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***Ab initio* Study of Cyclopropenone Formation in Interstellar Space** SEYEDSAEID AHMADVAND, RYAN ZAARI, SERGEY VARGANOV, Univ of Nevada - Reno, SERGEY A. VARGANOV TEAM — The recent discoveries of complex organic molecules such as cyclopropenone and glycoaldehyde in interstellar space have renewed the interest in astrochemical reaction mechanisms. We investigate three previously proposed reaction mechanisms for cyclopropenone formation in interstellar medium using ab initio quantum chemical methods. The nonadiabatic spin-forbidden reaction between atomic oxygen and cyclopropenylidene characterized by very small activation barrier and significant spin-orbit coupling between the lowest energies singlet and triplet states. We calculate the Landau-Zener probability of transition between the triplet and singlet states, and use nonadiabatic transition state theory to estimate the reaction rate constant of this spin-forbidden reaction. The reaction between acetylene and carbon monoxide, and between molecular oxygen and cyclopropenylidene, are two spin-allowed cyclopropenone formation pathways, also investigated in this work. Of the three studied reactions, the most probable mechanism of cyclopropenone formation in cold regions of interstellar space is between molecular oxygen and cyclopropenylidene since it is found to be a barrier free reaction.

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