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Modeling the chemical evolution and kinetics of pure H_2O Ices under various types of radiation employing the PROCODA code

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Abstract

Water is one of the most abundant molecules in space, especially in cold environments, where it is the main constituting of astrophysical ices. The space ionizing radiation affects these ices and induces chemical changes, including desorption to gas-phase, which increase the complexity of the interstellar medium. In this work, we employed the PROCODA code to investigate the behavior of several pure water ices under different type of ionizing radiation such as UV, X-rays, electrons and cosmic rays analogues. Here, we employ molecular column densities from laboratory and solved a set of coupled chemical reactions to calculated effective reaction rates (ERCs) and characterize the chemical equilibrium of water ices under high radiation fluences. Briefly, we monitored the evolution of nine species (including the observed ones H_2O, H_2O_2, and O_3, and the predicted ones H, O, H_2, OH, O_2, and HO_2). A discussion on the branching ratio for the considered reactions with the type of ionizing radiation is provided. Among the results, we observed that approximately 63% of the modeled molecules quantified at chemical equilibrium were non-observed species in the X-rays experiment, highlighting the importance of this work in providing insights into the processes that occur on the surface of icy interstellar grains exposed to cosmic radiation, including the formation and destruction of water ice. Accurate modeling of these processes can lead to a better understanding of the chemical evolution of interstellar and circumstellar environments, as well as offer insight into the formation and composition of celestial objects such as comets.

Keywords: Astrochemistry; Astrophysical ices; H_2O; PROCODA; Computational methodology

1. Introduction

Water is one of the most prevalent molecules in space, predominantly in solid form known as astrophysical ice (Gibb et al., 2004;). Water-rich ices are abundant on the surfaces of various outer bodies in the Solar System as well as the interstellar medium, including planets, satellites, planetary rings, and comets. The study of astrophysical ices is crucial in understanding the chemical and physical composition of these celestial bodies, making them significant in the investigation of planetary and solar system formation. Furthermore, they are also crucial in examining extreme environments and chemical processes under unusual conditions (Adriani et al., 2022), thus contributing to the development of astrobiology.

Numerous authors have conducted studies on astrophysical ice analogues in the presence of ionizing agents in laboratory settings, including Gerakines et al. (1996), Moore and Hudson (2000), Loeffler et al. (2006), Pilling et al. (2010), Pilling and Bergantini (2015), Zheng et al. (2006), Kulikov et al. (2019), Mejía et al. (2022). In summary, these studies have demonstrated that energetic particles can induce chemical and physical changes in water ice,

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