IUPAC RECOMMENDATIONS FOR NOTATIONS AND CONVENTIONS IN VIBRATIONAL-ROTATIONAL SPECTROSCOPY

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IUPAC Commission I.5 (the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division) is preparing a series of recommendations on notations and conventions in molecular spectroscopy, the first general treatment since Mulliken's report of 1955. The first three parts, on general and symmetry notation, were published last year.[a] Part 4, on rovibrational spectroscopy, is expected to appear in 1999. The outline of coverage is:

(1) Introduction: units; term values and spectroscopic constants; presentation of spectra. (2) Vibrational coordinates and force constants. (3) Vibrational states: diatomic molecules; designation of normal modes in polyatomic molecules; vibrational state labels; vibrational terms; resonances. (4) Vibrational transitions: types; notation. (5) Rotational states: rotational types; notation for linear molecules, and symmetric, spherical, and asymmetric tops. (6) Rotational transitions: notation; selection rules and transition formulas. (7) Rovibrational states, including state notation for use in electronic databases. (8) Rovibrational transitions. (9) Line shapes and intensities. (10) Possible additional topics.

The status of the project will be described, some particularly thorny issues discussed, and advice and input solicited.

[a] C. J. H. Schutte et al., *Pure Appl. Chem.* **69**, 1633–39, 141–49 (1997); P. R. Bunker et al., *ibid.* 1651–57.