

# Vibrational Bands of $H_xN_yO_z$ Molecules

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# Vibrational Bands of $H_xN_yO_z$ Molecules

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A compilation of experimental data is presented which covers all known molecular species fitting the  $^1H_x^{14}N_y^{16}O_z$  ( $y, z \neq 0$ ) chemical formula. The vibrational bands of these compounds in gas, liquid, solid, and matrix are listed together with their assignments and the relevant references. Most of the literature before October 1991 is covered.

**Key words:** atmospheric data; combination bands; fundamental bands; fundamental frequencies; infrared spectra; nitrogen acids; nitrogen oxides; overtone bands; polyatomic molecules; Raman spectra; vibration-rotation spectra; spectroscopic tables.

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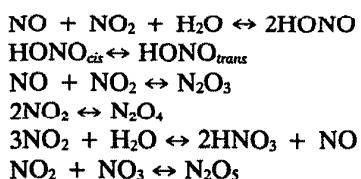
## 1. Introduction

As pointed out by L. Pauling<sup>1</sup> in his book on "The Nature of the Chemical Bond," nitric oxide (NO) is the most stable of the odd molecules. This notion of oddness, introduced by Lewis<sup>2</sup> in 1916, refers to the total number of electrons in the molecule. The notion of triple electron bond was introduced to explain the stability of such species. As a consequence, the latter were not expected to polymerize. It is nowadays established that NO-NO Van der Waals type bondings can be formed, under appropriate experimental conditions, thus somewhat in contradiction with that earlier statement. This holds even more firmly for the next member of this NO<sub>2</sub> family, nitrogen dioxide (NO<sub>2</sub>), known for a long time to be in thermodynamic equilibrium with the dimer N<sub>2</sub>O<sub>4</sub>. The geometrical structure of the dimer species is planar, but the various bond lengths and angles remain to be accurately deter-

mined. There is even a more basic structural problem about the next member of the family, nitrogen trioxide (NO<sub>3</sub>). Although it appears likely that the molecule is planar in its ground electronic state, it is not obvious whether the three N-O bonds are identical. The existence of the corresponding dimer (N<sub>2</sub>O<sub>6</sub>) is not even reported in the literature.

Even species of nitrogen and oxygen (N<sub>y</sub>O<sub>z</sub>,  $y = 2, 4, \dots$ ) are also known to exist. The simplest one, nitrous oxide (N<sub>2</sub>O), has been extensively studied and its stable linear geometry demonstrated. N<sub>2</sub>O<sub>2</sub>, N<sub>2</sub>O<sub>4</sub> (already mentioned), N<sub>2</sub>O<sub>3</sub>, and N<sub>2</sub>O<sub>5</sub> have been observed, but their structural and chemical properties remain to be well characterized. One can even postulate the existence of other larger species fitting the chemical formula N<sub>y</sub>O<sub>z</sub>.

In the presence of water (H<sub>2</sub>O), the N<sub>y</sub>O<sub>z</sub> species react with each other and form an extensive system with many chemical interplays. Indeed, several chemical equilibria take place, resulting into the formation of new, although connected species, such as nitrous acid (HONO) or nitric acid (HNO<sub>3</sub>). Examples of these reactions are as follows:



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Most of the above reactions are such that the species coexist each in reasonable abundance under a wide range of experimental conditions. This is certainly the case in the terrestrial atmosphere, and thus in any laboratory experiment performed under similar temperature and pressure conditions. It turns out that the role of the  $H_xN_yO_z$  species is central in various master physico-chemical processes occurring in our atmosphere. One can refer for instance to the balance of ozone ( $O_3$ ), or to the formation of acid rain, two of the atmospheric cycles in which some of the  $H_xN_yO_z$  species directly participate, as described in the book of Finlayson-Pitts and Pitts, Jr.<sup>3</sup> Because of the internal chemical connections we have mentioned, all members of the family are indirectly contributing. Thus the study of that chemical family as a whole is meaningful. It is actually of fundamental importance not only in the environmental context, but also in various other up to date chemical areas, such as those dealing with combustion, energy transfers or chemical bondings.

The basic role of infrared spectroscopy in probing the  $H_xN_yO_z$  molecules is well established, in particular in the atmospheric area. As a consequence of the trends we have pointed out, several of the family members are usually present in most realistic situations. Any related infrared spectrum will thus demonstrate the presence of various species through an extended series of bands. The bands will strongly overlap, not only because of their high density, but also because the probed molecules are very similar, and thus present very close vibrational frequencies. It appears critical to be able to fully assign such data in order to achieve an optimal diagnosis of the monitored sample *in situ* or in the laboratory. An exhaustive knowledge of the infrared spectrum of each individual species is therefore required. Of course, it is well known that spectral information recorded with high resolution will allow us in most cases to bypass this general prospect, and to immediately focus on some specific properties. However, such type of data are available for the lightest species only, and furthermore restricted to gas phase investigations.

The interest for a database collecting all the infrared spectral information appears consequently justified for many applications in atmospheric, fundamental, or analytical chemistry. It is the aim of the present compilation to provide such comprehensive and coherent information, at the stage of the literature existing nowadays.

The review by Laane and Ohlsen<sup>4</sup> provides interesting and complete background information on the role of the  $H_xN_yO_z$  molecules in various areas. Some spectroscopic infrared data are given in that earlier review. A more complete database has since been published by Jacox<sup>5</sup>, and compilations aimed at the investigation of the atmosphere are now also available [e.g., GEISA (Husson *et al.*<sup>6</sup>), HITRAN (Rothman *et al.*<sup>7</sup>), ATMOS (Brown *et al.*<sup>8</sup>)], which all are oriented towards infrared spectroscopy. In all cases, however, the spectroscopic content remains quite incomplete as only some of the species we are interested in are concerned, or only the fundamental frequencies are collected, or a very limited number of vi-

brational bands is provided. These previous works unfortunately do not really save the effort of a time consuming bibliographic research to produce exhaustive information on the vibrational bands of the members of the  $H_xN_yO_z$  chemical family, as we have actually experienced ourselves during our current research work.

Our present compilation is, in a way, an updating and an extension of the various tables provided in the book on infrared and Raman spectroscopy by Herzberg<sup>9</sup> (1st edition in 1949, new edition in preparation), which systematically lists some of the observed vibrational bands. We hope that the present tables will help scientists from different fields in their investigation on the  $H_xN_yO_z$  family of molecules, which we believe to be of central importance in chemistry.

## 2. Scope of Review and Guide to the Compilation

We have considered the various known neutral species fitting the  $H_xN_yO_z$  chemical formula, taking into account the main isotopic species only, i.e.,  $^1H$ ,  $^{14}N$ , and  $^{16}O$ . Their vibrational bands constitute the main information we have compiled. The energy range considered extends from the far infrared towards the near infrared, depending on the scientific publications on each species. Data from all phases are taken into account. The spectral information is presented in various forms in sets of tables. Each set concerns a different species. They are all built in a similar way. The first table in a set provides, for each known or postulated molecular geometry, the molecular point group, the symmetry and labeling of the corresponding normal modes of vibration, and their Raman and infrared activities. The labeling is the most conventional one usually reported in the various literature investigations. For each of the classes of isomeric forms of the species, the various modes of vibration are then briefly characterized in a second table in terms of the corresponding motions of the nuclei, and of their observed frequencies. The observed vibrational bands are listed in a final table.

The table of fundamental vibrational frequencies takes into account all wavenumbers found in the literature. Each of the listed frequencies, for each mode, usually corresponds, however, to a mean value whenever several literature data agree with each other within  $5\text{ cm}^{-1}$ . All the various references are mentioned, with appropriate remarks concerning the experimental medium used in the study. In some cases however, one of the values was preferred because it is the result of more accurate gas phase experiments. The corresponding work is then underlined in the list of references.

In the table collecting the *observed* vibrational bands, only one of the frequencies reported in the literature is given. Again, it corresponds to the gas phase result, when available. Otherwise, the selection is based on other criteria which are not detailed. The experiments reported in the literature are of various types, and, as already pointed out, may concern quite different media. The overall reso-

lution and accuracy is thus highly variable from one wavenumber to another in the table. In any case the remarks in the appropriate column in the table present the main characteristics of the related experiment. As a general rule, the wavenumbers correspond to the band origin, when arising from gas phase or matrix experiments. We also included the values for the R, Q, or P head measurements, when available in the literature. The band type is specified whenever it is detailed in the publications.

As already pointed out, the most accurate data arise from gas phase experiments; however, investigations on liquids may provide more complete information because of the stronger intensity of the bands, especially for those observed only through the Raman effect, while experiments performed in matrices are usually dedicated to the characterisation of less stable isomeric forms. The various wavenumbers may arise from totally different experimental techniques and the reader is referred to the original papers mentioned for further details.

We have noted in the tables whenever a list of rovibrational wavenumbers for a specified band appears in the atmospheric databases HITRAN (Rothman *et al.*<sup>7</sup>) and/or ATOMS (Brown *et al.*<sup>8</sup>). One should be aware that such a list usually corresponds to calculated wavenumbers. It also often happens that the corresponding measured wavenumbers are either directly provided or made available on request by the authors of the original paper, to which we always refer.

### 3. Units and Abbreviations

The usual spectroscopic unit for the wavenumber ( $\text{cm}^{-1}$ ) is used to characterize the spectral observations.

The following abbreviations are used throughout the tables:

#### Vibration type:

s-	symmetric
a-	asymmetric

#### Activity:

A	active band
I	inactive band

#### Experimental spectroscopic technique:

DL	Diode Laser
E	Infrared Emission (conventional or Fourier Transform Spectroscopy)
H	Heterodyne Frequency Measurements
IR	Infrared Absorption (conventional or Fourier Transform Spectroscopy)
LIF	Laser Induced Fluorescence
LMR	Laser Magnetic Resonance
LSS	Laser Stark Spectroscopy
MW	Microwave Spectroscopy
Ra	Raman Spectroscopy

#### Medium:

G	Gas
L	Liquid
LXe	Liquid Xenon
M	Matrix (see the referred paper for more details)
M:x,y	Matrix (medium specified as x,y,...; e.g., Ar, Ne, Xe, N <sub>2</sub> ...)
S	Solid

#### Band type:

(a,B)-	hybrid band; rotational envelope with some dominant B-type character
(A,b)-	hybrid band; rotational envelope with some dominant A-type character
(A,B)-	hybrid band; rotational envelope with evenly mixed A- and B-type character

## 4. Tables

## 4.1. NO

## Molecular Constants

	Vibrational constants (cm <sup>-1</sup> ) <sup>a</sup>	Spin-orbit constants (cm <sup>-1</sup> ) <sup>b</sup>	References, Remarks
$Y_0$	-948.5465(14)	123.25241(63)	c,d
$Y_1$	1904.1346(18)	-0.23570(48)	6,7(E,G)
$Y_2$	-14.08836(89)	-0.00408(10)	
$Y_3 \times 10^{+2}$	1.005(20)	-0.01863(74)	
$Y_4 \times 10^{+4}$	-1.53(22)		
$Y_5 \times 10^{+6}$	-9.8(1.4)	-0.252(18)	
$Y_6 \times 10^{+7}$	-1.91(43)	-0.0239(47)	
$Y_7 \times 10^{+9}$	-5.27(53)		
$\Delta G_{1/2}$	1875.98918(3)		c,d 3,4(IR,G); 10(H,G) See also 8,9 and references therein

<sup>a</sup>For  $v \leq 22$ , the vibrational level energies are expressed in terms of Dunham coefficients as following:

$$G(v) = \sum_{i=0} Y_i (v + 1/2)^i.$$

<sup>b</sup>For  $v \leq 22$ , the energy separation between  $X^2\Pi_{1/2}$  and  $X^2\Pi_{3/2}$  is roughly expressed in terms of Dunham coefficients as following:

$$\Delta(v) = \sum_{i=0} Y_i (v + 1/2)^i.$$

<sup>c</sup>Number in parentheses refers to the last quoted digits and represents one standard deviation.

<sup>d</sup>For other results or more details, see also Huber and Herzberg's tables<sup>5</sup>.

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	v'	v''	Assignment Transition	References	Remarks
1763.8766	5	4		8,9	
1791.8403	4	3		8,9	
1819.8392	3	2		8,9	
1847.8808	2	1		8,9	
1875.8804	1	0	$\Pi_{3/2} - \Pi_{3/2}$	3(IR,G)	Sub-band origin
1875.98918(3)	1	0		10(H,G)	<sup>b,c,d</sup> See also 3,4(IR,G)
1876.0897	1	0	$\Pi_{1/2} - \Pi_{1/2}$	3(IR,G)	Sub-band origin
1995.5917			$\Pi_{3/2} - \Pi_{1/2}$		
2993.5237	15	13		7(E,G)	e
3050.6806	14	12		7(E,G)	e
3107.4567	13	11		7(E,G)	e
3163.9320	12	10		7(E,G)	e
3220.1770	11	9		7(E,G)	e
3276.2541	10	8		7(E,G)	e
3332.2163	9	7		7(E,G)	e
3388.1105	8	6		7(E,G)	e
3443.9758	7	5		7(E,G)	e
3499.8472	6	4		7(E,G)	<sup>b,c,e</sup>
3555.7523	5	3		7(E,G)	<sup>b,c,e</sup>
3570.4331 R <sub>2</sub>	6	4	$\Pi_{3/2} - \Pi_{3/2}$	6(E,G)	
3570.8048 R <sub>1</sub>			$\Pi_{1/2} - \Pi_{1/2}$		
3611.7150	4	2		7(E,G)	<sup>b,c,e</sup> See also 1(E,G)
3667.7552	3	1		7(E,G)	<sup>b,c,e</sup> See also 1(E,G)

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	v'	Assignment v"	Transition	References	Remarks
3685.7860 R <sub>2</sub> } 3686.1018 R <sub>1</sub> }	4	2	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	6(E,G)	See also 1(E, G)
3723.85233(13)	2	0		4(IR,G)	<sup>b,c,d</sup> See also 1,6,7(E,G); 2(IR,G)
3743.5741 R <sub>2</sub> } 3743.8708 R <sub>1</sub> }	3	1	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	6(E,G)	See also 1(E,G)
3801.4564 R <sub>2</sub> } 3801.7282 R <sub>1</sub> }	2	0	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	6(E,G)	See also 1(E,G)
3907.2464 v <sub>0</sub> } 3933.996 R <sub>2</sub> } 3936.548 R <sub>1</sub> }	22	19		7(E,G)	<sup>e</sup>
4001.0060 v <sub>0</sub> } 4029.361 R <sub>2</sub> } 4031.631 R <sub>1</sub> }	21	18	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4092.9246 v <sub>0</sub> } 4122.836 R <sub>2</sub> } 4124.881 R <sub>1</sub> }	20	17	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4183.2654 v <sub>0</sub> } 4214.668 R <sub>2</sub> } 4216.527 R <sub>1</sub> }	19	16		7(E,G)	<sup>e</sup>
4272.2556 v <sub>0</sub> } 4305.126 R <sub>2</sub> } 4306.792 R <sub>1</sub> }	18	15	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4360.1038 v <sub>0</sub> } 4394.402 R <sub>2</sub> } 4395.907 R <sub>1</sub> }	17	14		7(E,G)	<sup>e</sup>
4446.9970 v <sub>0</sub> } 4482.661 R <sub>2</sub> } 4484.049 R <sub>1</sub> }	16	13	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4533.0999 v <sub>0</sub> } 4570.134 R <sub>2</sub> } 4571.364 R <sub>1</sub> }	15	12		7(E,G)	<sup>e</sup>
4618.5611 v <sub>0</sub> } 4656.894 R <sub>2</sub> } 4658.046 R <sub>1</sub> }	14	11	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4703.5082 v <sub>0</sub> } 4743.146 R <sub>2</sub> } 4744.176 R <sub>1</sub> }	13	10		7(E,G)	<sup>e</sup>
4788.0575 v <sub>0</sub> } 4828.949 R <sub>2</sub> } 4829.919 R <sub>1</sub> }	12	9	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>
4872.3056 v <sub>0</sub> } 4914.460 R <sub>2</sub> } 4915.329 R <sub>1</sub> }	11	8		7(E,G)	<sup>e</sup>
4956.3418 v <sub>0</sub> } 4999.717 R <sub>2</sub> } 5000.540 R <sub>1</sub> }	10	7	Π <sub>3/2</sub> — Π <sub>3/2</sub> Π <sub>1/2</sub> — Π <sub>1/2</sub>	7(E,G)	<sup>e</sup>

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )		Assignment		References	Remarks
	v'	v"	Transition		
5170.8 R <sub>1</sub>	8	5	Π <sub>1/2</sub> — Π <sub>1/2</sub>	1(E,G)	
5255.4 R <sub>1</sub>	7	4	Π <sub>1/2</sub> — Π <sub>1/2</sub>	1(E,G)	
5340.1 R <sub>1</sub>	6	3	Π <sub>1/2</sub> — Π <sub>1/2</sub>	1(E,G)	
5425.5 R <sub>1</sub>	5	2	Π <sub>1/2</sub> — Π <sub>1/2</sub>	1(E,G)	
5511.0 R <sub>1</sub>	4	1	Π <sub>1/2</sub> — Π <sub>1/2</sub>	1(E,G)	
5543.69160(19)	3	0		4(IR,G)	<sup>d</sup> See also 2(IR,G)
5595.1 R <sub>1</sub>	3	0		1(E,G)	
7335.158 }	4	0	Π <sub>3/2</sub> — Π <sub>3/2</sub>	2(IR,G)	Sub-band origins
7336.031 }			Π <sub>1/2</sub> — Π <sub>1/2</sub>		
~9100 v <sub>0</sub> }	5	0		11(IR,G)	
~9130 R }					

<sup>a</sup>Band origin; line positions calculated with the parameters obtained by 6(E,G).<sup>b</sup>Rotational line list available in HITRAN database (8).<sup>c</sup>Rotational line list available in ATMOS database (9).<sup>d</sup>Band origin calculated from rotational analysis; the number in parentheses refers to the last quoted digits and represents one standard deviation.<sup>e</sup>Band origin calculated from G(v) values: these latter vibrational energy values were obtained from a simultaneous least-squares fitting of the rovibrational data in the 1-0, 2-1, Δv = 2, and Δv = 3 bands [see 6.7(E,G) for more details].

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4.2. NO<sub>2</sub>

Species	Molecular point group	Normal modes		Activity	
		Symmetry	Vibrations	Raman	Infrared
	C <sub>2v</sub>	<i>A</i> <sub>1</sub> <i>B</i> <sub>2</sub>	<i>v</i> <sub>1</sub> , <i>v</i> <sub>2</sub> <i>v</i> <sub>3</sub>	<b>A</b> <b>A</b>	<b>A</b> <b>A</b>

Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A</i> <sub>1</sub>	<i>v</i> <sub>1</sub>	s-stretch	1319.770	3,24(LIF,G); 6(Ra,G); 13(Ra,M:Ar,Kr,Xe); 15,17(IR,G)
	<i>v</i> <sub>2</sub>	bend	749.6530	3,24(LIF,G); 4,5,15,23(IR,G); 6(Ra,G); 13(Ra,M:Ar,Kr,Xe); 14(LMR,G)
<i>B</i> <sub>2</sub>	<i>v</i> <sub>3</sub>	a-stretch	1616.85	3,24(LIF,G); 9,15(IR,G); 13(Ra,M:Ar,Kr,Xe)

Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
749.652961(29)	<i>v</i> <sub>2</sub> <i>B</i> -type band	23(IR,G)	<sup>a,b</sup> ( <i>v</i> <sub>1</sub> ,2 <i>v</i> <sub>2</sub> , <i>v</i> <sub>3</sub> ) + ( <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ,3 <i>v</i> <sub>2</sub> ). <sup>c,d</sup> See also 3,24(LIF,G); 4,5,15(IR,G); 6(Ra,G); 13(Ra,M); 14(LMR,G)
1319.77065(34)	<i>v</i> <sub>1</sub> <i>B</i> -type band	17(IR,G)	<sup>a,b</sup> ( <i>v</i> <sub>1</sub> ,2 <i>v</i> <sub>2</sub> , <i>v</i> <sub>3</sub> ) See also 3,24(LIF,G); 6(Ra,G); 13(Ra,M); 15(IR,G)
1498.3474(16)	2 <i>v</i> <sub>2</sub> <i>A</i> -type band	18(IR,G)	<sup>a,b</sup> ( <i>v</i> <sub>1</sub> ,2 <i>v</i> <sub>2</sub> , <i>v</i> <sub>3</sub> ), <sup>d</sup> See also 6(Ra,G); 9,15(IR,G); 13(Ra,M); 24(LIF,G)
1605.497	<i>v</i> <sub>3</sub> + <i>v</i> <sub>2</sub> - <i>v</i> <sub>1</sub> <i>A</i> -type band	15(IR,G)	<sup>d</sup> Calculation from ( <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ) and <i>v</i> <sub>2</sub> frequencies
1616.8535(20)	<i>v</i> <sub>3</sub> <i>A</i> -type band	15(IR,G)	<sup>a,b</sup> ( <i>v</i> <sub>1</sub> ,2 <i>v</i> <sub>2</sub> , <i>v</i> <sub>3</sub> ) + ( <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ,3 <i>v</i> <sub>2</sub> ), <sup>c,d</sup> See also 3,24(LIF,G); 9(IR,G); 13(Ra,M)
2063.11761(29)	( <i>v</i> <sub>1</sub> + <i>v</i> <sub>2</sub> ) <sup>0</sup> <i>B</i> -type band	20(IR,G)	*
2245.991(20)	3 <i>v</i> <sub>2</sub> <i>A</i> -type band	15(IR,G)	<sup>a,b</sup> (3 <i>v</i> <sub>2</sub> , <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ) See also 9(IR,G); 13(Ra,M); 24(LIF,G)
2355.1510(20)	( <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ) <sup>0</sup> <i>A</i> -type band	15(IR,G)	<sup>a,b</sup> (3 <i>v</i> <sub>2</sub> , <i>v</i> <sub>2</sub> + <i>v</i> <sub>3</sub> ) See also 9(IR,G); 24(LIF,G)

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
2627.3370(17)	$2v_1^0$ <i>B</i> -type band	5(IR,G)	<sup>a</sup> See also 6(Ra,G); 13(Ra,M); 24(LIF,G) Anomalies could be due to Coriolis interaction with $v_1 + v_3$
2805.512(17)	$(v_1 + 2v_2)^0$	12(IR,G)	<sup>a,b</sup> ( $v_1 + v_3, v_1 + 2v_2$ ), <sup>c,d</sup> See also 6(Ra,G); 13(Ra,M); 24(LIF,G)
2898.1930	$v_1 + v_3 + v_2 - v_2$	21,22	Calculated line positions See also 12(IR,G)
2906.0697(2)	$(v_1 + v_3)^0$ <i>A</i> -type band	12(IR,G)	<sup>a,b</sup> ( $v_1 + v_3, v_1 + 2v_2$ ), <sup>c,d</sup> See also 24(LIF,G)
2993.060	$4v_2^0$	9(IR,G)	See also 13(Ra,M); 24(LIF,G)
3092.48082(50)	$(2v_2 + v_3)^0$ <i>A</i> -type band	9(IR,G)	<sup>a,b</sup> ( $2v_2 + v_3, 2v_3$ ) See also 24(LIF,G)
3201.44395(39)	$2v_3^0$ <i>B</i> -type band	9(IR,G)	<sup>a,b</sup> ( $2v_2 + v_3, 2v_3$ ) See also 6(Ra,G); 13(Ra,M); 24(LIF,G)
3364.57	$(2v_1 + v_2)^0$	24(LIF,G)	<sup>e</sup> See also 6(Ra,G); 13(Ra,M)
3546.887(36)	$(v_1 + 3v_2)^0$	12(IR,G)	<sup>a,b</sup> ( $v_1 + 3v_2, v_1 + v_2 + v_3$ ) See also 6(Ra,G); 9(IR,G); 13(Ra,M); 24(LIF,G)
3637.84747(47)	$(v_1 + v_2 + v_3)^0$ <i>A</i> -type band	9(IR,G)	<sup>a,b</sup> ( $v_1 + 3v_2, v_1 + v_2 + v_3$ ) See also 12(IR,G); 13(Ra,M); 16(LMR,G); 24(LIF,G)
3738.6	$5v_2^0$	3(LIF,G)	See also 13(Ra,M); 24(LIF,G)
3829.34	$(3v_2 + v_3)^0$	24(LIF,G)	<sup>e</sup>
3922.61	$3v_1^0$	24(LIF,G)	<sup>e</sup> See also 6(Ra,G); 13(Ra,M)
3929.12	$(v_2 + 2v_3)^0$	24(LIF,G)	<sup>e</sup> See also 6(Ra,G); 13(Ra,M)
4100.150(18)	$(2v_1 + 2v_2)^0$	19(IR,G)	<sup>a,b</sup> ( $2v_1 + 2v_2, 2v_1 + v_3$ ) See also 6(Ra,G); 13(Ra,M); 24(LIF,G)
4179.9416(34)	$(2v_1 + v_3)^0$	19(IR,G)	<sup>a,b</sup> ( $2v_1 + 2v_2, 2v_1 + v_3$ ) See also 24(LIF,G)
4286.82	$(v_1 + 4v_2)^0$	24(LIF,G)	<sup>e</sup> See also 6(Ra,G); 13(Ra,M)
4369.10	$(v_1 + 2v_2 + v_3)^0$	24(LIF,G)	<sup>e</sup>
4461.07	$(v_1 + 2v_3)^0$	24(LIF,G)	<sup>e</sup> See also 6(Ra,G); 13(Ra,M)
4482.57	$6v_2^0$	24(LIF,G)	<sup>e</sup> See also 13(Ra,M)
4564.22	$(4v_2 + v_3)^0$	24(LIF,G)	<sup>e</sup>

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
4652.00	(3v <sub>1</sub> + v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e
4655.04(13)	(2v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>	19(IR,G)	<sup>a,b</sup> (2v <sub>2</sub> + 2v <sub>3</sub> ,3v <sub>3</sub> ) See also 6(Ra,G); 13(Ra,M); 24(LIF,G)
4754.20760(31)	3v <sub>3</sub> <sup>0</sup> <i>A</i> -type band	19(IR,G)	<sup>a,b</sup> (2v <sub>2</sub> + 2v <sub>3</sub> ,3v <sub>3</sub> ) See also 1(IR,G); 24(LIF,G)
4835.05	(2v <sub>1</sub> + 3v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G); 13(Ra,M)
4905.52	(2v <sub>1</sub> + v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5025.20	(v <sub>1</sub> + 5v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 13(Ra,M)
5098.00	(v <sub>1</sub> + 3v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5180.54	(v <sub>1</sub> + v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G); 13(Ra,M)
5205.81	4v <sub>1</sub> <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G); 13(Ra,M)
5224.55	7v <sub>2</sub> <sup>0</sup>	24(LIF,G)	e
5298.16	(5v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5377.91	(3v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5384.41	(3v <sub>1</sub> + 2v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G); 13(Ra,M)
5437.540(12)	(3v <sub>1</sub> + v <sub>3</sub> ) <sup>0</sup> <i>A</i> -type band	2(IR,G)	<sup>a</sup> See also 24(LIF,G)
5469.66	(v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5568.41	(2v <sub>1</sub> + 4v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 13(Ra,M)
5630.36	(2v <sub>1</sub> + 2v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5701.41	(2v <sub>1</sub> + 2v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G)
5762.23	(v <sub>1</sub> + 6v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G); 13(Ra,M)
5826.29	(v <sub>1</sub> + 4v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
5898.94	(v <sub>1</sub> + 2v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G)
5930.66	(4v <sub>1</sub> + v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e See also 6(Ra,G)
5965.61	8v <sub>2</sub> <sup>0</sup>	24(LIF,G)	e
5984.705(4)	(v <sub>1</sub> + 3v <sub>3</sub> ) <sup>0</sup> <i>A</i> -type band	1(IR,G)	<sup>a</sup> See also 24(LIF,G)
6030.71	(6v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
6101.80	(4v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	e
6112.11	(3v <sub>1</sub> +3v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	e
			See also 6(Ra,G)
6156.25	(3v <sub>1</sub> +v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>	24(LIF,G)	
6183.61	(2v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
6275.98	4v <sub>3</sub> <sup>0</sup>		
6299.70	(2v <sub>1</sub> +5v <sub>2</sub> ) <sup>0</sup>		
6351.40	(2v <sub>1</sub> +3v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
6414.16	(2v <sub>1</sub> +v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
6475.05	5v <sub>1</sub> <sup>0</sup>	24(LIF,G)	e
			See also 6(Ra,G)
6497.60	(v <sub>1</sub> +7v <sub>2</sub> ) <sup>0</sup>	24(LIF,G)	
6552.84	(v <sub>1</sub> +5v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
6616.53	(v <sub>1</sub> +3v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
6653.54	(4v <sub>1</sub> +2v <sub>2</sub> ) <sup>0</sup>		
6676.86	(4v <sub>1</sub> +v <sub>3</sub> ) <sup>0</sup>		
6693.12	(v <sub>1</sub> +v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
6705.23	9v <sub>2</sub> <sup>0</sup>		
6761.44	(7v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
6823.80	(5v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
6837.75	(3v <sub>1</sub> +4v <sub>2</sub> ) <sup>0</sup>		
6872.10	(3v <sub>1</sub> +2v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
6897.37	(3v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
6921.67	(3v <sub>1</sub> +2v <sub>3</sub> ) <sup>0</sup>		
6979.21	(v <sub>2</sub> +4v <sub>3</sub> ) <sup>0</sup>		
7029.48	(2v <sub>1</sub> +6v <sub>2</sub> ) <sup>0</sup>		
7072.23	(2v <sub>1</sub> +4v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7125.60	(2v <sub>1</sub> +2v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
7192.29	(2v <sub>1</sub> +3v <sub>3</sub> ) <sup>0</sup>		
7193.35	(5v <sub>1</sub> +v <sub>2</sub> ) <sup>0</sup>		
7231.06	(v <sub>1</sub> +8v <sub>2</sub> ) <sup>0</sup>		
7277.83	(v <sub>1</sub> +6v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7332.45	(v <sub>1</sub> +4v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
7374.57	(4v <sub>1</sub> +3v <sub>2</sub> ) <sup>0</sup>		
7386.33	(4v <sub>1</sub> +v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7403.04	(v <sub>1</sub> +2v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
7443.09	10v <sub>2</sub> <sup>0</sup>		
7478.02	(v <sub>1</sub> +4v <sub>3</sub> ) <sup>0</sup>		
7492.23	(8v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7544.62	(6v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
7562.47	(3v <sub>1</sub> +5v <sub>2</sub> ) <sup>0</sup>		
7587.04	(3v <sub>1</sub> +3v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7609.57	(4v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
7627.14	(3v <sub>1</sub> +v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
7681.49	(2v <sub>2</sub> +4v <sub>3</sub> ) <sup>0</sup>		
7730.08	6v <sub>1</sub> <sup>0</sup>		
7757.29	(2v <sub>1</sub> +7v <sub>2</sub> ) <sup>0</sup>		
7766.28	5v <sub>3</sub> <sup>0</sup>		
7791.18	(2v <sub>1</sub> +5v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
7834.97	(2v <sub>1</sub> +3v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
7888.16	(2v <sub>1</sub> +v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
7909.46	(5v <sub>1</sub> +2v <sub>2</sub> ) <sup>0</sup>		
7903.54	(5v <sub>1</sub> +v <sub>3</sub> ) <sup>0</sup>		
7962.27	(v <sub>1</sub> +9v <sub>2</sub> ) <sup>0</sup>		
8000.93	(v <sub>1</sub> +7v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
8046.44	(v <sub>1</sub> +5v <sub>2</sub> +2v <sub>3</sub> ) <sup>0</sup>		
8093.61	(4v <sub>1</sub> +4v <sub>2</sub> ) <sup>0</sup>		
8093.10	(4v <sub>1</sub> +2v <sub>2</sub> +v <sub>3</sub> ) <sup>0</sup>		
8110.13	(v <sub>1</sub> +3v <sub>2</sub> +3v <sub>3</sub> ) <sup>0</sup>		
8120.70	(4v <sub>1</sub> +2v <sub>3</sub> ) <sup>0</sup>		
8174.27	(v <sub>1</sub> +v <sub>2</sub> +4v <sub>3</sub> ) <sup>0</sup>		

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
8178.27	$11v_2^0$		
8218.84	$(9v_2 + v_3)^0$		
8264.28	$(7v_2 + 2v_3)^0$		
8284.17	$(3v_1 + 6v_2)^0$		
8299.45	$(3v_1 + 4v_2 + v_3)^0$		
8320.00	$(5v_2 + 3v_3)^0$		
8330.35	$(3v_1 + 2v_2 + 2v_3)^0$		
8374.58	$(3v_1 + 3v_3)^0$		
8382.64	$(3v_2 + 4v_3)^0$		
8441.44	$(6v_1 + v_2)^0$		
8457.15	$(v_2 + 5v_3)^0$		
8482.12	$(2v_1 + 8v_2)^0$		
8507.33	$(2v_1 + 6v_2 + v_3)^0$		
8542.25	$(2v_2 + 4v_2 + 2v_3)^0$		
8585.54	$(2v_1 + 2v_2 + 3v_3)^0$		
8608.92	$(5v_1 + v_2 + v_3)^0$		
8623.34	$(5v_1 + 3v_2)^0$		
8652.27	$(2v_1 + 4v_3)^0$		
8690.72	$(v_1 + 10v_2)^0$		
8721.11	$(v_1 + 8v_2 + v_3)^0$		
8758.28	$(v_1 + 6v_2 + 2v_3)^0$		
8797.95	$(4v_1 + 3v_2 + v_3)^0$		
8809.81	$(4v_1 + 5v_2)^0$		
8817.61	$(4v_1 + v_2 + 2v_3)^0$		
8816.65	$(v_1 + 4v_2 + 3v_3)^0$		
8868.35	$(v_1 + 2v_2 + 4v_3)^0$		
8911.29	$12v_2^0$		
8941.28	$(v_1 + 5v_3)^0$		
8944.50	$(10v_2 + v_3)^0$		
8968.55	$7v_1^0$		
8982.08	$(8v_2 + 2v_3)^0$		
9003.53	$(3v_1 + 7v_2)^0$		
9008.77	$(3v_1 + 5v_2 + v_3)^0$		
9029.44	$(6v_2 + 3v_3)^0$		
9031.81	$(3v_1 + 3v_2 + 2v_3)^0$		
9065.47	$(3v_1 + v_2 + 3v_3)^0$		
9082.71	$(4v_2 + 4v_3)^0$		
9101.27	$(6v_1 + v_3)^0$		
9151.35	$(6v_1 + 2v_2)^0$		
9148.84	$(2v_2 + 5v_3)^0$		
9203.99	$(2v_1 + 9v_2)^0$		
9220.73	$(2v_1 + 7v_2 + v_3)^0$		
9226.23	$6v_3^0$		
9247.78	$(2v_1 + 5v_2 + 2v_3)^0$		
9295.48	$(5v_1 + 2v_3)^0$		
9281.74	$(2v_1 + 3v_2 + 3v_3)^0$		
9310.32	$(5v_1 + 2v_2 + v_3)^0$		
9334.06	$(5v_1 + 4v_2)^0$		
9341.17	$(2v_1 + v_2 + 4v_3)^0$		
9416.05	$(v_1 + 11v_2)^0$		
9436.85	$(v_1 + 9v_2 + v_3)^0$		
9468.38	$(v_1 + 7v_2 + 2v_3)^0$		
9500.17	$(v_1 + 5v_2 + 3v_3)^0$		
9511.96	$(4v_1 + 2v_2 + 2v_3)^0$		
9524.14	$(4v_1 + 6v_2)^0$		
9518.26	$(4v_1 + 4v_2 + v_3)^0$		
9531.08	$(4v_1 + 3v_3)^0$		
9561.06	$(v_1 + 3v_2 + 4v_3)^0$		
9623.58	$(v_1 + v_2 + 5v_3)^0$		
9640.29	$13v_2^0$		
9672.18	$(7v_1 + v_2)^0$		
9654.17	$(11v_2 + v_3)^0$		
9696.16	$(9v_2 + 2v_3)^0$		
9716.70	$(3v_1 + 8v_2)^0$		

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
9713.52	(3v <sub>1</sub> + 6v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
9731.72	(3v <sub>1</sub> + 4v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
9736.30	(7v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
9753.30	(3v <sub>1</sub> + 2v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
9780.98	(5v <sub>1</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
9796.80	(3v <sub>1</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
9797.03	(6v <sub>1</sub> + v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
9836.38	(3v <sub>2</sub> + 5v <sub>3</sub> ) <sup>0</sup>		
9855.68	(6v <sub>1</sub> + 3v <sub>2</sub> ) <sup>0</sup>		
9904.99	(v <sub>2</sub> + 6v <sub>3</sub> ) <sup>0</sup>		
9920.43	(2v <sub>1</sub> + 10v <sub>2</sub> ) <sup>0</sup>		
9928.47	(2v <sub>1</sub> + 8v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
9950.41	(2v <sub>1</sub> + 6v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
9984.14	(5v <sub>1</sub> + v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
9976.50	(2v <sub>1</sub> + 4v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10007.48	(5v <sub>1</sub> + 3v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10025.10	(2v <sub>1</sub> + 2v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
10043.14	(5v <sub>1</sub> + 5v <sub>2</sub> ) <sup>0</sup>		
10081.20	(2v <sub>1</sub> + 5v <sub>3</sub> ) <sup>0</sup>		
10132.49	(v <sub>1</sub> + 12v <sub>2</sub> ) <sup>0</sup>		
10161.31	(v <sub>1</sub> + 10v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10184.66	8v <sub>1</sub> <sup>0</sup>		
10203.86	(4v <sub>1</sub> + 3v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10200.29	(v <sub>1</sub> + 6v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10214.37	(4v <sub>1</sub> + v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10231.98	(4v <sub>1</sub> + 7v <sub>2</sub> ) <sup>0</sup>		
10251.59	(v <sub>1</sub> + 4v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
10270.88	(7v <sub>1</sub> + v <sub>3</sub> ) <sup>0</sup>		
10304.69	(v <sub>1</sub> + 2v <sub>2</sub> + 5v <sub>3</sub> ) <sup>0</sup>		
10352.09	14v <sub>2</sub> <sup>0</sup>		
10375.23	(7v <sub>1</sub> + 2v <sub>2</sub> ) <sup>0</sup>		
10363.42	(12v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10399.71	(v <sub>1</sub> + 6v <sub>3</sub> ) <sup>0</sup>		
10415.48	(11v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10425.39	(3v <sub>1</sub> + 5v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10435.41	(3v <sub>1</sub> + 9v <sub>2</sub> ) <sup>0</sup>		
10445.42	(6v <sub>1</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10436.26	(8v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10478.49	(3v <sub>1</sub> + v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
10486.21	(6v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
10488.24	(6v <sub>1</sub> + 2v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10522.92	(4v <sub>2</sub> + 5v <sub>3</sub> ) <sup>0</sup>		
10557.69	(6v <sub>1</sub> + 4v <sub>2</sub> ) <sup>0</sup>		
10582.51	(2v <sub>2</sub> + 6v <sub>3</sub> ) <sup>0</sup>		
10632.76	(2v <sub>1</sub> + 11v <sub>2</sub> ) <sup>0</sup>		
10630.89	(2v <sub>1</sub> + 9v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10649.59	(5v <sub>1</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10659.32	7v <sub>3</sub> <sup>0</sup>		
10663.33	(2v <sub>1</sub> + 5v <sub>2</sub> + 3v <sub>3</sub> ) <sup>0</sup>		
10697.01	(5v <sub>1</sub> + 4v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10746.29	(5v <sub>1</sub> + 6v <sub>2</sub> ) <sup>0</sup>		
10763.15	(2v <sub>1</sub> + v <sub>2</sub> + 5v <sub>3</sub> ) <sup>0</sup>		
10850.34	(v <sub>1</sub> + 13v <sub>2</sub> ) <sup>0</sup>		
10876.58	(v <sub>1</sub> + 9v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10864.15	(v <sub>1</sub> + 11v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10900.00	(4v <sub>1</sub> + 4v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
10916.81	(4v <sub>1</sub> + 6v <sub>2</sub> + v <sub>3</sub> ) <sup>0</sup>		
10963.15	(v <sub>1</sub> + 5v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
11041.86	(v <sub>1</sub> + v <sub>2</sub> + 6v <sub>3</sub> ) <sup>0</sup>		
11063.22	(7v <sub>1</sub> + 3v <sub>2</sub> ) <sup>0</sup>		
11071.05	15v <sub>2</sub> <sup>0</sup>		
11096.84	(6v <sub>1</sub> + v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
11126.61	(3v <sub>1</sub> + 6v <sub>2</sub> + 2v <sub>3</sub> ) <sup>0</sup>		
11170.56	(3v <sub>1</sub> + 2v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		
11218.66	(7v <sub>2</sub> + 4v <sub>3</sub> ) <sup>0</sup>		

24(LIF,G) e,f

## Observed Infrared Bands -- Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
11200.80	$(5\nu_2 + 5\nu_3)^0$		
11259.79	$(6\nu_1 + 5\nu_2)^0$		
11251.48	$(3\nu_2 + 6\nu_3)^0$		
11290.61	$(5\nu_1 + 3\nu_2 + 2\nu_3)^0$		
11347.04	$(2\nu_1 + 8\nu_2 + 2\nu_3)^0$		
11364.34	$(2\nu_1 + 12\nu_2)^0$		
11376.13	$9\nu_1^0$		
11370.18	$(5\nu_1 + 5\nu_2 + \nu_3)^0$		
11401.71	$(8\nu_1 + \nu_3)^0$		
11423.13	$(2\nu_1 + 2\nu_2 + 5\nu_3)^0$	24(LIF,G)	c,f
11440.88	$(5\nu_1 + 7\nu_2)^0$		
11477.98	$(2\nu_1 + 6\nu_3)^0$		
11575.98	$(4\nu_1 + \nu_2 + 4\nu_3)^0$		
11557.26	$(4\nu_1 + 5\nu_2 + 2\nu_3)^0$		
11571.20	$(8\nu_1 + 2\nu_2)^0$		
11602.15	$(\nu_1 + 6\nu_2 + 4\nu_3)^0$		
11804.93	$(3\nu_1 + 7\nu_2 + 2\nu_3)^0$		
11933.35	$(4\nu_2 + 6\nu_3)^0$		
12101.1	$2\nu_1 + 11\nu_2 + \nu_3$ A-type band	8(IR,G)	Interaction with the $3\nu_2$ level of the low lying $\tilde{A}^2B_2$ electronic state
-12440	$\nu_1 + 14\nu_2 + \nu_3 - \nu_2$ or $16\nu_2 + \nu_3 - \nu_2$	11(IR,G)	
13179.45(71)	$(\nu_1 + 14\nu_2 + \nu_3)^0$ or $(16\nu_2 + \nu_3)^0$	11(IR,G)	
13511.057	$(2\nu_1 + 13\nu_2 + \nu_3)^0$ A-type band	10(IR,G)	Interaction with a vibrational level of the low lying $\tilde{A}^2B_2$ electronic state See also 7(IR,G)

<sup>a</sup>Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents one standard deviation.

<sup>b</sup>(x,y,...) : band origin and other molecular parameters are obtained from a global fit with other vibration-rotation data, in order to take into account a Coriolis interaction between x, y, ... levels.

<sup>c</sup>Rotational line list available in HITRAN database (21).

<sup>d</sup>Rotational line list available in ATMOS database (22).

<sup>e</sup>Supersonic molecular beam experiment; vibrational level energies calculated from the average of all the values obtained through the different transitions recorded as LIF features (band origins of these transitions measured to within 0.3 cm<sup>-1</sup>).

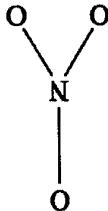
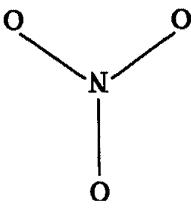
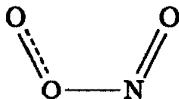
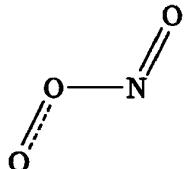
<sup>f</sup>Above 9000 cm<sup>-1</sup>, presence of various resonances between vibrational levels of the ground state. Numerous anomalies in the band positions (shifted by up to 30 cm<sup>-1</sup>) are also observed in this region; they are due to increasingly strong vibronic interaction with levels of the  $\tilde{A}^2B_2$  electronic state.

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### 4.3. NO<sub>3</sub>

Species	Molecular point group	Normal modes Symmetry	Vibrations	Raman	Activity Infrared
<i>symmetric</i>					
	D <sub>3h</sub>	<i>A'</i> <i>A''</i> <i>E'</i>	v <sub>1</sub> v <sub>2</sub> v <sub>3</sub> , v <sub>4</sub>	A I A	I A A
	C <sub>2v</sub>	<i>A</i> <i>B</i> <sub>1</sub> <i>B</i> <sub>2</sub>	v <sub>1</sub> → v <sub>3</sub> v <sub>4</sub> v <sub>5</sub> , v <sub>6</sub>	A A A	A A A
<i>asymmetric</i> (OONO)					
<i>cis</i>					
	C <sub>s</sub>	<i>A'</i> <i>A''</i>	v <sub>1</sub> → v <sub>5</sub> v <sub>6</sub>	A A	A A
<i>trans</i>					
	C <sub>s</sub>	<i>A'</i> <i>A''</i>	v <sub>1</sub> → v <sub>5</sub> v <sub>6</sub>	A A	A A

4.3.a. sym- $\text{NO}_3$ 

It is not yet absolutely clear whether the sym- $\text{NO}_3$  molecule belongs to  $D_{3h}$  or  $C_{2v}$  symmetry. Both experimental and theoretical works are divided about this point, even if several frequencies are commonly observed. The following table presents the correlation between the normal modes (and their symmetries) when one shifts from the  $D_{3h}$  to the  $C_{2v}$  symmetry.

$D_{3h}$			$C_{2v}$		
$A'_1$	$v_1$	N-O s-stretch	$A_1$	$v_1$	N-O s-stretch
$A''_2$	$v_2$	out of plane bend	$B_1$	$v_4$	out of plane bend
$E'$	$v_3$	N-O a-stretch	$\begin{cases} A_1 \\ B_2 \end{cases}$	$\begin{cases} v_2 \\ v_5 \end{cases}$	N-O s-stretch N-O a-stretch
$E'$	$v_4$	a-bend (in plane)	$\begin{cases} A_1 \\ B_2 \end{cases}$	$\begin{cases} v_3 \\ v_6 \end{cases}$	s-bend (in plane) a-bend (in plane)

Observed Fundamental Vibrational Frequencies

 $D_{3h}$ 

Sym.	Mode	Approximate type	Frequency ( $\text{cm}^{-1}$ )	References, Remarks
$A'_1$	$v_1$	N-O s-stretch	1050	1,6(LIF,G); attributed to $v_1$ ( $C_{2v}$ )
			1060	2(LIF,G)
			1080	7(result obtained from photo-electron spectrum of $\text{NO}_3^-$ )
$A''_2$	$v_2$	out of plane bend	749 (or 775)	6(LIF,G); attributed to $v_3$ and $v_4$ ( $C_{2v}$ )
			754	1(LIF,G); attributed to $v_3$ ( $C_{2v}$ )
			760	2(LIF,G)
			762.33	4(IR,G)
$E'$	$v_3$	N-O a-stretch (degenerated)	1480	2(LIF,G)
			1489	1(LIF,G); attributed to $v_2$ ( $C_{2v}$ )
			1492.393	3.5(DL,G); 4(IR,G) Could be a vibronic transition (5(DL,G))
			1498	6(LIF,G); attributed to $v_2$ ( $C_{2v}$ )
			360	1(LIF,G); attributed to $v_6$ ( $C_{2v}$ )
	$v_4$	O-N-O a-bend (in plane - degenerated)	366	7(result obtained from photo-electron spectrum of $\text{NO}_3^-$ )
			380	6(LIF,G); attributed to $v_6$ ( $C_{2v}$ )
				2(LIF,G)

The very latest results published in the literature seem to assess a  $D_{3h}$  structure to  $\text{NO}_3$ . Many anomalies have been observed in the  $\text{NO}_3$  spectrum. They mainly find an explanation in perturbations due to the two lowest excited electronic states  $\tilde{A}^2 E''$  and  $\tilde{B}^2 E'$ . For more details, see Ref. 7 (study of the photoelectron spectrum of  $\text{NO}_3^-$ ), and Refs. 8 and 9(DL,G).

## Observed Fundamental Vibrational Frequencies — Continued

 $C_{2v}$ 

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
$A_1$	$\nu_1$	N—O s-stretch	1050	1,6(LIF,G)
			1060	2(LIF,G); attributed to $\nu_1$ ( $D_{3h}$ )
			1080	7 (result obtained from photo-electron spectrum of $\text{NO}_3^-$ ); attributed to $\nu_1$ ( $D_{3h}$ )
$A_2$	$\nu_2$	N—O s-stretch	1480	2(LIF,G); attributed to $\nu_3$ ( $D_{3h}$ )
			1489	1(LIF,G)
			1492.393	3,5(DL,G); 4(IR,G); attributed to $\nu_3$ ( $D_{3h}$ ) Could be a vibronic transition (5(DL,G))
			1498	6(LIF,G)
$\nu_3$		s-bend (in plane)	749	6(LIF,G)
			754	1(LIF,G)
			760	2(LIF,G); attributed to $\nu_2$ ( $D_{3h}$ )
			762.33	4(IR,G); attributed to $\nu_2$ ( $D_{3h}$ )
$B_1$	$\nu_4$	out of plane bend	775	6(LIF,G)
$B_2$	$\nu_5$	N—O a-stretch	2000	1(LIF,G)
			2008	6(LIF,G)
$\nu_6$		a-bend (in plane)	360	1(LIF,G)
				7 (result obtained from photo-electron spectrum of $\text{NO}_3^-$ ); attributed to $\nu_4$ ( $D_{3h}$ )
			366	6(LIF,G)
			380	2(LIF,G); attributed to $\nu_4$ ( $D_{3h}$ )

## Observed Infrared Bands

Refs. 3,5(DL,G) analysed the  $\nu_3$  band ( $D_{3h}$  symmetry) and calculated the band origin:  $\nu_3^0 = 1492.3929$  (9)<sup>a</sup> cm<sup>-1</sup>. Ref. 4(IR,G) calculated  $\nu_2^0 = 762.327$  cm<sup>-1</sup> ( $D_{3h}$  symmetry). The other frequencies are presented below. The numbering of the fundamental frequencies refers to  $D_{3h}$  or  $C_{2v}$  assignments made in the previous tables.

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
679	$2\nu_6$ (?)	1(LIF,G)	$C_{2v}$ symmetry
759	$\nu_2 + \nu_4 - \nu_6$ (?)	4(IR,G)	$D_{3h}$ symmetry
1796	$\nu_1 + \nu_3$	1(LIF,G)	$C_{2v}$ symmetry
1910	$2\nu_4 + \nu_6$ (?)	1(LIF,G)	$C_{2v}$ symmetry
2024	$5\nu_4$	8(DL,G)	$D_{3h}$ symmetry
2126	$2\nu_1$	1(LIF,G)	$C_{2v}$ symmetry
2155	$\nu_1 + 3\nu_4$	8(DL,G)	$D_{3h}$ symmetry
2336	$\nu_5 + \nu_6$	1(LIF,G)	$C_{2v}$ symmetry
2486	$2\nu_1 + \nu_6$	1(LIF,G)	$C_{2v}$ symmetry
2523	$\nu_1 + \nu_3$	2(LIF,G)	$D_{3h}$ symmetry
			See also 5,8,9(DL,G)
2585	$3\nu_2 + \nu_4$ or $2\nu_1 + \nu_4$	8(DL,G)	$D_{3h}$ symmetry See also 5,9(DL,G)

<sup>a</sup>Number in parentheses refers to the last quoted digits and represents one standard deviation.

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4.3.b. *asym*-NO<sub>3</sub> (OONO)

Theoretical calculations of the six fundamental frequencies were made in Refs. 1 and 5. Only one band was observed and assigned to the N=O stretching motion by several authors:

Frequency (cm <sup>-1</sup> )	References
1830	3(IR,M:O <sub>2</sub> +N <sub>2</sub> )
1834.4 1837.5	4(IR,M:Ar)
1840*	1(IR,G)

\*This band was later reassigned by one of the authors to N<sub>2</sub>O<sub>3</sub> [2(IR,G), erratum on 1(IR,G)].

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4.4. N<sub>2</sub>O

Species	Molecular point group	Normal modes	Raman	Activity	Infrared
		Symmetry	Vibrations		
N—N—O	C <sub>nv</sub>	$\Sigma^+$ II	v <sub>1</sub> , v <sub>3</sub> v <sub>2</sub>	A A	A A

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
$\Sigma^+$	v <sub>1</sub>	N—O stretch	1284.9033	1,2 and references therein
II	v <sub>2</sub>	bend	588.7678	1,2 and references therein
$\Sigma^+$	v <sub>3</sub>	N—N stretch	2223.7567	1,2 and references therein

## Observed Infrared Bands

About seventy bands including fundamental, overtone and combination bands have been observed for <sup>14</sup>N<sub>2</sub><sup>16</sup>O between 525 and 5130 cm<sup>-1</sup>. The band origins and a list of rotational line positions are available in HITRAN<sup>1</sup> and ATMOS<sup>2</sup> databases. Since, to our knowledge, no major new contribution to these data exists, we only reproduce HITRAN<sup>1</sup> here the list ATMOS<sup>2</sup> of the observed infrared bands published by Ref. 1 and/or Ref. 2 without further references, in order to make these tables complete for the user. For more details, we refer the reader to the works mentioned in Ref. 1 and Ref. 2.

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment							
	Upper state		Lower state					
	v <sub>1</sub>	v <sub>2</sub>	v <sub>3</sub>	v <sub>1</sub>	v <sub>2</sub>	v <sub>3</sub>		
571.320	0	3	1	0	0	2	2	0
579.364	0	2	0	0	0	1	1	0
580.934	0	3	1	0	0	2	0	0
588.768	0	1	1	0	0	0	0	0
588.978	0	2	2	0	0	1	1	0
589.168	0	3	3	0	0	2	2	0
595.361	1	1	1	0	1	0	0	0
696.140	1	0	0	0	0	1	1	0
938.8534	0	0	0	1	1	0	0	0
1055.6245	0	0	0	1	0	2	0	0
1153.3768	0	4	2	0	0	2	2	0
1154.4408	0	4	0	0	0	2	0	0
1160.2973	0	3	1	0	0	1	1	0
1168.1323	0	2	0	0	0	0	0	0
1177.0931	1	2	0	0	1	0	0	0

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment				Lower state			
	Upper state							
	<i>v</i> <sub>1</sub>	<i>v</i> <sub>2</sub>	<i>l</i> <sub>2</sub>	<i>v</i> <sub>3</sub>	<i>v</i> <sub>1</sub>	<i>v</i> <sub>2</sub>	<i>l</i> <sub>2</sub>	<i>v</i> <sub>3</sub>
1177.7446	0	2	2	0	0	0	0	0
1278.4361	2	0	0	0	1	0	0	0
1284.9033	1	0	0	0	0	0	0	0
1285.5879	2	1	1	0	1	1	1	0
1291.4979	1	1	1	0	0	1	1	0
1293.8642	1	2	0	0	0	2	0	0
1297.0540	1	2	2	0	0	2	2	0
1297.1477	1	3	1	0	0	3	1	0
1301.8084	1	3	3	0	0	3	3	0
1395.2071	2	0	0	0	0	2	0	0
1620.5479	0	1	1	1	0	2	2	0
1630.1603	0	1	1	1	0	2	0	0
1634.9889	0	0	0	1	0	1	1	0
1733.8051	0	4	0	0	0	1	1	0
1742.3536	0	4	2	0	0	1	1	0
1749.0651	0	3	1	0	0	0	0	0
1868.4682	1	3	1	0	0	2	2	0
1873.2286	1	2	0	0	0	1	1	0
1878.0806	1	3	1	0	0	2	0	0
1880.2657	1	1	1	0	0	0	0	0
1880.9503	2	1	1	0	1	0	0	0
1886.0307	1	2	2	0	0	1	1	0
1890.9760	1	3	3	0	0	2	2	0
1974.5715	2	0	0	0	0	1	1	0
2079.0746	0	2	0	1	1	0	0	0
2181.3724	0	3	3	1	0	3	3	0
2181.6967	0	6	0	0	1	0	0	0
2181.7137	1	1	1	1	1	1	1	0
2182.1823	0	3	1	1	0	3	1	0
2189.5466	0	6	2	0	1	0	0	0
2193.6210	0	0	0	2	0	0	0	1
2195.3966	0	2	2	1	0	2	2	0
2195.8457	0	2	0	1	0	2	0	0
2195.9158	1	0	0	1	1	0	0	0
2209.5247	0	1	1	1	0	1	1	0
2223.7568	0	0	0	1	0	0	0	0
2309.0455	0	5	1	0	0	1	1	0
2322.5731	0	4	0	0	0	0	0	0
2331.1215	0	4	2	0	0	0	0	0
2452.8106	1	4	0	0	0	2	0	0
2453.8452	1	4	2	0	0	2	2	0
2457.4449	1	3	1	0	0	1	1	0
2461.9965	1	2	0	0	0	0	0	0
2463.3484	2	2	0	0	1	0	0	0
2474.7987	1	2	2	0	0	0	0	0
2551.4678	3	0	0	0	1	0	0	0
2563.3394	2	0	0	0	0	0	0	0
2566.1169	3	1	1	0	1	1	1	0
2577.0857	2	1	1	0	0	1	1	0
2580.1195	2	2	0	0	0	2	0	0

## Observed Infrared Bands — Continued

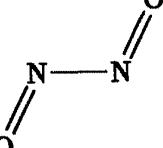
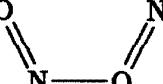
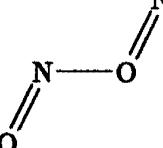
Frequency (cm <sup>-1</sup> )	Assignment				Lower state			
	Upper state							
	<i>v</i> <sub>1</sub>	<i>v</i> <sub>2</sub>	<i>l</i> <sub>2</sub>	<i>v</i> <sub>3</sub>	<i>v</i> <sub>1</sub>	<i>v</i> <sub>2</sub>	<i>l</i> <sub>2</sub>	<i>v</i> <sub>3</sub>
2586.7349	2	3	1	0	0	3	1	0
2588.3078	2	2	2	0	0	2	2	0
2668.2388	b	3	0	0	0	2	0	0
2753.5028	b	0	3	1	0	2	2	0
2763.1240	c	0	3	1	1	0	2	0
2770.5940	c	0	3	3	1	0	2	2
2775.2070	c	0	2	0	1	0	1	1
2777.0758	b	1	1	1	1	0	0	0
2784.3700	c	0	2	2	1	0	1	1
2798.2900	c	0	1	1	1	0	0	0
3342.491	0	3	1	1	0	1	1	0
3363.974	0	2	0	1	0	0	0	0
3445.921	2	0	0	1	1	0	0	0
3462.030	1	2	0	1	0	2	0	0
3464.713	1	2	2	1	0	2	2	0
3473.212	1	1	1	1	0	1	1	0
3480.821	1	0	0	1	0	0	0	0
3620.941	1	4	0	0	0	0	0	0
3747.031	2	3	1	0	0	1	1	0
3748.252	2	2	0	0	0	0	0	0
3836.373	3	0	0	0	0	0	0	0
3857.612	3	1	1	0	0	1	1	0
4061.979	1	1	1	1	0	0	0	0
4335.798	2	3	1	0	0	0	0	0
4388.928	0	1	1	2	0	1	1	0
4417.379	0	0	0	2	0	0	0	0
4630.164	1	2	0	1	0	0	0	0
4730.408	2	1	1	1	0	1	1	0
4730.828	2	0	0	1	0	0	0	0
4977.695	0	1	1	2	0	0	0	0
5026.34	3	2	0	0	0	0	0	0
5105.65	4	0	0	0	0	0	0	0

<sup>a</sup>Rotational line list available in HITRAN database<sup>1</sup> only.<sup>b</sup>Rotational line list available in ATMOS database<sup>2</sup> only.<sup>c</sup>Band origin measurements from ATMOS database<sup>2</sup>; other results are presented in HITRAN database<sup>1</sup>.

## References

- <sup>1</sup>The HITRAN database : 1986 edition, L. S. Rothman, R. R. Gamache, A. Goldman, L. R. Brown, R. A. Toth, H. M. Pickett, R. L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C. P. Rinsland, and M. A. H. Smith, Appl. Opt. 26, 4058 (1987).  
<sup>2</sup>Molecular line parameters for the Atmospheric Trace MOlecle Spectroscopy experiment, L. R. Brown, C. B. Farmer, C. P. Rinsland, and R. A. Toth, Appl. Opt. 26, 5154 (1987).

4.5. (NO)<sub>2</sub>

Species	Molecular point group	Normal modes Symmetry	Vibrations	Raman	Activity Infrared
<i>cis</i> -O=N-N=O					
	$C_{2v}$	$A_1$ $A_2$ $B_2$	$v_1 \rightarrow v_3$ $v_4$ $v_5, v_6$	A A A	A I A
<i>trans</i> -O=N-N=O					
	$C_{2h}$	$A_g$ $A_u$ $B_u$	$v_1 \rightarrow v_3$ $v_4$ $v_5, v_6$	A I I	I A A
<i>cis</i> -O=N-O=N					
	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_5$ $v_6$	A A	A A
<i>trans</i> -O=N-O=N*					
	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_5$ $v_6$	A A	A A

\*Not observed.

## 4.5.a. c/s-O=N-N=O

This species is reported as the most stable one. Useful information on the molecular structure of this isomer is presented in Ref. 8.

Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A</i> <sub>1</sub>	<i>v</i> <sub>1</sub>	N=O s-stretch	1861	IR : 1(L); 2(M:CO <sub>2</sub> ); 4(G); 6(S); 11(G) Ra : 1(L); 7(M:CO <sub>2</sub> )
			1868.252	IR : 1(S); 2(M:Ar); 3(M:N <sub>2</sub> ); 9(LXe); 13(G); 14(M:Ne) Ra : 5,6,10(S)
<i>v</i> <sub>2</sub>		N-N stretch	264	IR : 11(G)
			273	Ra : 1(L); 5,6,10(S); 7(M:CO <sub>2</sub> ) IR : 5(S)
	<i>v</i> <sub>3</sub>	N-N=O s-bend	161	Ra : 7(M:CO <sub>2</sub> )
			169	IR : 11(G)
			176	Ra : 1(L)
			187	Ra : 5(S) IR : 5(S) Ra : 6,10(S)
<i>A</i> <sub>2</sub>	<i>v</i> <sub>4</sub>	torsion	88.2 97	IR: 11(G); from <i>v</i> <sub>5</sub> - <i>v</i> <sub>4</sub> = 1700.8 cm <sup>-1</sup> Ra : 5,6(S); 10(S)
<i>B</i> <sub>2</sub>	<i>v</i> <sub>5</sub>	N=O a-stretch	1760	IR : 1,5,6(S); 9(LXe)
			1769	Ra : 1(L); 10(S)
			1776	IR : 1(L); 2(M:CO <sub>2</sub> )
			1778.7	IR : 2(M:Ar); 3(M:N <sub>2</sub> )
			1780.6 } 1789	IR : 14(M:Ne)
<i>v</i> <sub>6</sub>		N-N=O a-bend	199	IR : 4,11,12,13(G) IR : 11(G)
			214	Ra : 1(L); 6(S); 7(M:CO <sub>2</sub> ) Ra : 10(S)

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
97	$v_4$	10(Ra,S)	$T = 12$ K See also 5,6(Ra,S); 6(IR,S); 11(IR,G)
170	$v_3$	11(IR,G)	$T = 118 \rightarrow 138$ K See also 1(Ra,L); 5,6,10(Ra,S); 5(IR,S); 7(Ra,M)
198	$v_6$	11(IR,G)	$T = 118 \rightarrow 138$ K See also 1(Ra,L); 6,10(Ra,S); 7(Ra,M)
199	$2v_4$	10(Ra,S)	$T = 12$ K See also 6(Ra,S)
263	$v_2$	11(IR,G)	$T = 118 \rightarrow 138$ K See also 1(Ra,L); 5,6(IR,S); 6,10(Ra,S); 7(Ra,M)
347	$v_2 + v_4$	10(Ra,S)	$T = 12$ K
401	$2v_4 + v_6$ or $2v_6$	10(Ra,S)	$T = 12$ K; if $v_6 = 199$ cm <sup>-1</sup>
491	$v_2 + v_6$ or $2v_6$	10(Ra,S)	$T = 12$ K; if $v_6 = 214$ cm <sup>-1</sup> See also 1(Ra,L); 1(IR,S); 6(Ra+IR,S)
519	$2v_2$	1(IR,S)	
1506	$v_5 - v_2$	1(IR,L)	
1545	$v_5 - v_6$ (?)	1(IR,L)	
1600	$v_1 - v_2$	1(IR,L)	See also 1(IR,S)
1653	$v_1 - v_6$ (?)	4(IR,G)	
1700.8	$v_5 - v_4$ or $v_1 - v_3$ (?)	11(IR,G)	$T = 118 \rightarrow 138$ K See also 4(IR,G)
1732	$v_i + v_5 - v_i$ (?)	11(IR,G)	$T = 118 \rightarrow 138$ K
1759			
1770			
1774.6			
1789.15	$v_5$ A-type band	13(IR,G)	Q head See also 1(Ra+IR,L); 1,5,6(IR,S); 2,3,14(IR,M); 4,11,12(IR,G); 9(IR,LXe); 10(Ra,S)
1860	$v_1$	11(IR,G)	$T = 118 \rightarrow 138$ K See also 1(Ra+IR,L); 1,6(IR,S); 2,3,14(IR,M); 4(IR,G); 5,6,10(Ra,S); 7(Ra,M); 9(IR,LXe)
1868.2515(3)	$v_1^0$	13(IR,G)	"
1918	$v_3 + v_5$	1(IR,S)	
1965	$v_5 + v_6$	4(IR,G)	See also 1(IR,L+S)
2030	$v_2 + v_5$	4(IR,G)	See also 1(IR,L+S)
2042			
2124-2130	$v_1 + v_2$	1(IR,L+S)	
3551	$2v_5$	11(IR,G)	$T = 118 \rightarrow 138$ K; Q head See also 1(IR,L+S); 4(IR,G)
3559.32(10)	$2v_5^0$	15(IR,G)	"
3626	$v_1 + v_5$	11(IR,G)	$T = 118 \rightarrow 138$ K; Q head See also 1(IR,L+S); 4(IR,G); 9(IR,LXe)
3626.45(10)	$(v_1 + v_5)^0$	15(IR,G)	"
3708	$2v_1$	1(IR,L)	See also 1(IR,S); 9(IR,LXe)
5200±30	$3v_5$ (?)	1(IR,L)	See also 1(IR,S)
5390±30	$2v_1 + v_5$	1(IR,L)	See also 1(IR,S)

\*Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents one standard deviation.

## References

- <sup>1</sup>A. L. Smith, W. E. Keller, and H. L. Johnston, J. Chem. Phys. **19**, 189 (1951).
- <sup>2</sup>W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
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- <sup>10</sup>E. M. Nour, L. H. Chen, M. M. Strubo, and J. Laane, J. Phys. Chem. **88**, 756 (1984).
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- <sup>13</sup>Y. Matsumoto, Y. Ohshima, and M. Takami, J. Chem. Phys. **92**, 937 (1990).
- <sup>14</sup>M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
- <sup>15</sup>J. R. Hetzler, M. P. Casassa, and D. S. King, J. Phys. Chem. **95**, 8086 (1991).

4.5.b. *trans*-O=N-N=O

The only mode attributed to this species is the N=O a-stretch  $\nu_5$ . It has been observed through matrix experiments, in infrared spectra. Nevertheless, these assignments have to be considered rather cautiously :

Frequency (cm <sup>-1</sup> )	References
1740	1(IR, M:CO <sub>2</sub> )
1760.6 }	3(IR, M:Ne)
1762.5 }	2(IR, M:N <sub>2</sub> )

## References

- <sup>1</sup>W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 20 (1959).
- <sup>2</sup>W. A. Guillory and C. E. Hunter, J. Chem. Phys. **50**, 3516 (1969).
- <sup>3</sup>M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

4.5.c. *cis*-O=N-O=N

A "red species" has been observed, in special conditions, by only one group of workers<sup>1</sup>. It results from the reaction of NO with Lewis acids (BF<sub>3</sub>, BCl<sub>3</sub>, BBr<sub>3</sub>, SnCl<sub>4</sub>, SiF<sub>4</sub>, TiCl<sub>4</sub>), or with HCl, or with SO<sub>2</sub>, and it has been identified as the asymmetric *cis*-(NO)<sub>2</sub> species. Raman and infrared spectra have been recorded at 77 K. We reproduce here the fundamental frequencies obtained from Raman spectra of the products of the NO + BCl<sub>3</sub> reaction. Unless specified, the other frequencies (combination or overtone bands) were also obtained from these spectra.

The frequencies resulting from data recorded for different chemical conditions, detailed in Ref. 1, agree within 10 cm<sup>-1</sup> with those presented here.

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	Remarks
<i>A'</i>	$\nu_1$	-O=N stretch	1778	Could be $\nu_2$
	$\nu_2$	-N=O stretch	1690	Could be $\nu_1$
	$\nu_3$	-N-O- stretch	482	
	$\nu_4$	O=N-O= bend	184	Could be $\nu_5$
	$\nu_5$	N=O-N= bend	116	Could be $\nu_4$
	$\nu_6$	torsion	—	

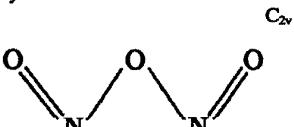
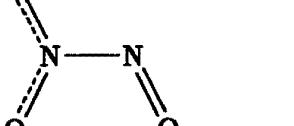
## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	Remarks
116	$\nu_5$	
184	$\nu_4$	
296	$\nu_4 + \nu_5$ or $\nu_3 - \nu_4$	
371	$2\nu_4$	
482	$\nu_3$	
552	$3\nu_4$	
593	$2\nu_3 - 2\nu_4$	
672	$\nu_3 + \nu_4$	
744	$4\nu_4$	
778	$2\nu_3 - \nu_4$	
849	$\nu_3 + 2\nu_4$	
925	$5\nu_4$	
962	$2\nu_3$	
1038	$\nu_2 + 3\nu_4$	NO + HCl
1151	$2\nu_3 + \nu_4$	NO + HCl
1197	$\nu_2 - \nu_3$	NO + HCl
1342	$2\nu_3 + 2\nu_4$	NO + HCl
1690	$\nu_2$	
1778	$\nu_1$	
1873	$\nu_2 + \nu_4$	
1957	$\nu_1 + \nu_4$	
1994	$\nu_2 + (\nu_4 + \nu_5)$ or $\nu_2 + (\nu_3 - \nu_4)$	
2061	$\nu_2 + 2\nu_4$	
2137	$\nu_1 + 2\nu_4$	NO + HCl
2176	$\nu_2 + \nu_3$	
2237	$\nu_2 + 3\nu_4$	
2345	$\nu_2 + (\nu_3 + \nu_4)$	NO + HCl
3363	$2\nu_2$	
3450	$\nu_1 + \nu_2$	NO + HCl; IR
3469	$2\nu_2 + \nu_5$	
3541	$2\nu_2 + \nu_4$	
3738	$2\nu_1 + \nu_4$ or $2\nu_2 + 2\nu_4$	NO + HCl; IR

## Reference

- <sup>1</sup>J. R. Ohlsen, and J. Laane, J. Am. Chem. Soc. **100**, 6948 (1978).

4.6.  $N_2O_3$ 

Species	Molecular point group	Normal modes Symmetry	Vibrations	Activity	
				Raman	Infrared
<i>Symmetric</i>					
	$C_{2v}$	$A_1$ $A_2$ $B_1$ $B_2$	$v_1 \rightarrow v_4$ $v_5$ $v_6$ $v_7 \rightarrow v_9$	A A A A	A A A A
					
<i>Asymmetric</i>					
	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_7$ $v_8, v_9$	A A	A A
					

4.6.a. *sym*- $N_2O_3$   
Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency ( $\text{cm}^{-1}$ )	References, Remarks
$A_1$	$v_1$	$N=O$ s-stretch	1740	Ra : 2(M:NO)
	$v_2$	$N-O$ s-stretch	967 973.6	IR : 1(M:N <sub>2</sub> ); 3(LXe) IR : 2(M:NO); 4(M:Ne) Ra : 2(M:NO)
	$v_3$	$N-O-N$ bend	375 388 395	IR : 3(LXe); could be $v_4$ IR : 1(M:N <sub>2</sub> ) Ra : 2(M:NO)
	$v_4$	$O=N-O$ s-bend	345 366 375	Ra : 2(M:NO) IR : 1(M:N <sub>2</sub> ) IR : 3(LXe); could be $v_3$
$A_2$	$v_5$	torsion	140	Ra : 2(M:NO)
$B_1$	$v_6$	torsion	105	Ra : 2(M:NO); calculated from $2v_6 = 210 \text{ cm}^{-1}$
$B_2$	$v_7$	$N=O$ a-stretch	1661 1679 1689 1697.2	IR : 1(M:N <sub>2</sub> ) Ra : 2(M:NO) IR : 1(M:N <sub>2</sub> ); 2(M:NO); 3(LXe) IR : 4(M:Ne)
	$v_8$	$N-O$ a-stretch	865 877	IR : 2(M:NO) IR : 1(M:N <sub>2</sub> )
	$v_9$	$O-N-O$ a-bend	705 710	IR : 1(M:N <sub>2</sub> ); 2(M:NO) Ra : 2(M:NO)

## Observed Infrared Bands

No other bands were observed, apart the fundamental ones mentioned above.

## References

- <sup>1</sup>E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
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**4.6.b. asym-N<sub>2</sub>O<sub>3</sub>**  
**Observed Fundamental Vibrational Frequencies**

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A'</i>	<i>v</i> <sub>1</sub>	N=O stretch	1829.54	IR : 3(G); 6(LXe); 8(M:Ne) Band origin calculated from band shape simulations
			1840	IR : 2(M:N <sub>2</sub> )
			1860	IR,Ra : 5(M:NO)
			1867	IR : 1(M:O <sub>2</sub> )
<i>v</i> <sub>2</sub>		NO <sub>2</sub> a-stretch	1594	IR : 1(M:O <sub>2</sub> ); 5(M:NO) Ra : 5(M:NO)
			1627	IR : 2(M:N <sub>2</sub> ); 6(LXe)
			1643.3	IR : 8(M:Ne)
			1652	IR : 3(G)
<i>v</i> <sub>3</sub>		NO <sub>2</sub> s-stretch	1288	Ra : 5(M:NO)
			1296	IR : 5(M:NO); 6(LXe)
			1302.5	IR : 1(M:O <sub>2</sub> ); 2(M:N <sub>2</sub> ); 3(G); 8(M:Ne)
<i>v</i> <sub>4</sub>		NO <sub>2</sub> bend	773.1	IR : 2(M:N <sub>2</sub> ); 3(G); 6(LXe) 8(M:Ne)
			788	IR : 1(M:O <sub>2</sub> ); 5(M:NO) Ra : 5(M:NO)
<i>v</i> <sub>5</sub>		NO <sub>2</sub> rock out of phase (or NO <sub>2</sub> rock)	395	IR : 5(M:NO)
			405	Ra : 5(M:NO)
			413	IR : 3(G); 6(LXe)
			420	IR : 2(M:N <sub>2</sub> )
<i>v</i> <sub>6</sub>		N-N stretch	243	IR : 3(G); 6(LXe)
			263	IR : 4(L); 5(M:NO)
				Ra : 5(M:NO)
<i>v</i> <sub>7</sub>		NO <sub>2</sub> rock in phase (or wag in plane)	160	IR : 4(L)
			203	IR,Ra : 5(M:NO)
<i>A''</i>	<i>v</i> <sub>8</sub>	NO <sub>2</sub> wag (out of plane)	615.5	IR : 6(LXe)
			626	IR,Ra : 5(M:NO)
<i>v</i> <sub>9</sub>		torsion	63	IR : 3(G)
			70	IR,Ra : 5(M:NO)
			76	IR : 4(L)

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
70	<i>v</i> <sub>9</sub>	5(Ra,M:NO)	<i>T</i> = 12 K See also 3(IR,G); 4(IR,L)
205	<i>v</i> <sub>7</sub>	5(Ra,M:NO)	<i>T</i> = 12 K See also 4(IR,L)
244(1)	<i>v</i> <sub>6</sub>	6(IR,LXe)	<sup>b</sup> <i>T</i> = 165 K See also 3(IR,G); 4(IR,L); 5(Ra + IR,M)
330 337 346 355	<i>v</i> <sub>5</sub> - <i>v</i> <sub>9</sub> + n <i>v</i> <sub>9</sub> - n <i>v</i> <sub>9</sub>	3(IR,G)	<i>T</i> = 220 K; Q heads C-type bands See also 6(IR,LXe)
370	<i>v</i> <sub>8</sub> - <i>v</i> <sub>6</sub>	5(Ra,M:NO)	<i>T</i> = 12 K

## Observed Infrared Bands -- Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
408 P 419 R	$v_5$ (a,B)-type band	3(IR,G)	$T = 220$ K See also 2,5(IR,M); 5(Ra,M); 6(IR,LXe)
455 462 469 477	$(v_5 + v_9) + 3v_9 - 3v_9$ $(v_5 + v_9) + 2v_9 - 2v_9$ $(v_5 + v_9) + v_9 - v_9$ $v_5 + v_9$	3(IR,G)	$T = 220$ K; Q heads C-type bands See also 6(IR,LXe); the authors attributed $2v_6$ to 477 cm <sup>-1</sup>
525(1)	$v_3 - v_4$ (?)	6(IR,LXe)	b $T = 165$ K; could be $v_4 - v_6$ (see below)
532 545 557 570	$v_4 - v_6$ $(v_4 - v_6) + v_9 - v_9$ $(v_4 - v_6) + 2v_9 - 2v_9$ $(v_4 - v_6) + 3v_9 - 3v_9$	3(IR,G)	$T = 220$ K; Q heads (A,b)- or (A,B)-type bands
565	$v_8 - v_9$ (?)	5(Ra,M:NO)	$T = 12$ K; could belong to the sequence above
615.5(1.0) $v_8$		6(IR,LXe)	b $T = 165$ K See also 5(Ra+IR,M)
767 P 779 R	$v_4$ (a,B)-type band	3(IR,G)	$T = 220$ K See also 1,2,5,8(IR,M); 5(Ra,M); 6(IR,LXe)
803(1)	$v_8 + v_7$	6(IR,LXe)	b $T = 165$ K
822(1)	$2v_5$	6(IR,LXe)	b $T = 165$ K
993 1001 1010	$(v_4 + v_6) + 2v_9 - 2v_9$ $(v_4 + v_6) + v_9 - v_9$ $v_4 + v_6$	3(IR,G)	$T = 220$ K See also 6(IR,LXe)
1298 P 1305 O 1313 R	$v_3$ (A,b)-type band	3(IR,G)	$T = 220$ K See also 1,2,5,8(IR,M); 5(Ra,M); 6(IR,LXe)
1378(1)	$v_4 + v_8$	6(IR,LXe)	b $T = 165$ K
1426(1)	$v_3 + v_7$ (?)	6(IR,LXe)	b If $v_7 = 160$ cm <sup>-1</sup> ; $T = 165$ K
1485(1)	$v_3 + v_7$ (?)	6(IR,LXe)	b If $v_7 = 203$ cm <sup>-1</sup> ; $T = 165$ K
1535(1)	$2v_4$ or $v_3 + v_6$	6(IR,LXe)	b $T = 165$ K
1646 P 1658 R	$v_2$ (a,B)-type band	3(IR,G)	$T = 220$ K See also 1,2,5,8 (IR,M); 5(Ra,M); 6(IR,LXe)
1826.0 1827.5	$(v_1 + 2v_9 - 2v_9)^0$ $(v_1 + v_9 - v_9)^0$	7(IR,G)	$T = 232$ K Band origins calculated from the shifts between Q heads in the $v_1$ band region
1827.7	$(v_1 + (v_7 + v_9) - (v_7 + v_9))^0$	7(IR,G)	Same remarks as for $v_1 + nv_9 - nv_9$
1828.9	$(v_1 + v_7 - v_7)^0$	7(IR,G)	Same remarks as for $v_1 + nv_9 - nv_9$

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
1829.535(2)	$v_1^0$	7(IR,G)	<sup>a,c</sup> $T = 232$ K
1821.3 P 1829.5 O 1838.3 R	$v_1$ (A,B)-type band	7(IR,G)	$T = 232$ K See also 1,2,5,8(IR,M); 3(IR,G); 5(Ra,M); 6(IR,LXe)
1829.9	$(v_1 + (v_6 + v_9) - (v_6 + v_9))^0$	7(IR,G)	Same remarks as for $v_1 + nv_9 - nv_9$
1831.6	$(v_1 + v_6 - v_6)^0$	7(IR,G)	Same remarks as for $v_1 + nv_9 - nv_9$
2028(1)	$v_2 + v_5$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
2072(1)	$v_1 + v_6$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
2444(1)	$v_1 + v_8$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
2580(1)	$2v_3$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
2598(1)	$v_1 + v_4$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
2900(1)	$v_2 + v_3$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
3123(1)	$v_1 + v_3$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
3227(1)	$2v_2$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
3456(1)	$v_1 + v_2$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
3618.7 3621.3 3624.4	$(2v_1 + 3v_9 - 3v_9)^0$ $(2v_1 + 2v_9 - 2v_9)^0$ $(2v_1 + v_9 - v_9)^0$	7(IR,G)	$T = 232$ K Band origins calculated from the shifts between Q heads in the $2v_1$ band region
3625.5(1.0)	$2v_1$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
3628.03(5)	$2v_1^0$	7(IR,G)	<sup>a,c</sup> $T = 232$ K
3633.3 3639.1	$(2v_1 + v_6 - v_6)^0$ $(2v_1 + 2v_6 - 2v_6)^0$	7(IR,G)	Same remarks as for $2v_1 + nv_9 - nv_9$
3866(1)	$3v_3$	6(IR,LXe)	<sup>b</sup> $T = 165$ K
5386.7	$(3v_1 + v_9 - v_9)^0$	7(IR,G)	$T = 232$ K Band origin calculated from the shifts between Q heads in the $3v_1$ band region
5392.6	$(3v_1 + v_7 - v_7)^0$	7(IR,G)	Same remarks as for $3v_1 + v_9 - v_9$
5394.124(10)	$3v_1^0$	7(IR,G)	<sup>a,c</sup> $T = 232$ K

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
5404.2	(3v <sub>1</sub> + v <sub>6</sub> - v <sub>5</sub> ) <sup>0</sup>	7(IR,G)	Same remarks as for 3v <sub>1</sub> + v <sub>9</sub> - v <sub>9</sub>
7128.5(1.0)	4v <sub>1</sub> <sup>0</sup>	7(IR,G)	b,c <i>T</i> = 232 K

<sup>a</sup>Number in parentheses refers to the last quoted digits and represents one standard deviation

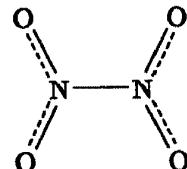
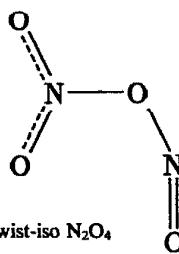
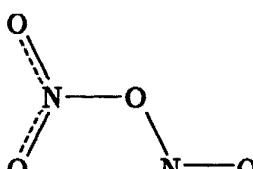
<sup>b</sup>Number in parentheses refers to the last quoted digits and represents the absolute accuracy of line position measurements

<sup>c</sup>Band shape simulation

## References

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- <sup>2</sup>E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
- <sup>3</sup>C. H. Bibart and G. E. Ewing, J. Chem. Phys. **61**, 1293 (1974).
- <sup>4</sup>G. M. Bradley, W. Siddall, H. L. Strauss, and E. L. Varetti, J. Phys. Chem. **79**, 1949 (1975).
- <sup>5</sup>E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. **87**, 1113 (1983).
- <sup>6</sup>R. F. Holland and W. B. Maier II, J. Chem. Phys. **78**, 2928 (1983).
- <sup>7</sup>L. A. Chewter, I. W. M. Smith, and G. Yarwood, Mol. Phys. **63**, 843 (1988).
- <sup>8</sup>M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

4.7. N<sub>2</sub>O<sub>4</sub>

Species	Molecular point group	Normal modes Symmetry Vibrations		Activity Raman Infrared	
<i>symmetric</i>					
	D <sub>2h</sub>	A <sub>1</sub> A <sub>u</sub> B <sub>1g</sub> B <sub>1u</sub> B <sub>2g</sub> B <sub>2u</sub> B <sub>3u</sub>	v <sub>1</sub> → v <sub>3</sub> v <sub>4</sub> v <sub>5</sub> , v <sub>6</sub> v <sub>7</sub> v <sub>8</sub> v <sub>9</sub> , v <sub>10</sub> v <sub>11</sub> , v <sub>12</sub>	A I A I A I I	I I I A I A A
sym-N <sub>2</sub> O <sub>4</sub> or D <sub>2h</sub> N <sub>2</sub> O <sub>4</sub>					
<i>staggered<sup>a</sup></i>					
cfr. symmetric, but the NO <sub>2</sub> planes are perpendicular to each other	D <sub>2d</sub>	A <sub>1</sub> B <sub>1</sub> B <sub>2</sub> E	v <sub>1</sub> → v <sub>3</sub> v <sub>4</sub> v <sub>5</sub> , v <sub>6</sub> v <sub>7</sub> → v <sub>9</sub>	A A A A	I I A A
<i>D-type<sup>b</sup></i>					
	C <sub>2</sub>	A' A''	v <sub>1</sub> → v <sub>9</sub> v <sub>10</sub> → v <sub>12</sub>	A A	A A
twist-iso N <sub>2</sub> O <sub>4</sub>					
<i>D'-type<sup>b</sup></i>					
	C <sub>2</sub>	A' A''	v <sub>1</sub> → v <sub>9</sub> v <sub>10</sub> → v <sub>12</sub>	A A	A A

<sup>a</sup>Not observed.<sup>b</sup>D and D'-types N<sub>2</sub>O<sub>4</sub> are often called *asym-* or *iso*-N<sub>2</sub>O<sub>4</sub>, without distinction. It is not yet obvious which molecular structure belongs to D or D'-type.

4.7.a. sym-N<sub>2</sub>O<sub>4</sub>

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
$A_g$	$v_1$	N–O s-stretch in phase	1380 1383 1387	Ra : 1,11(L); 6(S) 1,10(S); 4(M:Ar); 7(M:Ne) 7(M:Xe)
	$v_2$	NO <sub>2</sub> bend in phase	807 811 814	Ra : 1(L); 6(S); 7(M:Ne) 1,10(S); 11(L) 4(M:Ar); 7(M:Xe)
	$v_3$	N–N stretch	257 262 267 275 282	Ra : 7(M:Xe) 4(M:Ar) 1,11(L); 7(M:Ne) 1(S) 6,10,13(S)
$A_u$	$v_4$	torsion	79	Deduced from the band sequence around 540 cm <sup>-1</sup> (5(IR,G))
$B_{1g}$	$v_5$	N–O a-stretch out of phase	1712 1718 1725	Ra : 1(L) 7(M:Xe) 1,6,10(S)
	$v_6$	NO <sub>2</sub> rock out of phase (or NO <sub>2</sub> rock)	484 491 498	Ra : 1(L); 7(M:Xe) 1(S) 6,10,13(S); 7(M:Ne)
	$v_7$	NO <sub>2</sub> wag in phase (out of plane)	423 429 436	IR : 1(L); 5(G); 8(LXe) 1(G) 6,12(S)
$B_{2g}$	$v_8$	NO <sub>2</sub> wag out of phase (out of plane)	657 672 677	Ra : 7(M:Xe) 1(L) 6,10(S)
	$v_9$	N–O a-stretch in phase	1735 1742 1749.2 1756.76	IR : 1(L); 2(M:Ar); 3(M:N <sub>2</sub> ); 6(S) 8(LXe) 1(G); 2(M:O <sub>2</sub> ); 9(M:Ar); 12(S) 5,14, <u>15</u> (G)
	$v_{10}$	NO <sub>2</sub> rock in phase (or NO <sub>2</sub> wag in plane)	265 375 381 635	IR : 6(S); in agreement with the predicted value of 5(G) 8(LXe) 1(G) 12(S)
$B_{3u}$	$v_{11}$	N–O s-stretch out of phase	1250 1257 1261.1 1264	IR : 6,12(S); 8(LXe) 1(L); 2, <u>9</u> (M:Ar); <u>1,14</u> (G); 2(M:O <sub>2</sub> ); 3(M:N <sub>2</sub> ) 5(G)
	$v_{12}$	NO <sub>2</sub> bend out of phase	742 746 751.3	IR : 1(L); 6,12(S); 8(LXe) 2(M:Ar,O <sub>2</sub> ); 9(M:Ar) 1, <u>5,14</u> (G); 3(M:N <sub>2</sub> )

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
265(1)	$\nu_{10}$ (?)	6(IR,S)	<sup>a</sup> $T = 20$ K See below for other suggestions
281.3	$\nu_3$	10,13(Ra,S)	$T = 80$ and $20$ K respectively See also 1,6(Ra,S); 1,11(Ra,L); 4,7(Ra,M)
375	$\nu_{10}$ (?)	8(IR,LXe)	$T = 165$ K See also 1(IR,G)
370.3(2) 375.8(2) 380.1(2) 386.0(2)	$(\nu_2 - \nu_7) + n\nu_4 - n\nu_4$	5(IR,G)	<sup>a</sup> $T = 203$ K; Q heads C-type bands
404.7(2) 416.4(2) 420.7(2) 424.9(2) 429.5(2) 435.4(2) 442.2(2) 446.9(2) 451.9(2) 457.8(2)	$\nu_7 + n\nu_4 - n\nu_4$	5(IR,G)	<sup>a</sup> $T = 203$ K
435.8	$\nu_7$	12(IR,S)	$T = 20$ K See also 1(IR,L); 1,5(IR,G); 6(IR,S); 8(IR,LXe)
498.2	$\nu_6$	10(Ra,S)	$T = 80$ K See also 1(Ra,L); 1,6,13(Ra,S); 7(Ra,M)
522.5(2) 526.0(2) 529.0(2) 533.5(2) 538.3(2) 542.8(2) 547.7(2) 554.3(2)	$(\nu_6 + \nu_4) + 7\nu_4 - 7\nu_4$ $(\nu_6 + \nu_4) + 6\nu_4 - 6\nu_4$ $(\nu_6 + \nu_4) + 5\nu_4 - 5\nu_4$ $(\nu_6 + \nu_4) + 4\nu_4 - 4\nu_4$ $(\nu_6 + \nu_4) + 3\nu_4 - 3\nu_4$ $(\nu_6 + \nu_4) + 2\nu_4 - 2\nu_4$ $(\nu_6 + \nu_4) + \nu_4 - \nu_4$ $(\nu_6 + \nu_4)$	5(IR,G)	<sup>a</sup> $T = 203$ K; Q heads C-type bands
634.9	$\nu_{10}$ (?)	12(IR,S)	$T = 20$ K
676.8	$\nu_8$	10(Ra,S)	See also 1(Ra,L); 6(Ra,S); 7(Ra,M)
676.6(2) 683.9(2) 689.5(2) 695.7(2) 701.8(2) 709.1(2)	$(\nu_3 + \nu_7) + n\nu_4 - n\nu_4$	14(IR,G)	<sup>c</sup> Q heads See also 5(IR,G) See also 5(IR,G)
708	$\nu_3 + \nu_7$ (?)	8(IR,LXe)	$T = 165$ K See also 1(IR,G)
744(1) P 751(1) Q 759(1) R	$\nu_{12}$ A-type band	5(IR,G)	<sup>a</sup> $T = 203$ K See also 1(IR,L+G); 2,3,9(IR,M); 6,12(IR,S); $T = 203$ K See also 8(IR,LXe)

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
751.3(2)	$v_{12}^0$	14(IR,G)	b
761(1)	$v_6 + v_{10}$	5(IR,G)	a $T = 203$ K See also 6(IR,S) Suggested to form a Fermi diad with $v_{12}$ In 12(IR,S), a similar band at 752.1 cm <sup>-1</sup> is supposed to play the same role with $v = 736.6$ cm <sup>-1</sup> , but is attributed to $(v_{10} + v_{13})$
811.7	$v_2$	10(Ra,S)	See also 1,6(Ra,S); 1,11(Ra,L); 4,7(Ra,M)
1000	$v_3 + v_{12}$	8(IR,LXe)	$T = 165$ K
1004.6(2)	$\left. \begin{array}{l} 1011.1(2) \\ 1017.8(2) \\ 1036.4(2) \end{array} \right\} (v_3 + v_{12}) + nv_4 - nv_4$	14(IR,G)	c
1011.1(2)			Q heads
1017.8(2)			See also 5(IR,G)
1102.3(2)	$(v_7 + v_8)^0$	14(IR,G)	b See also 8(IR,LXe)
1194.0(2)	$\left. \begin{array}{l} 1197.3(2) \\ 1201.2(2) \\ 1205.5(2) \\ 1207.0(2) \\ 1210.4(2) \\ 1212.5(2) \\ 1215.7(2) \\ 1217.3(2) \\ 1221.9(2) \\ 1224.0(2) \\ 1227.7(2) \\ 1233.3(2) \end{array} \right\} (v_2 + v_7) + nv_4 - nv_4$ (?)	14(IR,G)	c
1197.3(2)			
1201.2(2)			
1205.5(2)			
1207.0(2)			
1210.4(2)			
1212.5(2)			
1215.7(2)			
1217.3(2)			
1221.9(2)			
1224.0(2)			
1227.7(2)			
1233.3(2)			
1237	$v_2 + v_7$ (?)	8(IR,LXe)	$T = 165$ K
1256(1) P	$v_{11}$	5(IR,G)	a
1264(1) Q	A-type band		See also 1(IR,L+G); 2,3,9(IR,M); 6,12(IR,S); 8(IR,LXe)
1272(1) R			8(IR,LXe)
1261.1(2)	$v_{11}^0$	14(IR,G)	b
1335.5	$2v_8$	10(Ra,S)	See also 1(Ra,L); 1,6(Ra,S) Fermi resonance is suggested with $v_1$
1382.3	$v_1$	10(Ra,S)	See also 1,6(Ra,S); 1,11(Ra,L); 4,7(Ra,M)
1491.4(2)	$(v_9 - v_3)^0$	14(IR,G)	b See also 1(IR,G); 8(IR,LXe)
1546	$v_2 + v_{12}$	8(IR,LXe)	$T = 165$ K See also 1(IR,L)
1681	$2v_8 + v_{10}$ (?) or $v_3 + v_8 + v_{12}$ (?)	8(IR,LXe)	$T = 165$ K See also 1(IR,L)
1723.5	$v_5$	10(Ra,S)	See also 1(Ra,L); 1,6(Ra,S); 7(Ra,M)
1733(1)	$(v_1 + v_{10})^0$ or $(v_6 + v_{11})^0$	14(IR,G)	b,d

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
1752(1) P 1764(1) R}	$v_9$ B-type band	5(IR,G)	a $T = 203$ K See also 1(IR,L+G); 2,3,9(IR,M); 6,12(IR,S); 8(IR,LXe) In 12(IR,S), the corresponding band at 1750.1 cm <sup>-1</sup> is supposed to form a Fermi diad with a band at 1727.9 cm <sup>-1</sup> attributed to $(v_6 + v_{11})$ ; see also 8(IR,LXe) for the same observation
1756.7650(15)	$v_9^0$	15(IR,G)	d,e See also 14(IR,G)
~1782	$v_4 + v_5$	8(IR,LXe)	$T = 165$ K
1802	$v_1 + v_7$	8(IR,LXe)	$T = 165$ K
1936.7(2)	$(v_8 + v_{11})^0$	14(IR,G)	b See also 1(IR,G); 8(IR,LXe)
2004(1)	$(v_3 + v_9)^0$	14(IR,G)	b See also 8(IR,LXe)
2063.0(2)	$(v_2 + v_{11})^0$	14(IR,G)	b See also 8(IR,LXe)
2125(1)	$(v_1 + v_{12})^0$ A-type band	14(IR,G)	b See also 1(IR,G); 8(IR,LXe)
2586.5(2)	$(2v_8 + v_{11})^0$	14(IR,G)	b See also 1(IR,G); 8(IR,LXe)
2631.5(2)	$(v_1 + v_{11})^0$ A-type band	14(IR,G)	b See also 1(IR,L+G); 8(IR,LXe)
2750.0(2)	$(v_{11} + 2v_{12})^0$	14(IR,G)	b See also 1(IR,G)
2973.0(2)	$(v_5 + v_{11})^0$ B-type band	14(IR,G)	b See also 1(IR,L+G); 8(IR,LXe)
3066(1)	$(2v_8 + v_9)^0$ B-type band	14(IR,G)	b See also 8(IR,LXe)
3088 3106	$v_1 + v_6 + v_{11}$ $v_1 + v_9$	8(IR,LXe) 8(IR,LXe)	Possible Fermi resonance See also 1(IR,L+G)
3117(1)	$(v_1 + v_9)^0$	14(IR,G)	b
3159(1)	$(2v_1 + v_7)^0$	14(IR,G)	b
3241(1)	$(v_2 + v_5 + v_{12})^0$ or $(v_3 + v_5 + v_{11})^0$	14(IR,G)	b
3416.5 3435	$v_5 + v_6 + v_{11}$ $v_5 + v_9$	8(IR,LXe) 8(IR,LXe)	Possible Fermi resonance See also 1(IR,L+G)
3442(1)	$(v_5 + v_9)^0$ A-type band	14(IR,G)	b
3773(1)	$(v_2 + v_5 + v_{11})^0$ B-type band	14(IR,G)	b
3910(?)	$v_1 + v_2 + v_9$ (?)	14(IR,G)	
3992(1)	$(2v_1 + v_{11})^0$	14(IR,G)	b
4251(1)	$(v_9 + 2v_{11})^0$	14(IR,G)	b See also 1(IR,G)
4330(1)	$(v_1 + v_5 + v_{11})^0$ B-type band	14(IR,G)	b

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
4478(1)	$(2v_1 + v_9)^0$	14(IR,G)	<sup>b</sup>
4668(1)	$(2v_5 + v_{11})^0$	14(IR,G)	<sup>b</sup> See also 1(IR,G)
4802(1)	$(v_1 + v_5 + v_9)^0$	14(IR,G)	<sup>b</sup>
5118(1)	$(3v_9)^0$ or $(2v_5 + v_9)^0$	14(IR,G)	<sup>b</sup> See also 1(IR,G)
6939(1)	$(2v_1 + v_2 + v_5 + v_9)^0$	14(IR,G)	<sup>b</sup>

<sup>a</sup>Number in parentheses refers to the last quoted digits and represents the accuracy of line position measurements.

<sup>b</sup>Number in parentheses refers to the last quoted digits and represents the accuracy of band origin measurements.

<sup>c</sup>Number in parentheses refers to the last quoted digits and represents the accuracy of head measurements.

<sup>d</sup>Supersonic molecular beam experiment.

<sup>e</sup>Band origin calculated from rotational analysis; number in parenthesis refers to the last quoted digits and represents one standard deviation.

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4.7.b. *asym-N<sub>2</sub>O<sub>4</sub>* : D-type

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A'</i>	<i>v</i> <sub>1</sub>	N=O stretch	1806	Ra : 4(M:Ne)
			1829	IR : 1(M:Ar,O <sub>2</sub> ); 3(M:O <sub>2</sub> ); 5(M:Ar)
			1850	Ra : 6(S)
			1861	IR : 2(M:N <sub>2</sub> )
<i>v</i> <sub>2</sub>		NO <sub>2</sub> a-stretch	1628	IR : 2(M:N <sub>2</sub> )
			1635	Ra : 4(M:Ne)
			1645	IR : 1(M:Ar,O <sub>2</sub> ); 3(M:O <sub>2</sub> ); 5(M:Ar) Ra : 4(M:Xe)
<i>v</i> <sub>3</sub>		NO <sub>2</sub> s-stretch	1279	IR : 2(M:N <sub>2</sub> )
			1290	IR : 1(M:Ar,O <sub>2</sub> ); 3(M:O <sub>2</sub> ); 5(M:Ar)
			1295	Ra : 4(M:Ne)
			1300	Ra : 4(M:Xe); 6(S)
<i>v</i> <sub>4</sub>		N-O stretch in O=N-O	904	IR : 1(M:O <sub>2</sub> ); 5(M:Ar)
			911	IR : 2(M:N <sub>2</sub> )
<i>v</i> <sub>5</sub>		NO <sub>2</sub> bend	783	IR : 1,3(M:O <sub>2</sub> )
			788	Ra : 4(M:Ne)
			792	IR : 1,5(M:Ar) Ra : 4(M:Xe) IR : 2(M:N <sub>2</sub> )
<i>v</i> <sub>6</sub>		O=N-O bend	624	Ra : 4(M:Ne,Xe)
			641	IR : 1,3(M:O <sub>2</sub> )
			647	Ra : 6,7(S) IR : 2(M:N <sub>2</sub> )
<i>A'</i>	<i>v</i> <sub>7</sub>	NO <sub>2</sub> rock (in plane)	488	IR : 1(M:O <sub>2</sub> ) The authors suggest two possible assignments: <i>v</i> <sub>7</sub> or <i>v</i> <sub>10</sub>
	<i>v</i> <sub>8</sub>	N-O-N bend	—	
<i>v</i> <sub>9</sub>		N-O stretch in O-NO <sub>2</sub>	—	
<i>A''</i>	<i>v</i> <sub>10</sub>	NO <sub>2</sub> wag (out of plane)	488	IR : 1(M:O <sub>2</sub> ) See remarks on <i>v</i> <sub>7</sub>
	<i>v</i> <sub>11</sub>	torsion	—	
<i>v</i> <sub>12</sub>		torsion	—	

One extra band at 304 cm<sup>-1</sup> was observed by Ref. 3 (IR,M:O<sub>2</sub>); it was tentatively assigned to D-type N<sub>2</sub>O<sub>4</sub>. The band at 263 cm<sup>-1</sup>, which was attributed to the *v*<sub>10</sub> mode of N<sub>2</sub>O<sub>4</sub> with D<sub>2h</sub> symmetry (see Ref. 6 (IR,S), in Sec. 4.7.a. *sym-N<sub>2</sub>O<sub>4</sub>*), has also been observed by Ref. 7 (Ra,S); the latter authors proposed that this band belongs to *D* or *D'*-type N<sub>2</sub>O<sub>4</sub>.

## Observed Infrared Bands

Apart from the fundamental bands listed above, only one other band is mentioned by Ref. 1 (IR,M:O<sub>2</sub>): (*v*<sub>2</sub>+*v*<sub>7</sub>) or (*v*<sub>2</sub>+*v*<sub>10</sub>) at 2132 cm<sup>-1</sup>.

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<sup>7</sup>A. Givan and A. Loewenschuss, J. Chem. Phys. **93**, 7592 (1990).

Mode	Frequency ( $\text{cm}^{-1}$ )	
	1(IR,M:O <sub>2</sub> )	2(IR,S)
$v_1$	1889–1899	2003
$v_2$	1584	1542
$v_3$	1290	1305
$v_4$	916	959
$v_5$	794	
$v_6$	660	
$v_7$ OR $v_{10}$	524	

4.7.c. asym-N<sub>2</sub>O<sub>4</sub> : D'-type

Besides the bands attributed to *D*-type N<sub>2</sub>O<sub>4</sub>, a few weak bands were observed and tentatively attributed to the *D'*-type by Ref. 1(IR,M:O<sub>2</sub>). Four peaks have also been attributed by Ref. 2(IR,S) to this isomer. We list here the assignments. The discrepancy between the observations of the two groups of workers is attributed "to the floppiness of these molecular forms, the frequencies being very sensitive to the environment" (see Ref. 2(IR,S)). These assignments for the *D'*-type N<sub>2</sub>O<sub>4</sub> obviously need further support.

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4.8. N<sub>2</sub>O<sub>5</sub>

The molecule is supposed to be planar, of C<sub>2v</sub> symmetry, but electron diffraction measurements (6), analyzed using a dynamical model, suggest a C<sub>2</sub> structure.

Species	Molecular point group	Normal modes		Activity	
		Symmetry	Vibrations	Raman	Infrared
<i>Planar</i>					
		$A_1$	$v_1 \rightarrow v_6$	A	A
		$A_2$	$v_7, v_8$	A	I
		$B_1$	$v_9, v_{10}$	A	A
		$B_2$	$v_{11} \rightarrow v_{15}$	A	A
<i>Non planar</i>					
	C <sub>2</sub>	A	$v_1 \rightarrow v_8$	A	A
		B	$v_9 \rightarrow v_{15}$	A	A

## Observed Fundamental Vibrational Frequencies\*

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A</i> <sub>1</sub>	<i>v</i> <sub>1</sub>	NO <sub>2</sub> a-stretch in phase	1716 1720 1728 1744 1752	9(G) 1,5(G) 2(G) 2(S); 3(M:N <sub>2</sub> ) 1(M:CO <sub>2</sub> )
	<i>v</i> <sub>2</sub>	NO <sub>2</sub> s-stretch in phase	1300 1305 1316 1337	4(M:O <sub>2</sub> ) 3(M:N <sub>2</sub> ) 1(M:CO <sub>2</sub> ) 2(G + S); 9(G)
	<i>v</i> <sub>3</sub>	NO <sub>2</sub> bend in phase	732 737 743	2(S) 1(M:CO <sub>2</sub> ); 3(M:N <sub>2</sub> ); 4(M:O <sub>2</sub> ); 7(M:Ar) 1,2,5,9(G)
	<i>v</i> <sub>4</sub>	NO <sub>2</sub> rock (in plane)	~600 ~614	2(S) 2(G)
	<i>v</i> <sub>5</sub>	N-O-N s-stretch	337 353	2(S) 2,10(G)
<i>A</i> <sub>2</sub>	<i>v</i> <sub>6</sub>	N-O-N bend	~85	2(S); from combination bands
	<i>v</i> <sub>7</sub>	NO <sub>2</sub> wag (out of plane)	—	—
<i>B</i> <sub>1</sub>	<i>v</i> <sub>8</sub>	NO <sub>2</sub> s-twist	—	—
	<i>v</i> <sub>9</sub>	NO <sub>2</sub> wag (out of plane)	557 562 577	5(G) 2(S) 2(G)
<i>B</i> <sub>2</sub>	<i>v</i> <sub>10</sub>	NO <sub>2</sub> a-twist	~50	10(G)
	<i>v</i> <sub>11</sub>	NO <sub>2</sub> a-stretch out of phase	1703 1718 1728	1(M:CO <sub>2</sub> ); 2(S); 3(M:N <sub>2</sub> ); 4(M:O <sub>2</sub> ); 7(M:Ar) 1,5,9(G) 2(G)
<i>v</i> <sub>12</sub>	NO <sub>2</sub> s-stretch out of phase	1241 1246	4(M:O <sub>2</sub> ) 1,2,5,9(G); 1(M:CO <sub>2</sub> ); 2(S); 3(M:N <sub>2</sub> ); 7(M:Ar)	
	<i>v</i> <sub>13</sub>	N-O-N a-stretch	853 860	2(S) 2,9(G)
<i>v</i> <sub>14</sub>	NO <sub>2</sub> bend out of phase	712 719 737 743	2(S) 1(M:CO <sub>2</sub> ) 3(M:N <sub>2</sub> ); 4(M:O <sub>2</sub> ); 7(M:Ar) 1,2,5,9(G)	
	<i>v</i> <sub>15</sub>	NO <sub>2</sub> rock (in plane)	337 353	2(S) 2,10(G)

\*All the observations were made with infrared techniques.

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
50	$\nu_{10}$	10(G)	
353	$\nu_5$ OR $\nu_{15}$	2(G)	See also 2(S); 10(G)
439	$\nu_5 + \nu_6$ (?)	2(G)	
577	$\nu_9$	2(G)	See also 2(S); 5(G)
614	$\nu_4$	2(G)	See also 2(S)
743.38 (2)	$\nu_3$ OR $\nu_{14}$	5(G)	a,b Q head; R,Q,P structure See also 1,2,9(G); 1,3,4,7(M); 2(S)
860	$\nu_{13}$	2.9(G)	See also 2(S)
986	$(\nu_1$ OR $\nu_{11}) - (\nu_3$ OR $\nu_{14})$ (?)	2(G)	
1245.86(6)	$\nu_{12}$	5(G)	a,b Q head; R,Q,P structure See also 1,2,9(G); 1,3,4,7(M); 2(S)
1338	$\nu_2$	2(G)	See also 1,3,4(M); 2(S); 9(G)
1430	$\nu_2 + \nu_6$ (?)	2(G)	b
1720	$\nu_1$ OR $\nu_{11}$	5(G)	See also 1,2,9(G); 1,3,4,7(M); 2(S)
2072	$(\nu_1$ OR $\nu_{11}) + \nu_5$ (?)	2(G)	
2314	$(\nu_1$ OR $\nu_{11}) + \nu_4$ (?)	2(G)	
2574	$\nu_2 + \nu_{12}$	2(G)	See also 5,9(G)
2954	$(\nu_1$ OR $\nu_{11}) + \nu_{12}$	2(G)	See also 5,9(G)
3053	$(\nu_1$ OR $\nu_{11}) + \nu_2$	2(G)	See also 5,9(G)
3424	$2\nu_1$ OR $2\nu_{11}$	2(G)	
3528	$(2\nu_1$ OR $2\nu_{11}) + \nu_6$	2(G)	

<sup>a</sup>Number in parentheses refers to the last quoted digits and represents the accuracy of line position measurements.

<sup>b</sup>Rotational line list available in ATMOS database<sup>8</sup>.

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4.9.  $(N_2O)_2$ 

Species	Molecular point group	Normal modes Symmetry	Vibrations	Activity	
				Raman	Infrared
(a)					
$N-N-O$	$N-N-O$	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_9$ $v_{10} \rightarrow v_{12}$	A A
(b)					
$N-N-O$	$N-N-O$	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_9$ $v_{10} \rightarrow v_{12}$	A A
(c)					
$N-N-O$	$N-N-O$	$C_s$	$A'$ $A''$	$v_1 \rightarrow v_9$ $v_{10} \rightarrow v_{12}$	A A
(a)					
$N-N-O$	$O-N-N$	$C_{2h}$	$A_g$ $A_u$ $B_g$ $B_u$	$v_1 \rightarrow v_5$ $v_6, v_7$ $v_8$ $v_9 \rightarrow v_{12}$	A I A I
(b)					
$N-N-O$	$O-N-N$	$C_{2h}$	$A_g$ $A_u$ $B_g$ $B_u$	$v_1 \rightarrow v_5$ $v_6, v_7$ $v_8$ $v_9 \rightarrow v_{12}$	I A I A

## Observed Fundamental Vibrational Frequencies

The (a) species of  $C_{2h}$  symmetry is now the unique one recognized by several authors. No Raman experiment seems to be reported. Therefore,  $v_1 \rightarrow v_5$  and  $v_8$  were not

observed. On the other hand, to our knowledge, only two fundamental frequencies have been observed in infrared spectra. They correlate with the  $v_1$  (N–O stretch) and  $v_3$  (N–N stretch) of  $N_2O$  and are of  $B_u$  symmetry. We will call them  $v_9$  and  $v_{10}$ .

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
$B_u$	$\nu_9$	out of phase N-O stretch	1279.711	4(IR,G)
	$\nu_{10}$	out of phase N-N stretch	2229.48	1,2(IR,G)

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
1279.7107(6)	$\nu_9^0$	4(IR,G)	<sup>a</sup> $T_{\text{rot}} = 5-10 \text{ K}$
~1277.7 P 1279.7 Q ~1281.7 R	$\nu_9$ (A,B)-type band	4(IR,G)	$T_{\text{rot}} = 5-10 \text{ K}$
2229.48	$\nu_{10}$	2(IR,G)	See also 1(IR,G)
3478.4357(30)	$(\nu_9 + \nu_{10})^0$	3(IR,G)	<sup>a</sup>

<sup>a</sup>Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents one standard deviation.

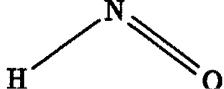
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## 4.10. HNO

Species	Molecular point group	Normal modes Symmetry	Vibrations	Activity Raman	Activity Infrared
	C <sub>2</sub>	A'	v <sub>1</sub> → v <sub>3</sub>	A	A

Useful information on the structure of this molecule is presented in Ref. 3.

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A'</i>	v <sub>1</sub>	N-H stretch	2683.9521 2716 2756	2,6,7(IR,G) 4(IR,M:Ar) 4(IR,M:N <sub>2</sub> )
	v <sub>2</sub>	bend	1500.819 1505 1511	2,6(IR,G); 5(LSS,G) 4(IR,M:Ar) 4(IR,M:N <sub>2</sub> )
	v <sub>3</sub>	N=O stretch	1565.348 1568.5	2,6(IR,G); 4(IR,M:Ar); 5(LSS,G) 1(IR,M:Ar); 4(IR,M:N <sub>2</sub> )

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
1500.8192(14)	v <sub>2</sub> <sup>0</sup> (A,B)-type band	5(LSS,G) 6(IR,G)	* Coriolis interaction with v <sub>3</sub> See also 2(IR,G); 4(IR,M)
1565.3481(4)	v <sub>3</sub> <sup>0</sup> (A,B)-type band	5(LSS,G) 6(IR,G)	* Coriolis interaction with v <sub>2</sub> See also 1,4(IR,M); 2(IR,G)
2665.3	2v <sub>1</sub> - v <sub>1</sub>	2(IR,G)	
2683.95210(8)	v <sub>1</sub> <sup>0</sup> (A,B)-type band	6,7(IR,G)	* See also 2(IR,G); 4(IR,M)
~3300	2v <sub>3</sub> ou v <sub>2</sub> + v <sub>3</sub> (?)	1(IR,M:Ar)	T = 20 K

\* Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents one standard deviation.

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4.11.  $HNO_2$ 

Species	Molecular point group	Symmetry	Normal modes Vibrations	Activity	
				Raman	Infrared
<i>trans</i> -HONO					
	$C_s$	$A'$	$\nu_1 \rightarrow \nu_5$	A	A
		$A''$	$\nu_6$	A	A
<i>cis</i> -HONO					
	$C_s$	$A'$	$\nu_1 \rightarrow \nu_5$	A	A
		$A''$	$\nu_6$	A	A

4.11.a. *trans*-HONO

This species is the most stable one.

Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency ( $\text{cm}^{-1}$ )	References, Remarks
$A'$	$\nu_1$	O-H stretch	3512	4(IR,S)
			3558	3(IR,M:N <sub>2</sub> )
			3590.770	1,2,4,7,8,10, <u>15</u> (IR,G)
	$\nu_2$	N=O stretch	1635	4(IR,S)
			1687	3(IR,M:N <sub>2</sub> ); 5,14(IR,M:Ar)
			1699.758	1,2,4,7,8,10,18(IR,G); 6(LSS,G); 9(DL,G)
	$\nu_3$	H-O-N bend	1421	4(IR,S)
			1298	3(IR,M:N <sub>2</sub> )
			1263.2069	1,2,4,7,8,10, <u>18</u> (IR,G); 5(IR,M:Ar); 13(DL,G)
	$\nu_4$	O-N stretch	790.1170	1,2,4,7,8,10,11, <u>17</u> (IR,G)
			795	14(IR,M:Ar)
			801	4(IR,S); 5(IR,M:Ar)
			815	3(IR,M:N <sub>2</sub> )
	$\nu_5$	O-N-O bend	595.620	1,2,4,8,10, <u>11</u> (IR,G)
			625	3(IR,M:N <sub>2</sub> )
			702	4(IR,S)
$A''$	$\nu_6$	torsion	499	4(IR,S)
			543.880	1,2,4,8,10, <u>11</u> (IR,G)
			550	5(IR,M:Ar)
			583	3(IR,M:N <sub>2</sub> )

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
543.880(4)	$v_6^0$	11(IR,G)	b,c Global fit with $v_5$ band rotational data, taking into account a Coriolis interaction between $v_5$ and $v_6$ levels. See also 8(IR,G)
540	$v_6$ C-type band	4(IR,G)	Q head See also 1,2,10(IR,G); 3,5(IR,M); 4(IR,S)
595.620(5)	$v_5^0$	11(IR,G)	b,c Global fit with $v_6$ band rotational data, taking into account a Coriolis interaction between $v_5$ and $v_6$ levels. See also 8(IR,G)
580 P 593 Q 607 R	$v_5$ A-type band	4(IR,G)	See also 1,2,10(IR,G); 3(IR,M); 4(IR,S)
790.117045(32)	$v_4^0$	17(IR,G)	a,c,e See also 8,11(IR,G)
777 P 791 Q 806 R	$v_4$ A-type band	4(IR,G)	See also 1,2,7,10(IR,G); 3,5,14(IR,M); 4(IR,S)
1263.20693(5)	$v_3^0$	18(IR,G)	a,c,e See also 8(IR,G); 13(DL,G)
1252 P 1265 Q 1278 R	$v_3$ (A,b)-type band	4(IR,G)	Perturbations due to resonance with $2v_5$ and $v_4 + v_6$ See also 1,2,7,10,18(IR,G); 3,5(IR,M); 4(IR,S)
1699.7582(6)	$v_2^0$	9(DL,G)	a,c,e See also 6(LSS,G); 8,18(IR,G)
1684 P 1699 Q 1715 R	$v_2$ (A,b)-type band	4(IR,G)	Perturbations due to resonance with $v_5 + 2v_6$ and $2v_5 + v_6$ See also 1,2,7,10,18(IR,G); 3,5,14(IR,M); 4(IR,S)
3372.12(6)	$2v_2^0$	8(IR,G)	a,d See also 18(IR,G)
3360 P 3372 Q 3392 R	$2v_2$ A-type band	4(IR,G)	See also 1,7,18(IR,G)
3590.77022(13)	$v_1^0$	15(IR,G)	a,c,e See also 8(IR,G)
3575 P 3588 Q 3605 R	$v_1$ (A,b)-type band	4(IR,G)	Coriolis interaction with $2v_3 + v_5 + v_6$ See also 1,2,7,10(IR,G); 3(IR,M); 4(IR,S)
4124	$v_2 + 2v_3$ A-type band	1(IR,G)	
4378.3	$(v_1 + v_4)^0$ (A,B)-type band	18(IR,G)	See also 1,16(IR,G)

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
4829.6	(v <sub>1</sub> + v <sub>3</sub> ) <sup>0</sup> A-type band	18(IR,G)	See also 1(IR,G)
5038	3v <sub>2</sub> <sup>0</sup> (?)	1(IR,G)	
6045.4	(v <sub>1</sub> + 2v <sub>3</sub> ) <sup>0</sup> A-type band	18(IR,G)	See also 1(IR,G)
7016.78895(20)	2v <sub>1</sub> <sup>0</sup> (A,b)-type band	18(IR,G)	<sup>a,c</sup> See also 1,16(IR,G)
10280.483(11)	3v <sub>1</sub> <sup>0</sup> (A,b)-type band	18(IR,G)	<sup>a,c</sup> See also 16(IR,G); possible resonance with 2v <sub>1</sub> + v <sub>2</sub> + 2v <sub>4</sub>
13385	4v <sub>1</sub> <sup>0</sup> (A,b)-type band	16(IR,G)	Possible resonance with 3v <sub>1</sub> + 2v <sub>3</sub> + v <sub>5</sub>

<sup>a</sup>Number in parentheses refers to the last quoted digits and represents one standard deviation.<sup>b</sup>Number in parentheses refers to the last quoted digits and represents the absolute accuracy of line position measurements.<sup>c</sup>Band origin calculated from rotational analysis.<sup>d</sup>Band origin calculated from band shape simulation.<sup>e</sup>Rotational line list available in ATMOS database (12).

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4.11.b. *cis*-HONO

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency (cm <sup>-1</sup> )	References, Remarks
<i>A'</i>	$v_1$	O-H stretch	3411	3(IR,M:N <sub>2</sub> ); 5(IR,M:Ar)
			3426.193	1,2,4,7,8,10, <u>17</u> (IR,G)
	$v_2$	N=O stretch	1611	4(IR,S)
			1628	1(IR,G)
			1633	3(M:N <sub>2</sub> ); 5,13(IR,M:Ar)
			1640.517	2,4,7(IR,G); <u>6</u> (LSS,G)
<i>v<sub>3</sub></i>		H-O-N bend	1261	4(IR,G); 5,13(IR,M:Ar)
	$v_4$	O-N stretch	851.9431	4,7,8,10,11, <u>15</u> (IR,G); 5,13(IR,M:Ar); 9(DL,G)
			857	1,2(IR,G); 4(IR,S)
			865	3(IR,M:N <sub>2</sub> )
<i>v<sub>5</sub></i>		O-N-O bend	609	4, <u>8</u> (IR,G); 5,13(IR,M:Ar)
			721	4(IR,S)
<i>A''</i>	$v_6$	torsion	518	4(IR,S)
			639	1,2,4, <u>8</u> (IR,G); 5,13(IR,M:Ar)
			658	3(IR,M:N <sub>2</sub> )

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
609.0(5)	$v_3^0$	8(IR,G)	<sup>a,c</sup>
608	$v_5$	4(IR,G)	Q head See also 4(IR,S); 5,13(IR,M)
638.5(5)	$v_6^0$	8(IR,G)	<sup>a,c</sup>
638	$v_6$	4(IR,G)	Q head See also 1,2(IR,G); 3,5,13(IR,M); 4(IR,S)
851.943054(32)	$v_4^0$	15(IR,G)	<sup>a,b,d</sup> See also 8,10,11(IR,G); 9(DL,G)
842 P 853 Q 868 R	$v_4$ (A,b)-type band	4(IR,G)	See also 1,2,7(IR,G); 3,5,13(IR,M); 4(IR,S)
1261	$v_3$ A-type band	4(IR,G)	Q head See also 5,13(IR,M)
1640.517(1)	$v_2^0$	6(LSS,G)	<sup>a,b,d</sup>
1640	$v_2$ (A,b)-type band	4(IR,G)	Q head See also 1,2,7(IR,G); 3,5,13(IR,M); 4(IR,S)
2493.00(5)	$(v_2 + v_4)^0$	8(IR,G)	<sup>a,c</sup> See also 1,7,16(IR,G)
3257.98(8)	$2v_2^0$ A-type band	8(IR,G)	<sup>a,c</sup> See also 1,7,16(IR,G)
3426.19275(40)	$v_1^0$ (A,B)-type band	17(IR,G)	<sup>a,b</sup> See also 1,2,4,7,8,10(IR,G); 3,5(IR,M)

## Observed Infrared Band -- Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
4281	$(v_1 + v_4)^0$ (A,B)-type band	14,16(IR,G)	
4829	$3v_3^0$ (A,b)-type band	14(IR,G)	Reassigned by 16(IR,G) to $(v_1 + v_3)^0$ for <i>trans</i> -HNO <sub>2</sub>
6664.5	$2v_1^0$ (a,B)-type band	16(IR,G)	See also 1,14(IR,G)

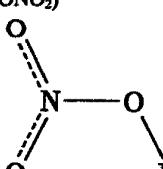
<sup>a</sup>Number in parentheses refers to the last quoted digits and represents one standard deviation.<sup>b</sup>Band origin calculated from rotational analysis.<sup>c</sup>Band origin calculated from band shape simulation.<sup>d</sup>Rotational line list available in ATMOS database (12).

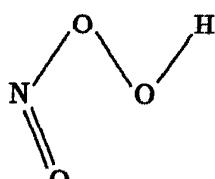
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<sup>8</sup>C. M. Deeley and I. M. Mills, J. Mol. Struct. **100**, 199 (1983).

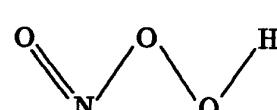
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<sup>14</sup>S. M. Holland, R. J. Stickland, M. N. R. Ashfold, D. A. Newnham, and I. M. Mills, J. Chem. Soc. Faraday Trans. **87**, 3461 (1991).  
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4.12. HNO<sub>3</sub>

Species	Molecular point group	Normal modes		Activity	
		Symmetry	Vibrations	Raman	Infrared
<i>Nitric acid</i> (HONO <sub>2</sub> )					
	C <sub>2</sub>	<i>A'</i>	$v_1 \rightarrow v_7$	A	A
		<i>A''</i>	$v_8, v_9$	A	A

*Peroxynitrous acid*  
(HOONO)*cis*

For the HOONO species, the O-H bond is nearly perpendicular to the O=N-O plane. These two molecular species are then non planar, and have no symmetry element.

*trans*

4.12.a. Nitric acid ( $\text{HONO}_2$ )

## Observed Fundamental Vibrational Frequencies

Sym.	Mode	Approximate type	Frequency ( $\text{cm}^{-1}$ )	References, Remarks
$A'$	$v_1$	O-H stretch	3106 3400 3410 3520 3550 3560	3(IR,S) 1(Ra,L) 3(Ra,L) 15(IR,M:Ar) 3(IR,G) 2(IR,G)
	$v_2$	$\text{NO}_2$ a-stretch	1646 1675 1698 1709.568	3(IR,S) 1,3(Ra,L) 15(IR,M:Ar) 2,3(IR,G); 5,10(DL,G)
	$v_3$	$\text{NO}_2$ s-stretch	1256 1300 1320 1325.735	3(IR,S) 1,3(Ra,L) 15(IR,M:Ar) 2,3,14(IR,G); 7(LSS,G)
	$v_4$	H-O-N bend	1303.518 1395 (?) 1420 (?)	3,14(IR,G); 15(IR,M:Ar) 3(Ra,L) 3(IR,S)
	$v_5$	$\text{NO}_2$ bend (in plane)	879.108 889.5 896.9 }	2,3(IR,G); 6(DL,G) 15(IR,M:Ar) 1,3(Ra,L) 3(IR,S)
	$v_6$	O- $\text{NO}_2$ stretch	646.826 680 722	3,12(IR,G) 1,3(Ra,L) 3(IR,S)
$A''$	$v_7$	O- $\text{NO}_2$ bend	580.304 610 707	2,3,12(IR,G) 1,3(Ra,L) 3(IR,S)
	$v_8$	$\text{NO}_2$ bend (out of plane)	763.154 769 773	2,3,12(IR,G); 15(IR,M:Ar) 1,3(Ra,L); estimated from $2v_8$ measurement 3(IR,S)
	$v_9$	O-H torsion	458.229 483	2,3,4,11(IR,G) 3(Ra,L)

## Observed Infrared Bands

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
376.5	$\nu_9 - \nu_9$	4(IR,G)	Q head
392.8	$\nu_9 - \nu_9$	4(IR,G)	Q head
410.5	$\nu_9 - \nu_9$	4(IR,G)	Q head; see also 3(IR,G)
422.1	$\nu_9 - \nu_9$	4(IR,G)	Q head; see also 3(IR,G)
438.5	$\nu_9 - \nu_9$	4(IR,G)	Q head; see also 3(IR,G)
458.2287(5)	$\nu_9^0$	11(IR,G)	
457.8 P } 475.0 R }	$\nu_9$ C-type band	4(IR,G) 3(IR,G)	See also 2(IR,G); 3(Ra,L)
580.3035(5)	$\nu_9^0$	12(IR,G)	
561.0 P } 579.0 Q } 590.2 R }	$\nu_7$ (A,b)-type band	3(IR,G)	See also 1,3(Ra,L); 2(IR,G); 3(IR,S)
641.3 646.8262(5)	$\nu_6 + \nu_9 - \nu_9$ $\nu_6^0$	3(IR,G) 12(IR,G)	
634.0 P } 646.6 Q } 657.2 R }	$\nu_6$ A-type band	3(IR,G)	See also 1,3(Ra,L); 3(IR,S)
747.0 763.1542(5)	$\nu_8 + \nu_9 - \nu_9$ $\nu_8^0$	3(IR,G) 12(IR,G)	
745.0 P } 762.2 Q } 783.2 R }	$\nu_8$ C-type band	3(IR,G)	See also 1,3(Ra,L); 2(IR,G); 3(IR,S); 15(IR,M)
879.1082(5)	$\nu_5^0$	6(DL,G)	a,b,c
869.4 P } 878.6 O }	$\nu_5$ A- or (A,b)-type band	3(IR,G)	Fermi resonance with $2\nu_9$ See also 1,3(Ra,L); 2(IR,G); 3(IR,S); 15(IR,M)
896.4187	$2\nu_9^0$	8,9	Calculated line positions See also 3(IR,G); 15(IR,M)
845-909	$3\nu_9 - \nu_9$	8	Fermi resonance with $\nu_5$
847-905	$\nu_5 + \nu_9 - \nu_9$	8	Calculated line positions
1033	$\nu_7 + \nu_9$	3(IR,G)	Calculated line positions
1099	$\nu_6 + \nu_9$	3(IR,G)	
1205.7070(5)	$(\nu_8 + \nu_9)^0$ A-type band	13(IR,G)	
1218 1303.5183(15)	$\nu_6 + \nu_7$ $\nu_8^0$ (A,B)-type band	3(IR,G) 14(IR,G)	See also 2,3(IR,G); 3(IR,S); 15(IR,M) Interaction with $\nu_6 + \nu_7$ Interaction with $\nu_8 + \nu_9$ a,b,d
1311 1324.9	P } $\nu_3$ Q } A- or (A,b)-type band	3(IR,G)	See also 3(IR,G + S); 3(Ra,L); 15(IR,M) See also 1,3(Ra,L); 2(IR,G); 3(IR,S); 15(IR,M)

## Observed Infrared Bands — Continued

Frequency (cm <sup>-1</sup> )	Assignment	References	Remarks
1325.7354(10)	$v_3^0$	14(IR,G)	a,b,d
1330.7	$v_5 + v_9$ (?)	3(IR,G)	See also 7(LSS,G) See also 2(IR,G); 3(Ra,L); 3(IR,S)
1380.3	$v_7 + v_8$ (?)	15(IR,M:Ar)	T = 12 K
1455	$v_5 + v_7$	3(IR,G)	
1470	$v_7 + v_8$	3(IR,S)	T = 85 K
1515	$2v_8$	3(IR,G)	See also 1,3(Ra,L); 3(IR,S)
1521	$v_5 + v_6$	3(IR,G)	
1709.5675(5)	$v_2^0$	5,10(DL,G)	a,b,c
1693.0 P 1705.6 Q 1711.8 Q 1720.0 R	$v_2$ B- or (a,B)-type band	3(IR,G)	See also 1,3(Ra,L); 2(IR,G); 3(IR,S); 15(IR,M)
1787	$v_3 + v_9$	3(IR,G)	See also 15(IR,M)
1905	$2v_5$	3(IR,S)	T = 85 K
2038	$v_4 + v_8$	3(IR,S)	T = 85 K
2163	$v_2 + v_9$	3(IR,G)	
2194	$v_3 + v_5$	3(IR,G)	
2200	$v_4 + v_5$	3(IR,S)	T = 85 K
2290	$v_2 + v_4$	3(IR,S)	T = 85 K
2585	$v_2 + v_5$	2(IR,G)	See also 15(IR,M)
2632	$2v_4$	3(IR,G)	See also 2(IR,G)
2643	$v_3 + v_4$	3(IR,G)	
2656	$2v_3$	3(IR,G)	See also 15(IR,M)
2999	$v_2 + v_3$ or $v_2 + v_4$	3(IR,G)	See also 2(IR,G); 15(IR,M)
3093	$v_1 - v_9$	3(IR,G)	
3400	$2v_2$	3(IR,G)	See also 2(IR,G)
3538.0 P 3550.0 Q 3562.0 R	$v_1$	3(IR,G)	See also 1,3(Ra,L); 2(IR,G); 3(IR,S); 15(IR,M)
3967.0	$v_1 + v_9$	15(IR,M:Ar)	T = 12 K

<sup>a</sup>Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents the absolute accuracy of line position measurements.

<sup>b</sup>Rotational line list available in HITRAN database (8).

<sup>c</sup>Rotational line list available in ATMOS database (9).

<sup>d</sup>The origins as well as the rotational parameters were calculated taking into account Fermi and Coriolis interactions between  $v_3$  and  $v_4$ ; other perturbations due to unknown levels were also observed.

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4.12.b. *cis*-HOONO

## Observed Fundamental Vibrational Frequencies

This species is supposed to be the most stable of the HOONO species. Five of the nine normal modes have been observed by Ref. 2(IR,M:Ar,N<sub>2</sub>), and attributed by comparison with calculations (1). No other infrared band seems to be reported.

Approximate type	Observations (cm <sup>-1</sup> )		Calculations (cm <sup>-1</sup> )
	Frequency	Medium	
O-H stretch	3541.7 3545.5	N <sub>2</sub> Ar	3677
N=O stretch	1701.4 1703.6	N <sub>2</sub> Ar	1692
H-O-O bend	1364.4 1394.9	Ar N <sub>2</sub>	1398
O-O stretch	952.0 960.5	Ar N <sub>2</sub>	946
O-N=O bend	772.8 793.6	Ar N <sub>2</sub>	814
O-N stretch	—		439
O-N=O torsion O-O-N bend	—		{ 384 337
H-O-O torsion	—		211

<sup>a</sup>According to Ref. 1, these two modes are coupled and cannot be exclusively assigned.

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4.12.c. *trans*-HOONO

## Observed Fundamental Vibrational Frequencies

Five frequencies observed by Ref. 1(IR,M:Ar) have been assigned as fundamental modes of this species.

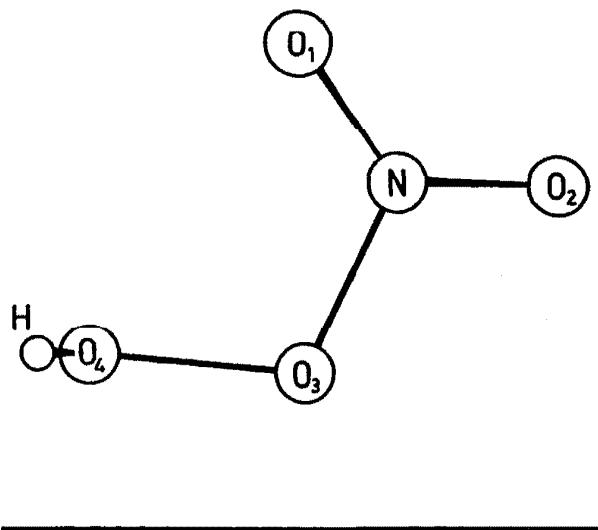
Approximate type	Frequency (cm <sup>-1</sup> )
O-H stretch	3563.3
N=O stretch	1708.3
H-O-O bend	1372.7
O-O stretch	957.4
O-N=O bend	782.9

## Reference

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4.13.  $\text{HNO}_4$  ( $\text{HO}_2\text{NO}_2$ )

The molecule is supposed to be non planar, and thus to have no symmetry element. The  $\text{O}_3$  atom is nearly coplanar with  $\text{O}_1\text{--N--O}_2$ ; the  $\text{O}_4$  atom is below the plane, and the H atom is above the plane (see Ref. 5).



## Observed Fundamental Vibrational Frequencies

Seven of the twelve normal modes have been observed and assigned by comparison with calculations. Two weak bands at  $722$  and  $919\text{ cm}^{-1}$  have been observed by Ref. 8 (IR,G). They have been attributed to combination or hot bands of  $\text{HNO}_4$ , since the fundamental frequencies which remain unknown are supposed to lie at lower energies.

Approximate type (Following (4))	Frequency	Observations ( $\text{cm}^{-1}$ ) References, Remarks	Calculations ( $\text{cm}^{-1}$ )		
			(4)	(5)	
$\text{O--NO}_2$ torsion	$\sim 145$	6(MW,G)	125	117	145
$\text{HO--O}$ torsion	—		200	285	302
$\text{O--O--H}$ bend	—		400	391	436
$\text{NO}_2$ rock	—		500	592	652
$\text{N--O}$ stretch	—		633	727	821
$\text{NO}_2$ wag	—		735	810	896
$\text{NO}_3$	802.56(5)	a,b 9(IR,G) Band called $v_6$ by 9(IR,G) c		922	1046
	802.7	1,2,3(IR,G) 8(IR,G) c	880	1050	1215
$\text{O--O}$ stretch	940			1405	1576
$\text{NO}_3$	1304.2	1,2,3(IR,G)			
$\text{O--H}$ bend	1396.9	c		1540	1615
		1,2,3,9(IR,G) Band called $v_3$ by 9(IR,G) c			
$\text{NO}_3$	1728.3	1,2,3(IR,G)		1705	1960
$\text{O--H}$ stretch	3540.1	c		3910	4100
		1,3(IR,G)			

<sup>a</sup>Rotational line list available in ATMOS database (7).

<sup>b</sup>Band origin calculated from rotational analysis; number in parentheses refers to the last quoted digits and represents the absolute accuracy of line position measurements.

<sup>c</sup>Q branch appears as a doublet; the value refers to the mean calculated from the positions of the two peaks.

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