Collision-induced Raman scattering and the peculiar case of neon: Anisotropic spectrum, anisotropy, and the inverse scattering problem

Titre	Collision-induced Raman scattering and the peculiar case of neon: Anisotropic spectrum, anisotropy, and the inverse scattering problem
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Résumé en anglais	Owing in part to the p orbitals of its filled L shell, neon has repeatedly come on stage for its peculiar properties. In the context of collision-induced Raman spectroscopy, in particular, we have shown, in a brief report published a few years ago [M. Chrysos et al., Phys. Rev. A 80, 054701 (2009)], that the room-temperature anisotropic Raman lineshape of Ne–Ne exhibits, in the far wing of the spectrum, a peculiar structure with an aspect other than a smooth wing (on a logarithmic plot) which contrasts with any of the existing studies, and whose explanation lies in the distinct way in which overlap and exchange interactions interfere with the classical electrostatic ones in making the polarizability anisotropy, $\alpha_{\parallel} - \alpha_{\perp}$. Here, we delve deeper into that study by reporting data for that spectrum up to 450 cm^{-1} and for even- and odd-order spectral moments up to M 6, as well as quantum lineshapes, generated from SCF, CCSD, and CCSD(T) models for $\alpha_{\parallel} - \alpha_{\perp}$, which are critically compared with the experiment. On account of the knowledge of the spectrum over the augmented frequency domain, we show how the inverse scattering problem can be tackled both effectively and economically, and we report an analytic function for the anisotropy whose quantum lineshape faithfully reproduces our observations.
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