Accurate absorption intensities of ozone in a wide IR spectral range from experimental measurements and \textit{ab initio} calculations

1 Introduction

Ozone ($\text{O}_3$) plays an important role for protecting life on Earth and in the climate formation. On the other hand, it acts as a harmful pollutant in the troposphere that must be controlled. Accurate spectroscopic data are mandatory for the global remote sensing of ozone using satellite and ground based observations. For a reliable determination of the real-time ozone variation in the atmosphere it is crucial to have precise and reliable laboratory data in a wide spectral range to make it possible observations with independent instruments.

We summarize recent results of our groups aimed at providing consistent data both for far- and mid-infrared vibration-rotation bands and for vibronic bands near 1 micron.

2 Absorption cross-sections in the near IR range of Wulf bands measured using the cw-CRDS laser spectrometer

![Graph showing absorption cross-section vs. wavenumber](https://example.com/figure1.png)

Fig.1. Example of the absorption cross-section, cm$^2$/molecule • 10$^{-23}$.
The cw-CRDS spectra recorded for the first time in the range above 10000 cm\(^{-1}\) with several partial pressures at medium and high resolutions (spectral steps of 0.1 cm\(^{-1}\) and 0.003 cm\(^{-1}\), respectively) showed a sequence of the narrow lines and broadened features due to the short lifetimes of the upper rovibronic states. A sample of the recorded spectrum is given in Fig 1. This spectral interval which falls in the water vapor transparency window can be used for the atmospheric remote sensing. A further step of the project is to determine the predissociative lines and broadened features due to the short lifetime and by factor 2.1 for atmospheric ground fluctuations of the retrievals have permitted to reduce the window consistency of ozone retrieval from 630 to 4900 cm\(^{-1}\) has been significantly improved among 37 spectral windows.

4 Consistency of the band intensity data in various spectral windows from MW to far-IR and mid-IR ranges

Another issue that remained unsolved for many decades is the consistency of the ozone atmospheric retrievals using various spectral intervals. When the laboratory databases were used in the past, the discrepancy could amount up to 15% depending on a selected IR interval [10]. The intensity calibration of about thirty bands using our \textit{ab initio} calculations [11] has permitted to make the spectral line list much more homogeneous. Moreover, the independent experimental validation (by G.Toon [10]) of these results (included in the last version of the S&MPO databank, https://smpo.tsu.ru) has shown that the consistency of the ozone retrieval from 630 to 4900 cm\(^{-1}\) has been significantly improved among 37 spectral windows.

A comparison of these independent data has permitted obtaining a sub-percent accuracy for the strongest fundamental and overtone bands (as illustrated in Fig. 2) that was confirmed by comparisons with other accurate experiments [8-9].