OZONE: THE KNOWLEDGE OF THE (204) VIBRATIONAL STATE THROUGH THE OBSERVATION OF THE 2ν₁+4ν₂ AND 2ν₁+4ν₁-ν₃ BANDS

M.-R. DE BACKER-BARILLY, Groupe de Spectrométrie Moléculaire et Atmosphérique, U.M.R. CNRS 6089,
Université de REIMS, Moulin de la Housse, B.P. 1039, 51687 REIMS cedex 2, FRANCE; A. BARBE,
X. THOMAS, P. VON DER HEYDEN, VL.G. TUYTEREV, Groupe de Spectrométrie Moléculaire et Atmo-
sphérique, U.M.R. CNRS 6089, Université de REIMS, Moulin de la Housse, B.P. 1039, 51687 REIMS cedex 2,
FRANCE.

The (204) vibrational state of ozone, early labelled (006), was considered as dark in a previous analyse of the ν₁+5ν₂ band . Since that time, the improvement of signal/noise ratios reaching 5000 in the 5000 cm⁻¹ spectral range allows now to observe very weak features which may be tentatively assigned. A first spectrum has been recorded, in the 4700 cm⁻¹ spectral range with the FTS of GSMA, with a path length of 36 metres and a pressure of 41.0 Torr. The transitions are derived with a precision better than 1 × 10⁻³ cm⁻¹ for wavenumbers and 10% for the intensities.

A typical A-type band shape has been assigned to the 2ν₁+4ν₁-ν₃ band. The ASSIGN code has allowed assigning lines up to J = 20 and Ka = 4, leading to available rotational constants for the (204) state. With these ones, we have searched for the cold 2ν₁+4ν₃ band in other spectra in the 5700 cm⁻¹ spectral range. Despite many difficulties, we finally succeed to assign lines corresponding to Ka = 0 and 1, and relatively large values of J. Using suitable Hamiltonian model taking account of resonances with the (105) and (312) vibrational states, we finally assign 18 lines up to Jmax = 26, Ka = 0, 1 for the cold band and 125 transitions, with Jmax = 25, Kmax = 8 for the hot band.

Concerning the intensities, accounting of the weakness of the transitions, only a rough estimation of µₓ = 0.8 × 10⁻⁴ φₓ (Debye) is given for the cold band. For the hot band, a fit on 72 transitions has been performed, leading to the value of µₓ = 0.1166 × 10⁻³ φₓ (Debye). We present here all the results for the spectroscopic parameters, effective transition moment operators, integrated band intensities, portion of created line lists available for databanks and examples of agreements between observed and calculated spectra.

This work is financially supported by VAMDC EU Project