Abstract Submitted
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Application of accurate molecular spectra for studying molecular collisions and interactions HUBERT JOZWIAK, Nicolaus Copernicus University Torun, Poland, FRANCK THIBAULT, Universite de Rennes 1, Rennes, France, PIOTR WCISLO, Nicolaus Copernicus University Torun, Poland — Accurate measurements of the shapes of molecular resonances provide information about molecular dynamics and validate the potential energy surfaces for various collisional systems. This is due to the fact that the collision-perturbed velocity distribution of the optical coherence manifests itself as the perturbation of the shape of such resonance. We present a theoretical description of this process, using state-of-the-art potential energy surfaces and quantum scattering calculations for diatom-atom and diatom-diatom systems. Not only does this approach properly describe the internal and translational motions of the molecules, but also correlations between them. This results in the subpercent agreement between the calculated and measured spectral line profiles. These theoretical developments are important for reducing systematic errors in optical metrology based on molecular spectroscopy (for instance, they allow for more accurate determination of rovibrational splitting in molecular hydrogen and, hence, for accurate tests of quantum electrodynamics for molecules). Accurate theoretical models of the collision-perturbed molecular spectra will be used for populating line-by-line spectroscopic databases and providing reference spectra for the studies of planetary atmospheres.

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