# Super-Oxygenation of Naphthalene: The break-Down Reaction

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Polycyclic aromatic hydrocarbons (PAHs) are interstellar molecules ubiquitous in the Universe that lock up ~15% of the C in space. If this C can be made available, it may play a role in the formation of complex organic molecules (COMs) [1]. While COM formations start with the activation of CO through hydrogenation reactions, the break-down reaction of PAHs may provide an alternative route for COM formations in space [1]. Atomic O has an abundance of ~$10^{-4}$ with respect to atomic H and 35% of O abundance is missing in cold regions of interstellar medium (ISM) with respect to the total O abundance in the ISM [2]. If atomic O binds with PAHs, it might contribute to form COMs and, thus, this might explain the lack of O abundance. PAHs are known to react with atomic H becoming super hydrogenated [3]. However, studies on the reaction of PAHs with atomic O are currently missing.

Here, using density functional theory (DFT), I predicted the formation of possible intermediates of the reaction of atomic O with naphthalene (Fig. 1). DFT calculations predict O attachment sequence equal to the first hydrogenation of naphthalene [4]. The energy barrier for the first O attachment is 0.13 eV, which is lower than the first H attachment in PAHs such as coronene (0.19 eV) and pyrene (0.22 eV) [5,6]. Once atomic O reacts with the first C atom of naphthalene, intersystem crossing (ISC) occurs from the triplet to the singlet spin state. In the singlet state, the O will bridge two adjacent carbon atoms of the naphthalene. The resulting O bridge catalyzes the barrier-less break-down reaction of the C-C bond that the O is bridging, forming a seven-membered heterocyclic ring. A second O radical will bind onto the adjacent carbon atom bound with the first O atom, which barrier-less breaks the CO bond catalyzing the opening of the aromatic ring. The second oxygenation causes the loss of the PAH structure, which is the first step to understand the formation of PAH's daughters that contribute to form COMs in star-forming regions. COMs are important reagents for the formation of building blocks of life [1]. The results of this work might also explain the lack of 35% of O observed in the ISM [2].

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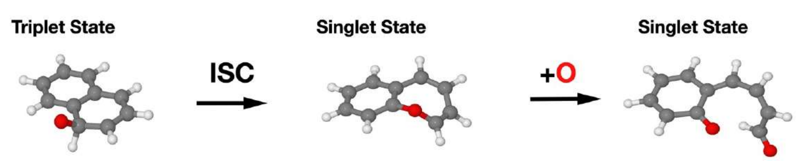


Fig. 1. Super-Oxygenation (in red) of naphthalene leading to opening the aromatic ring.

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