



Collisional ab initio hyperpolarizabilities in computing hyper-Rayleigh spectra of noble gas heterodiatomics

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Auteur	Głaz, Waldemar [1], Bancewicz, Tadeusz [2], Godet, Jean-Luc [3], Maroulis, George [4], Haskopoulos, Anastasios [5]
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Résumé en anglais	We review some recent studies on the theoretical and computational aspects of collision-induced nonlinear properties and phenomena, such as: the first hyperpolarizability of inert gas heteroatomic pairs (He-Ne, He-Ar, N-Ar and Kr-Xe) and spectral properties of hyper-Rayleigh scattered light in such systems. The hyperpolarizability data obtained by means of a variety of methods of quantum chemistry were applied to calculate spectral HR profiles. Computations are performed both quantum-mechanically and classically for two temperature values $T=95$ K and $T:295$ K. Resulting tensorial properties and spectra are presented and discussed.
URL de la notice	http://okina.univ-angers.fr/publications/ua14060 [11]
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