EFFECT OF SILICATE-SURFACES IN AEROSOL PARTICLES ON THE OXIDATION OF ATMOSPHERIC FORMIC ACID. A QUANTUM CHEMISTRY INVESTIGATION

C. IGNACIO SAINZ-DIAZ[1]*, CRISTINA IUGA[2], ANNIK VVIER-BUNGE[3]

[1]*instituto Andaluz De Ciencias De La Tierra (CSIC-UGR), Av. Fuentenueva s/n, Granada, 18002, Spain*
[2]*Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, Mexico, 18002, Mexico*
[3]*Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, Mexico, 18002, Mexico*
csorico@yahoo.com.mx

Heterogeneous reactions of atmospheric volatile organic compounds (VOCs) on aerosol particles may play an important role in atmospheric chemistry. Silicate particles are present in air-borne mineral dust in atmospheric aerosols, and radical reactions can be different with the presence of these mineral particles. The formic acid (HCOOH) is the most abundant carboxylic acid in the troposphere. Atmospheric HCOOH influences pH dependent chemical reactions in clouds and is a major acidic component of rain. Humans are exposed to formic acid in ambient air and food, as well as via inhalation and dermal contact. In the presence of atmospheric aerosols, the reactivity of adsorbed formic acid with OH free radicals is expected to be different than the one in the gas phase. The adsorption of formic acid molecule on models of silicate surface is studied with quantummechanical methods. The effects of this adsorption on the spectroscopic properties of this system are also analysed reproducing the experimental results and predicting new insights for future research. The reaction of hydroxyl free radical with formic acid adsorbed on silicate surface was studied. The mechanism and kinetics have been determined focusing on the oxidation pathway. The presence of mineral surface catalyses the reaction decreasing the activation free energy and silicates act as a sink of these organic pollutants.

Keywords: airborne mineral dust, formic acid, modelling