

Complex Robert-Bonamy line shape parameters for N₂-broadening of water using accurate *ab initio* rovibrational wavefunctions

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The calculations of the half-widths, their temperature dependence, and the line shifts were made for N₂-broadening of water using the semiclassical Complex Robert-Bonamy (CRB) approach [1,2]. Our calculations were done for rotational quantum numbers up to $J''=20$ in the rotational band of H₂¹⁶O using a converged potential and an exact trajectory model [3]. In this work, reduced matrix elements were calculated for the vibrational ground state from accurate *ab initio* rovibrational wavefunctions determined by Partridge and Schwenke [4]. These reduced matrix elements will be compared to the effective ones previously determined from an effective Watson Hamiltonian [5]. The comparison of the calculated line shape parameters with the effective ones [3] will also be discussed. These results open promising perspectives for taking into consideration rovibrational resonances within the CRB formalism for the strongly interacting states, in particular for transitions with high quantum numbers assignments.

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