Intermolecular polarizabilities in H2-rare-gas mixtures (H2–He, Ne, Ar, Kr, Xe): Insight from collisional isotropic spectral properties

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Résumé en anglais	The report presents results of theoretical and numerical analysis of the electrical properties related to the isotropic part of the polarizability induced by interactions within compounds built up of a hydrogen H2 molecule and a set of noble gas atoms, Rg, ranging from the least massive helium up to the heaviest xenon perturber. The Cartesian components of the collisional polarizabilities of the H2–Rg systems are found by means of the quantum chemistry methods and their dependence on the intermolecular distance is determined. On the basis of these data, the spherical, symmetry adapted components of the trace polarizability are derived in order to provide data sets that are convenient for evaluating collisional spectral profiles of the isotropic polarized part of light scattered by the H2–Rg mixtures. Three independent methods of numerical computing of the spectral intensities are applied at room temperature (295 K). The properties of the roto-translational profiles obtained are discussed in order to determine the role played by contributions corresponding to each of the symmetry adapted parts of the trace polarizability. By spreading the analysis over the collection of the H2–Rg systems, evolution of the spectral properties with the growing masses of the supermolecular compounds can be observed.
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