HIGH-RESOLUTION FAR INFRARED SPECTROSCOPY AND ANALYSES OF TRIOXANE

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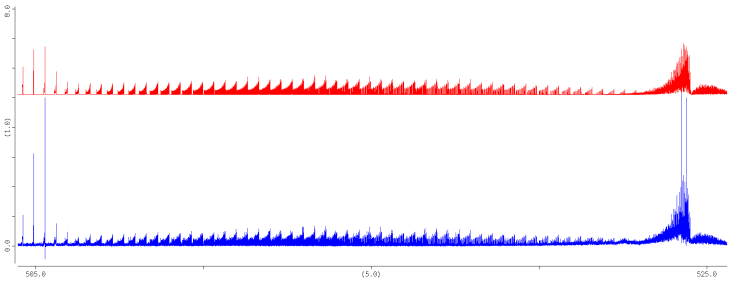
Trioxane, $(H_2CO)_3$, is a symmetric top that belongs to the C_{3v} symmetry group. The molecule owns 20 fundamental modes that are dispatched as 7 symmetric vibrations of type A1, 3 vibrations of type A2 and 10 doubly degenerate vibrations of type E.



Infrared spectra of trioxane have been recorded in the 50–650 cm^{-1} range using a high resolution Bruker IFS 125 interferometer located at the AILES beamline of the SOLEIL synchrotron facility. Owing to its higher brilliance in the far-infrared region, the SOLEIL synchrotron radiation was used to improve the signal-to-noise ratio of the spectrum at the maximal resolution of 0.001 cm^{-1}.

We present here a detailed analysis and modeling of intense OCO deformation ν_7 and ν_{19} modes as well as weaker CH_2 torsion ν_{20} mode and its first overtone $2\nu_{20}$. Thanks to the formalism and programs developed in Dijon, we could determine accurately the effective Hamiltonian parameters for these 3 modes.