



Supporting Information

© Wiley-VCH 2011

69451 Weinheim, Germany

Spectroscopic Observation of Matrix-Isolated Carbonic Acid Trapped from the Gas Phase**

*Jürgen Bernard, Markus Seidl, Ingrid Kohl, Klaus R. Liedl, Erwin Mayer, Óscar Gálvez,
Hinrich Grothe,* and Thomas Loerting**

anie_201004729_sm_miscellaneous_information.pdf

Supporting Information

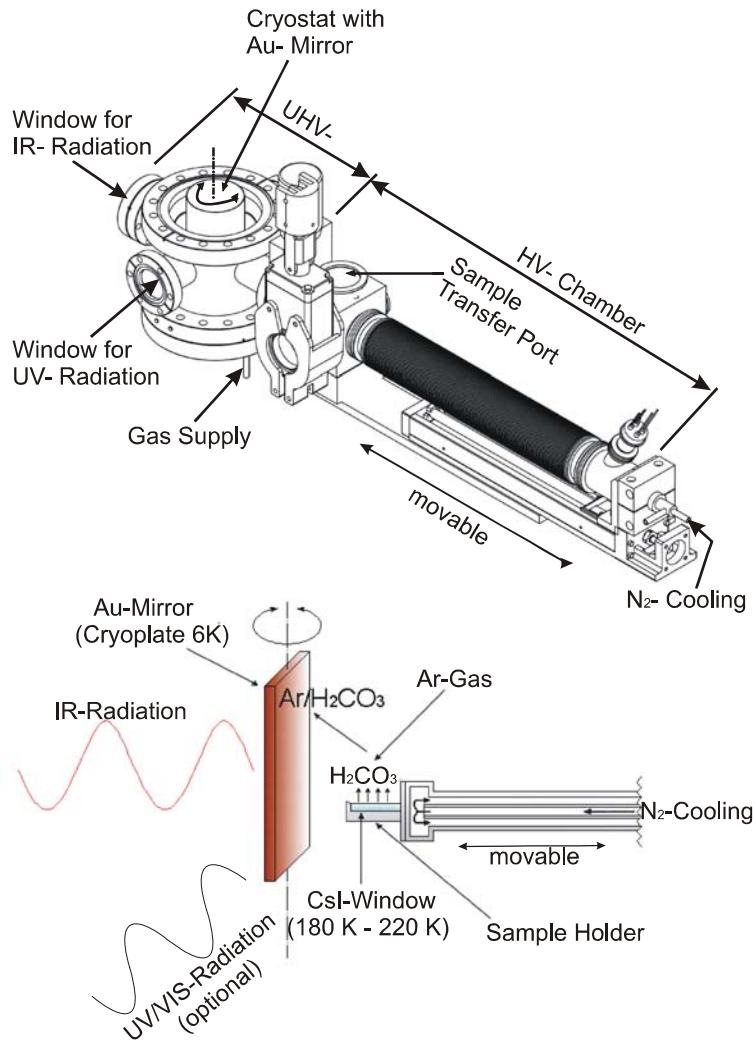


Figure 1. Transfer system and chamber at TU Vienna used for the purpose of matrix isolation viewed from the outside (top) and the inside (bottom). An infrared-transparent window (diameter 25 mm) covered with a thin crystalline film of $\alpha\text{-H}_2\text{CO}_3$ was prepared at Uni Innsbruck according to the well-established protocol described in detail in ref. [22]. This sample is transferred from a liquid nitrogen Dewar via the sample transfer port into the high-vacuum (HV)-chamber, where hexagonal ice is removed, which has condensed onto the sample during transfer. Using the movable transfer rod the sample is moved to the differentially pumped ultrahigh-vacuum (UHV)-chamber. There, the carbonic acid film is sublimed at 210 K for 60 minutes and carried together with high-purity gaseous argon (neon) to the rotatable Au-mirror. The distance between the sample window and Au-mirror is about 6 cm. The Au-mirror has a temperature of 6 K, at which argon and carbonic acid vapour condense as a solid. The ratio of argon (neon) to carbonic acid can be varied, but is typically 1000:1. Infrared spectra are taken in reflection after a rotation of the Au-mirror by 180°.

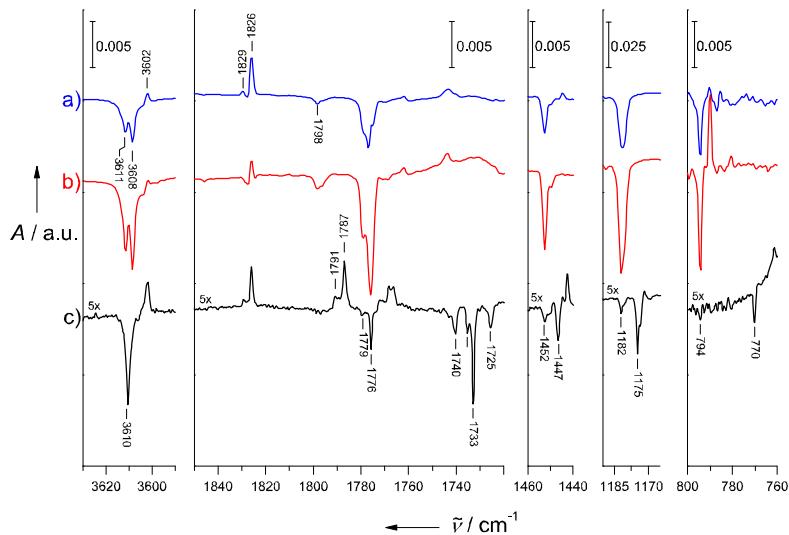


Figure 2. Changes in the spectrum after keeping the argon-trapped carbonic acid a) for 15 min at 20 K and b) for additional 15 minutes at 30 K (cf. Fig.2c), or c) after irradiation of ^{13}C -substituted carbonic acid (cf. Fig.2b) with a 300 W UV-VIS lamp (230 – 850 nm, maximum at 500 nm). Difference spectra are shown in the way that species that are accumulating show peaks pointing upward and shifted for clarity. The spectra suggest that monomeric carbonic acid isomerizes from C_{2v} to C_5 -symmetry both by heating the matrix and under the influence of UV-radiation (cf. assignment in Tab.1).

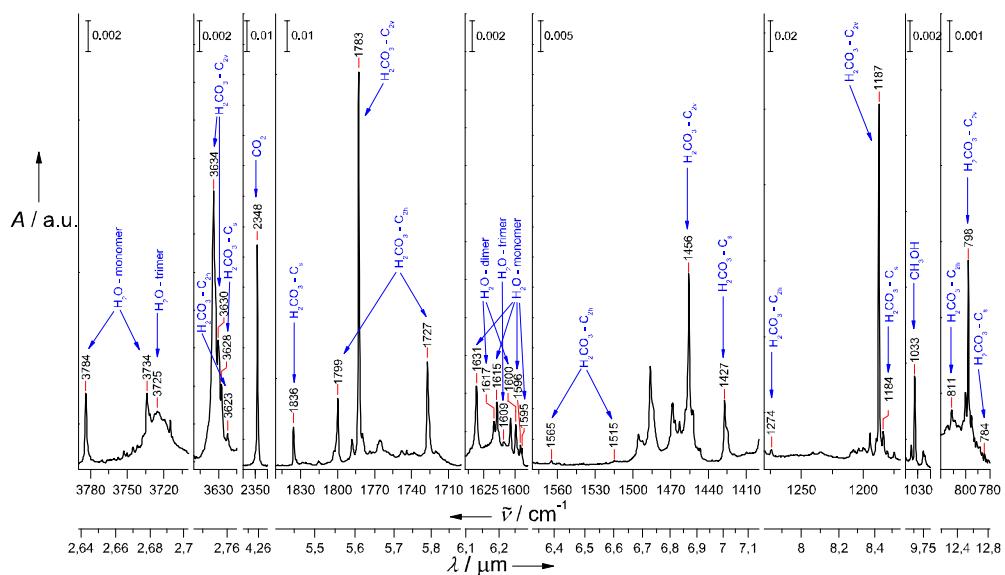


Figure 3. Infrared-spectrum of carbonic acid vapour after sublimation of crystalline α -H₂CO₃ at 210 K and isolation in neon matrix at 6 K. Assignment of the water monomer,^[36] water dimer,^[36,37] water trimer,^[38] carbon dioxide,^[39] and methanol^[40] is based on literature data. Assignment of carbonic acid (C_{2v}-monomer, C_S-monomer and C_{2h}-dimer) as discussed in the main text (cf. also Tab.1).

- [36] D. Forney, M. E. Jacox, W. E. Thompson, *J. Mol. Spectrosc.* **1993**, *157*, 479-493.
 - [37] J. Ceponkus, B. Nelander, *J. Phys. Chem. A* **2004**, *108*, 6499-6502.
 - [38] J. Ceponkus, G. Karlstroem, B. Nelander, *J. Phys. Chem. A* **2005**, *109*, 7859-7864.
 - [39] L. Wan, L. Wu, A.-W. Liu, S.-M. Hu, *J. Mol. Spectrosc.* **2009**, *257*, 217-219.
 - [40] J. P. Perchard, F. Romain, Y. Bouteiller, *Chem. Phys.* **2008**, *343*, 35-46.