\*\* basis set. Vibrational frequencies have been computed at the same level of theory to characterize stationary points as local minima or transition states, to obtain zero-point vibrational energy corrections (ZPE), and to be utilized in partition function calculations. Further, the wB97XD optimized geometries were used to refine single-point energies by the MOLPRO package. Temperature- and pressure-dependent rate constants for the reactions considered were evaluated within the framework of RRKM theory in combination with the Master Equation approach (RRKM-ME).

Based on the results of the study, the potential energy surface (PES) of the reaction of triplet propynylidene with molecular oxygen was constructed, and the rate constants of this interaction were determined. The calculated rate constants at different pressures were fitted by the modified Arrhenius expressions, which are proposed for kinetic modeling of propynylidene reactions in combustion.