

Data treatment

The Rosetta Orbiter Spectrometer for Ion and Neutral Analysis/Double Focusing Mass Spectrometer (ROSINA/DFMS) made in situ measurements of the coma of 67P/Churyumov-Gerasimenko. DFMS separated the species based on their mass-to-charge (Mass/Q) ratio. The particles associated with a given Mass/Q were detected by the microchannel plate/Linear Detector Array (MCP/LEDA) consisting of 2 rows (Row A and Row B). Each row consists of 512 pixels aligned in such a way that different Mass/Q fall on different pixels¹⁻⁵.

For each row of each individual mass spectrum (Fig. S1) corresponding to the species of interest in this study, we performed a peak fitting routine to produce time series files containing the counts representative of the abundance of each species. After locating blocks of pixels (may include more than one species, referred to as ‘peaks’) with count rates that exceed a pre-determined threshold related to standard deviation of the mean, we fit the peaks with one or multiple Gaussians. For each block, we used smoothing (averaging) and first, second derivatives to identify localized maxima and changes in slopes, identifying potential overlapping species in an automated fashion. If multiple potential overlapping species were identified, then we sorted the indices from smallest abundance to largest abundance. If a successful fit could not be found and the smallest local maximum (or change in slope) was less than e.g., 0.1 of the next smallest, then it was not considered to be a real species (i.e., noise), and was removed. We then determined how many Gaussians to fit to each species and to the overall peak (large local maxima are fit with 2 Gaussians with common center; see H₂O, CO₂, CO and O₂ in Fig. S1). The integrated count rates for each species were then stored in time series files (Supplementary Data).

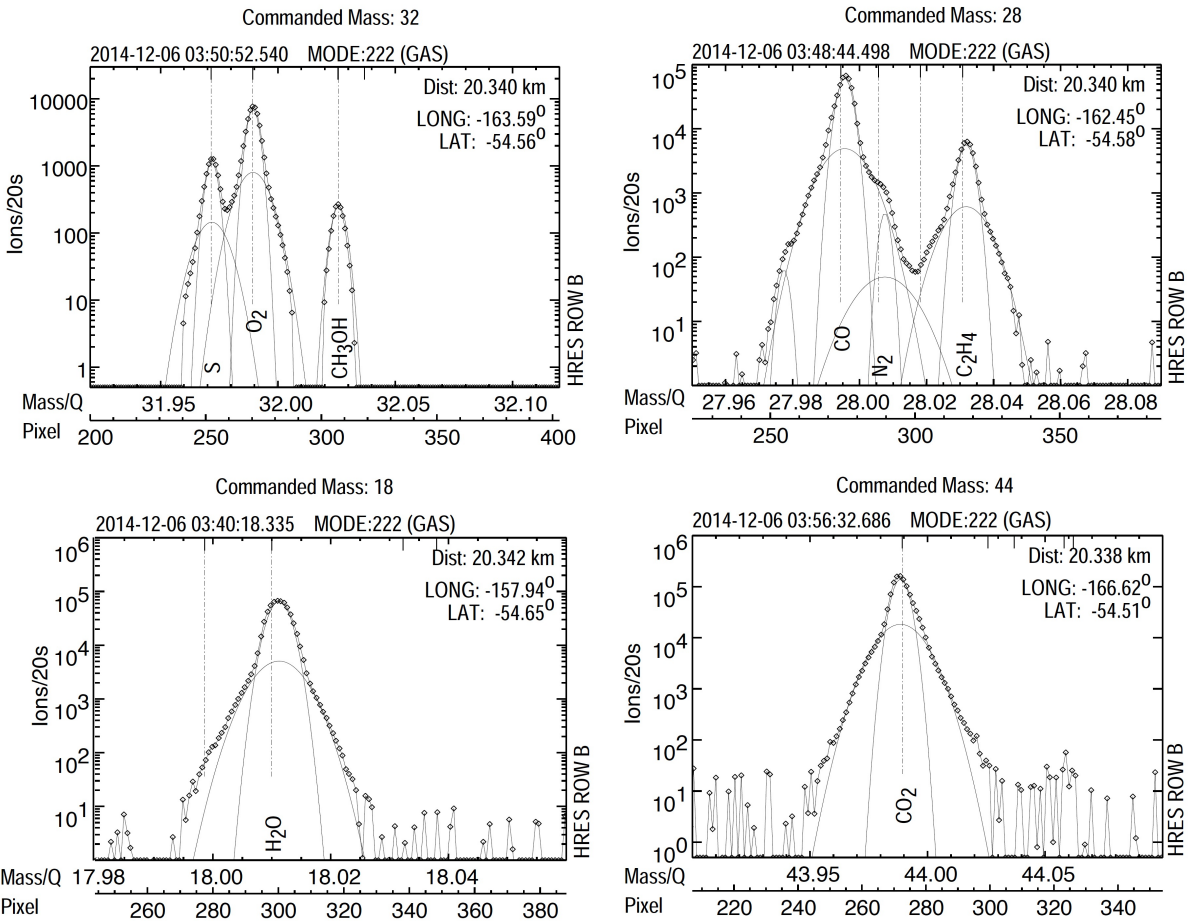


Figure S1. Example high-resolution ROSINA/DFMS spectra with spectral fits. O₂: top left, H₂O: top right, CO: bottom left, and CO₂: bottom right. The diamonds show the number of particles for an integration time of 20 seconds detected by one of the two rows (Row B) of the position-dependent Microchannel Plate/Linear Detector Array (MCP/LEDA). The vertical dash-dot lines indicate the expected position of the marked species on the MCP. The area under the Gaussians (black curves fitted to the diamond symbols) gives the signal associated with the species at a given moment.

Modeling gas trapping in solid H₂O

Table S1. Stabilization energy (eV) of O₂ (triplet state) in typical voids within the ice (4-bilayer model). ‘n’ is the number of missing H₂O molecules in the ice matrix. The density of voids (n) in the bulk is 2 times larger for Porosity 1 than for Porosity 2.

Process	n	Void position	Molecule	E_{stab}	
				Porosity 1	Porosity 2
Adsorption	0	-	O ₂ singlet	-0.83	-
Adsorption	0	-	O ₂ triplet	0.12	-
Inclusion	1	any	O ₂ triplet	-0.06	-
Inclusion (a)	2	2 adjacent bi-layers	O ₂ triplet	0.20	-
Inclusion (b)	2	same bi-layer	O ₂ triplet	0.24	-
Inclusion (c)	4	2 adjacent bi-layers	O ₂ triplet	0.27	0.25
Inclusion (d)	4	2 adjacent bi-layers	O ₂ triplet ×2	0.35	0.32
Inclusion (e)	4	2 adjacent bi-layers	O ₂ dimer (singlet)	0.43	0.40

Table S2. Stabilization energy (eV) of CO and CO₂ in typical voids within the ice (4-bilayer model). ‘n’ is the number of missing H₂O molecules in the ice matrix.

Process	n	Void position	Molecule	E_{stab} Porosity 1
Adsorption	0	-	CO	0.20
Inclusion (a)	2	2 adjacent bi-layers	CO	0.27
Inclusion (c)	4	2 adjacent bi-layers	CO	0.30
Adsorption	0	-	CO ₂	0.22
Inclusion (c)	4	2 adjacent bi-layers	CO ₂	0.43

References

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