

# HITRAN2024 supplementary material:

## Description of upper-state 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 been originally described in HITRAN2004 [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 outline the quantum number formats (as of HITRAN2024 [2]) that are provided as part of the traditional (default) “.par” output format (see [www.hitran.org/1b1/](http://www.hitran.org/1b1/)) of HITRAN2024. 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 schema (explained at <https://amdis.iaea.org/cbc/>), 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/](http://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 HITRAN2024, 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 often 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  $i^{\text{th}}$  normal mode is indicated as  $v_i$ , with  $l_j$  providing the vibrational angular momentum quantum number associated with the degenerate bending mode  $j$ .

The following bullet points provide additional information on the upper-state quanta for each class of molecule given in Table S1:

- Diatomic molecules (Class 1) with  $^2\Pi$  electronic ground states (e.g., NO, OH, ClO), or different electronic states (e.g., O<sub>2</sub>, SO, S<sub>2</sub>), 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,  $\Omega$ , 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<sub>2</sub>, the  $\Omega$  parameter is also needed for unique identification.
- Class 2a describes CO<sub>2</sub>, which contains large Fermi resonances and therefore requires the additional *r* ranking identifier (see Ref. [6], Sect. 2a). Standardized notation for additional linear molecules in HITRAN are given in Class 2b.
- Class 3 includes the normal vibrational modes of non-linear triatomic molecules.
- Class 4 describes the notation for pyramidal tetratomic molecules. For Class 4a, *S* provides the symmetry of the level. The notation used for <sup>14</sup>NH<sub>3</sub> was expanded in HITRAN2012 [4] and was also adopted for <sup>15</sup>NH<sub>3</sub> in HITRAN2024 [2] (see also Ref. [7] for additional descriptions of the quantum notation).
- Linear polyatomic molecules in Class 5 require separate descriptions due to the number of active vibrational modes. For C<sub>2</sub>H<sub>2</sub> (Class 5a) the parity *u/g* of the vibrational level is provided in the *S* field, with the symmetry type of  $\Sigma$  vibrational states ( $l_3 + l_4 = 0$ ) indicated with  $+/-$ . For C<sub>4</sub>H<sub>2</sub> (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<sub>2</sub>N<sub>2</sub> (Class 5d), the Pliva notation [8, 9], previously used for acetylene, is retained, where  $l = |l_3 + l_4|$  and *r* is a ranking number.
- Class 6 includes the normal vibrational modes of asymmetric top molecules. The notation specifically used for H<sub>2</sub>O<sub>2</sub> is described in Class 6b, where the torsional quanta *n* and  $\tau$  are included and described in Refs. [10, 11].
- Planar symmetric molecules are described in Class 7. SO<sub>3</sub> was first added to HITRAN for the 2012 edition [4] (further descriptions of the symmetries are given in Ref. [12]). CH<sub>3</sub> was added for HITRAN2024 and has the same format as SO<sub>3</sub>, but H<sub>3</sub><sup>+</sup> includes the total state symmetry following the notation described in Ref. [13].
- 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 ( $d$  or  $q$  when denoting magnetic dipole or electric quadrupole transitions for  $N_2$  and  $H_2$ ).

The following bullet points provide additional information on the lower-state quanta for each symmetry group of molecules described in Table S2:

- 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. The  $Sym''$  field for  $H_2O$  is used to identify magnetic dipole or quadrupole transitions ( $q$ ). For  $NO_2$  and  $HO_2$ , the total rotational angular momentum ( $N$ ) is used in the field for  $J$  and the  $Sym$  field is used to represent the  $J$ -coding (where + indicates that  $J = N + 1/2$  and - indicates that  $J = N - 1/2$ ). In addition, the  $Sym''$  field for HONO is used to differentiate between trans ( $t$ ) and cis ( $c$ ) isomers.
- For Group 2a molecules, the  $m$  descriptor is included to identify magnetic dipole transitions of  $CO_2$  introduced in HITRAN2020. For  $N_2$  and  $H_2$ , the  $Sym''$  field identifies electric quadrupole or magnetic dipole transitions as  $q/m$ . 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  $\alpha$  are described in Ref. [14]. Since  $\alpha$  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. [15, 16]. For ammonia (Group 4b), the notation was expanded for  $^{14}NH_3$  in HITRAN2012 [4] and for  $^{15}NH_3$  in HITRAN2024 [2], 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 [17].
- For planar symmetric molecules (Group 5), additional descriptions of the symmetries used for  $SO_3$  and  $CH_3$  are given in Ref. [12]. The notation used for  $H_3^+$  (Group 5b) is described in Bowsman et al. [13]. It requires  $G$  (see Ref. [18]) and also follows the  $U$ -notation of Watson [19] to differentiate between states with equivalent vibrational,  $J$ , and  $G$  assignments. Here,  $U$  identifies the upper/lower ( $u/l$ ) energy levels of the same assignment, with  $m$  identifying levels when the distinction is not required.
- 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 HITRAN2024.

Class definition for HITRAN molecules	Upper- and lower-state “global” quanta													
<b>Class 1: Diatomic molecules</b>														
a) CO, HF, HCl, HBr, HI, N <sub>2</sub> , NO <sup>+</sup> , H <sub>2</sub> , CS						$\overline{13X}$	v I2							
b) O <sub>2</sub> , NO, OH, ClO, SO, S <sub>2</sub>	$\overline{6X}$	X A2	$\Omega$ A3			$\overline{2X}$	v I2							
<b>Class 2: Linear triatomic molecules</b>														
a) CO <sub>2</sub>	$\overline{6X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	$l_2$ I2	v <sub>3</sub> I2	$r$ I1								
b) N <sub>2</sub> O, OCS, HCN, CS <sub>2</sub>	$\overline{7X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	$l_2$ I2	v <sub>3</sub> I2									
<b>Class 3: Non-linear triatomic molecules</b>														
H <sub>2</sub> O, O <sub>3</sub> , SO <sub>2</sub> , NO <sub>2</sub> , HOCl, H <sub>2</sub> S, HO <sub>2</sub> , HOBr				$\overline{9X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2							
<b>Class 4: Pyramidal tetratomic molecules</b>														
a) PH <sub>3</sub> , NF <sub>3</sub>				$\overline{5X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	v <sub>4</sub> I2	S A2					
b) <sup>14</sup> NH <sub>3</sub> , <sup>15</sup> NH <sub>3</sub> ,	$\overline{1X}$	v <sub>1</sub> I1	v <sub>2</sub> I1	v <sub>3</sub> I1	v <sub>4</sub> I1	$l_3$ I1	$l_4$ I1	$l$ I1	$\Gamma_{\text{vib}}$ A4					
<b>Class 5: Linear polyatomic molecules</b>														
a) C <sub>2</sub> H <sub>2</sub>				$\overline{1X}$	v <sub>1</sub> I1	v <sub>2</sub> I1	v <sub>3</sub> I1	v <sub>4</sub> I2	v <sub>5</sub> I2	$l_4$ I2	$l_5$ I2	$\pm$ A1	S A1	
b) C <sub>4</sub> H <sub>2</sub>	$\overline{1X}$	v <sub>1</sub> I1	v <sub>2</sub> I1	v <sub>3</sub> I1	v <sub>4</sub> I1	v <sub>5</sub> I1	v <sub>6</sub> I1	v <sub>7</sub> I1	v <sub>8</sub> I1	v <sub>9</sub> I1	$Sym$ A1	$\overline{1X}$	S A2	
c) HC <sub>3</sub> N				$\overline{2X}$	v <sub>1</sub> I1	v <sub>2</sub> I1	v <sub>3</sub> I1	v <sub>4</sub> I1	v <sub>5</sub> I1	v <sub>6</sub> I1	v <sub>7</sub> I1	$l_5$ I2	$l_6$ I2	$l_7$ I2
d) C <sub>2</sub> N <sub>2</sub>					v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	v <sub>4</sub> I2	v <sub>5</sub> I2	$l$ I2	$\pm$ A1	$r$ I1	S A1	
<b>Class 6: Asymmetric top molecules</b>														
a) H <sub>2</sub> CO, COF <sub>2</sub> , COCl <sub>2</sub>				$\overline{3X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	v <sub>4</sub> I2	v <sub>5</sub> I2	v <sub>6</sub> I2				
b) H <sub>2</sub> O <sub>2</sub>				$\overline{3X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	$n$ I1	$\tau$ I1	v <sub>5</sub> I2	v <sub>6</sub> I2			
<b>Class 7: Planar symmetric molecules</b>														
a) SO <sub>3</sub> , CH <sub>3</sub>					v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	$l_3$ I2	v <sub>4</sub> I2	$l_4$ I2	$\Gamma_{\text{vib}}$ A3			
b) H <sub>3</sub> <sup>+</sup>							v <sub>1</sub> $\overline{5X}$	v <sub>2</sub> I2	$l_2$ I2	$\overline{1X}$	$\Gamma_{\text{tot}}$ A3			
<b>Class 8: Spherical top molecules/isotopologues</b>														
<sup>12</sup> CH <sub>4</sub> , <sup>13</sup> CH <sub>4</sub> , CF <sub>4</sub> , GeH <sub>4</sub>				$\overline{3X}$	v <sub>1</sub> I2	v <sub>2</sub> I2	v <sub>3</sub> I2	v <sub>4</sub> I2	$n$ A2	$C$ A2				
<b>Class 9: The following molecules/isotopologues have explicit global quantum number notation</b>														
<sup>12</sup> CH <sub>3</sub> D, <sup>13</sup> CH <sub>3</sub> D, HNO <sub>3</sub> , CH <sub>3</sub> Cl, C <sub>2</sub> H <sub>6</sub> , SF <sub>6</sub> , HCOOH, ClONO <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , CH <sub>3</sub> OH, CH <sub>3</sub> Br, CH <sub>3</sub> CN, CH <sub>3</sub> F, CH <sub>3</sub> I, COFCl, HONO, ClNO <sub>2</sub>											Vibrational band A15			

Table S2: Notation and format for the seven groups of local quanta identification used in HITRAN2024.

Group classification and HITRAN molecules	Upper-state “local” quanta					Lower-state “local” quanta				
<b>Group 1: Asymmetric rotors</b>										
H <sub>2</sub> O <sup>a</sup> , O <sub>3</sub> , SO <sub>2</sub> , NO <sub>2</sub> <sup>b</sup> , HNO <sub>3</sub> , H <sub>2</sub> CO, HOCl, H <sub>2</sub> O <sub>2</sub> , COF <sub>2</sub> , H <sub>2</sub> S, HCOOH, HO <sub>2</sub> <sup>b</sup> , ClONO <sub>2</sub> , HOBr, C <sub>2</sub> H <sub>4</sub> , COCl <sub>2</sub> , COFCl, HONO <sup>c</sup> , ClNO <sub>2</sub>	<i>J'</i>	<i>K'<sub>a</sub></i>	<i>K'<sub>c</sub></i>	<i>F'</i>	<i>Sym'</i>	<i>J''</i>	<i>K''<sub>a</sub></i>	<i>K''<sub>c</sub></i>	<i>F''</i>	<i>Sym''</i>
	I3	I3	I3	A5	A1	I3	I3	I3	A5	A1
<b>Group 2: Closed-shell diatomic and linear molecules</b>										
a) CO <sub>2</sub> , N <sub>2</sub> O, CO, HF, HCl, HBr, HI, OCS, N <sub>2</sub> <sup>d</sup> , HCN, C <sub>2</sub> H <sub>2</sub> , NO <sup>+</sup> , HC <sub>3</sub> N, H <sub>2</sub> <sup>d</sup> , CS, C <sub>2</sub> N <sub>2</sub> , CS <sub>2</sub>			<i>m</i>		<i>F'</i>		<i>Br</i>	<i>J''</i>	<i>Sym''</i>	<i>F''</i>
			A1	$\overline{9X}$	A5	$\overline{5X}$	A1	I3	A1	A5
b) C <sub>4</sub> H <sub>2</sub>	<i>l'<sub>6</sub></i>	<i>l'<sub>7</sub></i>	<i>l'<sub>8</sub></i>	<i>l'<sub>9</sub></i>		<i>l''<sub>6</sub></i>	<i>l''<sub>7</sub></i>	<i>l''<sub>8</sub></i>	<i>l''<sub>9</sub></i>	
	A2	A2	A2	A2	$\overline{7X}$	A2	A2	A2	A2	$\overline{1X}$
							<i>Br</i>	<i>J''</i>	<i>Sym''</i>	
							A1	I3	A1	$\overline{1X}$
<b>Group 3: Spherical rotors</b>										
<sup>12</sup> CH <sub>4</sub> , <sup>13</sup> CH <sub>4</sub> , SF <sub>6</sub> , CF <sub>4</sub> , GeH <sub>4</sub>		<i>J'</i>	<i>C'</i>	<i>α'</i>	<i>F'</i>		<i>J''</i>	<i>C''</i>	<i>α''</i>	<i>F''</i>
	$\overline{2X}$	I3	A2	I3	A5	$\overline{2X}$	I3	A2	I3	A5
<b>Group 4: Symmetric rotors</b>										
a) <sup>12</sup> CH <sub>3</sub> D, <sup>13</sup> CH <sub>3</sub> D, CH <sub>3</sub> Cl, PH <sub>3</sub> , CH <sub>3</sub> OH, CH <sub>3</sub> Br, CH <sub>3</sub> CN, CH <sub>3</sub> F, CH <sub>3</sub> I, NF <sub>3</sub>	<i>J'</i>	<i>K'</i>	<i>l'</i>	<i>C'</i>	<i>Sym'F'</i>	<i>J''</i>	<i>K''</i>	<i>l''</i>	<i>C''</i>	<i>Sym''F''</i>
	I3	I3	I2	A2	A1 A4	I3	I3	I2	A2	A1 A4
b) <sup>14</sup> NH <sub>3</sub> , <sup>15</sup> NH <sub>3</sub>	<i>J'</i>	<i>K'</i>	<i>l'</i>		<i>Γ'<sub>rot</sub></i>	<i>Γ'<sub>tot</sub></i>				
	I2	I3	I2	$\overline{1X}$	A3	A3	$\overline{1X}$	A3	A3	$\overline{1X}$
c) C <sub>2</sub> H <sub>6</sub>	<i>J'</i>	<i>K'</i>	<i>l'</i>		<i>Sym'F'</i>		<i>J''</i>	<i>K''</i>	<i>l''</i>	<i>Sym''F''</i>
	I3	I3	I2	A3	A4		I3	I3	I2	A3 A4
<b>Group 5: Planar symmetric molecules</b>										
a) SO <sub>3</sub> , CH <sub>3</sub>	<i>J'</i>	<i>K'</i>		<i>Γ'<sub>rot</sub></i>	<i>Γ'<sub>tot</sub></i>		<i>J''</i>	<i>K''</i>	<i>Γ''<sub>rot</sub></i>	<i>Γ''<sub>tot</sub></i>
	I3	I3	$\overline{2X}$	A3	A3	$\overline{1X}$	I3	I3	$\overline{2X}$	A3 A3
b) H <sub>3</sub> <sup>+</sup>	<i>J'</i>	<i>Sym'</i>	<i>G'</i>	<i>U'</i>	<i>K'</i>		<i>J''</i>	<i>Sym''</i>	<i>G''</i>	<i>U''</i>
	I3	A2	I3	A2	A3	$\overline{2X}$	I3	A2	I3	A2 A3
<b>Group 6: Open-shell diatomics with <sup>3</sup>Σ ground electronic states</b>										
O <sub>2</sub> , SO, S <sub>2</sub>					<i>F'</i>		<i>Br</i>	<i>N''</i>	<i>Br</i>	<i>J''</i>
					$\overline{10X}$	A5	$\overline{1X}$	A1	I3	A1
								<i>J''</i>	<i>F''</i>	M
								A1	A5	A1
<b>Group 7: Open-shell diatomics with <sup>2</sup>Π ground electronic states</b>										
a) NO, ClO			<i>m</i>		<i>F'</i>			<i>Br</i>	<i>J''</i>	<i>Sym''</i>
			A1	$\overline{9X}$	A5		$\overline{2X}$	A2	F5.1	A1
									<i>F''</i>	A5
b) OH <sup>e</sup>					<i>F'</i>			<i>Br</i>	<i>J''</i>	<i>Sym''</i>
					$\overline{10X}$	A5	$\overline{1X}$	A2	F5.1	A2
									<i>F''</i>	A5

<sup>a</sup> For H<sub>2</sub>O, the *Sym''* field is used to indicate electric quadrupole transitions (q).

<sup>b</sup> For NO<sub>2</sub> and HO<sub>2</sub>, *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  $J = N - 1/2$ .

<sup>c</sup> For HONO, the *Sym''* field is used to indicate between trans (t) and cis (c) isomers.

<sup>d</sup> For N<sub>2</sub> and H<sub>2</sub>, the *Sym''* field is used to indicate electric quadrupole (q) and magnetic dipole (m) transitions.

<sup>e</sup> For OH, the format of *Sym* field in the lower-state quanta accommodates the upper- and lower-state symmetry (e or f).

## References for HITRAN2024 supplementary material

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