RAPID AND ACCURATE CALCULATION OF THE VOIGT FUNCTION

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A new algorithm for computation of both the real and imaginary parts of the Voigt (complex error) function is presented. This algorithm sacrifices a small amount of memory space for a considerable gain in speed and accuracy. Changes in the order of computation that take advantage of typical use in spectroscopy provide some of the gain in speed. 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 in a manner similar to many published algorithms. For most other cases a third order Taylor series expansion about the nearest point in a precomputed table is used. This technique is more efficient than it would seem due to some relationships among the various derivatives. 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 10^6 of the value of the function itself for Doppler widths less than about 50 000 times the Lorentz width and always accurate to an absolute value of 10^{-12}. In addition, the derivative of the function with respect to the distance from line center and the derivative of the function with respect to the ratio of Lorentz to Doppler halfwidths are computed. The algorithm is significantly faster than the Drayson[a] or Humlicek[b] algorithms and about two orders of magnitude more accurate.
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[a]S. R. Drayson, *JQSRT* **16**, 611 (1976).
[b]J. Humlicek, *JQSRT* **27**, 437 (1982).