
Spectroscopic Nomenclature

The Editors have received the following letter, about vibrational numbering in polyatomic molecules, from a group of 15 distinguished spectroscopists and photochemists.

The vibrational numbering of bands in the spectra of polyatomic molecules

In discussions of the vibrational assignments of bands of polyatomic molecules, extensive use has been made of the nomenclature introduced by Brand *et al.* [1], e.g. $2_0^2 4_0^1$, $6_0^1 16_1^1$, which first appeared in refs. 2 and 3. The principal numbers refer to the vibrations excited and the superscripts and subscripts refer to the number of quanta involved in the upper and lower states respectively. No confusion has arisen when these symbols are written but there has been some confusion when they are spoken. This unfortunate situation may have been caused by the need in some journals to stagger the superscripts and subscripts.

We *strongly recommend* that, when spoken, the superscript should precede the subscript in conformity with the recognized convention in molecular spectroscopy that the upper state precedes the lower state [4, 5]. We also recommend that, when staggering is necessary in print, the same order be followed, e.g. 4_0^1 . Reading from left to right, the assignment is then read as four-one-zero, in conformity with standard spectroscopic usage for molecules.

- 1 J. C. D. Brand, J. H. Callomon and J. K. G. Watson, personal communication, circulated to participants at the 35th Discuss. Faraday Soc. on the Structure of Electronically Excited Species in the Gas-phase, Queen's College, University of St. Andrews, April 2 - 3, 1963.
- 2 J. K. G. Watson, *Ph.D. Thesis*, University of Glasgow, 1962.
- 3 J. H. Callomon and K. K. Innes, *J. Mol. Spectrosc.*, 10 (1963) 166 - 181.
- 4 G. Herzberg, *Molecular Spectra and Molecular Structure*, Vol. I, *Spectra of Diatomic Molecules*, Van Nostrand, Princeton, NJ, 2nd edn., 1950; *Molecular Spectra and Molecular Structure*, Vol. II, *Infrared and Raman Spectra of Polyatomic Molecules*, Van Nostrand, Princeton, NJ, 1945; *Molecular Spectra and Molecular Structure*, Vol. III, *Electronic Spectra of Polyatomic Molecules*, Van Nostrand, Princeton, NJ, 1967.
- 5 R. S. Mulliken, Report on notation for the spectra of polyatomic molecules, *J. Chem. Phys.*, 23 (1955) 1997 - 2011.

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(Received April 12, 1983)