

AB INITIO QUANTUM SCATTERING CALCULATIONS FOR O₂-PERTURBED R(0) 0-0 LINE IN HCl

A. OLEJNIK, H. JOZWIAK, M. GANCEWSKI, P. WCISLO, *Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland*; **R. DAWES, E. QUINTAS-SANCHEZ**, *Department of Chemistry, Missouri University of Science and Technology, Rolla, Missouri 65409-0010, USA*

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 O₂, 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-O₂ 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 spectroscopic 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}

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