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Laboratory simulations of pre-cometary ice processes: thermal desorption, UV and X-ray irradiation

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Abstract

The formation of ice mantles on pre-cometary dust grains was simulated experimentally under ultrahigh vacuum conditions. An ice mixture containing H_2O, CO, CO_2, CH_3OH, and NH_3 was deposited at 8 K. The ice layer was either irradiated by UV or X-rays, or warmed up in a controlled way. The ice was monitored by infrared spectroscopy in transmittance and the species in the gas phase were detected by quadrupole mass spectroscopy (QMS). The temperature programmed desorption (TPD) of a complex ice mixture with up to five molecular components can aid to interpret the data collected by mass spectrometers on board cometary missions like Rosetta during the flyby. The irradiation experiments led to the formation of many photo-products. We will focus on those made by irradiation of ices containing H_2S to study the formation of the detected sulfur-bearing species in comets, such as S_2.

1. Introduction

There is a considerable number of publications dedicated to UV-photoprocessing and warm-up of ices of astrophysical interest, but there is almost no literature on soft X-ray irradiation of these ices. In addition, most of the UV-irradiation experiments performed so far were under high vacuum, $< 10^{-8}$ mbar, where background water accretion is a problem for the study of surface processes. We present new data obtained using our Interstellar Astrochemistry Chamber (ISAC) setup, base pressure in the 10^{-11} mbar range, see [4] for description of the setup. Thanks to a novel design of the gas line for the preparation of gas mixtures, which works dynamically using a QMS and electrovalves to control the flow of the gas components, we were able to control more precisely the composition of the ice mixture. The optimum vacuum conditions allowed the performance of UV and X-ray experiments at very low photon doses, leading to the detection of photo-products at very low abundances. In the case of X-ray experiments that was crucial since the available X-ray sources provide very low fluxes.

2. Results

The TPD experiments of ice mixtures clearly show how intermolecular forces operate in the ice matrix, leading to desorption temperatures that often differ significantly from those of pure ices. An example is shown in Fig. 1. There is co-desorption of CO, NH_3 and CO_2 around 135 K and co-desorption of the most polar species, CH_3OH and H_2O, with a maximum at 165 K.

The chemistry induced by UV photons in H_2S-containing ice mixtures is complex. Among the numerous UV-photoproducts are S-polymers, from S_2 to S_8 [2]. The soft X-ray irradiation (0.3 keV photon energy) of pure H_2S ice at very low dose led to the formation of H_2S_2 [3]. This species is common to the UV experiments using similar low doses.

3. Summary and Conclusions

The data collected during the TPD experiments will be compared to the results obtained by the COSAC mass spectrometer on board Rosetta described in [1].

Based on these experiments, we can predict the time sequence for the detection of volatile species as they desorb from the comet and arrive to the COSAC spectrometer. Because the temperature of the comet nucleus increases gradually as it approaches the Sun, it is expected that the first molecules detected will be the most volatile ones like CO, O_2, etc. At temperatures well above 100 K other ice species desorb including H_2O or CH_3OH. Less obvious is the estimation of the desorption temperatures when the molecular ice components are well mixed in the nucleus. In that case, the more volatile species will be trapped in the ice matrix and co-desorb with the more refractory species at temperatures much higher than expected. This is illustrated in the experimental data of Fig. 1. For instance, pure CO ice desorbs around 28 K in the laboratory, but if CO is mixed with H_2O and other molecules, a fraction of the CO molecules co-desorbs at much higher temperatures. It was found that the intermolecular forces between some species in the ice mixture were negligible while others make relatively strong bonds, which explains the observed co-desorption. The morphology and composition of the cometary ice will therefore affect strongly the detection times of the different volatiles by COSAC.

We proposed that irradiation of H_2S, either with UV or X-rays, leading to H_2S_2 and, by photodissociation, to S_2 formation, could explain the observed S_2 abundances in comets like IRAS-Araki-Alcock 1983d and Hyakutake [3]. We discuss that this formation route for S_2 should dominate over the formation via CS_2 as the parent molecule.

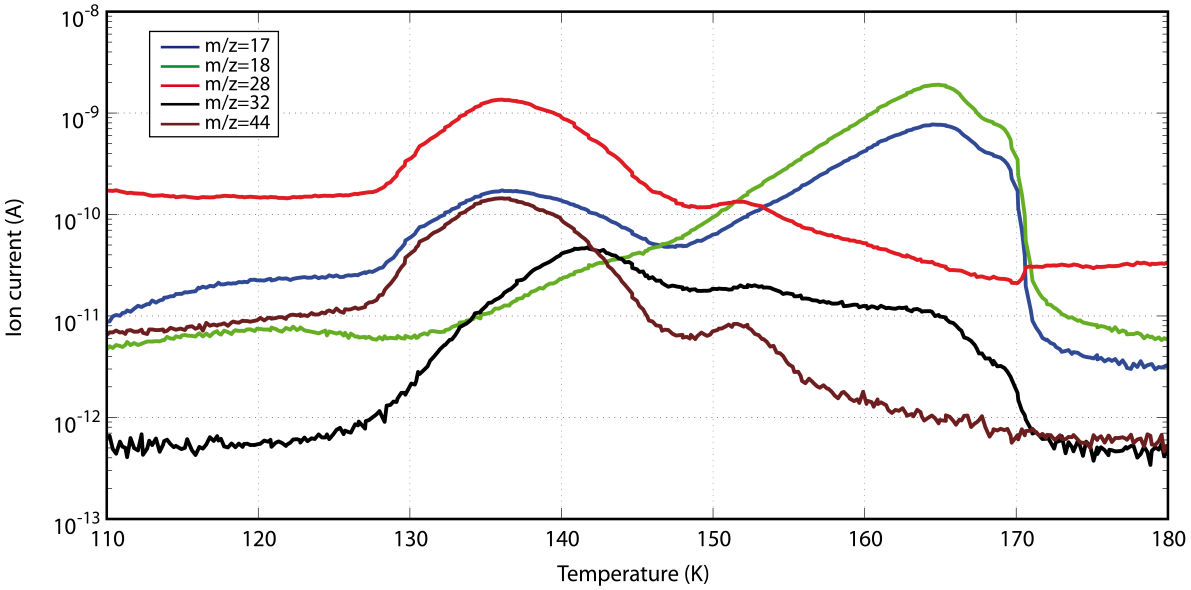

Figure 1: Temperature programmed desorption of molecules in the 110 to 180 K range for the ice mixture H_2O:CO:CO_2:CH_3OH:NH_3 = 37:25:25:7:6. There is an increase in the partial pressures of m/z = 28, 17, 44 with a maximum near 135 K, corresponding to the co-desorption of CO, NH_3 and CO_2. Methanol (m/z = 32) desorbs at a slightly higher temperature, 140 K, and triggers the desorption of H_2O (m/z = 18). The m/z = 17 is common to NH_3 and H_2O, but the maximum near 165 K with a similar behaviour as m/z = 18 indicates that only water desorbs at that temperature in this experiment, accompanied by the remaining CH_3OH (m/z = 32).

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