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PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE AND SPECTROSCOPY*
SUBCOMMITTEE ON NOTATIONS AND CONVENTIONS FOR MOLECULAR SPECTROSCOPY

# NOTATIONS AND CONVENTIONS IN MOLECULAR SPECTROSCOPY: PART 1. GENERAL SPECTROSCOPIC NOTATION

(IUPAC Recommendations 1997)

*Prepared for publication by*

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# Notations and conventions in molecular spectroscopy: Part 1. General spectroscopic notation (IUPAC Recommendations 1997)

Abstract -- The field of *Molecular Spectroscopy* was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is *Part 1* in a series, establishes the notations and conventions used for *general spectroscopic notations* and deals with *quantum mechanics*, *quantum numbers* (vibrational states, angular momentum and energy levels), *spectroscopic transitions*, and *miscellaneous notations* (e.g. spectroscopic terms). Further parts will follow, dealing *inter alia* with *symmetry notation*, *permutation* and *permutation-inversion symmetry notation*, *vibration-rotation spectroscopy* and *electronic spectroscopy*.

## PREAMBLE

The sub-committee on Notations and Conventions in Molecular Spectroscopy was initiated by Commission I.5, the Commission on Molecular Structure and Spectroscopy, to establish and recommend a set of conventions and symbols from those that are in common use in the spectroscopic literature.

The relevant literature was surveyed and compared with the Jenkins [1] and Mulliken [2] recommendations, as well as with the IUPAP [3] and IUPAC [4] manuals of symbols and terminology. The present document contains the recommendations with respect to General Spectroscopic Notation. Further sets of recommendations will be issued covering specialized areas.

Note: It is customary to distinguish between operators, vectors, tensors, scalar quantities, etc. by means of typography. The IUPAP [3] and IUPAC [4] typographical conventions are followed: physical quantities are indicated by italics, vectors and matrices by bold italics, tensors by sans-serif bold italic characters and symbols for units in Roman (upright) type. An operator is printed with a hat (or circumflex), ^, when the hat is helpful or is necessary to avoid confusion.

## Part 1. GENERAL SPECTROSCOPIC NOTATION

1.1 Quantum Mechanics
1.2 Quantum Numbers
1.3 Spectroscopic Transitions
1.4 Miscellaneous

Symbols used in this paper

Note: Symbols such as $n$ for a general integer and $x$ for a general variable are not listed.

| Greek Alphabet and Symbols | | | |
|---|---|---|---|
| $\alpha$ | 1.1.14 | $\Omega$ | 1.2.2.15, 1.2.2.16 |
| $\beta$ | 1.1.15 | $\lvert\,\rangle$ | 1.1.5 |
| $\gamma$ | 1.1.15 | $\langle\,\rvert$ | 1.1.6 |
| $\lambda$, $\lambda_i$ | 1.3.3; 1.2.2.2 | $\langle\ \rangle$ | 1.1.7 |
| $\Lambda$ | 1.2.2.12 | $\langle\,\rvert\,\rvert\,\rangle$ | 1.1.7 |
| $\mu$, $\mu$ | 1.1.12, 1.1.13; 1.1.22 | [ , ] | 1.1.10 |
| $\nu$ | 1.3.1 | $[\ ,\ ]_+$ | 1.1.11 |
| $\tilde{\nu}$ | 1.3.2 | $'$ | 1.3.6 |
| $\Sigma$ | 1.2.2.14 | $''$ | 1.3.7 |
| $\psi$, $\psi_n$, $\psi^*$ | 1.1.3, 1.1.4 | —, ←, → | 1.3.9 |
| $\omega_i$ | 1.2.2.3 | † | 1.1.2 |



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| Latin Alphabet | | | |
|---|---|---|---|
| $\hat{A}$, $\langle A \rangle$, $A_{ij}$ | 1.1.2, 1.1.7, 1.1.9 | $\boldsymbol{L}$, $L$ | 1.1.16, 1.2.2.4, 1.2.2.12 |
| $a,b,c$ | 1.1.17.5 | $\boldsymbol{m}$, $m$ | 1.1.13; 1.1.20 |
| $c$, $c_0$ | 1.3.4 | $M_r$ | 1.1.21 |
| $D_e$, $D_0$ | 1.4.1 | $M$, $M_{subscript}$ | 1.2.2.11 |
| $\langle E \rangle$, $\Delta E$ | 1.1.8, 1.3.8 | $\boldsymbol{N}$, $N$ | 1.1.16, 1.2.2.7, 1.2.2.13 |
| $\boldsymbol{F}$, $F$ | 1.1.16, 1.2.2.9, 1.4.5 | $\boldsymbol{p}$ | 1.1.12 |
| $G$ | 1.4.4 | $P$ | 1.2.2.16 |
| $h$, $\hbar$ | 1.3.5 | $\boldsymbol{R}$, $R$ | 1.1.16, 1.2.2.5 |
| $H$, $\hat{H}$ | 1.1.1 | $\boldsymbol{S}$, $S$ | 1.1.16, 1.2.2.6 |
| $I$, $I_a$, $I_A$ | 1.1.23; | $T$, $T_e$ | 1.1.19, 1.4.2, 1.4.3 |
| $\boldsymbol{I}$, $I_i$, $I_X$ | 1.1.16, 1.2.2.10, 1.2.2.17 | $V$ | 1.1.18 |
| $\boldsymbol{J}$, $J$ | 1.1.16, 1.2.2.8 | $v_i$ | 1.2.1.1 |
| $J_{K_a K_c}$ | 1.2.3.3 | $v_i^+$, $v_i^-$ | 1.2.1.2 |
| $(J, K)$ | 1.2.3.2 | $v_i^{\ell_i}$, $v_i^{\ell_i m_i}$ | 1.2.1.5, 1.2.1.6 |
| $(J, K, M)$ | 1.2.3.1 | $X'$, $X$, $x$ | 1.1.17.1, 1.1.17.2, 1.1.17.3 |
| $k$, $K$, | 1.2.1.4, 1.2.2.13 | $Y'$, $Y$, $y$ | 1.1.17.1, 1.1.17.2, 1.1.17.3 |
| $\boldsymbol{l}$, $\ell$, $l$ | 1.1.16, 1.2.1.4, 1.2.2.1 | $Z'$, $Z$, $z$ | 1.1.17.1, 1.1.17.2, 1.1.17.3 |
| $\ell_i$, $l_i$ | 1.2.1.3; 1.2.2.1 | | |

## 1.1 QUANTUM MECHANICS

| | | |
|---|---|---|
| 1.1.1 | Hamiltonian operator | $H$, $\hat{H}$ |
| 1.1.2 | Hermitian conjugate of operator $\hat{A}$ | $\hat{A}^\dagger$ |
| 1.1.3 | Eigenfunction of operator $\hat{H}$ | $\psi$, $\psi_n$ |
| 1.1.4 | Complex conjugate of $\psi$ | $\psi^*$ |
| 1.1.5 | Dirac ket, a right-hand state function | $\lvert\,\rangle$ |
| 1.1.6 | Dirac bra, a left-hand state function | $\langle\,\rvert$ |

| | | |
|---|---|---|
| 1.1.7 | Expectation value of operator $\hat{A}$<br>$\langle \hat{A} \rangle = \langle j \mid \hat{A} \mid j \rangle$ or $\langle \hat{A} \rangle = \int \psi_j^* \hat{A} \psi_j \, \mathrm{d}\tau$ | $\langle A \rangle$ |
| 1.1.8 | Expectation value of energy | $\langle E \rangle$ |
| 1.1.9 | Matrix element of operator $\hat{A}$<br>$A_{ij} = \langle i \mid \hat{A} \mid j \rangle$ or $A_{ij} = \int \psi_i^* \hat{A} \psi_j \, \mathrm{d}\tau$ | $A_{ij}$ |
| 1.1.10 | Commutator of operators $A$ and $B$<br>$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ | $[\hat{A},\hat{B}]$ |
| 1.1.11 | Anticommutator of operators $A$ and $B$<br>$[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$ | $[\hat{A},\hat{B}]_+$ |
| 1.1.12 | Electric dipole moment | $\boldsymbol{p}$, $\mu$ |
| 1.1.13 | Magnetic dipole moment | $\boldsymbol{m}$, $\mu$ |
| 1.1.14 | Polarizability tensor | $\alpha$ |
| 1.1.15 | Hyperpolarizability tensors | $\beta$, $\gamma$ |
| 1.1.16 | Reduced angular momenta (angular momenta divided by $\hbar$) | $\boldsymbol{L}, \boldsymbol{l}, \boldsymbol{J}, \boldsymbol{S}, \boldsymbol{N}, \boldsymbol{F}, \boldsymbol{I}, \boldsymbol{R}$ |
| 1.1.17 | Right-handed cartesian coordinates | |
| 1.1.17.1 | space-fixed axes | $X', Y', Z'$ |
| 1.1.17.2 | centre-of-mass fixed axes, which are parallel to $X'Y'Z'$ and translate with molecule | $X, Y, Z$ |
| 1.1.17.3 | rotating axes (molecule-fixed axes) | $x, y, z$ |
| | Note: The orientation of $x,y,z$ with respect to the nuclei must be specified, since it is important for the symmetry species notation [2,3]. | |
| 1.1.17.4 | cartesian displacement coordinates | $\Delta x$, $\Delta y$, $\Delta z$ |
| 1.1.17.5 | principal axes of inertia | $a, b, c$ |
| 1.1.18 | Potential energy | $V$ |
| 1.1.19 | Kinetic energy | $T$ |
| 1.1.20 | Mass | $m$ |
| 1.1.21 | Relative molar mass | $M_r$ |
| 1.1.22 | Reduced mass | $\mu$ |
| 1.1.23 | Principal moments of inertia ($I_a \leq I_b \leq I_c$) | $I$ ; $I_a$, $I_b$, $I_c$ ; $I_A$, $I_B$, $I_C$ |

## 1.2 QUANTUM NUMBERS

### 1.2.1 Vibrational States

| | | |
|---|---|---|
| 1.2.1.1 | vibrational | $v_i$ |
| 1.2.1.2 | vibrational, with inversion doubling | $v_i^+, v_i^-$ |
| 1.2.1.3 | component of vibrational angular momentum around molecular axis for degenerate vibration $v_i$ of linear or symmetric top molecule | $\ell_i, l_i$ |
| 1.2.1.4 | resultant vibrational angular momentum for linear molecule | $k, \ell, l$ |
| 1.2.1.5 | for doubly degenerate vibrations $v_i$ of linear, symmetric or spherical top molecules with quantum number $l_i$ for vibrational angular momentum around molecular axis | $v_i^{\ell_i}$ |
| 1.2.1.6 | for triply degenerate vibrations of spherical top molecules with quantum numbers $\ell_i$ and $m_i$ for the vibrational angular momentum and its axial component, respectively | $v_i^{\ell_i m_i}$ |

### 1.2.2 Angular Momenta

In this section the three symbols at the end of each line are quantum numbers for, in order, diatomic, linear polyatomic, and non-linear polyatomic molecules. For the last type, the molecular axis is the symmetry axis for symmetric tops, but may be arbitrarily chosen for asymmetric or spherical tops.

| | | | | |
|---|---|---|---|---|
| 1.2.2.1 | orbital angular momentum $\boldsymbol{l}$ for single electron $i$ | $\ell_i$ | $\ell_i$ | $\ell_i$ |
| 1.2.2.2 | component of the orbital angular momentum $\boldsymbol{l}$ of a single electron $i$ parallel to the molecular axis | $\lambda_i$ | $\lambda_i$ | $\lambda_i$ |
| 1.2.2.3 | projection of the total angular momentum of a single electron $i$ on the molecular axis (Rydberg-type case c) | $\omega_i$ | $\omega_i$ | $\omega_i$ |
| 1.2.2.4 | total orbital angular momentum; $\boldsymbol{L}$ | $L$ | $L$ | $L$ |
| 1.2.2.5 | rotational angular momentum; $\boldsymbol{R}$ | $R$ | $R$ | $R$ |
| 1.2.2.6 | total electron spin angular momentum; $\boldsymbol{S}$ | $S$ | $S$ | $S$ |
| 1.2.2.7 | total angular momentum excluding electron and nuclear spins; $\boldsymbol{N}$ | $N$ | $N$ | $N$ |
| 1.2.2.8 | total angular momentum of the molecule excluding nuclear spins; $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$ | $J$ | $J$ | $J$ |
| 1.2.2.9 | total angular momentum; $\boldsymbol{F}$ | $F$ | $F$ | $F$ |
| 1.2.2.10 | angular momentum of nuclear spin $\boldsymbol{I}$ for one nucleus $i$ (subscript may be left out) | $I_i$ | $I_i$ | $I_i$ |

| | | | | |
|---|---|---|---|---|
| 1.2.2.11 | projection of an angular momentum on axis of (axially-symmetrical) electric or magnetic field* | | | |
| | (a) for $\boldsymbol{L}$ | $M_L$ | $M_L$ | $M_L$ |
| | (b) for $\boldsymbol{S}$ | $M_S$ | $M_S$ | $M_S$ |
| | (c) for nuclear spin $\boldsymbol{I}$ | $M_I$ | $M_I$ | $M_I$ |
| | (d) for $\boldsymbol{N}$ | $M_N$ | $M_N$ | $M_N$ |
| | (e) for $\boldsymbol{J}$ | $M_J$ | $M_J$ | $M_J$ |
| | or, when unambiguous | $M$ | $M$ | $M$ |
| | (f) for $\boldsymbol{F}$ | $M_F$ | $M_F$ | $M_F$ |

* In the NMR literature the symbol $m$ is used instead of $M$. The lower case symbol is useful for signed quantum numbers, with $M = |m|$

| | | | | |
|---|---|---|---|---|
| 1.2.2.12 | projection of the resultant orbital angular momentum $\boldsymbol{L}$ on the molecular axis (Hund's cases (a) and (b) in the case of a diatomic molecule) | $\Lambda$ | $\Lambda$ | $\Lambda$ |
| 1.2.2.13 | component of the angular momentum $\boldsymbol{N}$ along the axis of a symmetric (or quasi-symmetric) rotor; for linear molecules $K$ describes the component of the vibronic angular momentum (excluding spin) along the axis | $\Lambda$ | $K, k$ | $K, k$ |
| 1.2.2.14 | projection of $\boldsymbol{S}$ on the molecular axis; for $K \neq 0$ the sign of $\Sigma$ is + or – depending on whether the component of vector $\boldsymbol{S}$ has the same or opposite direction to the axial component of $\boldsymbol{N}$ | $\Sigma$ | $\Sigma$ | $\Sigma$ |
| 1.2.2.15 | component of the total electronic angular momentum $\boldsymbol{L}+\boldsymbol{S}$ on the molecular axis (cases (a) and (c)) | $\Omega$ | $\Omega$ | $\Omega$ |
| 1.2.2.16 | component of the total angular momentum $\boldsymbol{J}$ along the principal symmetry axis when vector $\boldsymbol{S}$ is tightly coupled to latter; for linear molecules $P = \sum_i \ell_i + \Lambda + \Sigma$ and for symmetric or quasi-symmetric rotors $P = \sum_i \ell_i + K + \Sigma$ | $\Omega$ | $P$ | $P$ |
| 1.2.2.17 | resultant angular momentum of nuclear spins of equivalent atoms with atomic symbol X | $I_X$ | $I_X$ | $I_X$ |

1.2.3 Energy Levels

| | | |
|---|---|---|
| 1.2.3.1 | energy levels and states are referred to by their set of relevant quantum numbers, e.g. | $(J, K, M)$ |
| 1.2.3.2 | symbol for quantized rotational levels of symmetric rotors | $(J, K)$ |
| 1.2.3.3 | symbol for quantized rotational levels of asymmetric rotors | $J_{K_a K_c}$ |

## 1.3 SPECTROSCOPIC TRANSITIONS

| | | |
|---|---|---|
| 1.3.1 | Transition frequency | $\nu$ |
| 1.3.2 | Transition wavenumber* | $\tilde{\nu}$ |
| 1.3.3 | Transition wavelength | $\lambda$ |
| 1.3.4 | Speed of light, speed of light in vacuum | $c$, $c_0$ |
| 1.3.5 | Planck constant, Planck constant divided by $2\pi$ | $h$, $\hbar$ |
| 1.3.6 | Upper state quantities, right superscript | $'$ |
| 1.3.7 | Lower state quantities, right superscript | $''$ |
| 1.3.8 | Numerical difference between upper state and lower state quantities,** e.g., $\Delta E = E' - E''$ | e.g., $\Delta E$, $\Delta J$ |
| 1.3.9 | Signs indicating a transition between levels $a'$ and $a''$ ** | |
| | (a) general transition | $a' - a''$ |
| | (b) absorption (when needed) | $a' \leftarrow a''$ |
| | (c) emission (when needed) | $a' \rightarrow a''$ |

## 1.4 MISCELLANEOUS

| | | |
|---|---|---|
| 1.4.1 | Dissociation energy | |
| | (a) referred to potential energy minimum | $D_e$ |
| | (b) referred to vibrational ground level | $D_0$ |
| 1.4.2 | Total term value*** $T = T_e + G + F$ | $T$ |
| 1.4.3 | Electronic term value | $T_e$ |
| 1.4.4 | Vibrational term value | $G$ |
| 1.4.5 | Rotational term value | $F$ |

* The customary unit of wavenumber is $cm^{-1}$ in molecular spectroscopy. $\tilde{\nu}$ is used to denote wavenumber in vacuum, i.e., $\tilde{\nu} = \nu / c_0$.

** The upper state ( $'$ ) should *always* be written first and the lower state ( $''$ ) second, irrespective of whether absorption or emission is intended.

***The name "term value" is generally used to denote energies represented in wavenumber units (usually $cm^{-1}$), but pure rotational or hyperfine term values may be expressed in frequency units (usually kHz, MHz, or GHz). In general, the context will make it clear whether wavenumber or frequency units are implied; if a distinction is required, a tilde may be added to wavenumber quantities as in the equations $\nu = c_0\tilde{\nu}$, $B = c_0\tilde{B}$, $T = c_0\tilde{T}$, etc.

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