AB INITIO QUANTUM SCATTERING CALCULATIONS FOR O_2-PERTURBED R(0) 0-0 LINE IN HCl

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Accurate knowledge of the spectroscopic parameters of hydrogen halides is important in the quantitative analysis of the Earth's atmosphere. A particularly important hydrogen halide is HCl, which indirectly contributes to the depletion of the ozone layer.[1] Monitoring their presence in the stratosphere can aid in characterizing the distribution of ozone and controlling the state of the ozone layer. HF and HCl are also components of volcanic gases.[2] Collisions with O_2, the second most abundant molecule in the Earth's atmosphere, perturb the spectral lineshape of other molecules, including HCl,[3] making the interpretation of atmospheric observations challenging.

We report the results of the first fully quantum scattering calculations for the R(0) line in HCl molecules. The calculations are performed using the new four-dimensional potential energy surface for the HCl-O_2 system. The spectroscopic parameter calculations were conducted using our new computational package, BIGOS, developed in our group. The scattering matrices (S-matrices) obtained from the calculations are used to calculate the spectroscropic cross sections, which determine line broadening and shifting due to collisions.[4] The theoretical results show good agreement with experimental data.[5,6,7,8]

[1] United Nations. *Vienna convention for the protection of the ozone layer*. In: United Nations TS, editor. Vienna, 293 (1985).

[2] W. Stremme, I. Ortega, C. Siebe and M. Grutter, Earth Planet Sci. Lett. **301**, 502–510 (2011).

[3] J. M. Hartmann, C. Boulet and D. Robert, *Collisional Effects on Molecular Spectra Elsevier*, Amsterdam (2021).

[4] L. Monchick and L. W. Hunter, J. Chem. Phys. **85**, 713 (1986).

[5] B. J. Drouin, J. Quant. Spectrosc. Radiat. Transf. **83**, 321 (2004).

[6] I. Morino and K. M. T. Yamada, J. Mol. Spectrosc. **233**, 77 (2005).

[7] L. Zu, P. A. Hamilton, K. V. Chance and P. B. Davies, J. Mol. Spectrosc. **220**, 107 (2003).

[8] J. P. Houdeau, M. Larvor and C. Haeusler, Can. J. Phys. **58**, 318 (1980).

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