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Sublimation of cometary ices in the presence of organic volatiles

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Evolution of the surfaces of cometary nuclei is determined by the sublimation of ice. The rate of sublimation is commonly calculated using the simple Hertz–Knudsen formula, which should be corrected by a temperature dependent sublimation coefficient α_s (Kossacki et al., 1999; Gundlach et al., 2011; Kossacki and Leliwa–Kopystynski, 2014). In this work influence of C_3H_6O (acetone), and CH_3OH (methanol) present in cometary ice on the sublimation coefficient is investigated. We have found, that the mass fraction of admixtures $\leq 2\%$ in water ice is sufficient for an increase of α_s by a factor about 5, depending on the temperature. The sublimation coefficient is sensitive to very small concentrations of admixtures. When the admixture is acetone and the mass fraction $f = 0.005$ is $\alpha_s(215\ K) \sim 0.46$ instead of ~ 0.18 for pure water ice. When $f = 0.01$ is $\alpha_s(215\ K) \sim 0.74$, and when $f = 0.02$ is $\alpha_s(215\ K) \sim 0.78$. The presence of 0.01 mass fraction of methanol has similar influence on the sublimation coefficient as the presence of 0.01 mass fraction of acetone. At temperatures $T > 235$ K for all investigated compositions of ice $\alpha_s \sim 0.15$.

1. Introduction

There is no doubt that water in the frozen form is one of the main components of cometary nuclei. Molecular abundance of water considerably prevails over the other volatiles all together. Typically, the most abundant molecules apart of water are: carbon monoxide CO, carbon dioxide CO_2, and molecular oxygen, while methane, ammonia, and other are minors (e.g. Mall et al., 2016). The determined molecular ratios strongly vary from comet to comet. In Table 1 abundances of molecules detected in selected comets 1P/Halley, C/1996 B2 Hyakutake, C/195 Hale-Bopp, C/2001 A2 LINEAR, 77P/Schwassmann–Wachman 3, and 67P/Churyumov–Gerasimenko are presented (Mumma and Charnley, 2011; Goesmann et al., 2015; Mall et al., 2016).

It should be noted that the concentrations presented by Goesmann et al. (2015) were determined from the data provided by the evolved gas analyzer Cometary Sampling and Composition (COSAC) experiment aboard Rosetta's Philae lander, about twenty five minutes after Philae's first touchdown. The investigated molecules were ejected from the comet during impact, so the concentrations are measured in-situ.

The rate of sublimation is typically calculated using the classical Hertz–Knudsen equation. Originally, the equation was derived assuming equilibrium distribution of the velocities of molecules when the system is not in equilibrium. This makes the Hertz–Knudsen equation only approximate (Kossacki et al., 1999). Inaccuracy of the Hertz–Knudsen formula was shown also in relation to the evaporation of liquids (Holyst et al., 2015). The Hertz–Knudsen equation can be corrected by a temperature dependent sublimation coefficient (Kossacki et al., 1999; Gundlach et al., 2011; Kossacki and Leliwa-Kopystynski, 2014). In Kossacki and Leliwa-Kopystynski (2014) it was shown, that presence of a small amount of admixtures in the water ice can significantly affect the sublimation coefficient.

This work is intended to investigate the temperature dependence of the sublimation coefficient of H_2O ice with selected admixtures detected in comets. We present results for C_3H_6O (acetone), and CH_3OH (methanol).

2. Sublimation coefficient

The Hertz–Knudsen equation can be improved by introducing a temperature dependent sublimation coefficient α_s. Hence, the formula for the sublimation driven recession rate of the surface becomes

$$\frac{dz}{dt}(T) = \frac{\alpha_s(T)}{\varrho}\left(\frac{\mu}{2\pi R_g T}\right)^{0.5}(p_{sat} - p). \quad (1)$$

(Kossacki and Leliwa-Kopystynski, 2014). The symbol T denotes the surface temperature of a sample, ϱ is the density of the subliming material, p is the pressure over the subliming surface, p_{sat} is the equilibrium saturation pressure at temperature T, μ is the molar mass of ice, and R_g is the universal gas constant.

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Table 1
Molecular ratios of selected molecules detected in comets relative to water (data from [1] Mumma and Charnley (2011), [2] Goesmann et al. (2015), and [3] Mall et al. (2016)). The values are normalized to 100, so for pure H_2O ice the molecular ratio is 100.

Molecule	Molecular ratios					
	1P/ Halley [1]	C/1996 B2 Hyakutake [1]	C/1995 Hale-Bopp [1]	C/2001 A2 LINEAR [1]	77P/ SW3 [1]	67P/ C-G [2, 3]
H_2O	100	100	100	100	100	100
CO	3.5–11	14–30	12–23	4	0.5	1.2
CO_2	3–4	–	6	–	–	< 4.5[3]
CH_4	< 0.8	0.8	1.5	1.2	< 0.25	0.5[2]
C_2H_2	0.3	0.2–0.5	0.1–0.3	0.5	< 0.04	–
C_2H_6	0.4	0.6	0.6	1.7	0.14	–
CH_3OH	1.8	2	2.4	2.8-3.9	0.22	–
C_3H_6O (acetone)	–	–	–	–	–	0.3[2]
H_2CO	4	1	1.1	0.24	0.14	–
HCOOH	–	–	0.09	–	–	–
$HCOOCH_3$	–	–	0.08	–	–	–
CH_3CHO	–	–	0.02	–	–	0.5[2]
$(CH_2OH)_2$	–	–	0.25	–	–	–
CH_3OCH_3	–	–	< 0.5	–	–	–
NH_2CHO	–	–	0.015	–	–	–
NH_3	1.5	0.5	0.7	–	< 0.3	–
HCN	0.1	0.1-0.2	0.25	0.1-0.6	0.25	0.9[2]
HNC	–	0.01	0.04	0.0066	< 0.0013	–
HNCO	–	0.07	0.1	–	–	0.3[2]
$HCONH_2$	–	–	–	–	–	1.8[2]
CH_3CN	–	0.01	0.02	0.028	0.03	0.3[2]
CH_3NH_2		–	–	–	–	0.6[2]
CH_3NCO	–	–	–	–	–	1.3[2]
$C_2H_5NH_2$		–	–	–	–	0.3[2]
C_2H_5CHO			–	–	–	0.1[2]
CH_3CONH_2		–	–	–	–	0.7[2]
CH_2OHCHO		–	–	–	0.4[2]	
H_2S	0.4	0.8	1.5	1.15	0.25	–
S_2	–	0.005	–	–	–	–

[3] In coma, at heliocentric distance 2.3 AU (Mall et al., 2016).

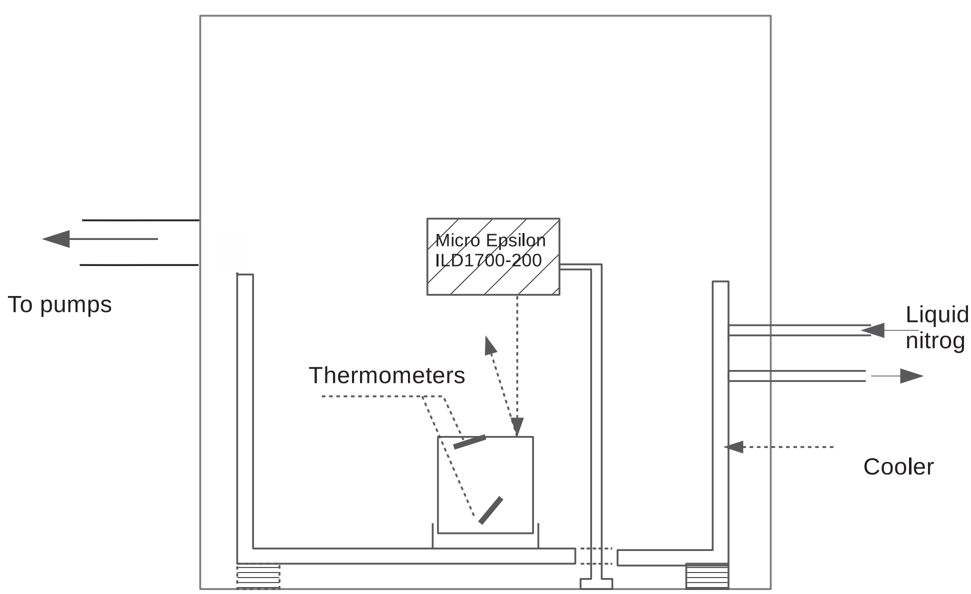

Fig. 1. Sketch of the experimental setup.

For the temperature dependent sublimation coefficient one can use the equation

$$\alpha_s = (1 - \frac{1}{a_1}) + \frac{1}{a_1} \tanh\left[-a_3 \tan\left(\pi \frac{T - a_2}{273 - a_2} - \frac{\pi}{2}\right)\right] \qquad (2)$$

(Kossacki et al., 1999). The values of the numerical coefficients improved by Kossacki and Leliwa-Kopystynski (2014) are: $a_1 = 2.33 \pm 0.08$, $a_2 = 138.72 \pm 0.94$, and $a_3 = 9.30 \pm 2.05$. Gundlach et al. (2011) proposed an alternative formula for $\alpha_s(T)$.

3. Experiments

The experiments presented in this report were performed using the experimental set-up described in Kossacki and Leliwa-Kopystynski (2014). In Fig. 1 a sketch of the experimental setup

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