The OC-HOCO Complex: Identification and Implications for ISM Chemistry

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Abstract

Water (H_2O) and carbon monoxide (CO) are two of the most abundant molecular constituents of ices that accrete onto dust grains in the interstellar medium (ISM) [1]. Irradiation of such ices increases the chemical complexity of the ISM through generation of molecules such as carbon dioxide (CO_2), formaldehyde (H_2CO), and methanol (CH_3OH) [2]. While the study of such ices in the laboratory can easily identify end products, reaction mechanisms are often much harder to determine experimentally in ices. The reactions of reactive intermediates can, however, be investigated by using a combination of matrix-isolation spectroscopy and theoretical chemistry.

In the present work, we identified the formation of an OC-HOCO complex in argon matrices using infrared spectroscopy. The complex is formed in the matrix after deposition of a discharged dilute mixture of H_2O and CO in argon at 6 K.

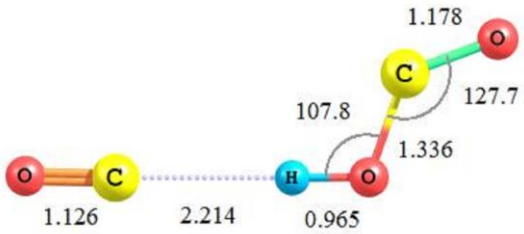

Figure 1: The structure of the OC-HOCO complex as was determined at the CCSD/cc-pVTZ theory level. Bond lengths and bond angles are given in Å and degrees, respectively.

The proposed mechanism of formation involves the reaction between a hydroxyl (OH) radical and CO, and so should also occur in the irradiated CO/H_2O ices. This reactive intermediate is likely a key participant in the formation of CO_2 in CO-rich ices through a proton-transfer reaction resulting in HCO and CO_2 production.

$$OC\text{-}HOCO \rightarrow HCO + CO_2$$

The OH/2CO potential energy surface has been investigated theoretically and shows that the exothermic decomposition of the OC-HOCO to CO_2 is likely. This previously unrecognized complex could be an important intermediate in the formation of CO_2 in CO-rich ices.

References

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