

### **Detailed work plan of the STSM**

#### **Spectroscopic characterization of the HOC(O)O radical for its identification in Earth's atmosphere**

15.4-23.4 : The best approaches for determining accurate spectroscopic parameters that can guide future detection and experimental characterization of the atmospherically relevant HOC(O)O radical will be discussed.

In particular, we will consider state-of-the-art coupled-cluster approaches that include corrections for basis set incompleteness and account for core correlation effects.

For the ground state and lowest-lying excited state, vibrationally corrected rotational constants that include quartic and sextic centrifugal distortion terms will be calculated.

The IR spectrum of the ground state will be simulated with an approach based on second order vibrational perturbation theory that includes anharmonic effects in both energies and intensities. The results of this research may be helpful for the detection of this radical by means of high-resolution spectroscopic techniques in the IR, microwave and millimeter-wave domains.