

# <sup>16</sup>O<sub>3</sub> Integrated Band Intensities, and Dipole Transition Moment Operator Constants for the $4\nu_1 + 2\nu_2 + \nu_3$ , $4\nu_1 + 2\nu_2 + \nu_3 - \nu_2$ and the $2\nu_1 + 5\nu_3$ A-Type Bands

Natural isotopic abundance: 0.992728.

Reference	[2008Cam]
Method	Continuous wave – cavity ring down spectroscopy.
Equations	Equations 47 and 52 in chapter “Introduction”.
Statistical errors	One standard deviation in units of the least significant full size digits.
Remarks	The calculated integrated intensities are given in cm/molecule at 296 K. The parameters of the dipole transition moment operators are given in Debye. Calculated constants are purposely given with a supplementary digit, in index form, in order to reproduce the line intensities to experimental accuracy. Spectroscopic parameters are given in chapter “ <sup>16</sup> O <sub>3</sub> Vibrational Energy and Rotational and Centrifugal Distortion Constants for the Dark (304), the (421), the (205) and the Dark (350) Interacting States” The isotopic composition of the elements used for the calculation of the natural isotopic abundance is taken from [2007Coh].
Abbreviation	{A,B} = AB + BA

Band	Integrated intensity	Transformed dipole transition moment operators	Parameters
$4\nu_1 + 2\nu_2 + \nu_3$ A-type band	$0.94 \times 10^{-24}$	$\varphi_z \times 10^4$ $\{\varphi_z, J^2\} \times 10^8$	0.12385 <sub>6</sub> (94)
$2\nu_1 + 5\nu_3$ A-type band	$2.00 \times 10^{-24}$	$\varphi_z \times 10^4$ $\{\varphi_z, J^2\} \times 10^8$	0.3850 <sub>4</sub> (37) −0.480 <sub>6</sub> (45)
$4\nu_1 + 2\nu_2 + \nu_3 - \nu_2$ A-type band	No data	$1/2[\{\varphi_x, iJ_y\} - \{i\varphi_y, J_x\}] \times 10^7$ $\varphi_z \times 10^3$	−0.37 <sub>0</sub> (14) 0.010 <sub>0</sub> (20)

## Symbols and abbreviations

Short form	Full form
$v_1 v_2 v_3$	Upper vibrational level in normal mode notation
$J_x, J_y, J_z$	Molecule-fixed components of J
SE	Statistical error

## References

- [2007Coh] Cohen, E.R., Cvitaš, T., Frey, J.G., Holmström, B., Kuchitsu, K., Marquardt, R., Mills, I., Pavese, F., Quack, M., Stohner, J., Strauss, H.L., Takami, M., Thor, A.J.: Quantities, Units and Symbols in Physical Chemistry. The IUPAC Green Book, 3rd Ed., Cambridge: RSC Publishing, 2007.
- [2008Cam] Campargue, A., Barbe, A., De Backer-Barilly, M.R., Tyuterev, V.G., and Kassi, S.: The near infrared spectrum of ozone by CW-cavity ring down spectroscopy between 5850 and 7000 cm<sup>−1</sup>: new observations and exhaustive review. Phys. Chem. Chem. Phys. 10 (2008) 2925–2946.