HIGH RESOLUTION THZ AND FIR SPECTROSCOPY OF $SOCl_2$

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Thionyl chloride ($SOCl_2$) is an extremely powerful oxidant widely used in industrial processes and playing a role in the chemistry of the atmosphere[a]. In addition, it has a molecular configuration similar to that of phosgene ($COCl_2$), and is therefore of particular interest for security and defense applications. Low resolution vibrational spectra of gas phase $SOCl_2$[b] as well as high resolution pure rotational transitions up to 25 GHz[c] have previously been investigated. To date no high resolution data are reported at frequencies higher than 25 GHz.

We have investigated the THz absorption spectrum of $SOCl_2$ in the spectral region 70–650 GHz using a frequency multiplier chain coupled to a 1 m long single path cell containing a pressure of about 15 μbar. At the time of the writing, about 8000 pure rotational transitions of $SO^{35}Cl_2$ with highest J and K_a values of 110 and 50 respectively have been assigned on the spectrum.
We have also recorded the high resolution FIR spectra of $SOCl_2$ in the spectral range 50–700 cm^{-1} using synchrotron radiation at the AILES beamline of SOLEIL facility. A White-type cell aligned with an absorption path length of 150 m has been used to record, at a resolution of 0.001 cm^{-1}, two spectra at pressures of 5 and 56 μbar of $SOCl_2$. On these spectra all FIR modes of $SOCl_2$ are observed (ν_2 to ν_6) and present a resolved rotational structure. Their analysis is in progress.

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[c] H. S. P. Müller and M. C. L. Gerry, *J. Chem. Soc. Faraday Trans.* 90, 3473 (1994)