



Morphology of collisional nonlinear spectra in H₂-Kr and H₂-Xe mixtures

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Résumé en anglais

This article reports new results of theoretical and numerical studies of spectral features of the collision-induced hyper-Rayleigh light scattered in dihydrogen-noble gas (H₂-Rg) mixtures. The most massive and polarizable scattering supermolecules with Rg = Kr and Xe have been added to the previously considered systems in order to gain a more complete insight into the evolution of the spectral properties. The symmetry adapted components of the first collisional hyperpolarizabilities are obtained by means of the quantum chemistry numerical routines supplemented with appropriate theoretical methods. Roto-translational spectral lines are calculated on the grounds of the quantum-mechanical as well as semi-classical approach. The role of particular hyperpolarizability components in forming the line shapes is discussed. The intensities of the lines are compared with those obtained for less massive scatterers. Advantages of prospective application of the new scattering systems for experimental detection of the nonlinear collisional effects are indicated.

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