New insights for O₂ 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 O₂ 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 O₂ were linked to H₂O 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 O₂ with H₂O, CO₂ 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 O₂.

O₂ trapping in and release from the 2 distinct nucleus reservoirs

(a) Trapping of O₂ in the porous near-surface H₂O ice beyond 3.3 au. O₂ is released from a deep, primordial reservoir. The insets show possible calculated arrangements of the H₂O 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 H₂O where O₂ can be incorporated and stabilized.

(b) Release of large amounts of accumulated, water-trapped O₂ with H₂O sublimation closer than 3.3 au (arbitrary scales).

Computational evaluations of O₂ trapping in water ices

<table>
<thead>
<tr>
<th>Process</th>
<th>Void of n H₂O</th>
<th>Void position</th>
<th>Trapped molecule</th>
<th>E_stabilization (eV)</th>
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<tr>
<td>Adsorption</td>
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<td>-</td>
<td>O₂ triplet</td>
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<td>O₂ triplet</td>
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</tr>
<tr>
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<td>2 adjacent bi-layers</td>
<td>O₂ triplet</td>
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<tr>
<td>Inclusion (d)</td>
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<td>O₂ triplet 2</td>
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<tr>
<td>Inclusion (e)</td>
<td>4</td>
<td>2 adjacent bi-layers</td>
<td>O₂ dimer (singlet)</td>
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</tbody>
</table>

Solid model

Calculations done with the Vienna ab initio simulation package (VASP) (Kresse, G. & Hafner, J. 1993, PhRvB, 46, 5413; 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 H₂O sublimation beyond ~3.3 au is low, the trapped O₂ may be bound to the H₂O structure and unable to leave until the next onset of H₂O sublimation. In that case, the O₂ measured in the coma is O₂ released from depth together with CO and CO₂. This O₂ coming from the deeper nucleus layers may either leave the nucleus or keep accumulating in the near-surface H₂O ice (away from the Sun) as long as there is O₂ release happening at depth and there are enough cavities in the near-surface H₂O ice to trap it.

b) As 67P makes its way back toward the next pre-perihelion equinox, H₂O sublimation gradually turns on and the trapped O₂ is released together with the sublimating H₂O. This release of accumulated O₂ from the secondary, water-trapped reservoir closer to the surface by the sublimation of H₂O ice explains the surprisingly high O₂ relative abundances measured early in the mission. While O₂ at depth continues to be released along with CO₂ and CO, the accumulated O₂ source in H₂O ice is significantly stronger; hence the strong correlation between O₂ and H₂O up until the H₂O sublimation begins to turn off.

These new insights imply that O₂ 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 O₂ correlations with other minor volatile species may help to finally unravel the origin of O₂ in 67P.