An isolated line-shape model to go beyond the Voigt profile in spectroscopic databases and radiative transfer codes

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We demonstrate that the partially-Correlated quadratic-Speed Dependent Hard-Collision (pCqSDHC) model opens the route for the inclusion of refined non-Voigt profiles in spectroscopic databases and atmospheric radiative transfer codes. Indeed, this model fulfils many essential requirements: (i) It takes both velocity changes and the speed dependences of the pressure-broadening and -shifting coefficients into account. (ii) It leads to accurate descriptions of the line shapes of very different molecular systems. Tests made [1,2] for pure H_2, CO_2 and O_2 and for H_2O diluted in N_2 show that residuals are down to $\square\, 0.2\%$ of the peak absorption, (except for the untypical system of H_2 where a maximum residual of ±3% is reached), thus fulfilling the precision requirements of the most demanding remote sensing experiments. (iii) It is based on a limited set of parameters for each absorption line that have known dependences on pressure and can thus be stored in databases. (iv) Its calculation requires very reasonable computer costs, only a few times higher than that of a usual Voigt profile. Its inclusion in radiative transfer codes will thus induce bearable CPU time increases. (v) It can be extended in order to take line-mixing effects into account, at least within the so-called first-order approximation.

FORTRAN subroutines for the calculation of the pCqSDHC model and of its two limits: the quadratic-Speed-Dependent Voigt (qSDV) and the quadratic-Speed-Dependent Hard-Collision (qSDHC) profiles are also provided. Numerical tests successfully confirm the analytically derived fact that all these profiles can be expressed as combinations of complex Voigt probability functions. Based on a slightly improved version of the CPF subroutine [3] for the calculation of the complex probability function, we show that the pCqSDHC, qSDHC and qSDV profiles can be quickly calculated with an accuracy better than 10^{-4} [4].

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