QUANTUM SCATTERING CALCULATIONS FOR ACCURATE MODELING OF COLLISION-PERTURBED MOLECULAR SPECTRA

H. JÓŹWIAK, M. GANCEWSKI, A. OLEJNIK, A. ZADROŻNY P. WCISŁO,
Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, ul Grudziadzka 5, 87-100 Toruń, Poland)

Reliable interpretation of molecular spectra requires taking into account subtle collisional effects that extend beyond the Voigt profile. Such effects include spatial confinement of molecules due to frequent velocity-changing collisions, which gives rise to the Dicke narrowing phenomenon,[1] and the speed dependence of collisional broadening and shift.[2]

I will present a theoretical description of the shapes of molecular resonances, based on *ab initio* potential energy surfaces, quantum scattering calculations, and an advanced statistical model of collisional perturbation of the optical coherence. This approach has been successfully validated on cavity-enhanced spectra of H_2 perturbed by collisions with He atoms[3] and H_2-perturbed D_2 lines. I will discuss the challenges in performing quantum scattering calculations in diatom-diatom systems and the computational tools developed in our group. I will present the application of the theoretical approach in accurate spectroscopy of hydrogen for fundamental studies[4] and the importance of beyond-Voigt line-shape effects in the context of astrophysical spectral analysis and terrestrial atmospheric studies. In particular, I will highlight our results for resonances in CO,[5,6] O_2[7] and HCl, perturbed by collisions with the most abundant species of the Earth's atmosphere: N_2 and O_2.

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