Vibrational study of methyl formate $(HCOOCH_3)_n$:$(H_2O)_m$ complexes in solid neon. First observation of three isomers for each of the 2:0, 1:1, and 1:2 complexes.

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Methyl formate (MF) is an important interstellar medium molecule and it has been the subject of several theoretical and experimental studies in literature. The experimental study of the complexation of this molecule with water has never been undertaken from a vibrational point of view as well as the homodimer $(MF)_2$.

We highlight for the first time the presence of three isomers for the $(MF)_2$, MF-H_2O and MF-$(H_2O)_2$ complexes in solid neon. For the MF-H_2O complex, we observe without ambiguity three isomers: two where the carbonyl oxygen served as the proton acceptor and one where the alkoxy oxygen was the proton acceptor. For the MF-$(H_2O)_2$ complex, we clearly observe three isomers especially by the observation of large frequency shifts of two MF modes.

Theoretical calculations at MP2- aug-cc-pVTZ level have been performed to obtain the equilibrium geometries and vibrational spectra at the harmonic level and comparison with experimental data allows us to give structures of observed complexes.