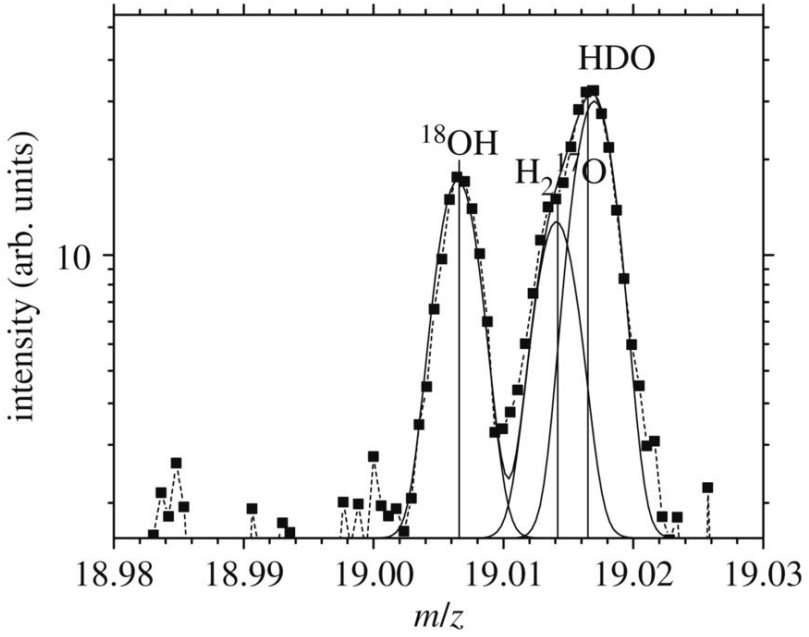
H_2O, HDO and D_2O

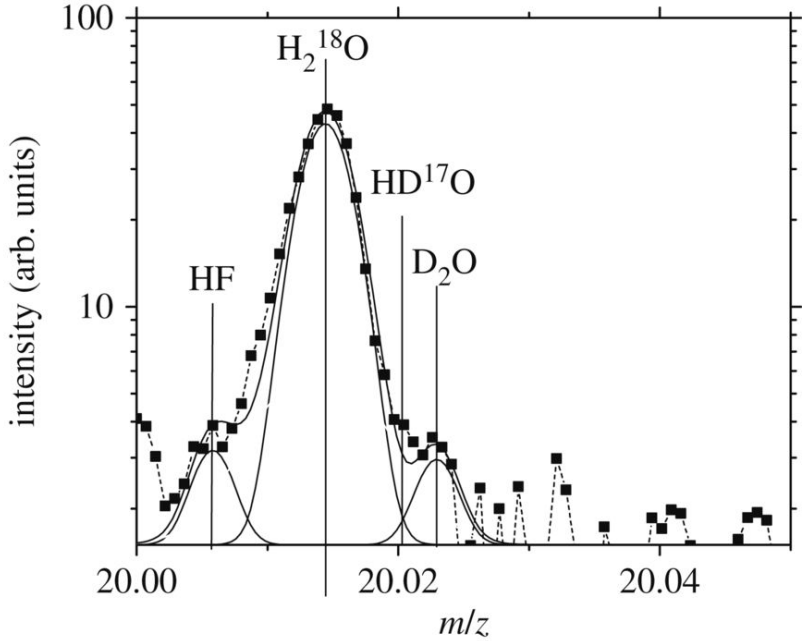
D1 = HDO

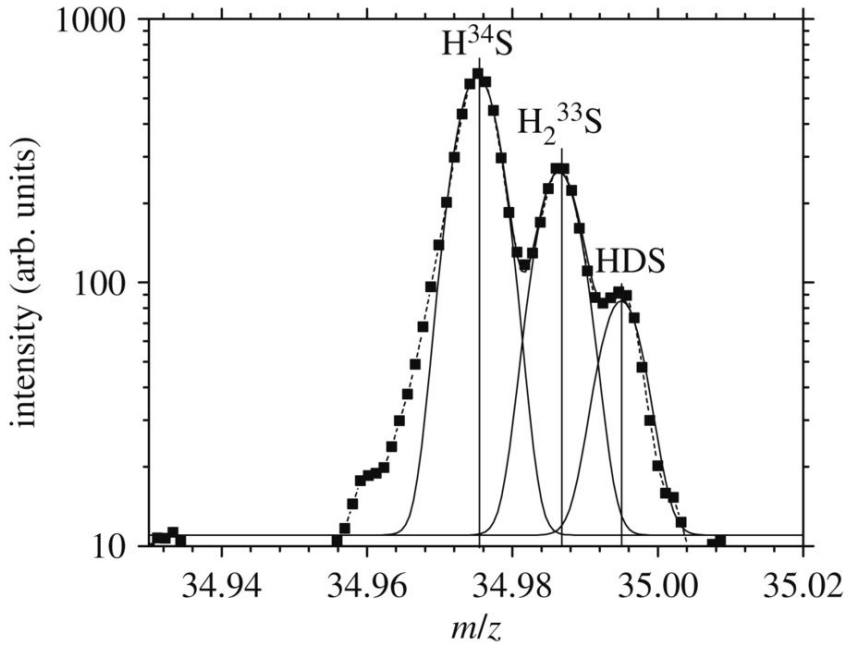
D2=D_2O

f_{D1}=HDO/H_2O

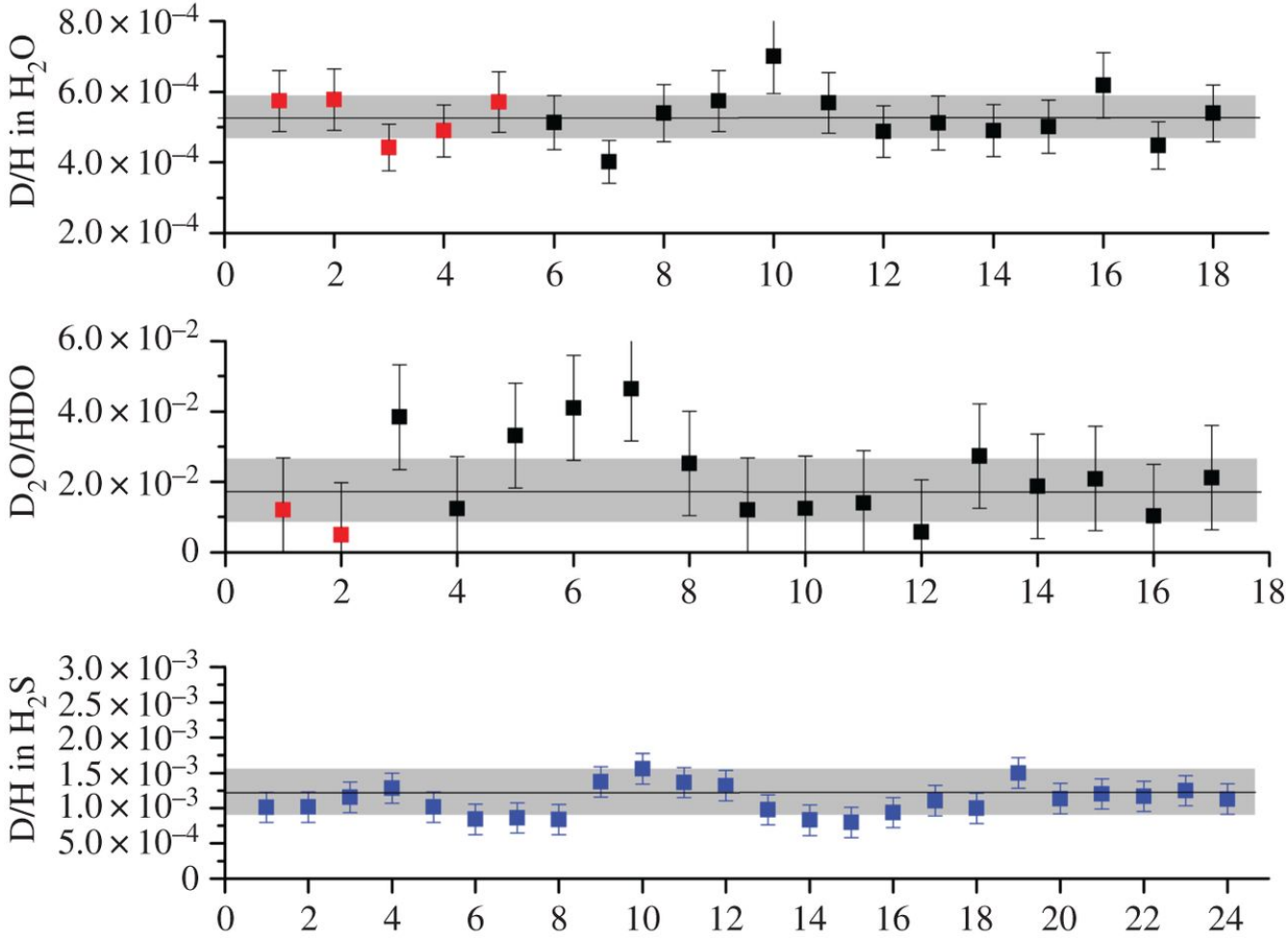
f_{D2}=D_2O/HDO







Altwegg, K., Balsiger, H., Berthelier, J. J., Bieler, A., Calmonte, U., De Keyser, J., ... & Owen, T. (2017). D2O and HDS in the coma of 67P/Churyumov–Gerasimenko. *Phil. Trans. R. Soc. A*, *375*(2097), 20160253.



From top to bottom: D/H in [H2O], [D2O]/[HDO], D/H in [H2S] measured in the coma of 67P during December 2015 (red)/March 2016 (black) and May 2016 (blue), respectively. For time stamp and geometrical information see table 2.

Furuya, K., Van Dishoeck, E. F., & Aikawa, Y. (2016). Reconstructing the history of water ice formation from HDO/H2O and D2O/HDO ratios in protostellar cores. *Astronomy & Astrophysics*, *586*, A127.

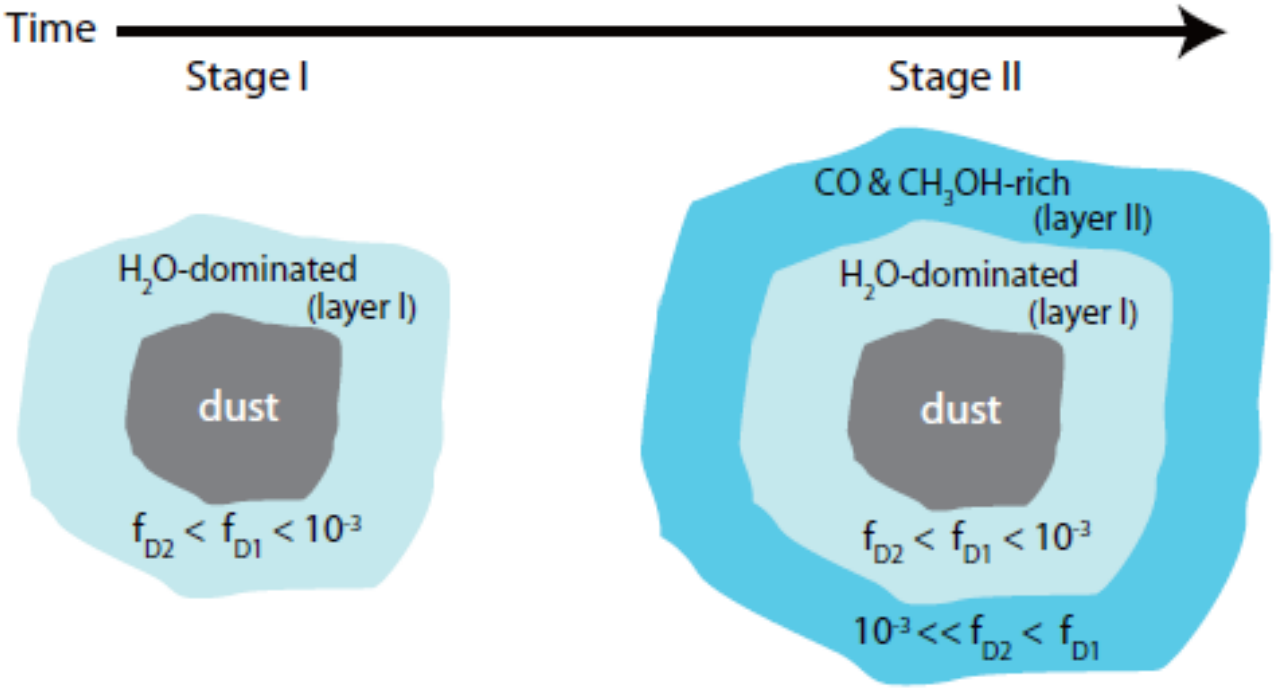


Fig. 1. Schematic view of our scenario and the layered ice structure. Stage I) The main formation stage of H_2O ice. Water deuteration is not efficient, $f_{D2} < f_{D1} < 10^{-3}$. The majority of oxygen is locked in O-bearing molecules in this stage. Stage II) CO/CH_3OH-rich outer ice layers are formed, while the formation of water ice continues with much reduced efficiency compared to Stage I. Nevertheless, the formation of HDO and D_2O ices is more efficient than in Stage I, due to the enhanced deuteration processes, $10^{-3} \ll f_{D2} < f_{D1}$.

H2 rather than CO is the key regulator of deuterium chemistry driven by H_3^+ +HD ⇋ H_2D^++H_2, as long as OPR(H2)/x(CO) > 40 at temperatures of <20 K

Initially, most oxygen is locked up in CO and water ice with bulk ice ratios of HDO/H2O and D2O/HDO of ∼10−4. In the static phase and during the collapse at T < 20 K, the environment is favorable for deuteration:
the low temperature, 10-20 K, and the relatively low OPR(H2), ∼10−3, and the weak UV radiation field

Table 1. Initial Abundances of Selected Species with respect to Hydrogen Nuclei.

Species	MC1	MC2	MC3	AT1	AT2	AT4
o-H_2	2.4(-2)	1.1(-3)	2.4(-4)	4.5(-2)	5.0(-3)	5.0(-5)
p-H_2	4.8(-1)	5.0(-1)	5.0(-1)	4.5(-1)	5.0(-1)	5.0(-1)
HD	1.4(-5)	1.4(-5)	1.1(-5)	1.5(-5)	1.5(-5)	1.5(-5)
H I	5.2(-4)	7.3(-5)	5.1(-5)	-	-	-
D I	7.6(-7)	9.5(-7)	2.3(-6)	-	-	-
H_2O	6.9(-9)	5.2(-9)	9.2(-9)	-	-	-
HDO	1.2(-12)	3.7(-11)	1.3(-9)	-	-	-
D_2O	–	2.9(-13)	8.1(-11)	-	-	-
iH_2O	8.4(-5)	1.1(-4)	1.2(-4)	-	-	-
iHDO	1.1(-8)	1.3(-8)	3.4(-8)	-	-	-
iD_2O	6.9(-13)	7.1(-13)	1.8(-11)	-	-	-
O I	2.2(-5)	1.7(-6)	2.3(-7)	1.8(-4)	1.8(-4)	1.8(-4)
O_2	1.9(-9)	4.0(-10)	3.2(-10)	-	-	-
iO_2	-	-	-	-	-	-
CO	6.1(-5)	3.6(-5)	5.1(-6)	-	-	-
iCO	1.2(-5)	3.1(-5)	4.7(-5)	-	-	-

Notes. $a(-b)$ means $a \times 10^{-b}$. o-H_2 indicates ortho-H_2, while p-H_2 indicates para-H_2. iX indicates species X in the bulk ice mantle. - indicates that abundances are less than 10^{-13}.

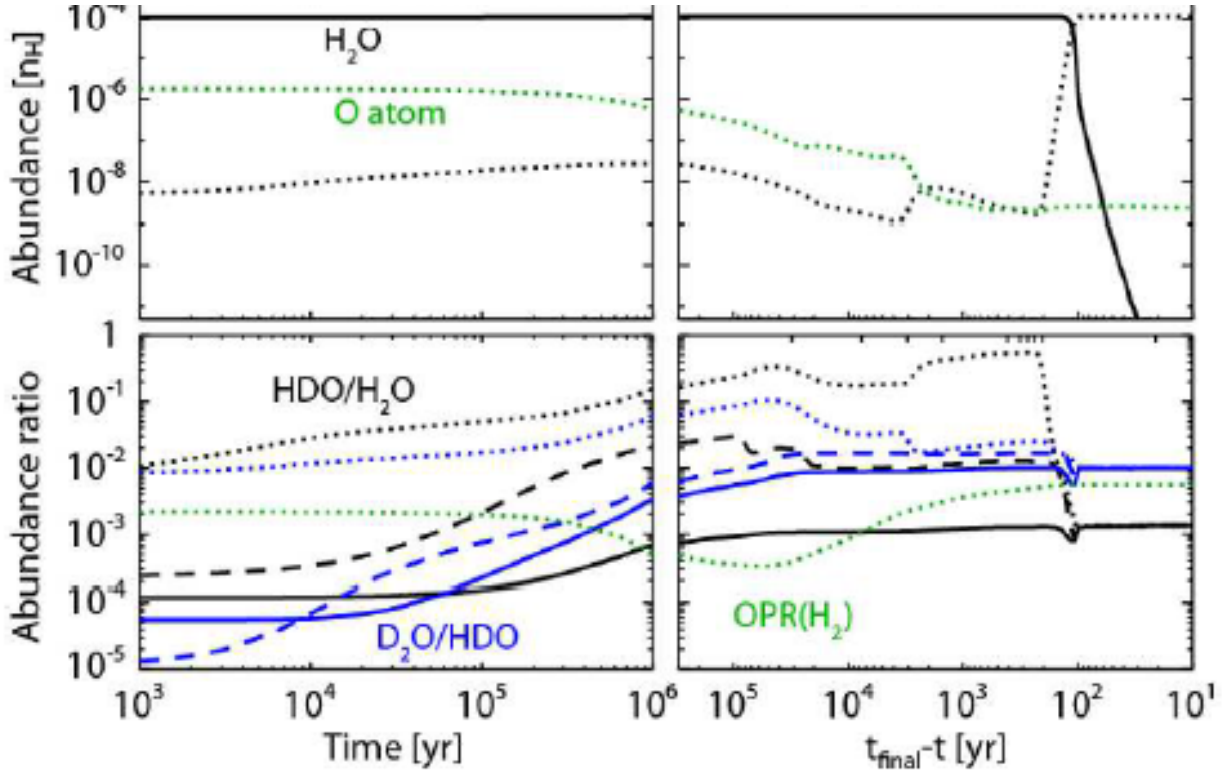


Fig. 3. Temporal variations of molecular abundances (top) and abundance ratios (bottom) in the static phase (left) and during the collapse (right) in model MC2B in the fluid parcel, which reaches $R = 5$ AU at the final time of the simulation. Before the collapse begins, the temperature is 10 K and the number density of hydrogen nuclei (n_H) is 2.3×10^4 cm^{-3}. The horizontal axis of the right panels is set to be $t_{final} - t$, where t_{final} represents the final time of the simulation and $t = 0$ corresponds to the onset of the collapse. The solid lines, the dashed lines, and the dotted lines represent molecules in the bulk ice mantle, molecules in the surface ice layers, and gaseous molecules, respectively.