

# $^{16}\text{O}_3$ Coriolis and Darling-Dennison Coupling Parameters for the Interacting Triad $\{(012), (210), (111)\}$ and Dark $(040)$ Vibrational States

Natural isotopic abundance: 0.992728.

Reference	[99Mik2]
Method	Fourier transform spectroscopy.
Equations	Equations 6, 7, 19, and 20 in chapter “Introduction”.
Statistical errors	One standard deviation.
Remarks	All values are given in $\text{cm}^{-1}$ . Molecular constants determined in the same fit are given in chapter “ $^{16}\text{O}_3$ Vibrational Energy and Rotational and Centrifugal Distortion Constants for the Interacting Triad $\{(012), (210), (111)\}$ and Dark $(040)$ Vibrational States. Coupling Interaction Between the $(111)$ and the Dark $(040)$ States”. The Darling-Dennison interaction between the $(012)$ and $(210)$ states is included in the fit with only one fixed parameter taken equal, as in chapter “ $^{16}\text{O}_3$ Coriolis and Darling-Dennison Coupling Constants for the $(002), (101),$ and $(200)$ Vibrational States”, to $-27.0 \text{ cm}^{-1}$ . Actually, no rotation corrections are needed since the mixing coefficients due to this interaction are small and practically constant. A weak discrepancy for eight energy levels of the $(111)$ state is found and assigned to a Coriolis interaction with the $(040)$ state. The corresponding parameter $C_{001}$ value is equal to $1.09 \cdot 10^{-3} \text{ cm}^{-1}$ . The isotopic composition of the elements used for the calculation of the natural isotopic abundance is taken from [2007Coh].
Abbreviation	SE: Statistical error.

Parameter		<111 H 012>		<111 H 210>	
		Value	SE	Value	SE
$C_{001}$	$\times 10$	-3.35		3.3	
$C_{011}$	$\times 10^2$	-1.76072	0.00041	-1.4159	0.0021
$C_{021}$	$\times 10^5$			-6.41	0.14
$C_{201}$	$\times 10^6$	2.257	0.024		
$C_{031}$	$\times 10^6$	6.926	0.029		
$C_{211}$	$\times 10^7$			-2.153	0.068

## Symbols and abbreviations

Short form	Full form
$C_y, C_{yz}$	Coriolis coupling parameter
SE	Statistical error

## References

- [99Mik2] Mikhailenko, S., Barbe, A., Plateaux, J.J., and Tyuterev, V.G.: New Analysis of  $2\nu_1 + \nu_2, \nu_1 + \nu_2 + \nu_3,$  and  $\nu_2 + 2\nu_3$  Bands of Ozone in the  $2600\text{--}2900 \text{ cm}^{-1}$  Region. *J. Mol. Spectrosc.* **196** (1999) 93–101.
- [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.