



Are asymmetric stretch Raman spectra by centrosymmetric molecules depolarized ? : The 2v3 overtone of CO2

Submitted by Emmanuel Lemoine on Mon, 06/02/2014 - 18:28

Titre	Are asymmetric stretch Raman spectra by centrosymmetric molecules depolarized ? : The 2v3 overtone of CO2
Type de publication	Article de revue
Auteur	Chrysos, Michel [1], Verzhbitskiy, I.-A. [2], Rachet, Florent [3], Kouzov, A.-P. [4]
Editeur	American Institute of Physics
Type	Article scientifique dans une revue à comité de lecture
Année	2011
Langue	Anglais
Date	01/2011
Numéro	4
Volume	134
Titre de la revue	Journal of Chemical Physics
ISSN	0021-9606
Mots-clés	(hyper)polarizability [5], carbon-dioxide [6], dipole [7], fermi resonance region [8], frequency-shifts [9], isotopic [10], moment [11], Polarizability [12], polyatomic-molecules [13], scattering [14], variants [15]
Résumé en anglais	Molecular vibrations that are not totally symmetrical give rise to depolarized lines [P. Atkins and J. de Paula, Atkins Physical Chemistry (Oxford University Press, UK, 2006), p. 464]. But in the case of stretching vibrations in centrosymmetric molecules, the statement has so far not been conclusively verified. It is the purpose of this article to report a rigorous experimental and theoretical analysis of the 2 nu(3) band of CO2-the first overtone of the asymmetrical stretch vibration. The anisotropic spectrum was extracted and its spectral moment calculated from light-scattering measurements, taken at room temperature and for a wide range of CO2-gas densities. Evidence for a near-entirely depolarized Raman band is provided, with integrated depolarization ratio $\eta(\text{int}) = 6/7.16$, closely approaching the upper bound $\eta(\text{max}) = 6/7$. Agreement with theoretical predictions is found, on the basis of quality ab initio data for polarizability properties, provided that electro-optical and mechanical anharmonicity and intermode coupling effects between symmetric nu(1) and antisymmetric nu(3) stretching vibrations are incorporated.
URL de la notice	http://okina.univ-angers.fr/publications/ua3146 [16]
DOI	10.1063/1.3535599 [17]

Liens

[1] <http://okina.univ-angers.fr/michel.chrysos/publications>

[2] [http://okina.univ-angers.fr/publications?f\[author\]=4472](http://okina.univ-angers.fr/publications?f[author]=4472)

[3] <http://okina.univ-angers.fr/florent.rachet/publications>

- [4] [http://okina.univ-angers.fr/publications?f\[author\]=2657](http://okina.univ-angers.fr/publications?f[author]=2657)
- [5] [http://okina.univ-angers.fr/publications?f\[keyword\]=6903](http://okina.univ-angers.fr/publications?f[keyword]=6903)
- [6] [http://okina.univ-angers.fr/publications?f\[keyword\]=6899](http://okina.univ-angers.fr/publications?f[keyword]=6899)
- [7] [http://okina.univ-angers.fr/publications?f\[keyword\]=6902](http://okina.univ-angers.fr/publications?f[keyword]=6902)
- [8] [http://okina.univ-angers.fr/publications?f\[keyword\]=6897](http://okina.univ-angers.fr/publications?f[keyword]=6897)
- [9] [http://okina.univ-angers.fr/publications?f\[keyword\]=6909](http://okina.univ-angers.fr/publications?f[keyword]=6909)
- [10] [http://okina.univ-angers.fr/publications?f\[keyword\]=6907](http://okina.univ-angers.fr/publications?f[keyword]=6907)
- [11] [http://okina.univ-angers.fr/publications?f\[keyword\]=6911](http://okina.univ-angers.fr/publications?f[keyword]=6911)
- [12] [http://okina.univ-angers.fr/publications?f\[keyword\]=4937](http://okina.univ-angers.fr/publications?f[keyword]=4937)
- [13] [http://okina.univ-angers.fr/publications?f\[keyword\]=6906](http://okina.univ-angers.fr/publications?f[keyword]=6906)
- [14] [http://okina.univ-angers.fr/publications?f\[keyword\]=6910](http://okina.univ-angers.fr/publications?f[keyword]=6910)
- [15] [http://okina.univ-angers.fr/publications?f\[keyword\]=6908](http://okina.univ-angers.fr/publications?f[keyword]=6908)
- [16] <http://okina.univ-angers.fr/publications/ua3146>
- [17] <http://dx.doi.org/10.1063/1.3535599>

Publié sur *Okina* (<http://okina.univ-angers.fr>)