New insights for O_2 origin in comet 67P

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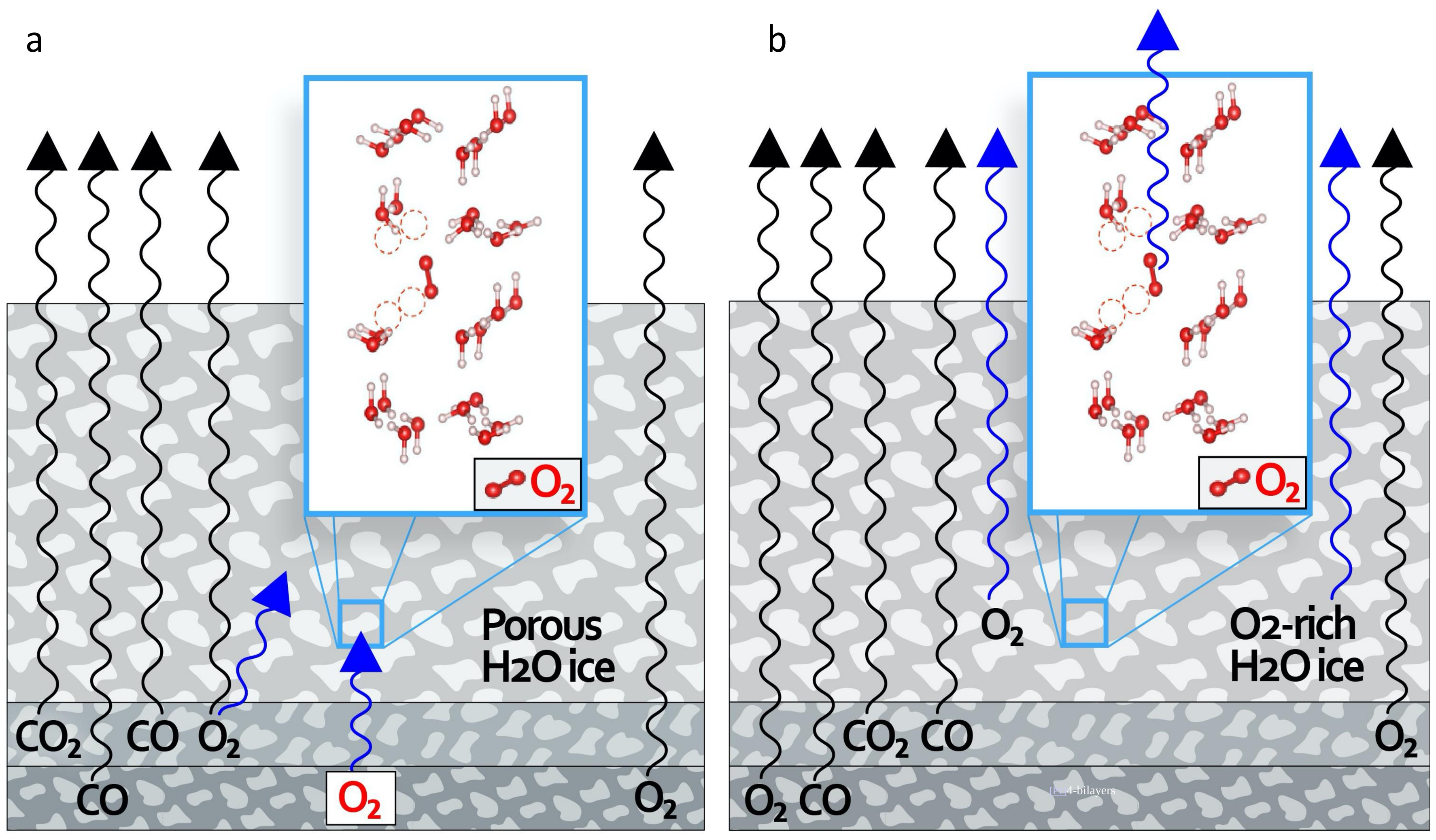
Scenarios for a sensitive determination

One of the biggest surprises of the Rosetta mission was the detection of O_2 in the coma of 67P/Churyumov–Gerasimenko in remarkably high abundances [Bieler, A. et al. , 2015, Nature 526, 678–681]. For the last years the consensus was that the source and release of cometary O_2 were linked to H_2O at all times [Luspay-Kuti, A. et al. , 2018, Space Sci. Rev. 214, 1–24]. A deeper analysis of the ROSINA observations, in particular along time and position of the comet, gave a previously unrecognized change in the correlations of O_2 with H_2O, CO_2 and CO that contradicts this prevailing notion [Altwegg, K. et al. , 2020, MNRAS 498, 5855–5862 ; Luspay-Kuti, A. et al. , 2019, A&A 630, A3].

The findings can be explained only by the presence of two distinct reservoirs of O_2.

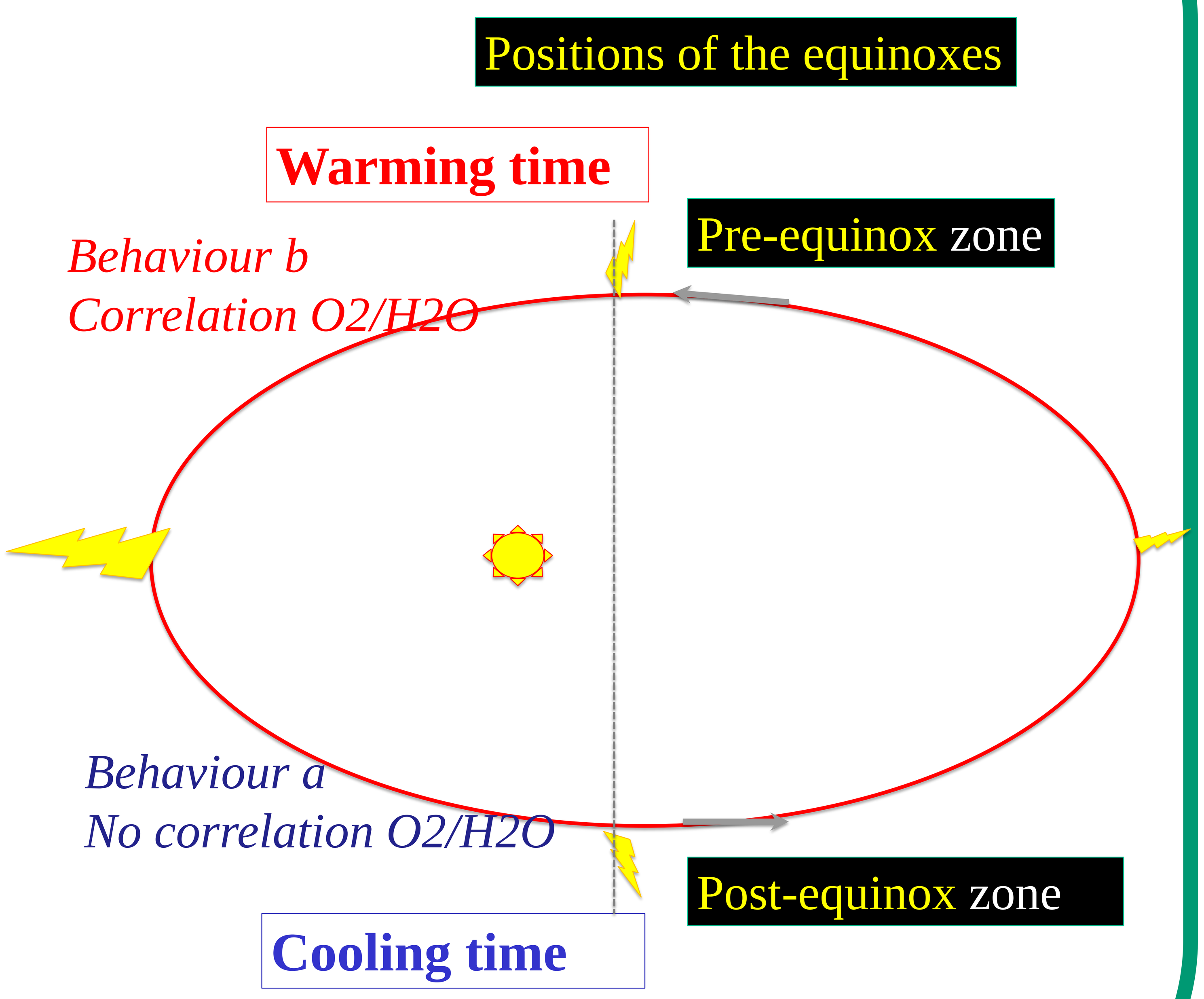
O_2 trapping in and release from the 2 distinct nucleus reservoirs

Luspay-Kuti, A. et al. , 2022, Nature Astronomy, 724–730



(a) Trapping of O_2 in the porous near-surface **H_2O ice beyond 3.3 au.** O_2 is released from a deep, primordial reservoir.

(b) Release of large amounts of accumulated, water-trapped O_2 with H_2O sublimation **closer than 3.3 au** (arbitrary scales).



The insets show possible calculated arrangements of the H_2O ice molecules on a microscopic scale based on a first-principle DFT periodic model (see below). The red dashed circles indicate the locations of missing H_2O where O_2 can be incorporated and stabilized.

Computational evaluations of O_2 trapping in water ices

Process	Void of n H_2O	Void position	Trapped molecule		$E_{stabilization}$ (eV)
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**
Inclusion (d)	4	2 adjacent bi-layers	O_2 triplet × 2		**0.35**
Inclusion (e)	4	2 adjacent bi-layers	O_2 dimer (singlet)		**0.43**

Solid model

Calculations done with the Vienna ab initio simulation package (VASP) (Kresse, G., & Hafner, J. 1993, PhRvB, 48, 13115 ; 1994, PhRvB, 49, 14251), using the hybrid functional (PBE + 50% HF exchange) with Grimme correction (D2) included for dispersion effects (Perdew, J. P. et al. 1996, PhRvL, 77, 3865). Core electrons are frozen and replaced by pseudo-potentials generated by the plane augmented wave method (PAW).

Scenario: Two mechanisms imbricated

a) Since H_2O sublimation beyond ~3.3 au is low, the trapped O_2 may be bound to the H_2O structure and unable to leave until the next onset of H_2O sublimation. **In that case, the O_2 measured in the coma is O_2 released from depth together with CO and CO_2.** This O_2 coming from the deeper nucleus layers may either leave the nucleus or keep accumulating in the near-surface H_2O ice (away from the Sun) as long as there is O_2 release happening at depth and there are enough cavities in the near-surface H_2O ice to trap it.

b) As 67P makes its way back toward the next pre-perihelion equinox, H_2O sublimation gradually turns on and the trapped O_2 is released together with the sublimating H_2O. This release of accumulated O_2 from the secondary, water-trapped reservoir closer to the surface by the sublimation of H_2O ice explains the surprisingly high O_2 relative abundances measured early in the mission. While O_2 at depth continues to be released along with CO_2 and CO, **the accumulated O_2 source in H_2O ice is significantly stronger; hence the strong correlation between O_2 and H_2O up until the H_2O sublimation begins to turns off**.

These new insights imply that O_2 must have been incorporated into the nucleus in a solid and distinct phase during accretion in significantly lower abundances than previously assumed.
Further analysis of O_2 correlations with other minor volatile species may help to finally unravel the origin of O_2 in 67P.