THE ROTATIONAL *g* FACTOR IN ANALYSIS OF INFRARED AND RAMAN SPECTRA OF SMALL MOLECULES IN GASEOUS SAMPLES

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Although long recognised by practitioners of experiments on molecular beams and microwave spectra, the importance of effects played by the rotational *g* factor in infrared and Raman spectra measured under conditions of great resolution tends to be neglected. Both experimental and computational methods to obtain values of this quantity are well developed.[a,b] Watson included within an expression for reduced mass a correction for net electric charge on a molecular ion,[c] but numerator and denominator of this expression are intrinsically inconsistent: the function of this correction is properly assigned to the rotational *g* factor of such ions. We discuss some examples of deduction of values of the rotational *g* factor from infrared spectra of diatomic and triatomic molecular compounds, and illustrate how these values can assist and improve reduction of frequencies and wave numbers of many spectral lines to few parameters in radial functions.

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[a] J. F. Ogilvie, J. Oddershede and S. P. A. Sauer, *Adv. Chem. Phys.* **111**, 475–535 (2000)

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

[c] J. K. G. Watson, *J. Mol. Spectrosc.* **80**, 411–421 (1980)