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## Ozone spectroscopy in the electronic ground state: High-resolution spectra analyses and update of line parameters since 2003



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### ABSTRACT

The state of the art analyses of high-resolution ozone spectra and a critical discussion of line parameters updated since the previous review by Rinsland et al. [J Quant Spectrosc Radiat Transfer 2003;82:207–18] are presented. We focus on recent works revisiting improved measurements and analyses of Fourier transform spectra below 5600 cm<sup>-1</sup> and review Cavity Ring-Down Spectroscopy measurements and analyses in the 5850–7920 cm<sup>-1</sup> spectral region which have been performed for <sup>16</sup>O<sub>3</sub> and all <sup>18</sup>O enriched ozone isotopologues. Various issues related to resonance perturbations due to dark states are discussed as well as the issues concerning the accuracy of the experimental parameters, the data modelling and the data reduction. Comparisons of vibration levels determined from spectra analyses with predictions for calculated line lists are described and the "intricate" question of absolute intensity determination is overviewed. Also, a review of deficiencies, challenge for improvements, and related works in progress are reported.

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## 1. Introduction

Spectroscopic parameters of ozone are important for the characterization of molecular properties related to the ozone dynamics as well as for various applications. As strongest absorber in the UV spectral range, ozone protects the Earth (human and plants) from harmful radiation. Ozone also acts as a pollutant in the troposphere. Moreover, ozone is an important reactant in the climate system. Therefore, global and regional monitoring of the evolution of the ozone layer and of tropospheric ozone is essential, for which spectroscopic methods are indispensable. This

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explains the large number of studies over the past several decades with complete lists of references given in the information system "Spectroscopy and Molecular Properties of Ozone" S&MPO [1]. In order to monitor ozone in the atmosphere from spectral analyses, a precise knowledge of line parameters is required. For remote retrieval of ozone profiles, selected lines optimized for the different instruments and methods require target accuracies of the order of 0.001 cm<sup>-1</sup> on line positions and about 1% on line intensities [2]. But an overall understanding of ozone absorbance over a very large spectral range is also necessary. This is most important for subtracting the ozone contribution in order to characterize spectral signatures of other molecules, especially those of atmospheric trace species or pollutants, which cause only very weak absorptions. Other parameters such as pressure-broadened halfwidths and pressure shifts and their temperature dependence also play a role, with accuracy requirements being specific for different applications.

Ozone remote sensing satellite programs, such as MetOp (IASI, GOME), MTG, TOVS, TOMS, UARS, IMG, AURA, ENVISAT (GOMOS, MIPAS, SCIAMACHY), SCISAT/ACE, TEMPO (see Refs. [2–7] and references therein), have been conducted in the past decades by Europe, USA, Canada, Russia and Japan. Ground-based spectroscopic measurements (e.g. the Dobson, Brewer, and NDACC networks) are being performed world-wide to monitor the evolution of the ozone layer. These activities show the strong interest of the international community in the fundamental issues related to the ozone photochemistry and dynamics, in the context of atmospheric change.

The details of the formation of the ozone molecule in the Earth's atmosphere are not yet completely understood [8]. Atmospheric and laboratory ozone investigations show an anomalous isotopic enrichment, which can be linked to the molecular dynamics at the dissociation limit. Despite numerous experimental and theoretical investigations, a fully consistent picture has not yet been established. Accurate knowledge of highly excited rovibrational quantum states of the ozone isotopologues near the dissociation limit are extremely helpful for the understanding of these isotopic effects. The spectral analyses reported in this work are part of the investigations in framework of the project Isotopic and Dynamic Effects in Excited Ozone (IDEO: symmetry breaking, high energy states and dissociation [9]) currently in progress that may help advance the state of knowledge in this domain. In particular, the very sensitive Cavity Ring Down Spectroscopy (CRDS) measurements of all <sup>18</sup>O enriched isotopologues close to the dissociation limit in combination with the corresponding spectral analyses will be particularly helpful for answering some of these questions. Information on high energy levels retrieved from the CRDS spectra in the 5850-7920 cm<sup>-1</sup> spectral region is expected to be important for the validation of the molecular potential energy surface (PES) and for the study of non-Local Thermodynamic Equilibrium (LTE) effects in the upper atmosphere.

In this work we present the state of art in analyses of high-resolution ozone spectra and give a critical discussion of updated line parameters since the previous review by Rinsland et al. on this subject [10] published in 2003. A part of these studies has contributed to the line lists implemented in the last editions of S&MPO [1], HITRAN [11,12] and GEISA [13] databanks, but we give here a larger panorama of ozone analyses including more recent works and spectra investigations currently in progress.

# 2. Rotational transitions within the ground vibrational state

An accurate reinvestigation of the rotational transitions in the ground vibrational state of ozone was reported in 2005 by Colmont et al. [14]. For this study, the group of Mader in Kiel measured the microwave spectrum by means of waveguide Fourier Transform Spectroscopy. Spectrometers in the ranges 8-18 GHz and 18-26.5 GHz were used yielding an exceptional accuracy of typically 0.1–10 kHz for the line centre frequency, depending on the strength of the line. The millimeterwave and submillimeterwave spectra have been measured in Lille in the group of Demaison in the range 180–650 GHz with the accuracy of the central frequency better than 50 kHz for most lines. Previously available 1036 rotational transitions completed by 266 more accurate measurements cited above were fitted together. An improvement of standard errors in fitted parameters suggests that the ground state rotational constants, quartic and sextic centrifugal distortion constants were more accurate than in previous determinations. However these accurate data correspond to less extended set of levels in comparison with infrared measurements, in particular information on transitions with large  $K_a$  values is still missing. Some additional measurements were also carried out in Köln [15]. Information on high J and  $K_a$  levels could be obtained from weak transitions in the THz range, but such measurements are not yet available.

# 3. The 700–5800 cm<sup>-1</sup> spectral domain investigated by Fourier Transform Spectroscopy

### 3.1. FTS experiments

All the spectra, which were used for recent analyses in the 700–5800 cm<sup>-1</sup> range, reported here, have been recorded with the Fourier Transform Spectrometer (FTS) at GSMA laboratory in Reims. The instrumental characteristics corresponding to the original experimental setup were given in Refs. [16,17]. Since that time, several improvements have been achieved, by using two detectors and new components with higher performances leading to much better signal to noise (S/N) ratios. At present the characteristics of the spectrometer allow determining line positions with the precision of  $\sim 8 \times 10^{-5} \text{ cm}^{-1}$  and line intensities with the precision of  $\sim$  1% for best cases of well isolated lines for stable molecules. In the case of dense ozone spectra, the accuracy of line positions can degrade to  $\sim 6 \times 10^{-4} \text{ cm}^{-1}$  for weak transitions corresponding to high I,  $K_a$  quantum numbers or somewhat worse for blended lines. Errors in relative intensity measurements are on average of 1-3% for strong lines. They crucially depend on the density of surrounding lines and could drop to 5-15% or even worse in cases of congested spectra and Download English Version:

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