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Adsorption of glycine on cometary dust grains: II—Effect of amorphous water ice

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ABSTRACT

In recent years glycine, the simplest amino acid, has become a topic of great importance in astrobiology owing to its unambiguous detection in comet 81P/Wild 2 dust by Stardust mission. A possible end state for glycine in comets is by forming a molecular bond with some species of cometary dust. Many questions remain about how glycine survives the extreme conditions prevailing in the interstellar medium (ISM). The detailed chemical interactions occurring on the dust grain surfaces with organic molecules are of great interest, as they shed light on possible routes of life to Earth from extraterrestrial space. In a previous work we simulated the interaction between glycine molecules and a forsterite surface and found that the interaction occurs through a chemisorption process. In this paper, we try to describe a more realistic situation, by adding an ice component to the mixture. We propose two models for that interaction. In the first model, neutral glycine is adsorbed on a mineral surface covered by a thin layer of amorphous ice, while in the second model neutral glycine and ice are adsorbed simultaneously onto the mineral surface. We find that this second model is the most likely scenario, although the particular adsorption process depends on the kind of surface. For a dipolar surface the adsorption proceeds through an associative process. In the case of a non-dipolar surface the adsorption process is both associative and dissociative and the chemisorption process is stronger. For the stable systems, we calculated the infrared frequencies to characterize the most reactive sites in the chemisorption processes. We observed important shifts frequencies that have relationship with the position of the main vibrational modes of the C=O and COO⁻ moieties, which react chemically with the mineral surface.

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1. Introduction

Comets are the most primitive bodies of the Solar System. It is generally believed that comets played a major role in bringing

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organic matter to the early Earth, enabling the prebiotic synthesis of the biochemical compounds. The dust particles in comets are composed of a heterogeneous mixture of amorphous and crystalline silicates, organic material, and other minor constituents such as iron sulfides and oxides. These dust grains are embedded in a matrix of various ices, such as H₂O, CO, CO₂, NH₃, and CH₄. The grains are released from the ice matrix when sublimate. At large heliocentric distances, species such as CO and CO₂ drive the cometary activity, while at short heliocentric distances, H₂O sublimation is dominant (Bockelee-Morvan et al., 2004; Hanner and Bradley, 2004). Recently, it has been discovered the presence of glycine and cometary amines in the comet 81P/Wild 2 dust embedded in the aerogel panel returned by the Stardust mission (Elsila et al., 2009; Glavin et al., 2008). The glycine returned by Stardust has an extraterrestrial carbon isotope signature, indicating that was formed in space. Additionally, these results indicated the presence of both free and bonded glycine in the comet. Elsila et al. (2009) proposed that in the bonded form, the amine group (–NH₂) of glycine may have been covalently bonded to some species. This discovery has raised several questions about how glycine can be present under the physical conditions of the interstellar medium (low temperature, irradiation and cosmic rays) and what are the chemical interactions with the mixture of the amorphous water ice that takes place on grain surface.

This discovery has great significance in the theories of the origin of life on Earth, because the amino acids contained in grains of cosmic dust might be deposited on the surface of young planets following comet and asteroid impacts, making viable the extra-terrestrial hypothesis of the origin of life.

On Earth, glycine has been found in the carbonaceous chondrites of several meteorites, such as Murchison and Tagish Lake (Cronin and Pizzarello, 1997; Herd et al., 2011). However glycine has not yet been detected spectroscopically in comets from the ground or with space-borne instrumentation. In comets Hale-Bopp and Hyakutake only upper limits of ~0.3% glycine by mass in cometary amorphous ice, or 0.05% glycine by mass in cometary material, with a dust to amorphous ice ratio of 5, have been established (Crovisier et al., 2004). The lack of cometary glycine detection is due probably to insufficiently sensitive spectroscopic detection methods (Cronin and Pizzarello, 1997; Ehrenfreund et al., 2001).

On the other hand, the presence of minerals in space may be of great importance in prebiotic synthesis. Within the minerals that constitute the dust grains, olivine is the most abundant, and has been detected spectroscopically showing up as prominent emission bands in the mid-infrared (Campins and Ryan, 1989). Olivine consists of magnesium, iron and silicate that form a complete solid solution between two endmembers: forsterite (Mg-rich olivine) and fayalite (Fe-rich olivine). On Earth, olivine is common in mafic and ultramafic rocks, and is one of the main components of the Earth's mantle. Forsterite has an orthorhombic structure in the *Pbnm* space group with the crystallographic parameters of $a=4.756$, $b=10.207$, $c=5.980$ Å with $\gamma=\beta=\alpha=90^\circ$ (Smyth and Hazen, 1973), and consists of independent SiO₄ tetrahedra linked by divalent cations with octahedral coordination (Fig. 1). Forsterite, has been investigated experimentally and theoretically (de Leeuw et al., 2000; Price et al., 1987b; Smyth and Hazen, 1973; Stimpfl et al., 2006). There is evidence that the (100) surface is more reactive for water adsorption (Muralidharan et al., 2008; Stimpfl et al., 2006). Preliminary theoretical studies for water adsorbed on forsterite surfaces showed that steps, terrace, and corners are produced on the surfaces with low coordination of Mg atoms. These sites are associated with high reactivity (King et al., 2010).

The detailed chemical interactions on the surface of the minerals with organic molecules in comets and other extraterrestrial bodies are of great importance to the understanding of the

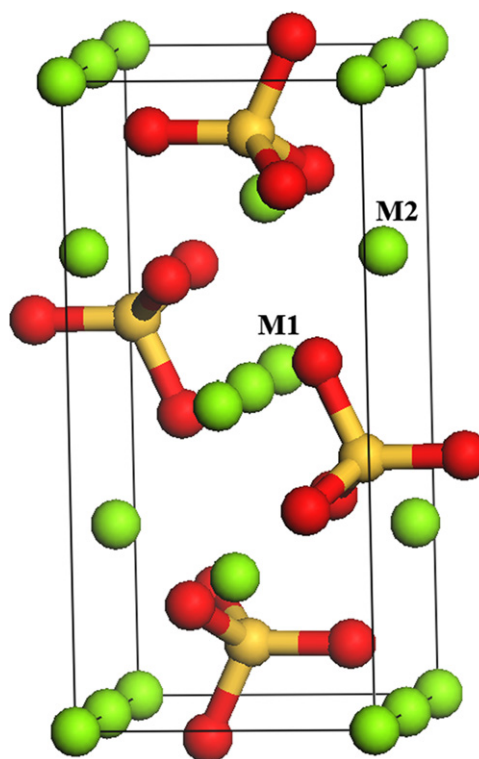


Fig. 1. Bulk model of the Forsterite, with M2 and M1 sites. O, Si and Mg atoms are displayed as red, yellow and green spheres, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

origin of life on Earth. It is probably that the mineral surface can catalyze the organic molecules for their subsequent polymerization in the prebiotic synthesis (Bernal, 1949). It is therefore very important to study the grain-surface chemistry processes by ISM molecules. The chemical reaction in gas-phase of several organic molecules to produce glycine in the ISM has been studied from the theoretical side (Barrientos et al., 2012; Lattelais et al., 2011; Woon, 2001a, 2001b). However, the studies of chemical reactions on the dust grain surfaces are scarce.

In a previous work (Escamilla-Roa and Moreno, 2012), we simulated the interaction between glycine molecules and a forsterite surface and found that the interaction occurs through a chemisorption process. In this work, we improve the previous model by considering the addition of amorphous water ice as a fundamental component in the mixture, in order to mimic the real environment more closely. We perform the electronic structure calculations by means of the Density Functional Theory (DFT) to describe and detail several interactions of glycine and ice in cometary dust. The main aim of this paper is to perform a detailed study of the effect the amorphous water ice has in the adsorption processes of glycine.

2. Descriptions of the models

In our previous work (Escamilla-Roa and Moreno, 2012), we found that glycine in gas phase was chemisorbed in dry environments onto dipolar and non-dipolar (100) surfaces of forsterite, under conditions similar to those prevailing in the ISM. In this work we propose to study a more realistic scenario of a ternary system consisting of one neutral glycine molecule, amorphous water ice, and two forsterite (100) surfaces.

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