

Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Mercredi 30 Mars à 10:30

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Rôle du solvant aqueux dans la réactivité des polyphénols vis à vis du radical superoxide

Superoxide radical anion has a great importance in biochemical processes and atmospheric chemistry. For a long time, literature has focused on the deleterious character of reactive species derived from oxygen (ROS) since oxidative damage contributes to the pathology of a lot of human diseases such as cancer and atherosclerosis. But, nowadays, it is admitted that the field is far more complex than that.

The balance between the formation of ROS and the antioxidant defense is essential in maintaining good health. This balance is assured by several mechanisms that produce antioxidants in situ (endogenous antioxidants) or by exogenous antioxidants supplied through foods (essentially polyphenols).

The reactivity of polyphenols with superoxide radical can be studied by ab-initio dynamics using CPMD software. Calculations show that it depends largely on the environment of the hydroxyl group giving its hydrogen atom, the geometry of the first water layer and the presence of a certain number of water molecules in the second layer, indicating a great influence of the solvent on the reactivity.