

¹⁶O₃ Coriolis and Anharmonic Coupling Parameters of the (114), (213), Dark (080) and (321) Interacting States

Natural isotopic abundance: 0.992728.

Reference	[2012Bar]
Method	Fourier transform spectroscopy.
Equations	Equations 14, 15, and 16 in chapter “Introduction”.
Statistical errors	One standard deviation in units of the least significant full size digits.
Remarks	<p>All values are given in cm⁻¹.</p> <p>Molecular constants determined in the same fit are given in chapter “¹⁶O₃ Vibrational Energy and Rotational and Centrifugal Distortion Constants for the (213), (114), (321), and for the Dark (080)* Vibrational States”.</p> <p>Calculated constants are purposely given with a supplementary digit, in index form, in order to reproduce the energy levels to experimental accuracy.</p> <p>The perturbing (080) vibrational state is supposed to be a dark state.</p> <p>The isotopic composition of the elements used for the calculation of the natural isotopic abundance is taken from [2007Coh].</p>
Abbreviations	SE: Statistical error.

	Coriolis type coupling parameters			Anharmonic type coupling parameters			
	<114 H 213>	<080 H 213>	<321 H 213>	Value	SE	Value	SE
C ₀₁₁	-0.4786 ₃ × 10 ⁻²	31	-0.1027 × 10 ⁻³	19	F ₀₂₀	0.0506 ₅	16
C ₀₃₁			-0.3136 × 10 ⁻⁴	18	F ₀₀₂	0.6550 ₀ × 10 ⁻³	76
C ₂₁₁	-0.2012 ₆ × 10 ⁻⁵	49	-0.936 × 10 ⁻⁶	13			

Symbols and abbreviations

Short form	Full form
C _y , C _{yz}	Coriolis coupling parameter
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.
- [2012Bar] Barbe, A., De Backer, M.R., Starikova, E., Tashkun, S.A., Thomas, X., and Tyuterev, V.G.: FTS high resolution spectra of ¹⁶O₃ in 3500 and 5500 cm⁻¹ regions. First example of new theoretical modelling for a polyad of strongly coupled states. J. Quant. Spectrosc. Radiat. Transfer. **113** (2012) 829–839.