EPSC Abstracts
Vol. 14, EPSC2020-318, 2020
https://doi.org/10.5194/epsc2020-318
Europlanet Science Congress 2020

Monitoring the Reactivity of Formamide on Amorphous SiO2 by In-Situ UV-Raman Spectroscopy and DFT Modeling

Stefano Pantaleone[1,2], Matteo Signorile[1], Nadia Balucani[2], Francesca Bonino[1], Gianmario Martra[1], and Piero Ugliengo[1]

[1]Dipartimento di Chimica and Nanostructured Interfaces and Surfaces (NIS) Centre, Università degli Studi di Torino, via P. Giuria 7, IT-10125 Torino, Italy (stefano.pantaleone@unito.it)

[2]Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, I-06123 Perugia, Italy

Formamide has been recognized in the literature as a key species in the formation of the complex molecules of life, such as nucleobases. Furthermore, several studies reported the impact of mineral phases as catalysts for its decomposition/polymerization processes, increasing the conversion and also favoring the formation of specific products. Despite the progresses in the field, in situ studies on these mineral-catalyzed processes are missing. In situ UV-Raman characterization of the chemical evolution of formamide over amorphous SiO_2 samples, selected as a prototype of silicate minerals, was performed. The experiments were carried out after reaction of formamide at 160 °C on amorphous SiO_2 (Aerosil OX50) either pristine or pre-calcined at 450 °C, to remove a large fraction of surface silanol groups. Our measurements, interpreted on the basis of density functional B3LYP-D3 calculations (Figure 1), allow to assign the spectra bands in terms of specific complex organic molecules, namely, diaminomaleonitrile (DAMN), 5-aminoimidazole (AI), and purine, showing the role of the mineral surface on the formation of relevant prebiotic molecules.