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Second Harmonic Elastic Light Scattering by Gases Composed of Centrosymmetric Molecules. The Case of H2-Ar.

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Auteur	Głaz, Waldemar [1], Bancewicz, Tadeusz [2], Godet, Jean-Luc [3], Maroulis, George [4]
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Mots-clés	Collision theories [5], Elasticity [6], Light scattering [7], Semiclassical theories [8], Tensor methods [9]
Résumé en anglais	A numerical and theoretical study of nonlinear collisional electrical and/or optical properties of near van der Waals weakly bound complexes is presented. The molecular systems considered are composed of a linear nonpolar molecule (H_2 taken as an example) and a spherical atomic entity (Ar)—a supermolecule of symmetry of one step lower than that considered before. The basic stage of the procedure developed consists of computational quantum chemistry efforts of determining values of the first hyperpolarizability tensor for several intermolecular configuration arrangements. Subsequent theoretical discussion includes these quantities within a routine developed in order to produce symmetry adapted (SA) components of the hyperpolarizability tensor, which are finally used so that the spectral distributions of the collision-induced hyper-Rayleigh (CIHR) light scattering could be determined. Translational parts of these functions have served as an assessment tool to judge about the role played by a particular SA contribution in the overall tensorial property. In particular, the convergence of the series expansion of the hyperpolarizability dependence on intermolecular distances has been investigated. Three computational methods based on quantum and semiclassical approach have been compared.
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