**Highlights**

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* Quantum study at B3LYP / 6-311 ++ G (d, p) level and ELF analysis
* Forrmation of propynal and cyclopropenone in interstellar medium.
* Molecules obtained from reactions between carbon monoxide (CO) and acetylene (C2H2) in the cold conditions of interstellar clouds.
* Reaction paths are elaborated and discussed here.
* Propadienone, another isomer, not detected, found as stable triplet ground state with a weak dipole moment.