Contribution ID: 45

# Analysis of the structure massoia lactone through light-matter interaction

We propose to investigate the same compound, massoia lactone (MAL), using two spectroscopic techniques, Fourier transform infrared (FTIR) spectroscopy and Fourier transform microwave (FTMW) spectroscopy to analyze and compare their spectral features. Massoia lactone (MAL) is the intermediary product between 6-amyl- $\alpha$ -pyrone and delta-decalactone, both molecules important in several fields of industry. Although both 6-amyl-alpha-pyrone and delta-decalactone have been widely studied with different spectroscopic techniques, there is almost no study about MAL. Our goal is to explore the structural landscape and to identify the intramolecular interactions of MAL, to better understand its physical and chemical properties by using two powerful spectroscopic techniques. In FTIR spectra, the observation of certain bands can be associated with the presence of specific functional groups in the molecule arising from their vibrations. The FTMW spectra are denser with hundreds of lines arising from transitions between two rotational levels and corresponding to many conformers present at the same time. The rotational constants extracted from the analysis of the FTMW spectra are directly related to the arrangement of the atoms in the molecule. Thus, rotational spectroscopy allows identifying several conformers and determining very precisely their molecular structures. MAL features several functional groups and a great conformational flexibility, which make it interesting to study using both FTIR and FTMW spectroscopy. We aim that the student will get a hands-on experience on quantum-chemical calculations, on instrumentation using two instruments, with the rotational spectrometer being home-built, and to analyze the spectra from two spectroscopic techniques that provide complementary information to each other.

# Field

A2: Molecular sciences (application oriented)

## **DESY Place**

Hamburg

# **DESY Division**

FS

## **DESY Group**

SMP

## **Special Qualifications:**

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