NITROSYL IODIDE, INO: MILLIMETER-WAVE SPECTROSCOPY GUIDED BY *AB INITIO* QUANTUM CHEMICAL COMPUTATION

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In the series of the nitrosyl halides, XNO (where X = F, Cl, Br, I), the millimeter-wave spectrum of INO remains so far unknown. We report our investigation on the first high-resolution rotational spectroscopy of nitrosyl iodide, INO.

One of the motivation for this work comes from the growing need in developing a more complete understanding of atmospheric chemistry, especially halogen and nitrogen oxides chemistry that adversely impacts ozone levels. In the family of the nitrogen oxyhalides such as nitrosyl (XNO), nitryl (XNO), nitrite (XONO), and nitrate (XON0$_2$) halides, those with X = F, Cl, Br have been well studied, both theoretically and experimentally. However, relatively little is known about the iodine-containing analogues, although they also are of potential importance in tropospheric chemistry. In 1991, the Fourier-transform IR spectroscopic detection of INO, INO_2 and $IONO_2$ in the gas phase has been reported[a].

The INO molecule was generated by *in situ* mixing continuously I_2 and NO in a 50-cm long reaction glass tube whose outlet was connected to the absorption cell using a teflon tube. At the time of writing this abstract, 68 μ_a-type transitions ($K_a = 0 - 10$), all weak, have been successfully assigned. The hyperfine structures due to both I and N nuclei will also be presented.

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[a]I. Barnes, K. H. Becker and J. Starcke, J. Phys. Chem. 1991, 95, 9736-9740.