HITRAN2020 supplementary material:
Description of upper- and lower-state quanta

1. Summary

The identifications of quantum numbers of energy levels or states provided in the line-by-line section of the HITRAN database have previously been described in the HITRAN2004 paper [1]. Since then, many new molecules have been added to the HITRAN database, and adjustments have been made to the formats of some molecules and isotopologues to include additional information. The following tables will outline the quantum number formats (as of HITRAN2020 [2]) that are provided as part of the traditional (default) ".par" output format (see `www.hitran.org/lbl/`) of HITRAN2020. It should be noted that ".par" is a fixed-length ASCII format; therefore some molecules required individual solutions for fitting all the available quantum information in the limited space. The relational structure of the database also supports the XSAMS format (explained at `http://www.vamdc.org/documents/cbc-1.0/`), which can be retrieved by creating a custom output format, and has the capability to store more detailed quantum information.

2. Format overview

The quantum numbers are divided into "global" and "local", each with an upper-state and lower-state field. These fields constitute 15 alphanumeric characters and contain the information used to identify specific transitions. For users of HITRAN Application Programming Interface (HAPI) [3] (`www.hitran.org/hapi/`), the fields are named `global_upper_state`, `global_lower_state`, `local_upper_state`, and `local_lower_state`. Traditionally the global quanta were used to describe the vibrational (and occasionally, electronic) states, whereas the local quanta were used to describe the rotational, fine, and hyperfine structure levels. While this is generally still the case for the majority of molecules in HITRAN2020, for some molecules (e.g., C_4H_2) the information is shared between the global and local fields due to a large number of vibrational modes and space limitations in the global quanta fields.

The tables and descriptions below provide the format details of the global and local fields for each molecule. It should be noted that not all quantum numbers are completed for all transitions of a specific molecule. In some instances, every quantum number is not necessary for unique identifications, or are unavailable for transitions of a molecule (e.g., hyperfine structure quanta are not provided when it is not resolved). For unassigned lines, the quanta are typically blank. In the case of partially assigned transitions for H_2O, CO_2, and $H^{13}CN$, a negative integer "-2" is used to indicate the lack of vibrational assignments. In addition, negative integers are also used in place of K_a and K_c rotational quanta for H_2O to provide symmetry information as described in the HITRAN2012 paper [4]. For NH_3, special characters have been used to identify partial assignments (see Table 7 of Ref. [4]).

2.1. Global quanta in Table S1

Table S1 describes the notation and format of the upper and lower global quantum identifications (i.e., `global_upper_state` and `global_lower_state`). The molecules have been separated into nine classes (broadly based on molecular symmetry), with each class further subdivided where necessary. The right-hand column describes the specific quantum identifications used for each molecule, with their FORTRAN descriptors given beneath each variable (blank characters are indicated, for example, as $\overline{13X}$ for thirteen blank characters). In each class, the vibrational quantum number associated with the ith normal mode is indicated as v_i, with l_j providing the vibrational angular momentum quantum number associated with the degenerate bending mode j. Diatomic molecules with $^2\Pi$ electronic ground

states (e.g., NO, OH, ClO), or different electronic states (e.g., O_2, SO), require X to designate the electronic state of the molecule. For instance, the letter notation for the electronic states of OH are X for ground electronic state, and A for the excited electronic state. In addition, for the $^2\Pi$ molecules, the projection of total (orbital plus electron spin) angular momentum, Ω, can equal $\frac{1}{2}$ or $\frac{3}{2}$, which means that $N = J \pm \frac{1}{2}$ depending on the molecule [5, pp. 223–234]. For some ultraviolet bands of O_2, the Ω parameter is also needed for unique identification. Class 2a describes CO_2, which contains large Fermi resonances and therefore requires the additional r ranking identifier (see Ref. [6], Sect. 2a). Class 4a describes the notation for pyramidal tetratomic molecules, where S is the symmetry of the level. The notation used in HITRAN for $^{14}NH_3$ was expanded in HITRAN2012 [4], see also Ref. [7] for additional descriptions. Linear polyatomic molecules in Class 5 require separate descriptions due to the number of active vibrational modes. For C_2H_2 (Class 5a) the parity u/g of the vibrational level is provided in the S field, with the symmetry type of Σ vibrational states ($l_3 + l_4 = 0$) indicated with $+/-$. For C_4H_2 (Class 5b), the e/f symmetry is given by Sym, but the bending mode quantum numbers (l_6, l_7, l_8, and l_9) are provided in the local quanta (see Table S2). For C_2N_2 (Class 5d), the Plíva notation [8, 9], previously used for acetylene, is retained, where $l = |l_3 + l_4|$ and r is a ranking number. The notation used for H_2O_2 is described in Class 6b, where the torsional quanta n and τ are included and described in Refs. [10, 11]. SO_3 is a planar symmetric molecule (Class 7) and was first added to HITRAN for the 2012 edition [4]; further descriptions of the symmetries are given in Ref. [12]. For spherical top molecules/isotopologues in Class 8, n is a multiplicity index and C is the symmetry. For molecules in Class 9, the upper- and lower-state global information is explicitly described and aligned to the right of the field (example notation includes: `V1`, `2V2`, `V3+V4`, and `GROUND`).

2.2. Local quanta in Table S2

Table S2 describes the notation and format of the upper and lower local quantum identifications (i.e., `local_upper_state` and `local_lower_state`). The molecules have been separated into seven broad groups (again based on molecular symmetry), with each class further subdivided where necessary. The second and third columns describe the specific upper-state (indicated with $'$) and lower-state (indicated with $''$) local quantum numbers, with their FORTRAN descriptors given beneath each variable (blank characters are indicated, for example, as $\overline{10X}$ for ten blank characters). In each group, J is the quantum number associated with the total angular momentum, excluding nuclear spin, and F is the quantum number associated with the total angular momentum including nuclear spin. When included, Br is used to note the branch (i.e., O, P, Q, R, or S) and Sym identifies the symmetry/parity as e/f (rotationless parity) for l-type doubling, but can also be $+/-$ for required symmetry symbols (or d/q when denoting magnetic dipole or electric quadrupole transitions for N_2 and H_2). For asymmetric rotors (Group 1), the projections of angular momentum on the molecular a and c axes (i.e., K_a and K_c) are also included. For Group 2a molecules, the m descriptor is included to identify magnetic dipole transitions of CO_2 introduced in HITRAN2020. The notation used for C_4H_2 (Group 2b) includes the vibrational bending mode quantum numbers l_6, l_7, l_8, and l_9, which for other molecules are included in the global quanta. For spherical rotors (Group 3), the notations C and α are described in Ref. [13]. Since α is not always consistent between different reference sources, all values of $\alpha \geq 999$ are set to equal 999. For symmetric rotors belonging to Group 4a, l and the symmetry C are described in Refs. [14, 15]. For $^{14}NH_3$ (Group 4b), the notation was expanded in HITRAN2012 [4], with additional descriptions of the symmetries given in Ref. [7]. For C_2H_6 (Group 4c), the symmetry notation is explained in the HITRAN2008 paper [16]. For planar symmetric molecules (Group 5), additional descriptions of the symmetries are given in Ref. [12]. For molecules with $^3\Sigma$ ground electronic states (Group 6), the M field is used to identify the magnetic dipole transitions, electric quadrupole transitions, and far wing absorption (denoted d, q, and g, respectively), and the branches (Br) of the total orbital angular momentum N and J are included separately. For molecules with $^2\Pi$ ground electronic states (Group 7), the branch (Br) field describes both N and J, and the symmetry for OH (Group 7b) contains the upper- and lower-state values (e/f).

Table S1: Notation and format for the nine classes of global quanta identifications used in HITRAN2020.

Class definition for HITRAN molecules	Upper- and lower-state "global" quanta

Class 1: Diatomic molecules

a) CO, HF, HCl, HBr, HI, N_2, NO^+, H_2, CS

$\overline{13X}$	v_1
	I2

b) O_2, NO, OH, ClO, SO

$\overline{6X}$	X	Ω	$\overline{2X}$	v_1
	A2	A3		I2

Class 2: Linear triatomic molecules

a) CO_2

$\overline{6X}$	v_1	v_2	l_2	v_3	r
	I2	I2	I2	I2	I1

b) N_2O, OCS, HCN, CS_2

$\overline{7X}$	v_1	v_2	l_2	v_3
	I2	I2	I2	I2

Class 3: Non-linear triatomic molecules
H_2O, O_3, SO_2, NO_2, HOCl, H_2S, HO_2, HOBr

$\overline{9X}$	v_1	v_2	v_3
	I2	I2	I2

Class 4: Pyramidal tetratomic molecules

a) $^{15}NH_3$, PH_3, NF_3

$\overline{5X}$	v_1	v_2	v_3	v_4	S
	I2	I2	I2	I2	A2

b) $^{14}NH_3$

$\overline{1X}$	v_1	v_2	v_3	v_4	$\overline{1X}$	l_3	l_4	$\overline{1X}$	l	$\overline{1X}$	Γ_{vib}
	I1	I1	I1	I1		I1	I1		I1		A4

Class 5: Linear polyatomic molecules

a) C_2H_2

$\overline{1X}$	v_1	v_2	v_3	v_4	v_5	l_4	l_5	$\pm$	$\overline{1X}$	S
	I1	I1	I1	I2	I2	I2	I2	A1		A1

b) C_4H_2

$\overline{1X}$	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	$\overline{1X}$	Sym	$\overline{1X}$	S
	I1	I1	I1	I1	I1	I1	I1	I1	I1		A1		A2

c) HC_3N

$\overline{2X}$	v_1	v_2	v_3	v_4	v_5	v_6	v_7	l_5	l_6	l_7
	I1	I1	I1	I1	I1	I1	I1	I2	I2	I2

d) C_2N_2

v_1	v_2	v_3	v_4	v_5	l	$\pm$	r	S
I2	I2	I2	I2	I2	I2	A1	I1	A1

Class 6: Asymmetric top molecules

a) H_2CO, COF_2, $COCl_2$

$\overline{3X}$	v_1	v_2	v_3	v_4	v_5	v_6
	I2	I2	I2	I2	I2	I2

b) H_2O_2

$\overline{3X}$	v_1	v_2	v_3	n	τ	v_5	v_6
	I2	I2	I2	I1	I1	I2	I2

Class 7: Planar symmetric molecules
SO_3

v_1	v_2	v_3	l_3	v_4	l_4	Γ_{vib}
I2	I2	I2	I2	I2	I2	A3

Class 8: Spherical top molecules/isotopologues
$^{12}CH_4$, $^{13}CH_4$, CF_4, GeH_4

$\overline{3X}$	v_1	v_2	v_3	v_4	n	C
	I2	I2	I2	I2	A2	A2

Class 9: The following molecules/isotopologues have explicit global quantum number notation

$^{12}CH_3D$, $^{13}CH_3D$, HNO_3, CH_3Cl, C_2H_6, SF_6, HCOOH, $ClONO_2$, C_2H_4, CH_3OH, CH_3Br, CH_3CN, CH_3F, CH_3I

Vibrational band
A15

Table S2: Notation and format for the seven groups of local quanta identification used in HITRAN2020.

Group classification and HITRAN molecules	Upper-state local quanta	Lower-state local quanta

Group 1: Asymmetric rotors
H_2O^a, O_3, SO_2, $NO_2{}^b$, HNO_3, H_2CO, HOCl, H_2O_2, COF_2, H_2S, HCOOH, $HO_2{}^b$, $ClONO_2$, HOBr, C_2H_4, $COCl_2$

	J'	K'_a	K'_c	F'	Sym'		J''	K''_a	K''_c	F''	Sym''
	I3	I3	I3	A5	A1		I3	I3	I3	A5	A1

Group 2: Closed-shell diatomic and linear molecules

a) CO_2, N_2O, CO, HF, HCl, HBr, HI, OCS, $N_2{}^c$, HCN, C_2H_2, NO^+, HC_3N, $H_2{}^c$, CS, C_2N_2, CS_2

	m		F'		Br	J''	Sym''	F''
	A1	$\overline{9X}$	A5	$\overline{5X}$	A1	I3	A1	A5

b) C_4H_2

	l'_6	l'_7	l'_8	l'_9		l''_6	l''_7	l''_8	l''_9		Br	J''	Sym''	
	A2	A2	A2	A2	$\overline{7X}$	A2	A2	A2	A2	$\overline{1X}$	A1	I3	A1	$\overline{1X}$

Group 3: Spherical rotors
$^{12}CH_4$, $^{13}CH_4$, SF_6, CF_4, GeH_4

		J'	C'	α'	F'			J''	C''	α''	F''
	$\overline{2X}$	I3	A2	I3	A5		$\overline{2X}$	I3	A2	I3	A5

Group 4: Symmetric rotors

a) $^{12}CH_3D$, $^{13}CH_3D$, $^{15}NH_3$, CH_3Cl, PH_3, CH_3OH, CH_3Br, CH_3CN, CH_3F, CH_3I, NF_3

	J'	K'	l'	C'	Sym'	F'		J''	K''	l''	C''	Sym''	F''
	I3	I3	I2	A2	A1	A4		I3	I3	I2	A2	A1	A4

b) $^{14}NH_3$

	J'	K'	l'		Γ'_{rot}	Γ'_{tot}			J''	K''	l''		Γ''_{rot}	Γ''_{tot}	
	I2	I3	I2	$\overline{1X}$	A3	A3	$\overline{1X}$		I2	I3	I2	$\overline{1X}$	A3	A3	$\overline{1X}$

c) C_2H_6

	J'	K'	l'	Sym'	F'		J''	K''	l''	Sym''	F''
	I3	I3	I2	A3	A4		I3	I3	I2	A3	A4

Group 5: Planar symmetric molecules
SO_3

		J'	K'		Γ'_{tot}				J''	K''		Γ''_{rot}	
	$\overline{3X}$	I3	I3	$\overline{2X}$	A3	$\overline{1X}$		$\overline{3X}$	I3	I3	$\overline{2X}$	A3	$\overline{1X}$

Group 6: Open-shell diatomics with $^3\Sigma$ ground electronic states
O_2, SO

	F'		Br	N''	Br	J''	F''	M
	$\overline{10X}$ A5	$\overline{1X}$	A1	I3	A1	I3	A5	A1

Group 7: Open-shell diatomics with $^2\Pi$ ground electronic states

a) NO, ClO

	m		F'		Br	J''	Sym''	F''
	A1	$\overline{9X}$	A5	$\overline{2X}$	A2	F5.1	A1	A5

b) OH^d

	F'		Br	J''	Sym''	F''
	$\overline{10X}$ A5	$\overline{1X}$	A2	F5.1	A2	A5

[a] For H_2O, the Sym'' field is used to indicate electric quadrupole transitions (q).

[b] For NO_2 and HO_2, N (the total rotational angular momentum) is used in place of J. The Sym field is used to represent the J-coding where $+$ indicates that $J = N + 1/2$ and $-$ indicates that $J = N - 1/2$.

[c] For N_2 and H_2, the Sym'' field is used to indicate magnetic dipole (d) and electric quadruple (q) transitions.

[d] For OH, the format of Sym field in the lower-state quanta accommodates the upper- and lower-state symmetry (e/f).

References for supplementary material

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