

## COLLISIONAL EFFECTS IN THE SPECTRA OF HYDROGEN HALIDES: TOWARDS RELIABLE *AB INITIO* MODELING OF THE TERRESTRIAL-ATMOSPHERIC MOLECULAR SPECTRA

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It has been long recognized that the spectroscopy of hydrogen halides (such as HF, HCl, HBr, and HI) provides a valuable tool, with atmospheric and astrophysical, as well as industrial applications [*J. Quant. Spectrosc. Radiat. Transf.* **130**, 284 (2013)]. As far as the terrestrial-atmospheric studies are concerned, two halide species – HF and HCl – may be considered the most important of the bunch. Being the main reservoirs of fluorine and chlorine, HF and HCl are used as pollutant trace gases in the determination of the anthropogenic chlorofluorocarbons' concentration in the Earth's atmosphere. Since these molecular species are of the pollutant-type, their atmospheric spectra must necessarily be considered as perturbed by intermolecular interactions involving the main constituents of our planet's atmosphere – N<sub>2</sub> and O<sub>2</sub>. Indeed, the process of ozone depletion is mainly induced by Cl and ClO, which result from the photodissociation of HCl. Therefore, to be applicable in atmospheric science, the spectra of the terrestrial hydrogen halides must be considered in the presence of the surrounding molecular bath of N<sub>2</sub> and O<sub>2</sub>.

Here, we take a fully *ab initio* approach to the theoretical determination of atmospheric spectra of hydrogen halides, starting from the O<sub>2</sub>-induced line shape perturbations. Taking the state-of-the-art potential energy surfaces (PESs) as our starting point, we perform close-coupling calculations of HF-O<sub>2</sub> and HCl-O<sub>2</sub> quantum scattering. We take a novel approach to the construction of the energy-level basis used in the close-coupling computations, and we study the convergence of the calculated cross sections against the size of the employed basis in full detail. Further, we calculate the temperature-dependent line shape parameters of the O<sub>2</sub>-perturbed rotational R(0) line in HCl. The PESs used in this study were constructed automatically using the AUTOSURF code [*J. Chem. Inf. Model.* **59**, 262 (2018)].