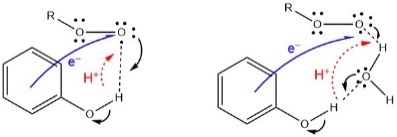
**WATER-MEDIATED REACTION OF PHENOL ANTIOXIDANT WITH PEROXYL RADICALS**

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**Abstract**

****The reaction of phenols with alkylperoxyl radicals is of fundamental importance in oxidation processes and is difficult to investigate in water. The trapping of peroxyl radicals was found to follow different mechanism, depending on the pH. At large pH, SPLET-like mechanism is favoured which consists of acidic dissociation of phenols prior to their reaction with ROO• radicals. At low pH, direct H-atom transfer can take place, in which water seems to be involved as proton relay in the rate-determining steps [1].

This theoretical work is a first approach to answer the question whether a water-mediated mechanism is taking place. The phenol molecule is presented to react with MeOO• in water. Density functional calculations are performed with a network of water using 1, 2, and 3 explicit water molecules between the phenol OH group and the radical. From the transition state of the H-transfer, conclusions on the reaction barrier and the kinetics will be drawn.

**References.**

[1] R. Amorati, A. Baschieri, G. Morroni, R. Gambino, L. Valgimigli, Chem. Eur. J. 2016, 22, 7924-7923.