The depolarized Raman 2 nu(3) overtone of CO2: A line-mixing shape analysis

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Titre	The depolarized Raman 2 nu(3) overtone of CO2: A line-mixing shape analysis
Type de publication	Article de revue
Auteur	Verzhbitskiy, I.-A. [1], Kouzov, A.-P. [2], Rachet, Florent [3], Chrysos, Michel [4]
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Résumé en anglais	In a recent article we showed that the 2 nu(3) transition of CO2 gives rise to a Raman spectrum that is almost entirely depolarized [M. Chrysos, I. A. Verzhbitskiy, F. Rachet, and A. P. Kouzov, J. Chem. Phys. 134, 044318 (2011)]. In the present article, we go further forward in the study of this overtone by reporting a first-principles shape analysis of its depolarized spectrum at room temperature. As a first step in our analysis, a model assuming isolated Lorentzian line shapes was applied, which at low gas densities turns out to be sufficient for qualitative conclusions. As the next step, a sophisticated approach was developed on the basis of the extended strong-collision model in order to properly account for the heavy line mixing between rotational lines. Whereas a marked deviation between model and measured spectra was observed upon application of the simpler model, striking agreement even at the highest CO2 density was found on applying the sophisticated one. Accurate calculated data were used for the rotational line broadening coefficients without resort to arbitrary parameters. Values for the vibrational shift scaling linearly with the density of the gas are given.
URL de la notice	http://okina.univ-angers.fr/publications/ua3164 [15]
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