ID de Contribution: **149** Type: **Contribution orale**

Theoretical study of primary ozonolysis in oleic acid aerosol phase

vendredi 7 juillet 2023 10:00 (15 minutes)

In the Earth atmosphere, the chemical and structural processing of each reaction steps influence the overall outcome of the products and understanding of each step requires vigorous investigation molecular level. Therefore, in this study, the formation of the primary ozonide generated by the attack of the ⍰ bond of oleic acid is studied in gas and aerosol phases using ab initio, density functional and classical modelling approaches. The presence of water is also considered. Reaction rates are obtained using variational transition state theory including tunnelling effect. For surface processes, both Eley-Rideal and Langmuir-Hinshelwood mechanisms are considered. The results are compared to available experimental obtained in both laboratory and field conditions.

Affiliation de l'auteur principal

Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille, F-59000 Lille, France

Auteur principal: DUFLOT, Denis (Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille, F-59000 Lille, France)

Co-auteurs: M. RAJAMANI, Akilan (Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille, F-59000 Lille, France); Mme ABOUHAIDAR, Rawan (Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille, F-59000 Lille, France); M. ROOSE, Antoine (Paul Scherrer Institute, Switzerlandd); Mme TOUBIN, Céline (Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille)

Orateur: DUFLOT, Denis (Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM) —UMR 8523 —Univ. Lille, F-59000 Lille, France)

Classification de Session: Mini-colloques: MC13 Effets d'environnement et de solvatation sur les processus moléculaires

Classification de thématique: MC13 Effets d'environnement et de solvatation sur les processus moléculaires