

CRDS measurements and *ab initio* calculations of collisional effects in pure D₂.

Mikołaj Zaborowski^{1,*}, Piotr Wcisło¹, Franck Thibault², Szymon Wójtewicz¹, Agata Cygan¹,
Grzegorz Kowzan¹, Piotr Masłowski¹, Daniel Lisak¹, and Roman Ciuryło¹

1. Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland

2. Institut de Physique de Rennes, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, Bât.11B, F-35042 Rennes, France

* zaborowski@fizyka.umk.pl

Recent progress in theoretical calculations of dissociation energies of H₂, HD and D₂ [1–2] gives predictions of the transition frequencies with uncertainty exceeding the level of 10⁻³ cm⁻¹ for the first overtone band (2–0) [3]. Such predictions open a way for testing relativistic and quantum electrodynamics corrections. They give also the opportunity for searching for new physics like additional long-range hadron-hadron interactions [4]. At this level of accuracy the uncertainty of the H₂ (or its isotopologues) line position determination in Doppler limit becomes considerably affected by the line-shape effects [5] including asymmetry of the line shapes. Spectral line shapes of D₂ transitions are atypical and difficult to model. First strategy for overcoming this problem is measuring the spectra at low pressures, where collisional effects are negligible [3]. However, it is experimentally challenging due to exceptionally low intensities of the quadrupole lines. Another approach is recording them at higher pressures and describe the collisions in a more sophisticated way. Here as an example of the second strategy, we present our preliminary results applied for very weak S(2) transition of deuterium in the 2-0 band, using *ab initio* calculations. Transition has been measured with the frequency-stabilized cavity ring-down spectroscopy (FS-CRDS) assisted by an optical-frequency comb [6,7], using experimental setup described in [8]. The line positions at high pressures, up to 1000 Torr, were measured with sub-MHz accuracy.

Furthermore, to validate *ab initio* model, we extended our experiments to a wide range of temperatures. We compare it with *ab initio* quantum scattering calculations, where we obtain the generalized spectroscopic cross sections. The real and imaginary parts provide the speed-dependent collisional broadening $\gamma(v)$ and shifting $\delta(v)$. The velocity-changing collisions, in turn, are described by hard-sphere approximation of the *ab initio* potential which is called the speed-dependent billiard-ball profile (SDBBP) [9].

References

- [1] K. Pachucki *et al*, Phys. Chem. Chem. Phys. **12**, 9188 (2010)
- [2] K. Pachucki *et al*, J. Chem. Phys. **143**, 034111 (2015)
- [3] D. Mondelain *et al*, J. Mol. Spectrosc. **in press** (2016)
- [4] E. Salumbides *et al*, J. Mol. Spectrosc. **300**, 65 (2014)
- [5] P. Wcisło *et al*, Phys. Rev. A **93**, 022501 (2016)
- [6] J. Domysławska *et al*, J. Chem. Phys. **136**, 024201 (2012)
- [7] D. Long *et al*, Chem. Phys. Lett. **536**, 1 (2012)
- [8] A. Cygan *et al*, Meas. Sci. Technol. **27**, 045501 (2016)
- [9] P. Wcisło *et al*, Phys. Rev. A **91**, 052505 (2015)