Double vibrational collision-induced Raman scattering by SF6–N2: Beyond the point-polarizable molecule model

Titre	Double vibrational collision-induced Raman scattering by SF6–N2: Beyond the point-polarizable molecule model
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Auteur	Verzhbitskiy, I.-A. [1], Chrysos, Michel [2], Kouzov, A.-P. [3]
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Résumé en anglais	Collision-induced Raman bandshapes and zeroth-order spectral moments are calculated both for the depolarized spectrum and for the extremely weak isotropic spectrum of the SF6(ν1) +N2(ν1) double-Raman-scattering band. A critical comparison is made with experiments conducted recently by the authors [Phys. Rev. A 81 012702 (2010) 81 042705 (2010)]. The study of this transition, hitherto restricted to the model framework of two point-polarizable molecules, is now completed to incorporate effects beyond the point-molecule approximation. Whereas the extended model offers a few percent improvement in the depolarized spectrum, it reveals a huge 80% increase in the isotropic spectrum and its moment, owing essentially to the polarizability anisotropy of N2. For both spectra, agreement between quantum-mechanical calculations and our experiments is found, provided that the best ab initio data for the (hyper)polarizability parameters are used. This refined study shows clearly the need to include all mechanisms and data to a high level of accuracy and allows one to decide between alternatives about difficult and controversial issues such as the intermolecular potential or the sensitive Hamaker force constants.
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