

High resolution infrared spectrum of the $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ ozone isotopologue recorded by FTS in the 4300-6000 cm^{-1} spectral range: Analyses of two new bands.

Alain Barbe^a, Marie-Renée De Backer^a, Xavier Thomas^a, Vladimir G. Tyuterev^a, Evgeniya N. Starikova^{a,b}

^a Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 7331, UFR Sciences, BP 1039, 51687 Reims Cedex 2, France, tel. : +33 326918777, Fax : +33 326913147, E-mail : alain.barbe@univ-reims.fr mr.debacker@univ-reims.fr vladimir.tyuterev@univ-reims.fr

^b Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics SB RAS 1, Akademician Zuev square, 634021 Tomsk, Russia, E-mail: starikova_e@iao.ru

This work is a continuation of our systematic studies of high resolution near infrared spectra of ozone in the electronic ground state. A recent review of all the data has recently been published [1], concerned with the analyses of all ^{16}O , ^{17}O and ^{18}O enriched isotopologues. As the highest analysed bands recorded by FTS for non homogeneous species was 4824 cm^{-1} [2] and the lowest in energy analysed from CRDS spectra was 5964 cm^{-1} [3], it was important, to test the validity of theoretical predictions and follow the evolution of spectroscopic parameters with respect to energy, to fill the gap 4800-6000 cm^{-1} .

Thanks to the improvements of the signal to noise ratio (S/N) of the Reims FTS, new spectra have been recorded in this relevant spectral range.

Two different mixtures ($\text{O}^{18}=35.1\%$ - $\text{O}^{16}=64.9\%$ and $\text{O}^{18}=65.7\%$ - $\text{O}^{16}=34.3\%$) have been used in order discriminate between $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ and $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ on one side, and $^{18}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ on the other side. The optical path length was 40.22 metres and the total pressure on the order of 25 torr, for both mixtures.

A total of almost 15 characteristic features of A-type bands (very compressed R-branches) are observed, most of them being very weak.

Two of them, which are assigned to $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ are fully analysed. A first band centred at 4624 cm^{-1} , and assigned to the $\nu_1+\nu_2+3\nu_3$ where 939 rovibrational transitions are assigned, with $J_{max} = 37$ and $K_{a\ max} = 9$, the final root mean square being $4.5 \times 10^{-3} \text{ cm}^{-1}$, the analysis including 3 dark states.

A second one, centred at 4908 cm^{-1} (vibrational label has to be confirmed) has 653 transitions assigned, with $J_{max} = 34$ and $K_{a\ max} = 12$, the *rms* being $3.2 \times 10^{-3} \text{ cm}^{-1}$.

For both bands, we present hamiltonian and dipole moment parameters, statistics of the fits, both for positions and intensities, and comparisons of derived band centres and rotational constants with theoretical predictions [4].

We also present examples of agreements between synthetic spectra, using derived spectroscopic parameters and observed spectra.

[1] A. Barbe, S. Mikhailenko, E. Starikova, M.-R. De-Backer, V.I.G. Tyuterev, D. Mondelain, S. Kassi, A. Campargue, C. Janssen, S. Tashkun, R. Kochanov, R. Gamache, J. Orphal, *J. Quant. Spectrosc. Radiat. Transfer* **2013**, under press.

[2] M.-R. De Backer-Barilly, A. Barbe, S. Tashkun, V.I.G. Tyuterev, A. Chichery, *Mol. Phys.* **2002**, **100**, 3499-506.

[3] M.-R. De-Backer-Barilly, A. Barbe, E. Starikova, V.I.G. Tyuterev, D. Mondelain, S. Kassi, A. Campargue, *J. Quant. Spectrosc. Radiat. Transfer* **2013**, doi.org/10.1016/j.jqsrt.2013.04.005.

[4] V.I.G. Tyuterev, R. Kochanov, S. Tashkun, Proceedings of the XVII International Symposium HighRus-2012, <http://symp;iao.ru/en/hrms/17/proceedings>.