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Effects of anisotropic interaction-induced properties of hydrogen-rare gas compounds on rototranslational Raman scattering spectra: Comprehensive theoretical and numerical analysis

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Titre	Effects of anisotropic interaction-induced properties of hydrogen-rare gas compounds on rototranslational Raman scattering spectra: Comprehensive theoretical and numerical analysis
Type de publication	Article de revue
Auteur	Głaz, Waldemar [1], Bancewicz, Tadeusz [2], Godet, Jean-Luc [3], Gustafsson, Magnus [4], Haskopoulos, Anastasios [5], Maroulis, George [6]
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Mots-clés	collision-induced scattering (CIS) [7], Hydrogen-rare gases compounds [8]
Résumé en anglais	A comprehensive study is presented of many aspects of the depolarized anisotropic collision induced (CI) component of light scattered by weakly bound compounds composed of a dihydrogen molecule and a rare gas (Rg) atom, H2–Rg. The work continues a series of earlier projects marking the revival of interest in linear light scattering following the development of new highly advanced tools of quantum chemistry and other theoretical, computational, and experimental means of spectral analyses. Sophisticated ab initio computing procedures are applied in order to obtain the anisotropic polarizability component's dependence on the H2–Rg geometry. These data are then used to evaluate the CI spectral lines for all types of Rg atoms ranging from He to Xe (Rn excluded). Evolution of the properties of CI spectra with growing polarizability/masses of the complexes studied is observed. Special attention is given to the heaviest, Kr and Xe based, scatterers. The influence of specific factors shaping the spectral lines (e.g., bound and metastable contribution, potential anisotropy) is discussed. Also the share of pressure broadened allowed rotational transitions in the overall spectral profile is taken into account and the extent to which it is separable from the pure CI contribution is discussed. We finish with a brief comparison between the obtained results and available experimental data.
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