Spectroscopic and computational characterization of the HCO···H_2O complex.

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Streszczenie

The complexes of HCO with water are prepared in a Kr matrix and characterized by IR spectroscopy with the aid of ab initio calculations. The calculations at the UCCSD(T)/aug-cc-pVTZ level of theory predict three structures of the HCO···H_2O complex. In the "linear" structure **I**, a hydrogen atom of water interacts with the oxygen atom of HCO. In structure **II**, the hydrogen atom of HCO interacts with the oxygen atom of water. The "cyclic" structure **III** has the C–H···O and O–H···O hydrogen bonds simultaneously. In the experiment, the HCO···H_2O complex is produced by photolysis of HCOOH/HY/Kr (Y = Br and Cl) matrices followed by thermal annealing at about 30 K, which promotes the H + CO···H_2O → HCO···H_2O reaction. The analysis of the spectroscopic data shows that the main product has structure **III** whereas the formation of structure **II** is less efficient. The experiments show no evidence of the weakest structure **I**. The experiments with deuterated formic acid (DCOOH) provide additional support of the proposed assignment.

Adres publiczny

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https://www.acs.org/content/acs/en.html