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Mapping the evolution of pure CO_2 ices irradiated by ions, UV, and electrons using the upgraded PROCODA code (employing an effective rate constant ordering by thermochemistry data)

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Abstract

Chemical reactions and desorption processes are being triggered by incoming ionizing radiation over astrophysical ices in cold space environments. The quantification of these processes is crucial to achieve a detailed understanding of the underlying chemistry occurring within the ice. With this goal, we have upgraded the PROCODA code (Pilling et al. 2022a) which solves a system of coupled differential equations and describes the evolution of the molecular abundances under processing by radiation, now including an effective rate constant (ERCs) ordering by employing thermochemistry data taken from literature. This methodology helps to identify the most important reactions within the reaction network and therefore decreases the degeneracy of the solutions and enhancing the accuracy of the calculations. Here, we described the chemical evolution of four irradiated pure CO_2 considering 11 different chemical species, 100 reaction routes and 11 radiation-induced desorption processes. The best-fit models provide the effective rate constants, several desorption parameters, as well as, the characterization of the chemical equilibrium (CE) phase. A comparison with previous code version was given and indicates that the ordering of rate constants by thermochemistry data is more important when more energy is deposited in the ice. The current work present more realistic values for the effective rate constants and a better characterization of the CE phase, such data can be used to refine astrochemical models to better describe cold space environments in the presence of incoming ionizing radiation field such molecular clouds and protoplanetary regions and the surface of comets and frozen moons and planets.

Keywords: ISM: molecules; Astrochemistry; Molecular data; Molecular processes; Software: simulations; Solid state: volatile

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1. Introduction

In cold space environments, chemical reactions and desorption processes are being triggered by incoming ionizing radiation impinging astrophysical ices (e.g. Muñoz Caro et al. 2002; Meinert et al. 2016). This radiation-induced processing leads to an increase in chemical complexity in the ices, as well as in their gaseous vicinity (e.g. van Dishoeck 2014; Boogert et al. 2015). Among the chemical inventory in the interstellar medium, carbon dioxide (CO_2), an apolar molecule with linear geometry, is ubiquitously found in the interstellar medium (e.g., de Graauw et al. 1996, Gerakines et al. 1999, Pontoppidan et al. 2008, Poteet et al. 2013, Ehrenfreund & Charnley 2000; Fraser et al. 2002, Öberg et al. 2011) and on icy moons of the solar system (Buratti et al. 2005, Cartwright et al. 2015). The irradiation of pure CO_2 ice by UV radiation has shown that other molecules, such as CO, O_3, and CO_3, can be formed in the ice (Gerakines et al. 1996). Addi-

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