PROCEDURES AND SUBROUTINES FOR ANALYSIS OF SPECTRAL DATA, OF TYPES BOTH FREQUENCY AND INTENSITY, OF DIATOMIC MOLECULAR SPECIES

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In collaboration with others, I have developed procedures and subroutines for digital computers for the purpose of facilitating comprehensive analysis of spectral data, of types both frequency and intensity, of diatomic molecular species. Subroutines[a] in Fortran have been readily available through Computer Physics Library since 1983 for use in conjunction with analysis of primarily frequency data in vibration-rotational spectra, or equivalent data from electronic spectra. Other procedures[b] in Maple, which can be readily translated for execution with other symbolic processors, are accessible through the applications library at Waterloo Maple software company, with application to data of types both frequency and intensity from spectra of diatomic molecules. I summarise the nature of this software and outline its prospective applications. Efficient utilisation of this software is facilitated through acquaintance of pertinent content of a monograph[c], but can be achieved independently thereof.

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[a] http://www.cpc.cs.qub.ac.uk/cpc

[b] http://www.maplesoft.com/apps/categories/science/chemistry/acchemistry.html

[c] J. F. Ogilvie, *The Vibrational and Rotational Spectrometry of Diatomic Molecules* [Academic Press, London U.K., 1998]