OPTIMIZED CALCULATION OF A QUADRATIC MODEL FOR SPEED DEPENDENT LINESHAPES

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A new algorithm for computation of a speed dependent lineshape function is presented. The lineshape that is calculated is based upon a quadratic model for the Lorentz width as a function of velocity. The calculation includes both real and imaginary parts of the lineshape for applications to line mixing and Dicke narrowing. This algorithm sacrifices a small amount of memory space for a considerable gain in speed and accuracy and employs methods similar to the techniques used to calculate the Voigt Profile as described by Letchworth and Benner[a]. For Lorentz widths greater than about five times the Doppler width and for points more than about five Doppler widths from the center of the spectral line, Gauss-Hermite quadrature is employed. For most other cases, a Taylor series expansion about the nearest point in a precomputed table is used. In some cases where the Doppler width is more than an order of magnitude larger than the Lorentz width, Lagrange interpolating polynomials are used with a table of precomputed points. The accuracy is one part in 10^5 of the value of the function itself. Optionally, derivatives with respect to certain lineshape parameters are also returned. The algorithm provides a good approximation for speed dependent lineshapes with a calculation time which is not significantly larger than the time required to calculate the Voigt Profile using the Drayson[b], Humlicek[c], and Letchworth and Benner routines.
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[a] K. L. Letchworth, D. C. Benner *J. Quant. Spectrosc. Radiat. Trans.* In Press.
[b] S. R. Drayson *J. Quant. Spectrosc. Radiat. Trans.* **16**, 611-614, 1976.
[c] J. Humlicek *J. Quant. Spectrosc. Radiat. Trans.* **27**, 437-444, 1982.