

# $^{16}\text{O}^{17}\text{O}^{17}\text{O}$ Dipole Transition Moment Operator Constants, Integrated Intensity for the $\nu_1$ and $\nu_3$ Bands

Natural isotopic abundance:  $2.88 \times 10^{-7}$ .

Reference	[]
Method	Fourier transform spectroscopy.
Equations	Equations 47, 52, and 53 in chapter “Introduction”.
Remarks	<p>The first order term moment operator constants, practically do not vary for the <i>A</i>- and <i>B</i>-type <math>\nu_1</math> and <math>\nu_3</math> bands with the isotopomer. The calculations of the line intensities have then been performed using the <math>^{16}\text{O}_3</math> values given in [87Fla2].</p> <p>The integrated intensities are given in units of <math>\text{cm}^{-1}/\text{molecule.cm}^{-2}</math> at 296 K. Their values correspond to the sum of their individual line intensities, calculated with a cut-off equal to <math>0.5 \times 10^{-22} \text{ cm}^{-1}/\text{molecule.cm}^{-2}</math> at 296 K.</p> <p>Band centers and vibrational energy and rotational and centrifugal distortion constants are given in chapter “<math>^{16}\text{O}^{17}\text{O}^{17}\text{O}</math> Vibrational Energy and Rotational and Centrifugal Distortion Constants. Band Center for the <math>\nu_1</math> and <math>\nu_3</math> Bands”.</p> <p>The isotopic composition of the elements used for the calculation of the natural isotopic abundance is taken from [2007Coh].</p>

Band	Integrated intensity	Transformed dipole transition moment operators	Parameters
$\nu_3$	$0.135 \times 10^{-16}$		
<i>A</i> -type band		$\varphi_Z$	-0.188232
$\nu_1$			
<i>B</i> -type band	$0.384 \times 10^{-18}$	$\varphi_X$	-0.0154509
<i>A</i> -type band	$0.179 \times 10^{-18}$		

## Symbols and abbreviations

Short form	Full form
$v_1 v_2 v_3$	Upper vibrational level in normal mode notation
SE	Statistical error

## References

- [87Fla2] Flaud, J.M., Camy-Peyret, C., Devi, V.M., Rinsland, C.P., and Smith, M.A.H.: The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities. *J. Mol. Spectrosc.* **124** (1987) 209–217.
- [2000Per2] Perrin, A., Flaud, J.M., Valentin, A., Camy-Peyret, C., Gbaguidi, N., and N’Gom, A.: The  $\nu_1$  and  $\nu_3$  bands of the  $^{16}\text{O}^{17}\text{O}^{17}\text{O}$  isotopomer of ozone. *J. Mol. Struct.* **517–518** (2000) 157–163.
- [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.