

## Molecular Line Parameters for the “MASTER” (Millimeter Wave Acquisitions for Stratosphere/Troposphere Exchange Research) Database

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**Abstract.** In order to investigate the upper troposphere/lower stratosphere (UTLS) region of the earth’s atmosphere, ESA/ESTEC (European space agency) is considering the opportunity to develop the spaceborne limb sounding millimeter sensor “MASTER” (millimeter wave acquisitions for stratosphere/troposphere exchange research). This instrument is part of the “atmospheric composition explorer for chemistry and climate interactions” (ACECHEM) project. In addition, ESA/ESTEC is developing the “MARSCHALS” (millimeter-wave airborne receiver for spectroscopic characterization of atmospheric limb sounding) airborne instrument which will demonstrate the feasibility of MASTER. The present paper describes the line-by-line database which was generated in order to meet at best the needs of the MASTER (or MARSCHALS) instrument. The linelist involves line positions, line intensities, line broadening and line shift parameters in the 294–305, 316–325, 342–348, 497–506 and 624–626 GHz spectral microwindows. This database was first generated for the target molecules for MASTER (H<sub>2</sub>O, O<sub>3</sub>, N<sub>2</sub>O, CO, O<sub>2</sub>, HNO<sub>3</sub>, HCl, ClO, CH<sub>3</sub>Cl, BrO). In addition, ten additional molecules (SO<sub>2</sub>, NO<sub>2</sub>, OCS, H<sub>2</sub>CO, HOCl, HCN, H<sub>2</sub>O<sub>2</sub>, COF<sub>2</sub>, HO<sub>2</sub> and HOBr) had also to be considered in the database as “possible interfering species” for the retrieval of the target molecules of MASTER. The line parameters were derived, depending on their estimated accuracy, (i) from a combination of spectral parameters included in the JPL and HITRAN catalogs (ii) from data taken into the literature or (iii) using data obtained through experimental measurements (and/or) calculations performed during the present study.

**Key words:** broadening coefficients, millimeter and submillimeter spectral domains, line intensities, line positions, spectroscopic database

## 1. Introduction

Millimeter and sub-millimeter wave techniques have been extensively used or are under development since many years in order to perform remote observations of the Earth's middle atmosphere. These studies involve ground-based microwave radiometers (de La Noë *et al.*, 1983; Nedoluha *et al.*, 1995; de La Noë *et al.*, 1998; Raffalski *et al.*, 1998), airborne (Titz *et al.*, 1995; De Valk *et al.*, 1997) and balloon-borne (Pardo *et al.*, 2000) sensors.

Remote sensing of the Earth's atmosphere from satellite platforms is essential for the understanding of stratospheric ozone chemistry and climatology because the spatial concentration of numerous trace gases can be monitored simultaneously on a global scale. The upper troposphere/lower stratosphere (UTLS) region is a major focus of interest for atmospheric research due to the importance of this region to climate radiative forcing, stratosphere/troposphere exchanges and tropospheric chemistry.

Although sensors working in the infrared (IR) or visible ultra violet (VIS-UV) spectral regions like the Michelson interferometer for passive atmospheric sounding (MIPAS) or the scanning imaging absorption spectrometer for atmospheric chartography (SCIAMACHY) on the environmental satellite (ENVISAT <http://envisat.esa.int/>) have potential to sound this region of the atmosphere, it is anticipated that the attributes of millimeter wave limb sounding would be especially well suited to the task since the quality of the retrievals is less affected by clouds and aerosols than in the infrared, visible or ultraviolet wavelengths. On the other hand, continuum emission from water and dry air limits this advantage. At present stratospheric limb sounding has already been demonstrated successfully by instruments like the microwave limb sounder (MLS) on the upper atmosphere research satellite (UARS) (Lahoz *et al.*, 1994; Eluszkiewicz *et al.*, 1996 Livesey *et al.*, 2003 and references therein) and more recently by the sub millimeter radiometer (SMR) on board the Odin satellite since February 2001 (Murtagh *et al.*, 2002; Eriksson *et al.*, 2002; Baron *et al.*, 2002; Merino *et al.*, 2002; Pardo *et al.*, 2002; Ridal *et al.*, 2002; Urban *et al.*, 2004). Also the NASA's Earth observation system microwave limb sounder (EOS-MLS) was launched in 2004. In addition, there exist new projects, like the heterodyne sub-millimeter receiver JEM/SMILES (superconducting sub-millimeter wave limb emission sounder) which would operate on the Japanese experimental module (JEM) on the International space station (ISS) (<http://smiles.tksn.nasda.go.jp/>).

The European space agency (ESA/ESTEC) investigates the possibility to develop the spaceborne limb sounding millimeter sensor "MASTER" (millimeter wave acquisitions for stratosphere/troposphere exchange research). This instrument is part of the "atmospheric composition explorer for chemistry and climate interactions" (ACECHEM) project. The mission objectives of MASTER are to perform limb measurements of spatially variable gases (see Table I) in the 294–626 GHz spectral region in appropriate altitude ranges and with adequate vertical

Table I. Primary instrument requirements for MASTER

Primary targets	Height domain	Band	Spectral coverage (GHz)	Spectral resolution (MHz)	NEBT/accuracy (K)	Vertical HPBW (Km)
O <sub>3</sub> , N <sub>2</sub> O, O <sub>2</sub> (pointing) HNO <sub>3</sub>	UT/LS	B	294.0–305.5	50	1.2/1.0	2.3
H <sub>2</sub> O, O <sub>3</sub>	UT/LS	C	316.5–325.5	50	1.3/1.0	2.3
CO, HNO <sub>3</sub> , BrO	UT/LS	D	342.25–348.75	50	0.5/1.0	2.3
ClO, O <sub>3</sub> , N <sub>2</sub> O, BrO, H <sub>2</sub> O, CH <sub>3</sub> Cl	LS	E	497.0–506.0	50	0.6/1.0	1.6
HCl, O <sub>3</sub>	LS	F	624.0–626.5	50	2.0/1.0	1.6

Note. LS = lower stratosphere, UT = upper troposphere, NEBT = noise equivalent brightness temperature, HPBW = antenna half-power beam width.

resolution. In parallel to MASTER studies, ESA has defined a program to develop and deploy MARSCHALS (millimeter-wave airborne receiver for spectroscopic characterisation of atmospheric limb sounding), an airborne simulator for the proposed spaceborne instrument MASTER. The primary objective of MARSCHALS is to demonstrate the feasibility of limb sounding at millimeter and sub-millimeter wavelength (microwindows B, C and D of Table I). The most innovative of MASTER’s capabilities, which MARSCHALS should seek to simulate as closely as possible, is that of UT limb sounding.

In order to retrieve the atmospheric parameters (pressure, temperature, concentration profiles, . . .) with the best possible accuracy, it is essential to have spectral parameters of high quality. Therefore, compilations of parameters which include for each transition the line position, the line intensity, the lower state energy, the vibrational and rotational assignments, various line shape parameters (depending on the databases), together with some error estimates and relevant literature data are constantly updated.

The main compilations in the microwave and millimeter wave (MW/MMW) domain are the HITRAN (high-resolution transmission) (Rothman *et al.*, 1983, 1992, 1998, 2003) database and the JPL (Jet Propulsion Laboratory) (Poynter and Pickett, 1985; Pickett *et al.*, 1998) catalog.

### 1.1. THE HITRAN DATABASE

The HITRAN database (Rothman *et al.*, 1983, 1992, 1998, 2003) is focused mainly on atmospheric applications. The line-by-line subsection which covers the 0–20,000 cm<sup>-1</sup> spectral range includes for each line the position, the intensity (at 296 K) for a sample with “natural” isotopic concentrations (de Bievre *et al.*, 1984), the lower state energy, the air- and self-pressure-broadening coefficients (Half Width at Half Maximum at 296 K), the *n*-temperature dependence of the air-broadening coefficient, the air-pressure shift coefficient, the vibrational and rotational assignments and indices giving errors estimates and relevant literature data.

## 1.2. THE JPL CATALOG

The JPL catalog (Poynter and Pickett, 1985; Pickett *et al.*, 1998) is devoted to the microwave and millimeter wave (MW/MMW) spectral range and was initially generated for astrophysical applications. This catalog includes line positions and line intensities quoted at 300 K for a pure isotopic sample for an extended set of molecules involving numerous isotopic species. There are also files with informations about the source of the molecular data, updates and partition functions. Actually as stressed by Pickett *et al.* (1998) for numerous (but not all) species, the JPL line intensities were generated using a partition function which accounts only for the rotation and nuclear spin (and/or) electron spin contributions  $Z_{\text{Spin-Rot}}(T)$  to the “total” partition function  $Z_{\text{Tot}}(T)$ . In fact the total partition function  $Z_{\text{Tot}}(T)$

$$Z_{\text{Tot}}(T) \approx Z_{\text{Spin-Rot}}(T) Z_{\text{vib}}(T) \quad (1)$$

includes also a “vibrational” contribution  $Z_{\text{vib}}(T)$  which, assuming the harmonic approximation takes the general form:

$$Z_{\text{vib}}(T) = \prod_{\text{Vib}} (1 - \exp^{-E_{\text{vib}}/kT})^{-d_{\text{vib}}} \quad (2)$$

where the product runs over the different modes of vibration of the molecule with  $d_{\text{vib}}$  as the associated degeneracy.

For that reason, the JPL intensities which are generated at 300 K are overestimated for a number of species by a factor equal to  $Z_{\text{vib}}(300 \text{ K})$  which is non negligible for molecules with rather low vibrational modes. Therefore, these line intensities have to be corrected before their introduction into databases of atmospheric interest, and this has been done for the databases generated for the ODIN satellite (Eriksson *et al.*, 2002) as well as in the present database. Finally all the line shape parameters (air- and self-broadening parameters and line air-pressure shift) are completely absent in the JPL catalog.

## 1.3. DATABASE GENERATED TO A DEDICATED INSTRUMENT

Apart from these general databases it is worth noticing that some databases were generated for a dedicated instrument. This was the case some years ago for the ATMOS (molecular line parameters for the atmospheric molecule trace spectroscopy) experiment (Brown *et al.*, 1987), for the SAO (Smithsonian Astrophysical Observatory) FIRS-2 balloon borne spectrometer (Chance *et al.*, 1994a), and, more recently, for the MIPAS instrument (Flaud *et al.*, 2003b) which is on board the ENVISAT satellite.

The present paper describes the line-by-line database which has been generated in order to meet the needs of the MASTER (or MARSCHALS) instrument. The parameters (line positions, line intensities, line broadening and pressure shifts) included in this database are provided both for the target molecules for MASTER,

namely, water (H<sub>2</sub>O), ozone (O<sub>3</sub>), nitrous oxide (N<sub>2</sub>O), carbon oxide (CO), oxygen (O<sub>2</sub>), nitric acid (HNO<sub>3</sub>), hydrogen chloride (HCl), chloride oxide (ClO), methyl chloride (CH<sub>3</sub>Cl), bromide oxide (BrO), see Table I) and for the possible interfering species, namely sulfur dioxide (SO<sub>2</sub>), nitrogen dioxide (NO<sub>2</sub>), carbonyl sulfide (OCS), formaldehyde (H<sub>2</sub>CO), hypochlorous acid (HOCl), hydrogen cyanide (HCN), hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), carbonyl fluoride (COF<sub>2</sub>), hydroperoxyl radical (HO<sub>2</sub>) and hypobromous acid (HOBr).

These line parameters were derived, depending on their availability and their estimated accuracy, (i) from a combination of parameters extracted from the JPL (Poynter and Pickett, 1985; Pickett *et al.*, 1998) and HITRAN (Rothman *et al.*, 1998, 2003) catalogs (ii) from data taken into the literature or (iii) using data obtained through experimental measurements and/or calculations performed during two recent studies (Bauer *et al.*, 1998a; Demaison *et al.*, 2004 and references therein).

Actually, the uncertainties in the knowledge of the spectroscopic parameters can lead to systematic errors during the retrieval of the atmospheric volume mixing ratio (VMR) and temperature profiles. To assess more precisely the parameters for which an improved accuracy is needed, a forward calculation accompanied by a detailed errors analysis with respect to the spectroscopic parameters was performed. These calculations (Verdes *et al.*, 2004, 2005) involve inversions of the atmospheric measurements performed for a realistic MASTER observation scenario using the formalism developed by Rodgers (2000).

As it will be seen in the following, the available line positions parameters are almost always accurate enough for MASTER. For some of the species under study, new line intensity calculations had to be performed. As expected, the air-broadening parameters (the air-broadening coefficients  $\gamma_{\text{air}}$  and their  $n$ -temperature dependences  $n_{\text{air}}$ ), existing in the literature are not often accurate enough. The self broadening coefficients  $\gamma_{\text{self}}$  are often unknown but, except for water and oxygen, have anyway a negligible effect on the quality of the retrieval analysis. Finally, the air line shifts are still rather sparse, but during the course of this study, it was established that the pressure shifts seem to lead to rather negligible effects for the MASTER retrievals. Therefore, unless explicitly specified, a zero default value was quoted in MASTER for the air pressure shift and the self broadening linewidth. Also the default value “ $n = 0.7$ ” was quoted for the temperature dependence of the air- and self-broadening parameters.

For the parameters for which the impact of the associated errors on the retrievals appear to be important, measurements had to be performed in some cases in Bologna (LMSB), Lille (PhLAM) and Wessling (Deutsches Zentrum für Luft- und Raumfahrt), the results of which are described in extensive reports (Bauer *et al.*, 1998a, Demaison *et al.*, 2004).

## 2. Description of the MASTER Database

In the MASTER database the line positions are in MHz and the lower state energies in  $\text{cm}^{-1}$ . The line intensities  $S_{\text{MASTER}}$  are quoted in  $\text{cm}^{-1}/(\text{molecule cm}^{-2})$  at  $T_{\text{Ref}} = 296$  K for a pure isotopic sample (contrary to HITRAN). The air pressure-broadening coefficients  $\gamma_{\text{air}}$  the self pressure-broadening coefficients  $\gamma_{\text{self}}$  and the air pressure-shifts  $\delta_{\text{air}}$  are given (in MHz/Torr) for a reference temperature  $T_{\text{Ref}} = 296$  K. However when they were measured these parameters are given at the temperature of the measurements  $T_{\text{meas}}$  which is also quoted in the database. Finally, the MASTER database includes also the coefficients  $n_{\text{air}}$  and  $n_{\text{self}}$  necessary to calculate the temperature dependence for air-broadening and self-broadening coefficients. It is important to underline that the line shape parameters were implemented assuming a Voigt profile for all the lines. Possible deviations from this “classical” line profile may occur (Puzzarini *et al.*, 2002; Rohart *et al.*, 2003) for some specific laboratory conditions. Two possible reasons can be responsible for these deviations: the velocity changing collisions (Dicke, 1953) leading to a Galatry profile (Galatry, 1961) or the speed dependence of the relaxation rates, and both profiles give a better fit to experimental data and lead to broadening coefficients in good agreement. However, in usual atmospheric conditions the collisional line broadening is significantly stronger, in the millimeter wave spectral range, than the Doppler linewidth and for this reason these deviations from the Voigt profile can be ignored. Finally, the line mixing effects (Liebe *et al.*, 1992; Tretyakov *et al.*, 2004) were not accounted for in this database because they are negligible for the frequencies and pressures ranges of interest.

The list of lines to be included in the MASTER database could not be limited to the spectral micro-bands (Table I) of MASTER since strong lines far away from the considered spectral bands can have a high contribution to the absorption coefficients. On the other hand it is important to have a reasonable number of lines in the database so that the computing time during the retrieval process remains reasonable. Therefore criteria were adopted for including a given transition in the database. They are as defined in the following:

For a given isotopic species with a “natural” isotopic abundance  $a_{\text{ISO}}$  (de Bievre *et al.*, 1984), the lines were introduced in the MASTER linelist if their intensity  $S_{\text{MASTER}}$  fulfills Equations (3) or (4) depending of the positions of these lines with respect to the MASTER spectral bands.

For the lines within the B, C, D, E and F microbands (Table I) or within  $\pm 3$  GHz of these bands:

$$S_{\text{MASTER}}a_{\text{iso}} \geq 0.1 \times 10^{-27} \text{ cm}^{-1}/(\text{molecule cm}^{-2}) \quad (3)$$

For the lines falling in the intervals [3–20] GHz away from these bands, the lower limit is:

$$S_{\text{MASTER}}a_{\text{iso}} \geq 0.1 \times 10^{-22} \text{ cm}^{-1}/(\text{molecule cm}^{-2}) \quad (4)$$

The exceptions are water and the  $^{16}\text{O}_2$  isotopic species of the oxygen molecule. For both molecules, it is necessary to account for the continuum contribution (Bauer *et al.*, 1986; Godon and Bauer, 1991, 1993, 1995, 1998b; Godon *et al.*, 1992; Liebe 1984, 1985, 1989; Ma *et al.*, 1990; Ma and Tipping, 1992; Ma and Tipping, 2002; Liebe *et al.*, 1992; Tipping and Ma, 1995; Rosenkrantz 1998, 1999; Kuhn *et al.*, 2002) during the retrievals. In order to well model these continua, it is necessary that the database includes a complete line-by-line description for these two molecules. Therefore the MASTER database contains the water lines and  $^{16}\text{O}_2$  lines which are present in the 0–2,500 and 45–1,870 GHz frequency ranges, respectively.

Since the problems are specific to each molecule, we describe in the following the choice of the spectral parameters, molecule-by-molecule, giving arguments sustaining the updates.

It is clear, however, that the strongest efforts were devoted to the target species which are gathered in Table I. Finally one should mention that the new database can be easily used to predict atmospheric absorption and radiative transfert in the framework of the public domain Atmospheric Radiative Transfer Simulator program (ARTS) (Buehler *et al.*, 2004).

### 3. Status for the Target Species for MASTER<sup>1</sup>

#### 3.1. WATER VAPOR ( $\text{H}_2\text{O}$ ): MOLECULE 1

It is clear that because of their rather broad absorption profile, even the water lines located far away from the MASTER microwindows will interfere with the target molecules of MASTER. In addition it is necessary to have a complete water line list in order to account for the water continuum (Liebe 1984, 1985, 1989). Therefore the complete set of water lines (857 transitions belonging to the  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{18}\text{O}$ ,  $\text{H}_2^{17}\text{O}$  and HDO four main isotopic species of water) present in HITRAN in the whole 0–2,500 GHz frequency range were introduced in the MASTER database.

##### 3.1.1. Line Positions and Line Intensities

For the water molecule the line positions implemented in the MASTER database are those quoted in the JPL database. This is justified since most of the JPL line positions for the microwave or millimeter wave spectral range are issued from very good line position measurements (de Lucia *et al.*, 1971, 1972a, 1972b, 1974; de Lucia and Helminger, 1975; Matsushima *et al.*, 1995; Messer *et al.*, 1983, 1984; Pearson *et al.*, 1991 and references therein).

On the other hand, it was not obvious to decide which set of water line intensities should be used for MASTER. The HITRAN intensities in the 0–2,500 GHz were generated using a classical rotational expansion for the dipole moment (Flaud *et al.*, 1981). Actually these intensities differ only marginally from the JPL ones as one could expect since the theoretical approach used to generate these data is

the same. Therefore in this study we have investigated the quality of the HITRAN intensities by comparing them with new values obtained using a theoretical model developed recently (Coudert, 1994).

*Theoretical background.* The water molecule is among the lightest molecules and it has very large  $A$ ,  $B$ , and  $C$  rotational constants equal to 27.88, 14.52, and 9.27  $\text{cm}^{-1}$ , respectively. As a consequence, it displays a strong vibration–rotation interaction arising because the rotational energy spacing for quantum numbers as low as eight is of the same order of magnitude than the vibrational energy spacing. The vibrational mode which is the most strongly coupled to the rotation is the bending  $\nu_2$  mode as it is the lowest energy vibrational mode ( $\sim 1,648 \text{ cm}^{-1}$ ) and as it leads to an infinitely large  $A$  rotational constant for a linear configuration of the molecule, i.e., when the bending angle is equal to  $180^\circ$ . This coupling leads to the so-called anomalous centrifugal distortion: when dealing with the rotational energies of water, the usual approach (expansion of the Hamiltonian as a power series of the components of the angular momentum  $J$ ) developed for rigid molecules cannot be safely used because such an expansion diverges for rotational levels with medium and large values of the rotational quantum numbers.

The theoretical approach developed recently (Coudert, 1994) accounts for the strong coupling between the bending  $\nu_2$  mode and the overall rotation of the molecule using a four dimensional Hamiltonian in which the overall rotation of the molecule as well as the bending mode are treated together. This approach was successfully used to calculate properly the rotational energies of water (Lanquetin *et al.*, 1999, 2001). In parallel, a model was developed for the line intensities (Coudert, 1999) leading to the determination of a set of dipole moment parameters which are able to reproduce very satisfactorily a large body of intensities from the literature (Toth, 1993a, 1993b, 1998; Rinsland *et al.*, 1991a; Brown and Plymate, 1996).

*Validation of the line intensities present in HITRAN.* The line intensities in the HITRAN database (denoted HIT in the following) were compared with the line intensities calculated (denoted CALC in the following) using the theoretical approach described above.

For the main isotopic species ( $\text{H}_2^{16}\text{O}$ ) the results may be summarized in the following way:

- For the pure rotational lines the ratio of intensities  $\text{HIT}/\text{CALC} = 1.007$  (0.016) shows that for the set of lines considered there is a very good agreement between the two line lists. This is understandable since the water lines considered here involve low or medium quantum numbers for which centrifugal distortion is rather weak.
- For the rotational lines in the first excited state the ratio of intensities  $\text{HIT}/\text{CALC} = 1.034$  (0.053) shows that for the set of lines considered there is still a very good agreement between the two line lists.



- For the rotational lines in the second excited state the ratio of intensities (HIT/CALC = 0.87(23)) shows that for the set of lines considered, the two calculations do not agree very well even if the standard deviation is rather large. It is however difficult to decide without new intensity measurements which line list is better.

For the less abundant isotopic species of H<sub>2</sub>O the lines involve rather low rotational quantum numbers as compared to H<sub>2</sub><sup>16</sup>O, and it can be expected that the usual approach (Flaud *et al.*, 1981) is working. This was checked on the H<sub>2</sub><sup>18</sup>O isotopomer by comparing the intensities of its lines to those of the main isotopomer H<sub>2</sub><sup>16</sup>O.

As a conclusion one can say that at this stage it is reasonable to use the HITRAN line intensities. For this reason, the line intensities in HITRAN were implemented for water in the MASTER database.

### 3.1.2. Line Broadening Coefficients

The air broadening ( $\gamma_{\text{air}}^0(T_{\text{Ref}})$  and  $n_{\text{air}}$ ) coefficients can be found in HITRAN, but these coefficients which are a mixture of a small number of measured values for which the confidence is not always very high (Gamache *et al.*, 1994) and of a larger amount of calculated or estimated values (Gamache and Davies, 1983) which have not been updated for many years are disputable. Furthermore, the self-broadening coefficients are completely missing in HITRAN for the 0–500 cm<sup>-1</sup> frequency range.

As a consequence we adopted the following strategy:

- When measurements exist, we use the experimental values. This is the case for:
  - The 183 GHz line: (at 298 K)  $\gamma_{\text{air}} = 3.84(4)$  MHz/Torr,  $n_{\text{air}} = 0.64(1)$ ,  $\gamma_{\text{self}} = 20.0(1)$  MHz/Torr and  $n_{\text{self}} = 0.85(5)$  (Bauer *et al.*, 1985, 1989; Goyette and De Lucia, 1990; Tretyakov *et al.*, 2003).
  - The 325.15 GHz line of H<sub>2</sub><sup>16</sup>O:  $\gamma_{\text{air}} = 3.633(30)$  MHz/Torr at 300 K,  $n_{\text{air}} = 0.640(93)$  (Colmont *et al.*, 1999).
  - The 380.2 GHz line of H<sub>2</sub><sup>16</sup>O:  $\gamma_{\text{air}} = 3.80(4)$  MHz/Torr at 300 K,  $n_{\text{air}} = 0.72(3)$  (Goyette *et al.*, 1993a) and  $\gamma_{\text{self}} = 20.61(7)$  MHz/Torr,  $n_{\text{self}} = 0.89(1)$  (Bauer *et al.*, 1987).
  - The 556 GHz line of H<sub>2</sub><sup>16</sup>O ( $\gamma_{\text{air}} = 4.92(6)$  MHz/Torr at 297 K (Markov and Krupnov, 1995).
  - The 203.41 GHz line of H<sub>2</sub><sup>18</sup>O:  $\gamma_{\text{air}} = 3.833(32)$  MHz/Torr at 300 K  $n_{\text{air}} = 0.900(38)$  (Colmont *et al.*, 1999).
  - The HDO lines at 225.896 GHz ( $\gamma_{\text{air}} = 3.85(4)$  MHz/Torr at 298 K,  $n_{\text{air}} = 0.75(2)$ ), 241.561 GHz ( $\gamma_{\text{air}} = 4.12(4)$  MHz/Torr at 298 K,  $n_{\text{air}} = 0.80(5)$ ), and 241.973 GHz ( $\gamma_{\text{air}} = 3.08(4)$  MHz/Torr at 298 K,  $n_{\text{air}} = 0.70(2)$ ) (Goyette *et al.*, 1993b).

- For the lines for which line broadening measurements are not available, we used, when the MASTER database was generated the calculated air-broadening and self broadening coefficients given at  $T = 300$  K together with their  $n$ -temperature dependence exponents (Bauer *et al.*, 1989). These calculations involve all the  $\text{H}_2^{16}\text{O}$  strong lines in the 0–1,000 GHz frequency range. In addition, these data were also used for the same rotational transitions of the  $\text{H}_2^{18}\text{O}$  and  $\text{H}_2^{17}\text{O}$  isotopic species.
- For future updates of the database it may be necessary to implement the air broadening coefficients issued from the recent calculations at 296 K of  $\text{N}_2$ - and  $\text{O}_2$ -broadening coefficients (Gamache and Fischer, 2003a, 2003b; Gamache and Hartmann, 2004) performed for  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{18}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , HDO and  $\text{D}_2\text{O}$  using the Complex Robert–Bonamy (CRB) formalism (Gamache *et al.*, 1998). These new calculations were successfully validated using an extended set of measurements (Gamache and Fischer, 2003b). Actually, although the  $\text{N}_2$ - and  $\text{O}_2$ - broadening parameters differ significantly in Gamache *et al.* (2003a) from those previously calculated (Bauer *et al.*, 1989), the difference is not so important for the air broadening halfwidths (less than 5%) for most of the transitions of interest for MASTER. The exceptions are for the transitions involving large  $K_a$  values ( $K_a \approx J \gg K_c$ ) which are weak lines: in this case the disagreement between the two calculations is larger (up to 8%). However, to our knowledge, this new calculation does not provide yet for the pure rotation band the  $n$ -temperature dependence of the air-broadening halfwidths and the self-broadening coefficients which are of importance for MASTER.
- Finally, for the weak lines of water which are in the 0–1,000 GHz range or for all the water lines which are above 1,000 GHz, which therefore are expected to interfere only weakly with the lines from the MASTER database, we implement the air-broadening coefficients quoted in HITRAN and the self-broadening coefficients which were deduced from the (empirical) expression (Gamache *et al.*, 1994):

$$\gamma_{\text{self}} = 5\gamma_{\text{air}}, \quad n_{\text{self}} = 1.12n_{\text{air}} \quad (5)$$

### 3.1.3. Line Shifts

The data on air shifts for the rotational lines of water are rather sparse. For all water lines for which this parameter is unknown the value  $\delta_{\text{air}} = 0$  was used in the database. The exceptions concern the lines for which these parameters are available (at about 300 K) namely, for  $\text{H}_2^{18}\text{O}$  the 203.4 GHz line ( $\delta_{\text{air}} = 0.126$  MHz/Torr, calculated in Colmont *et al.*, 1999), and for  $\text{H}_2^{16}\text{O}$ , the lines located at 183 GHz ( $\delta_{\text{air}} = -0.067(20)$  MHz/Torr, measured in Tretyakov *et al.*, 2003), 325.1 GHz ( $\delta_{\text{air}} = -0.15$  MHz/Torr, calculated in Colmont *et al.*, 1999) and 556 GHz ( $\delta_{\text{air}} = +0.300(4)$  MHz/Torr, measured in Markov and Krupnov, 1995). One should mention that an improvement in the UARS-MLS retrievals was ob-

tained when considering  $\delta_{\text{air}}$  for the 183 GHz line of water (Pumphrey *et al.*, 2000).

### 3.2. OZONE (O<sub>3</sub>): MOLECULE 3

#### 3.2.1. Line Positions

For the line positions and lower state energies, we used the JPL values (Depannemaeker and Bellet, 1977; Pickett *et al.*, 1985; Pickett *et al.*, 1988) with the exception of the  $2^1 \leftrightarrow 2^1$  transitions of the  $^{16}\text{O}^{18}\text{O}^{16}\text{O}$  and  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$  isotopic species for which the lower energy levels are incorrect. For these transitions we have used the HITRAN values (Flaud *et al.*, 1990a).

#### 3.2.2. Line Intensities

For ozone, the centrifugal distortion effects which affect the line intensities in the microwave spectral region appear as a rotational dependence of the dipole moment operator expansion in the ground vibrational state (Pickett *et al.*, 1985; Flaud *et al.*, 1990a; Flaud and Bacis, 1998a). Such an effect was accounted for by expanding the dipole moment up to the second order with respect to rotational operators (See the Table VIII in Flaud *et al.*, 1990a). The ozone line intensities resulting from this calculation (Flaud *et al.*, 1990a) are presently implemented in the HITRAN database. Since that time the main changes have concerned a likely better evaluation (Flaud *et al.*, 1990b; Birk *et al.* 1994a, 1994b; Claveau *et al.*, 2001; de Backer-Barilly and Barbe, 2001; Wagner *et al.*, 2002; Flaud *et al.*, 2003a) of the first derivatives of the dipole moment coefficients  ${}^{\alpha}\mu_m$  of Table VIII in Flaud *et al.* (1990a). Table II gives the new values of these coefficients as well as the previous ones and the corresponding changes.

Such changes (of the order of 1%) translate in analogous changes in the (second order) correcting rotational terms appearing in the expansion of the effective dipole moment in the ground state (Table VIII in Flaud *et al.*, 1990a).

Table II. Change in the values of the first order derivatives of the ozone dipole moment (in Debye)

Coefficient	New value (Claveau <i>et al.</i> , 2001; de Backer-Barilly <i>et al.</i> , 2001; Wagner <i>et al.</i> , 2002; Flaud <i>et al.</i> , 2003a)		Change (%)
		Previous value (Flaud <i>et al.</i> , 1990a)	
${}^x\mu_1$	−0.02150	−0.02185	−1.6
${}^x\mu_2$	−0.06483	−0.06529	−0.7
${}^z\mu_3$	−0.2630	−0.2662	−1.2

Given the order of magnitude of these terms, assuming maximum values of 80–100 for the rotational quantum numbers  $J$  or  $K_a$  leads to a change smaller than 0.1% in the line intensities and this for the weakest lines. As a consequence, given the present knowledge of the  $O_3$  dipole moment, one can say that the intensities quoted in HITRAN are the best that one can generate. As a consequence the HITRAN line intensities were introduced in the MASTER database.

### 3.2.3. Line Broadening Coefficients

As for  $H_2O$ , we have used, when available, experimental values for the air-broadening coefficients. More precisely for the lines of  $^{16}O_3$  located at 497.1, 498.7, 500.2, 501.8, 505.26 GHz we used the line broadening coefficients which were derived during a previous study (Bauer *et al.*, 1998a; Priem *et al.*, 2000b; Birk *et al.*, 1997). For the lines at 288.96, 610.37 and 625.37 GHz, we used calculated values for  $\gamma_{air}$  and  $n_{air}$  (Drouin *et al.*, 2004b). For the lines at 300.7, 301.8, 303.2, 317.2, 343.2 and 343.5 GHz we used the line broadening coefficients measured within the course of this study (Demaison *et al.*, 2004). All these data are collected in Table III.

It is generally recognized that the vibrational dependence of the line broadening coefficients for ozone is rather weak. Also the isotopic dependence for the broadening coefficients is assumed to be negligible. Accordingly, the available experimental  $\gamma_{air}$  values were used for the various hot bands transitions of ozone and for the less abundant isotopic species. Finally, for all the other lines the broadening coefficients are issued from the HITRAN database.

The  $n$ -temperature dependences of the linewidths which are collected in Table III were incorporated in the database. For the other lines, the value  $n_{air} = 0.76$  (as in HITRAN) was used for the  $n$ -temperature dependence of the air-halfwidths. Finally the self broadening coefficients  $\gamma_{self}$  quoted in HITRAN were implemented for the lines present in the MASTER database. For the ozone lines absent in HITRAN, we set  $\gamma_{self} \sim 4$  MHz/Torr together with  $n_{self} = 0.7$ , these values being the average values obtained recently (Larsen *et al.*, 2001).

### 3.2.4. Line Shifts

Table III collects the existing pressure shifts data for ozone in the microwave region for the lines of MASTER interest. Additional informations are also given in (Drouin *et al.*, 2004b). It is clear that this effect is rather weak and therefore the value  $\delta_{air} = 0$  was stated in the database for all lines of MASTER.

Table III. List of the line broadening data collected for ozone in the MASTER database

	$\nu$	$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$T$ (K)	$\gamma_{\text{air}}$	$n_{\text{air}}$	$\delta_{\text{air}}$
L	300685	13	4	10	14	3	10	238	3.730(18)		
L + B	301813	14	0	14	13	1	13	296	3.081(19)	0.676(20)	10(2)
L	303165	7	2	6	7	1	7	296	3.287(19)		
B + L	317195	5	3	3	6	2	4	296	3.427(29)		
B	317195	5	3	3	6	2	4	240	3.888(6)		13(1)
B	319997	20	1	19	20	0	20	296	2.951(10)	0.722(13)	28.2(5)
L	343238	26	2	24	25	3	23	240	3.583(26)		
L	343506	4	3	1	5	2	4	240	3.682(30)		
Ba	497098	23	2	22	23	1	23	240	3.27(3)	0.81(5)	
Ba	498747	24	1	23	23	2	22	240	3.34(1)	0.74(2)	
Ba	501771	48	4	44	48	3	45	240	3.28(3)	0.78(6)	
Ba	505257	5	4	2	6	3	3	240	3.10(4)	0.76(6)	
P	500433	34	2	32	34	1	33	240	3.362(20)	0.876(80)	
D	288959	9	1	9	8	0	8	296	3.172	0.806	-1
D	610365	25	1	25	24	0	24	296	2.756	0.790	-8
D	625371	15	6	10	16	5	11	296	3.011	0.77	-4

L and B: Measurements performed within the course of the experimental study performed in Lille (L) and Bologne (B) (Demaison *et al.*, 2004); P: Measurements from (Priem *et al.*, 2000b); Ba: Measurements from (Bauer *et al.*, 1998a); D: Calculated data from (Drouin *et al.*, 2004b);  $\bar{\nu}$ : line position in MHz,  $J'K_a'K_c'$   $J''K_a''K_c''$  upper and lower rotational quantum numbers;  $T$ : temperature for the measurements;  $\gamma_{\text{air}}$ : air-pressure broadening coefficient (in MHz/Torr);  $n_{\text{air}}$ : temperature dependence;  $\delta_{\text{air}}$ : air-pressure shift (in kHz/Torr).

### 3.3. NITROUS OXIDE (N<sub>2</sub>O): MOLECULE 4

#### 3.3.1. Line Positions

N<sub>2</sub>O has been the subject of numerous studies (Lovas, 1978; Reinartz *et al.*, 1978; Teffo *et al.*, 1994; Lyulin, 1995; Lovas, 2004). Therefore, the experimental line positions gathered in the compilations performed by Lovas (Lovas, 1978, 2004) have been included in the JPL database.

For the MASTER database which involves lines belonging to <sup>14</sup>N<sup>14</sup>N<sup>16</sup>O and to the two minor species, <sup>14</sup>N<sup>15</sup>N<sup>16</sup>O and <sup>15</sup>N<sup>14</sup>N<sup>16</sup>O, we have used the JPL line positions for the transitions within the ground vibrational state and within the first two excited states. For the N<sub>2</sub>O lines belonging to the (1 0° 0) ↔ (1 0° 0) band we have used the HITRAN line positions because such transitions are absent in the JPL database.

#### 3.3.2. Line Intensities

For nitrous oxide, the line intensities calculation for microwave transitions can be performed without considering Herman-Wallis effect. The line intensities in the

JPL catalog were generated using the value of the permanent dipole moment  $\mu_0$  which was measured with a good accuracy by Stark effect (Scharpen *et al.*, 1970). On the other hand, the vibrational contribution to the  $\text{N}_2\text{O}$  partition function which is  $Z_{\text{vib}}(T) = 1.1340$  at  $T = 300$  K was neglected, and therefore the line intensities in the JPL catalog are overestimated by  $\sim 13\%$ .

To solve this problem, a new intensity calculation was performed using the  $\text{N}_2\text{O}$  dipole moment (Scharpen *et al.*, 1970) and the HITRAN partition function. The new intensities are (as expected)  $\sim 13\%$  weaker than those in the JPL catalog, but on the other hand, also about  $\sim 7\%$  weaker than the HITRAN ones. The reasons for this disagreement are still not clear because we did not succeed to identify the origin of the HITRAN data.

Given these comments we have implemented in the MASTER database the  $\text{N}_2\text{O}$  intensities generated from this study.

### 3.3.3. Line Broadening Coefficients

For the air-broadening coefficients  $\gamma_{\text{air}}$  and its temperature dependence we used the values quoted in the HITRAN database. The exceptions are the lines of interest for MASTER for which broadening measurements exist, namely the 301.443 and 301.422 GHz lines (R11 lines of the  $^{14}\text{N}_2^{16}\text{O}$  and  $^{14}\text{N}^{15}\text{N}^{16}\text{O}$  isotopomers, respectively) for which we implemented the value  $\gamma_{\text{air}} = 3.148(14)$  MHz/Torr at 296 K (Demaison *et al.*, 2004), and the line at 627.751 GHz ( $\gamma_{\text{air}} = 2.87(10)$  MHz/Torr at 294 K) (Morino and Yamada, 2003). Outside MASTER frequency range, additional line broadening coefficients were measured for the 201, 552 and 577 GHz millimeter lines (Rohart *et al.*, 2003).

For the self-broadening coefficients and their temperature dependence, we used  $\gamma_{\text{self}} = 4$  MHz/Torr and  $n_{\text{self}} = 0.7$  which are mean values for these parameters according to various infrared (Lacome *et al.*, 1983; Toth 1993c) and microwave measurements (Colmont and Semmoud-Monnanteuil, 1987; Morino and Yamada, 2003).

## 3.4. CARBON MONOXIDE (CO): MOLECULE 5

Numerous line positions and intensities measurements were performed both in the microwave and in the infrared spectral range (Winnewisser *et al.*, 1997; Cazzoli *et al.*, 2002a, 2002b; Klapper *et al.*, 2000a, 2000b, 2001). As far as the MASTER database is concerned  $^{12}\text{C}^{16}\text{O}$  will be measured using the R2 line whose line position was measured at 345795.98(5) MHz with high accuracy by Nolt *et al.* (1987).

When dealing with line intensities, two measurements of the CO dipole moment were performed by Stark effect leading to fully compatible results (Muentner, 1975; Meerts *et al.*, 1977). These data were used to generate the accurate intensities quoted in the JPL database for CO.

For the 345.8 GHz line of CO, measurements of the N<sub>2</sub>- and O<sub>2</sub>- line broadening coefficients were performed (Priem *et al.*, 2000a; Birk *et al.*, 1997; Bauer *et al.*, 1998a) leading to the values  $\gamma_{\text{air}} = 2.728(17)$  MHz/Torr (at 296 K) and  $n_{\text{air}} = 0.864(36)$ .

### 3.5. MOLECULAR OXYGEN (THE <sup>18</sup>O<sup>16</sup>O, <sup>17</sup>O<sup>16</sup>O AND <sup>16</sup>O<sub>2</sub> ISOTOPIC SPECIES): MOLECULE 7

For the <sup>16</sup>O<sub>2</sub>, <sup>18</sup>O<sup>16</sup>O and <sup>17</sup>O<sup>16</sup>O isotopic species, we used the JPL line positions and intensities. These line positions are of excellent quality, since they were measured extensively (Krupenie 1972; Amano and Hirota, 1974; Steinbach and Gordy, 1975; Cazzoli *et al.*, 1981; Zink and Mizushima, 1987; Crownover *et al.*, 1990; Mizushima and Yamamoto, 1991; Golubiatnikov and Krupnov, 2003 and references therein), and the line intensities are in excellent agreement with the HITRAN’s ones.

For <sup>16</sup>O<sub>2</sub> we used<sup>2</sup> the N<sub>2</sub>- and O<sub>2</sub>-broadening coefficients measured recently (Krupnov *et al.*, 2002; Tretyakov *et al.*, 2004). For O<sup>18</sup>O<sup>16</sup>, the broadening coefficients were estimated from those of rotational transitions involving similar quantum numbers of the <sup>16</sup>O<sub>2</sub> isotopic species (Krupnov *et al.*, 2002; Tretyakov *et al.*, 2004). These values are quoted in Table IV for O<sup>18</sup>O<sup>16</sup>. For the less abundant O<sup>17</sup>O<sup>16</sup> species, the rotational dependence of the linewidths was not accounted for and the average values  $\gamma_{\text{N}_2} \approx 2.2$  MHz/Torr and  $\gamma_{\text{O}_2} \approx 2.10$  MHz/Torr were implemented for all the lines.

Finally, it has to be mentioned that the earth magnetic field leads to Zeeman effects which may modify the profile of oxygen lines. For example, a  $\pm 2.5$  MHz substructure for the 2<sub>1</sub> ← 0<sub>1</sub> rotational transition of <sup>16</sup>O<sup>18</sup>O located at 233.9 GHz was observed during ground measurement by the 2.5 m-radiotelescope POM-2 located at “Plateau de Bure” in the French Alps (Pardo *et al.*, 1995; Sandor and Clancy, 1997). In addition line mixing may occur in the Q-branches as it was also pointed out for <sup>16</sup>O<sub>2</sub> at 60 GHz (Liebe *et al.*, 1992) and 118 GHz (Tretyakov *et al.*, 2004). These two effects may be of importance for the retrievals.

Table IV. Broadening parameters (in MHz/TORR) implemented in MASTER for the <sup>18</sup>O<sup>16</sup>O ( $T = 295$  K)

Frequency in GHz	$\gamma_{\text{N}_2}$	$\gamma_{\text{O}_2}$	N', J' ← N'' J''
298	2.30	2.25	2 2 ← 0 1
345	2.21	2.19	3 2 ← 1 1
508	2.15	2.10	4 3 ← 2 2
627	2.15	2.10	4 4 ← 2 3

### 3.6. NITRIC ACID (HNO<sub>3</sub>): MOLECULE 12

For the description of the nitric acid contribution in the spectral ranges of MASTER it is necessary to take into account a large number of lines because of the low values of the rotational parameters of this molecule ( $A \sim B \sim 13$  GHz,  $C \sim 6.2$  GHz). In addition, the first vibrational states of nitric acid  $9^1$ ,  $7^1$ ,  $6^1$ ,  $8^1$ ,  $5^1$  and  $9^2$  are located at rather low energies, i.e. at 458, 580, 647, 763, 879, and 896 cm<sup>-1</sup> respectively. Therefore the transitions within  $9^1$ ,  $7^1$ ,  $6^1$ ,  $8^1$ ,  $5^1$  and  $9^2$  (hereafter referred as “hot” transitions) contribute at 296 K for about 23% to the total HNO<sub>3</sub> line intensities and are to be considered in addition to those within the ground vibrational state (hereafter referred as “cold transitions”).

Numerous recent microwave or millimeter studies involve line position studies for transitions not only in the ground vibrational state but also in the  $9^1$ ,  $7^1$ ,  $6^1$ ,  $8^1$ ,  $5^1$  and  $9^2$  vibrational states (Cazzoli and De Lucia, 1979; Crownover *et al.*, 1988; Paulse *et al.*, 1996; Goyette *et al.*, 1996; Petkie *et al.*, 2001, 2003; Perrin 1998b; Perrin *et al.*, 2004). It is important to underline that some of these studies had to take into the fact that the  $\nu_9$  mode located at 458 cm<sup>-1</sup> (OH torsional mode relative to the NO<sub>2</sub> moiety) is a “large amplitude motion”. This effect induces indeed splittings of about 2, 35 and 51 MHz for the energy levels in the  $9^1$ ,  $5^1$ , and  $9^2$  vibrational states, respectively.

#### 3.6.1. HNO<sub>3</sub> Line Positions and Intensities in the HITRAN and JPL Databases

In the JPL database the quoted lines involve hot transitions within  $9^1$ ,  $6^1$ ,  $7^1$ ,  $8^1$ ,  $5^1$  and  $9^2$  in addition with the cold transitions. However, the line positions for the  $9^1 \leftrightarrow 9^1$ ,  $5^1 \leftrightarrow 5^1$ ,  $9^2 \leftrightarrow 9^2$ ,  $5^1 \leftrightarrow 9^2$  and  $9^2 \leftrightarrow 5^1$  transitions are not accurate since the JPL calculations were performed around 1990 when the theoretical model able to handle the torsional effects was not yet developed.

The line intensities in the JPL catalog were generated using a dipole moment  $\mu_0$  derived from various Stark concurring measurements (Cox and Riveros, 1965; Kleiner *et al.*, 1987). On the other hand, and as for N<sub>2</sub>O only the rotational part of the partition function was accounted for in the JPL calculation: see Table V where a comparison of the partition functions used in HITRAN (Fischer *et al.*, 2003) and in the JPL catalog is given. Because of the existence of rather low vibrational states for HNO<sub>3</sub>, the vibrational part of the partition function contributes for about 30% at  $T = 296$  K ( $Z_{\text{vib}}(300 \text{ K}) \sim 1.3$ ) to the total partition function, leading to JPL intensities for HNO<sub>3</sub> overestimated by about 30%. The situation is not better in HITRAN since the positions and intensities parameters (Rothman *et al.*, 1983) are only a 1983 version of the JPL catalog.



Table V. Comparison of the partition function for nitric acid calculated in this work and in the HITRAN and JPL databases. For the present calculation, the vibrational and rotational contributions are given

Temp	$Z_{\text{Rot}}$	$Z_{\text{Vib}}$	$Z_{\text{Tot}}$	Z(JPL)	Z(HITRAN)
75	3493.79	1.00017	3494.39	3493.8	3496.2
150	9879.18	1.01933	10070.2	9878.7	10080.0
225	18151.0	1.11344	20210.1	18151.0	20244.7
296	27363.6	1.29952	35559.6		35687.8
300	27917.4	1.31316	36660.1	27938.3	36797.9

### 3.6.2. $\text{HNO}_3$ Line Positions and Intensities in the MASTER Database

Given the previous comments, a new list of  $\text{HNO}_3$  line positions and intensities was generated for MASTER. For the cold band and transitions within the  $6^1$ ,  $7^1$ , and  $8^1$  excited vibrational states, no perturbations had to be accounted for. Therefore we used a classical method of calculation both for line positions (Watson, 1977) and line intensities (Flaud *et al.*, 1981), and the rotational and centrifugal distortion parameters from Petkie *et al.* (2003), the  $\text{HNO}_3$  dipole moment (Cox and Riveros, 1965) and the partition function quoted in HITRAN (Fischer *et al.*, 2003). For the  $9^1 \leftrightarrow 9^1$ ,  $5^1 \leftrightarrow 5^1$ ,  $9^2 \leftrightarrow 9^2$ ,  $5^1 \leftrightarrow 9^2$  and  $9^2 \leftrightarrow 5^1$  transitions, we had to account for the torsional effect. This was done using the Internal Axis Method (IAM) both for the line position and line intensity calculations. For these computations we used the rotational, torsional and coupling parameters which are quoted by Paulse *et al.* (1996) and by Perrin *et al.* (2004) for the  $9^1$  and  $5^1, 9^2$  vibrational states respectively.

To illustrate these results, a comparison is performed in Table VI for the  $9^1 \leftrightarrow 9^1$  “hot” band of  $\text{HNO}_3$  in the 343,799–343,835 MHz region. In this case the line positions calculated using the parameters from (Paulse *et al.*, 1996) differ from those present in JPL because the torsional splitting is now accounted for correctly. Also, the JPL linelist involves eight transitions, but for symmetry reasons, only four transitions (instead of eight) actually exist (Paulse *et al.*, 1996).

### 3.6.3. $\text{HNO}_3$ Line Broadening Coefficients

The only existing  $\text{N}_2$ - and  $\text{O}_2$ -line broadening calculation was performed a long time ago by Tejwani and Yeung (1978). Since this early work performed using the Anderson theory, to our knowledge no new line broadening calculation was published.

There exist few line broadening measurements for  $\text{HNO}_3$ . The most accurate were performed in the microwave or submillimeter spectral region by Goyette *et al.* (1988a, 1991, 1998), Zu *et al.* (2002), and Colmont *et al.* (2003), because these measurements were performed for well-isolated lines. In order to complete

Table VI. Portion of the JPL line list for the  $9^1-9^1$  transitions of  $\text{HNO}_3$  in the 343.7–343.9 GHz region and comparison with the observed positions and with the calculation (positions and intensities) performed in the present study

$\tilde{\nu}_{\text{JPL}}$	Int $\times 10^{+23}$ JPL	$\nu_{\text{Obs}}$ (Paulse <i>et al.</i> , 1996)	$\nu_{\text{Calc}}$ (This work)	Int $\times 10^{+23}$ (This work)	$J'$	$K'_a$	$K'_c$	$J''$	$K''_a$	$K''_c$
343823.7959	0.19	343826.189	343826.056	1.46	18	9	9	17	10	8
343826.9947	0.19									
343826.1411	1.25	343827.162	343827.074	0.741	18	10	9	17	10	8
343826.1468	1.25									
343832.2270	1.25	343831.089	343831.164	0.741	18	9	9	17	9	8
343832.2326	1.25									
343831.3791	0.19	343832.219	343832.182	1.46	18	10	9	17	9	8
343834.5778	0.19									

Note. As compared to the JPL list, only every other line is existing for symmetry reasons. Other details on the intensity calculations are given in the text. All the intensities are in  $\text{cm}^{-1}/(\text{molecule cm}^{-2})$  at 296 K.

these studies, air-broadening measurements were performed in Lille and Bologna (Demaison *et al.*, 2004; Cazzoli *et al.*, 2005). Depending on the rotational transition, the nitrogen- and oxygen-broadening coefficients range between 4.17 MHz/Torr and 4.88 MHz/Torr for  $\gamma_{\text{N}_2}$ , and between 2.31 MHz/Torr and 2.96 MHz/Torr for  $\gamma_{\text{O}_2}$ . Table VII gives a list of air broadening halfwidths for various pure rotational transitions in the microwave or millimeter regions, and it is clear also, from this table that there exists a rather clear rotational dependence of the air broadening coefficients which need to be modeled.

We used an empirical model which is defined as follows.

For low and medium  $J''$  values:

$$\gamma_{\text{air}} = a_{\text{air}} + b_{\text{air}}(J' + J'')/2 \quad (6)$$

For high  $J''$  values ( $(J' + J'')/2 > J^{\text{MAX}}$ ), we used (more or less) a “hard spheres” collisions model:

$$\gamma_{\text{air}} = \text{constant} \quad (7)$$

This model is presented in Figure 1. In order to determine  $a_{\text{air}}$ ,  $b_{\text{air}}$  and  $J^{\text{MAX}}$ , a least squares fit calculation was performed on the experimental data quoted in Table VII. The results of this computation are (in MHz/Torr for  $a_{\text{air}}$  and  $b_{\text{air}}$ ):

$$J^{\text{MAX}} = 34.402 \pm 5, \quad \alpha_{\text{air}} = 5.04875 \pm 0.20, \quad \text{and} \quad b_{\text{air}} = 0.0340645 \pm 0.009 \quad (8)$$

The inspection of Table VII and Figure 1 shows that the empirical model is working reasonably well. As a consequence Equations (6), (7) and (8) were used

Table VII. List of the air-broadening experimental coefficients used for the empirical description of the broadening coefficients of HNO<sub>3</sub>. Results of the calculation

$\nu$	$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\gamma_{\text{airObs}}$	$\gamma_{\text{airCalc}}$	Ref.
231778	14	d	10	13	d	9	4.599	4.589	(Goyette <i>et al.</i> , 1988a)
281782	19	d	16	18	d	15	4.311	4.419	(Goyette <i>et al.</i> , 1988a)
281685	22	d	22	21	d	21	3.909	4.316	(Goyette <i>et al.</i> , 1988a)
444556	26	d	17	25	d	16	4.11	4.180	(Goyette <i>et al.</i> , 1988a)
457042	27	9	18	26	9	17	3.989	4.146	(Goyette <i>et al.</i> , 1988a)
444284	35	d	35	34	d	34	3.851	3.877	(Goyette <i>et al.</i> , 1988a)
456784	36	d	36	35	d	35	3.954	3.877	(Goyette <i>et al.</i> , 1988a)
235168	11	9	3	10	9	2	4.355	4.691	(Goyette <i>et al.</i> , 1988a)
232179	12	6	6	11	6	5	4.93	4.657	(Goyette <i>et al.</i> , 1988a)
284871	13	11	2	12	11	1	4.566	4.623	(Goyette <i>et al.</i> , 1988a)
283003	14	8	6	13	8	5	4.590	4.589	(Goyette <i>et al.</i> , 1988a)
370541	18	12	7	17	12	6	4.428	4.453	(Goyette <i>et al.</i> , 1988a)
453822	20	15	5	19	15	4	3.747	4.384	(Goyette <i>et al.</i> , 1988a)
231627	18	d	18	17	d	17	4.353	4.453	(Goyette <i>et al.</i> , 1991)
369487	22	d	15	21	d	14	4.229	4.316	(Goyette <i>et al.</i> , 1991)
369258	29	d	29	28	d	28	3.929	4.078	(Goyette <i>et al.</i> , 1991)
206595	16	d	16	15	d	15	4.428	4.521	(Goyette <i>et al.</i> , 1998)
206663	14	d	12	13	2	11	4.752	4.589	(Goyette <i>et al.</i> , 1998)
206703	13	d	10	12	3	9	4.824	4.623	(Goyette <i>et al.</i> , 1998)
219037	24	d	17	24	8	16	4.215	4.231	(Goyette <i>et al.</i> , 1998)
218896	25	d	17	25	9	16	4.343	4.197	(Goyette <i>et al.</i> , 1998)
218739	26	10	17	26	10	16	4.221	4.163	(Goyette <i>et al.</i> , 1998)
206765	12	5	8	11	5	7	4.689	4.657	(Goyette <i>et al.</i> , 1998)
205120	30	14	16	30	14	17	4.198	4.027	(Goyette <i>et al.</i> , 1998)
686636	32	28	4	31	28	3	3.916	3.976	(Zu <i>et al.</i> , 2002)
686579	32	28	5	31	28	4	4.337	3.976	(Zu <i>et al.</i> , 2002)
686157	32	23	10	31	23	9	4.01	3.976	(Zu <i>et al.</i> , 2002)
684157	31	22	9	30	22	8	4.171	4.010	(Zu <i>et al.</i> , 2002)
316611	44	19	25	44	18	26	3.832	3.877	Lille
316902	43	19	25	43	17	26	3.82	3.877	Lille
344241	27	d	27	26	d	26	4.182	4.146	Lille + Bologna
470233	24	13	11	23	13	10	4.16	4.248	Lille
544365	38	5	33	37	5	32	3.92	3.877	Lille
206663	14	2	12	13	2	11	4.881	4.589	Lille
319221	25	0	25	24	0	24	4.192	4.214	Bologna
319897	27	2	25	27	1	27	4.282	4.129	Bologna
320005	26	1	25	26	0	26	4.211	4.163	Bologna
322348	15	13	3	14	13	2	4.574	4.555	Bologna

Note. *Meaning of the different columns:*  $\tilde{\nu}$ : frequency in MHz;  $J'$   $K_a'$   $K_c'$   $J''$   $K_a''$   $K_c''$ : upper and lower rotational quantum numbers, d is for degenerate doublets ( $K_a = J - K_c$  and  $J - K_c + 1$ );  $\gamma_{\text{air}}$  observed and calculated air-pressure broadening coefficients (in MHz/Torr at 296 K); Ref.: source of the data, Lille and Bologna are for the measurements described by Demaison *et al.* (2004).

Table VIII. Comparison between the BrO partition function achieved in this work and those quoted in the JPL catalog

$T$ (K)	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Rot}}^{3/2}(T) + Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$	$Z_{\text{JPL}}(T)$
$^{79}\text{BrO}$						
150	1965.33	0.184	1965.51	1.001	1967.42	1949.83
225	2941.8	6.074	2947.87	1.0099	2977.04	2932.18
300	3918.94	38.03	3956.97	1.0321	4084.13	3941.17
296	3866.81	35.24	3902.05	1.0306	4021.52	
$^{81}\text{BrO}$						
150	1973.40	0.184	1973.59	1.001	1975.50	1957.96
225	2953.95	6.099	2960.05	1.0099	2989.33	2944.41
300	3935.17	38.18	3973.35	1.0321	4101.03	3957.59
296	3882.82	35.38	3918.20	1.0306	4038.17	

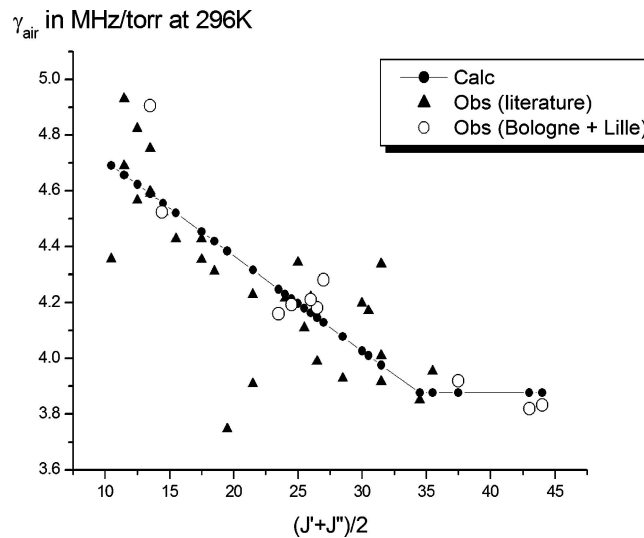


Figure 1. Air broadening parameter  $\gamma_{\text{air}}$  for  $\text{HNO}_3$  as a function of  $(J' + J'')/2$ .

to generate the air broadening coefficients for the whole set of  $\text{HNO}_3$  lines, except for the lines for which these broadening coefficients were measured: in this case we used the measured data instead of the calculated ones.

For the temperature dependence exponent, the only existing data vary from 0.57 to 0.74 for  $n_{\text{N}_2}$  and 0.67 to 0.85 for  $n_{\text{O}_2}$  (Goyette *et al.*, 1991, 1998), (Colmont *et al.*, 2003). When looking in more details at these studies it was not possible to set up a reasonable empirical description for the rotational dependence of  $n_{\text{air}}$ , and for this reason, the constant value  $n_{\text{air}} = 0.70$  was adopted for all the  $\text{HNO}_3$  lines in MASTER.

Finally the value which is quoted for the self-broadening coefficient  $\gamma_{\text{self}} \approx 31.8$  MHz/Torr is an average of the values measured in Zu *et al.* (2002).

#### 3.6.4. Pressure Shifts

Pressure shift measurements were performed in Bologna during this study for the 319.221, 319.897, 320.005, 322.348 and 344.241 GHz lines of HNO<sub>3</sub>, leading to rather low values for the pressure shifts ( $\delta_{\text{air}} = 17(4)$ ,  $-32(6)$ ,  $12(15)$ ,  $22(2)$  and  $4(2)$  kHz/Torr, respectively). In order to avoid systematic errors for the lines for which no information is available, it was decided to implement a zero value for all HNO<sub>3</sub> pressure shifts in the MASTER database.

### 3.7. HYDROGEN CHLORIDE (HCl): MOLECULE 15

#### 3.7.1. Line Positions and Line Intensities

For the hydrogen chloride molecule, it is necessary to take into account the hyperfine structure to get accurate line positions and line intensities in the microwave or submillimeter spectral region (Nolt *et al.*, 1987; Klaus *et al.*, 1998; Odashima *et al.*, 1999; Cazzoli and Puzzarini, 2004 and references therein). Two sets of HCl rotational transitions (with a triplet hyperfine structure) are observable at 625.0 GHz and 625.9 GHz within the channel F of MASTER: they correspond to the  $J' - J'' = 1 - 0$  transitions of the H<sup>37</sup>Cl and H<sup>35</sup>Cl isotopic species of hydrogen chloride, respectively.

The line positions that we used for MASTER are the experimental positions measured by Klaus *et al.*, (1998), which were confirmed by the very accurate measurements performed very recently by Cazzoli and Puzzarini (2004). These measurements are in excellent agreement with the line positions previously measured by Nolt *et al.* (1987).

The line intensities in the JPL, SAO and HITRAN databases were generated using the value of the HCl dipole moment measured by Stark effect (Kaiser, 1970; De DeLeeuw and Dymanus, 1973). On the other hand for both H<sup>35</sup>Cl and H<sup>37</sup>Cl the partition functions in HITRAN are smaller than those in the JPL catalog for the whole 70–300 K temperature range. For example at 300 K one has  $Z_{\text{JPL}}(300 \text{ K})/Z_{\text{HITRAN}}(300 \text{ K}) \approx 1.024$ , and for this reason, the intensities for HCl in the JPL catalog are  $\approx 2\%$  weaker than those in HITRAN. To resolve this discrepancy a new computation of the HCl partition function was performed during the present study which leads to an excellent agreement with the HITRAN values.

#### 3.7.2. Line Broadening and Line Shift Coefficients

Drouin (2004a) measured the N<sub>2</sub>- and O<sub>2</sub>-pressure broadenings and pressure shifts for the rotational  $J = 1 \leftarrow 0$  lines of H<sup>35</sup>Cl located near 625 GHz, respectively.

The N<sub>2</sub>- and O<sub>2</sub>-broadening coefficients were measured at different temperatures leading to the  $n$ -temperature dependences of these coefficients. Therefore the air-broadening coefficients  $\gamma_{\text{air}}(296\text{ K}) = 3.420(7)$  MHz/Torr and  $n_{\text{air}} = 0.73(3)$  issued from these results were implemented in the MASTER database for both H<sup>35</sup>Cl and H<sup>37</sup>Cl. It has to be pointed out that the broadening coefficients achieved by Park *et al.* (1991) for the  $J = 4 \leftarrow 3$  of H<sup>35</sup>Cl located near 2.5 THz are quite different from those obtained for the 625 GHz lines, but this is not a surprise considering the strong dependence on the  $m$  rotational number ( $m = -J$  and  $m = J + 1$  for the P- and R-lines, respectively) which was noticed for the  $1 \leftarrow 0$  fundamental band at 2,886 cm<sup>-1</sup> (Houdeau *et al.*, 1980; Pine and Fried, 1985; Pine and Looney, 1987; Ballard *et al.*, 1985; Chackerian *et al.*, 1985).

From the various existing self-broadening measurements (Pourcin 1972; Pourcin *et al.*, 1981), one can estimate that the HITRAN value  $\gamma_{\text{self}}(296\text{ K}) \approx 8.61$  MHz/Torr is reasonable. Finally the value of the air-pressure shift  $\delta_{\text{air}}(296\text{ K}) = 0.146(3)$  MHz/Torr obtained by Drouin (2004a) was also implemented in MASTER.

### 3.8. CHLORIDE MONOXIDE (ClO): MOLECULE 18

Numerous line position studies were performed recently in the infrared or microwave spectral regions (Cohen *et al.*, 1984; Rinsland *et al.*, 1992; Burkholder *et al.*, 1987; Drouin *et al.*, 2001b). The ClO linelist which is present in the JPL database was generated in 1991, using extensive and accurate measurements (Cohen *et al.*, 1984). The excellent quality of the line positions was confirmed by recent measurements (Drouin *et al.*, 2001b). The line intensities were computed using the ClO measured dipole moment (Yaron *et al.*, 1988). The partition function given in the JPL catalog, in HITRAN and calculated in the present study are in excellent agreement. Therefore, because of their excellent quality, the line positions and intensities quoted in the JPL catalog were implemented in the MASTER database.

For the air-broadening coefficients and their temperature dependences, we used the values which were measured at DLR (Bauer *et al.*, 1998a) for the 501.2 GHz lines ( $J' = 13.5 \leftarrow J'' = 12.5$  transition of <sup>35</sup>ClO), namely  $\gamma_{\text{air}} = 3.23(13)$  MHz/Torr @296 K and  $n_{\text{air}} = 0.69(6)$ . However, it has to be pointed out that these broadening coefficients are significantly higher than for the 204.4 ( $J' = 5.5 \leftarrow J'' = 4.5$  of <sup>35</sup>ClO) and 649.4 GHz lines ( $J' = 13.5 \leftarrow J'' = 12.5$  of <sup>35</sup>ClO) for which the values  $\gamma_{\text{air}} = 2.54(8)$  MHz/Torr @296 K (with  $n_{\text{air}} = 0.62(6)$ ) and  $\gamma_{\text{air}} = 2.11(6)$  MHz/Torr @296 K (with  $n_{\text{air}} = 0.85(9)$ ) respectively were obtained at JPL by Oh and Cohen (1994). Therefore, further air broadening measurements should be performed for ClO in order to validate more accurately the quality of the air-broadening coefficients.

3.9. METHYL CHLORIDE (CH<sub>3</sub>Cl): MOLECULE 243.9.1. *Line Positions and Intensities*

Numerous microwave measurements were performed for both the CH<sub>3</sub><sup>35</sup>Cl and CH<sub>3</sub><sup>37</sup>Cl isotopic species, and these results were completed by analyses performed in the  $\nu_3$  and  $\nu_6$  band (Wlodarczak *et al.*, 1985a, 1985b, 1986; Carpenter and Seo, 1985; Demaison *et al.*, 1994). Therefore, the accurate line positions present in the JPL catalog were included in the MASTER database.

The JPL catalog uses, for the line intensity calculation, the value of the permanent dipole moment of CH<sub>3</sub>Cl determined by laser-Stark spectroscopy (Wlodarczak *et al.*, 1985b). On the other hand, the partition function used in the JPL catalog for CH<sub>3</sub>Cl accounts only for its spin-rotational contribution and since  $Z_{\text{vib}}(300\text{ K}) = 1.050$  the intensities are overestimated by 5%. Consequently the line intensities present in the JPL catalog for CH<sub>3</sub>Cl were divided by  $Z_{\text{vib}}(300\text{ K}) = 1.050$  before their introduction in the MASTER database.

3.9.2. *Line Broadening Coefficients*

Numerous recent analyses were performed in the infrared region (Blanquet *et al.*, 1993a, 1993b; Bouanich *et al.*, 2001). The N<sub>2</sub>- and O<sub>2</sub>-broadening coefficients were measured at room temperature in the  $\nu_3$  band. Also theoretical calculations of these broadening coefficients were performed (Bouanich *et al.*, 1993). In both cases (theory and experiment) a variation with the  $J$  and  $K$  quantum numbers was pointed out. More precisely, the N<sub>2</sub>-broadening coefficients (resp. the O<sub>2</sub>-ones) vary from  $\gamma_{\text{N}_2} \approx 4.7$  MHz/Torr for  $J = 3$  to  $\gamma_{\text{N}_2} \approx 3.9$  MHz/Torr for  $J = 46$  (resp.  $\gamma_{\text{O}_2} \approx 3.7$  MHz/Torr for  $J = 3$  to  $\gamma_{\text{O}_2} \approx 2.9$  MHz/Torr for  $J = 46$ ). More recently, the temperature dependence of the N<sub>2</sub>-broadening coefficient was measured and in this case also a  $J$ -dependence was pointed out (Bakri *et al.*, 2002). According to these results a mean value for the air broadening can be estimated ( $\gamma_{\text{air}} = 0.79\gamma_{\text{N}_2} + 0.21\gamma_{\text{O}_2}$ ) leading the values  $\gamma_{\text{air}} \approx 4.04$  MHz/Torr and  $n_{\text{air}} = 0.7$  which were implemented in the MASTER database. Finally  $\gamma_{\text{self}} \approx 20$  MHz/Torr was used for the self-broadening parameter (Harde *et al.*, 1994, 1997a, 1997b).

## 3.10. BROMIDE MONOXIDE (BrO): MOLECULE 40

As it is the case for other halogen monoxides, BrO has a single vacancy in the  $p\pi$  antibonding orbital. This gives rise to an inverted doublet  $\Pi$  ground electronic state. More explicitly the  $X_1^2\Pi_{1/2}$  (with  $J \geq 1/2$ ) doublet component is located at  $\sim 970$  cm<sup>-1</sup> above the lower  $X_1^2\Pi_{3/2}$  (with  $J \geq 3/2$ ) component. The vibrational frequencies are  $\omega_0 = 723.41420$  cm<sup>-1</sup> and  $\omega_0 = 721.92715$  cm<sup>-1</sup> for the <sup>79</sup>BrO and <sup>81</sup>BrO species, respectively. To reproduce the rotational energy levels, one has to account for the various hyperfine effects, and since the nuclear spin of <sup>79</sup>Br and <sup>81</sup>Br is equal to  $I = 3/2$ , each rotational component (with a given  $J$  value) is split

in general into four  $F$  components corresponding to  $|F - J| = 3/2$  or  $1/2$ . Also it is necessary to account for the  $\Lambda$  doubling (Amano *et al.*, 1972; Brown *et al.*, 1972; Butler *et al.*, 1984; Cohen *et al.*, 1981; Drouin *et al.*, 2001a). For the MASTER database we used the line positions and line intensities quoted in the JPL catalog (Cohen *et al.*, 1981).

As BrO is missing in HITRAN, we have generated the partition functions for  $^{79}\text{BrO}$  and  $^{81}\text{BrO}$ , using:

$$Z_{\text{Tot}}(T) = Z_{\text{Vib}}(T)[Z_{\text{Rot}}^{3/2}(T) + Z_{\text{Rot}}^{1/2}(T)] \quad (9)$$

where  $Z_{\text{Vib}}(T)$  is the vibrational partition function and  $Z_{\text{Rot}}^{3/2}(T)$  and  $Z_{\text{Rot}}^{1/2}(T)$  are the individual contributions of the rotational partition function for the  $X^2\Pi_{3/2}$  and  $X^2\Pi_{1/2}$  spin components respectively.

One has:

$$Z_{\text{Rot}}^{3/2}(T) = \sum_{J \geq 3/2} \sum_F \sum_{\pm} (2F + 1) \exp\left(-E_{J,F,\pm}^{3/2,\text{Rot}}/kT\right) \quad (10)$$

$$Z_{\text{Rot}}^{1/2}(T) = \sum_{J \geq 1/2} \sum_F \sum_{\pm} (2F + 1) \exp\left(-E_{J,F,\pm}^{1/2,\text{Rot}}/kT\right) \quad (11)$$

In Equations (10) and (11) the summation is performed starting from  $J \geq 3/2$  and  $J \geq 1/2$  for  $Z_{\text{Rot}}^{3/2}(T)$  and  $Z_{\text{Rot}}^{1/2}(T)$ , respectively, for  $F$  such as  $|F - J| = 3/2$  or  $1/2$ , and for each of the two  $\pm$  lambda subcomponents. Actually it proved that the convergence of the summation is obtained at  $J \approx 85$  for temperatures up to  $T = 330 \text{ K}$ .<sup>4</sup> From the comparison which is performed in Table VIII, it appears that the partition functions calculated in the present study are systematically larger than the JPL ones. The source of this disagreement which occurs for all temperatures is not clear.

The JPL partition functions were used to generate the BrO intensities present in the JPL catalog which were introduced in the MASTER database. Therefore, provided that the present results on the BrO partition function are confirmed by further studies, the BrO intensities may be overestimated by  $\approx 3.6\%$  at 300 K and by  $\approx 1\%$  at 150 K (Table VIII).

For the air-broadening coefficients we used the values  $\gamma_{\text{air}}(296 \text{ K}) = 3.54(3)$  MHz/Torr and  $n_{\text{air}} = 0.45(18)$  as measured at DLR (Bauer *et al.*, 1998a) for the 499.6 GHz line of  $^{79}\text{BrO}$  ( $J = 19.5 \leftarrow 18.5$  transition). After the generation of the MASTER database, new  $\text{N}_2$ - and  $\text{O}_2$ -broadening measurements were performed simultaneously at Ibaraki University and at the Jet Propulsion laboratory (Yamada *et al.*, 2003) for the 624.768 and 650.178 GHz lines (the  $J = 24.5 \leftarrow 23.5$  and  $J = 25.5 \leftarrow 24.5$  rotational transitions in the  $X^2\Pi_{3/2}$  vibronic state of  $^{81}\text{BrO}$ ), leading to rather reasonable agreements for the broadening parameters measured in both laboratories. From these new measurements and using  $\gamma_{\text{air}} = 0.79\gamma_{\text{N}_2} + 0.21\gamma_{\text{O}_2}$  the air-broadening coefficients are  $\gamma_{\text{air}} = 3.05(5)$  MHz/Torr,  $n_{\text{air}} = 0.80(5)$ , and  $\gamma_{\text{air}} = 3.03(7)$  MHz/Torr,  $n_{\text{air}} = 0.81(7)$  for the 624.768 and 650.178 GHz lines,



respectively. These values are significantly weaker than those measured earlier at DLR for the  $J = 19.5 \leftarrow 18.5$  transition of  $^{79}\text{BrO}$ , indicating a very likely decreasing with  $J$  of the air-broadening parameters. This  $J$ -dependence should be investigated in more details by further air broadening measurements.

#### 4. The “Possible Interfering Species” in the MASTER Database

The following molecules were added in the linelist as possible interfering species for the target molecules of MASTER.

##### 4.1. SULFUR DIOXIDE ( $\text{SO}_2$ : MOLECULE 9), AND NITROGEN DIOXIDE ( $\text{NO}_2$ : MOLECULE 10)

For  $^{14}\text{N}^{16}\text{O}_2$  we used the line positions and intensities that were generated by Perrin *et al.* (1988, 1992, 1998a) for HITRAN: these parameters account for the hyper-fine structure and for the electron spin-rotation interaction. The partition function which was used to calculate the line intensities accounts for the spin-rotation and vibrational contributions. Therefore these data which involve both the ground and the first vibrational states are more complete than those available in the JPL catalog.

For  $^{32}\text{S}^{16}\text{O}_2$ ,  $^{34}\text{S}^{16}\text{O}_2$ ,  $^{32}\text{S}^{16}\text{O}^{18}\text{O}$ , and  $^{33}\text{S}^{16}\text{O}_2$ , the line positions quoted in the JPL catalog are of excellent quality owing to the numerous studies performed for this molecule (Lovas, 1985, 2004). On the other hand, before their implementation in the MASTER database, the line intensities present in the JPL catalog were divided by a factor equal to the vibrational partition function  $Z_{\text{vib}}(300\text{ K}) = 1.0965$ , since  $Z_{\text{vib}}$  was not considered in the JPL calculations.

For the air- and self-broadening coefficients, we used the values which were included in the 1998 version of HITRAN (Perrin *et al.*, 1998a)  $\gamma_{\text{air}} = 4.73\text{ MHz/Torr}$ ,  $\gamma_{\text{self}} = 15.8\text{ MHz/Torr}$  for  $\text{SO}_2$ , and  $\gamma_{\text{air}} = 2.64\text{ MHz/Torr}$  for  $\text{NO}_2$ . For  $\text{NO}_2$  this value is however lower than values measured by Goyette *et al.* (1988b),  $\gamma_{\text{air}} = 3.14(3)\text{ MHz/Torr}$  and  $\gamma_{\text{air}} = 3.00(5)\text{ MHz/Torr}$  for the 231.2 GHz and 247.4 GHz lines, respectively. Therefore an update for  $\text{NO}_2$  may have to be performed provided that these results are completed by a more extended set of broadening coefficients. Actually according to recent infrared measurements (Benner *et al.*, 2004) the rotational dependence for these broadening coefficients is far from being negligible. Finally, for  $\text{NO}_2$ , we used  $\gamma_{\text{self}} = 1.42\text{ MHz/Torr}$  as it was calculated by Tejwani (1972).

##### 4.2. CARBONYL SULFIDE ( $\text{OCS}$ : MOLECULE 19)

For  $\text{OCS}$ , the line positions and intensities quoted in the HITRAN are those given in the JPL catalog (Lovas, 1978). This means that the line intensities in both databases are overestimated by  $\sim 20\%$  because as already said the partition function used in the JPL catalog does not account for the vibrational contribution which at 300 K is

$Z_{\text{vib}}(300 \text{ K}) = 1.207$ . For this reason all the OCS intensities were divided by this 1.207 factor before their introduction in the MASTER database.

For the air-broadening and the self-broadening coefficients we used the values  $\gamma_{\text{air}} = 3.57 \text{ MHz/Torr}$  and  $\gamma_{\text{self}} = 5.9 \text{ MHz/Torr}$  which were deduced from the measurements performed by Bouanich *et al.* (1987) and Depannemaecker and Lemaire (1988), respectively.

#### 4.3. FORMALDEHYDE ( $\text{H}_2\text{CO}$ : MOLECULE 20)

The JPL line positions are of good quality (Bocquet *et al.*, 1996 and references therein). As far as the intensities are concerned, the JPL calculation was performed using the  $\text{H}_2\text{CO}$  dipole moment from (Fabricant *et al.*, 1977 and references therein). Again, the vibrational partition function was neglected, but for  $\text{H}_2\text{CO}$  this contribution is still negligible at 300 K (less than 5%). Therefore the line positions and intensities present in the JPL catalog for the  $\text{H}_2\text{CO}$  were implemented in the MASTER database.

For the air-broadening coefficients, the value  $\gamma_{\text{air}} = 4.70 \text{ MHz/Torr}$  which is issued from the existing air broadening measurements (Nadler *et al.*, 1987) is used in the MASTER database. This value differs slightly from the value  $\gamma_{\text{air}} = 4.22 \text{ MHz/Torr}$  presently given in HITRAN (Rothman *et al.*, 1998) and for which there is no information. For the self-broadening halfwidth, we used the measured  $\gamma_{\text{self}} = 23 \text{ MHz/Torr}$  (Nerf, 1975a). No value was found in the literature for the  $n$ -temperature dependence of the pressure linewidths which was set to  $n = 0.7$ . Let us notice that the rotational dependence of these broadening coefficients is presumably rather large as pointed out by the calculation (Tejwani and Yeung, 1977) and the measurements (Nerf, 1975a).

#### 4.4. HYPOCHLOROUS ACID, HYPOBROMOUS ACID ( $\text{HOCl}$ AND $\text{HOBr}$ : MOLECULES 21 AND 37)

The  $\text{HOCl}$  and  $\text{HOBr}$  molecules are non-linear molecules of  $C_s$  symmetry and therefore both A- and B-type transitions with ( $\Delta K_a = \text{even}$  and  $\Delta K_c = \text{odd}$ ) and ( $\Delta K_a = \text{odd}$  and  $\Delta K_c = \text{odd}$ ) selection rules, are observable in the microwave, submillimeter or far infrared regions for these two molecules (Singbeil *et al.*, 1984; Gillis *et al.*, 1984; Koga *et al.*, 1989; Flaud *et al.*, 1998b).  $\text{HOCl}$  and  $\text{HOBr}$  lines exhibit a hyperfine structure which is non negligible for the low rotational quantum numbers. This hyperfine structure is explicitly taken into account in the JPL database. On the other hand in HITRAN the hyperfine structure of  $\text{HOCl}$  was ignored and no parameters are available for  $\text{HOBr}$  in the millimeter region.

For  $\text{HOCl}$  and  $\text{HOBr}$  the line intensities given in the JPL catalog were generated using the parameters obtained by Singbeil *et al.* (1984) and Yoga *et al.* (1989) and a partition function which accounts only for the spin and rotational contributions. Therefore the intensities are (weakly) overestimated by a factor equal to the

vibrational contribution at 300 K to the partition function ( $^{\text{HOCl}}Z_{\text{vib}}(300 \text{ K}) = 1.035$  and  $^{\text{HOBr}}Z_{\text{vib}}(300 \text{ K}) = 1.058$ ). As far as HOCl is concerned, this was also evidenced during the line intensity calculation performed for the far infrared region (Flaud *et al.*, 1998b). Since these intensity corrections are rather weak the line positions and line intensities given in the JPL database were implemented in the MASTER database.

The air broadening coefficients and its  $n$ -temperature dependence which are quoted in HITRAN for HOCl, (namely:  $\gamma_{\text{air}} = 2.37 \text{ MHz/Torr}$  (at 296 K) and  $n_{\text{air}} = 0.5$ ) are the original default values which were quoted for all molecules in the first version of the AFGL-HITRAN database and therefore have no real physical meaning. Therefore, we have followed the recommendations for the MIPAS (Flaud *et al.*, 2003b) database and have implemented for HOCl the value  $\gamma_{\text{air}} = 3.94 \text{ MHz/Torr}$  (at 296 K) which is the average values of two lines measured recently in the  $\nu_2$  band (Shorter *et al.*, 1997). Also the temperature dependence coefficient has been set to 0.7, a value which seems more reasonable for this molecule than the value 0.5 quoted in the HITRAN database. These values were also used for HOBr which is rather similar to HOCl.

#### 4.5. HYDROGEN CYANIDE (HCN: MOLECULE 23)

For the line positions and line intensities, we used the parameters quoted in the HITRAN database. In fact the line intensities in the HITRAN database are  $\sim 7\%$  weaker than those quoted in the JPL catalog. This is consistent with the fact that the vibrational contribution of the partition ( $Z_{\text{vib}}(300 \text{ K}) = 1.0725$ ) is not considered during the JPL line intensity calculation leading to intensities overestimated by this factor.

Also the air-broadening coefficients that we used are the HITRAN values: these values were deduced from the results of Lemaire *et al.* (1996). Finally the self broadening  $\gamma_{\text{self}} \approx 24 \text{ MHz/Torr}$  was measured by Nerf and Sonnenberg (1975b).

#### 4.6. HYDROXYL PEROXIDE ( $\text{H}_2\text{O}_2$ : MOLECULE 25)

For the line positions and intensities we used the parameters that were generated by Perrin *et al.* (1996). In this calculation, the large amplitude OH torsional mode was accounted for both for the line positions and line intensities, leading to parameters more complete and accurate than those available in the JPL catalog or in HITRAN. For the air broadening halfwidth, we used the value  $\gamma_{\text{air}} = 3.94 \text{ MHz/Torr}$  which is an average value deduced from the measurements of Malathy Devi *et al.* (1986). This air broadening halfwidth is more or less in agreement with the results given by Goyette *et al.* (1988b):  $\gamma_{\text{air}} = 4.45(12) \text{ MHz/Torr}$  and  $\gamma_{\text{air}} = 3.92(7) \text{ MHz/Torr}$  for the 223.1 and 229.8 GHz lines, respectively.

#### 4.7. CARBONYL FLUORIDE (COF<sub>2</sub>: MOLECULE 29)

The JPL line positions which were generated using the spectroscopic constants given by Carpenter (1974) and Cohen and Lewis-Bevin (1991) were introduced in the MASTER database. The JPL line intensities were generated using the COF<sub>2</sub> permanent dipole moment measured by Laurie and Pence (1962) and a partition function which accounts only for the rotational contribution, leading to intensities overestimated by a factor equal to  $Z_{\text{vib}}(300 \text{ K}) = 1.166$ : these line intensities were introduced in the MASTER database after a division by this factor.

According to the recommendations of Rinsland *et al.* (1992) we used, for the air-broadening, the self-broadening coefficients and their  $n$ -temperature dependence, the values  $\gamma_{\text{air}} = 3.33 \text{ MHz/Torr}$   $\gamma_{\text{self}} = 6.90 \text{ MHz/Torr}$  and  $n = 0.94$  (at  $T = 296 \text{ K}$ ) achieved by May (1992).

#### 4.8. HYDROPEROXYL RADICAL (HO<sub>2</sub>: MOLECULE 33)

For the line positions and intensities we used the parameters quoted in the JPL database. For the air broadening coefficients, the values obtained recently in the microwave (Chance *et al.*, 1994b) and in the infrared region (Nelson and Zahniser, 1994) differ by about 30%. We decided to include in the database the microwave value  $5.6 \text{ MHz/Torr}$  (Chance *et al.*, 1994a) which is likely more accurate than the infrared one (Nelson and Zahniser, 1994).

### 5. Conclusion

This paper describes the MASTER database. The spectral line parameters (line positions, line intensities and line broadening coefficients) were derived, depending of their estimated accuracy, (i) by combining parameters coming from the JPL and HITRAN catalogs (ii) from data taken into the literature or (iii) using experimental data and theoretical results obtained within this study. The line positions available in the JPL catalog or in the literature are almost always adequate for the MASTER retrievals. For some of the species under study the line intensities had to be re-computed since they are incorrect for atmospheric applications in the usual public access databases. Finally, as expected, the existing air-broadening coefficients  $\gamma_{\text{air}}$  and  $n_{\text{air}}$  were not always at the required accuracy in the literature and for this reason, measurements had to be performed at Bologna, Lille and Wessling (Bauer *et al.*, 1998a; Demaison *et al.*, 2004). Since the HNO<sub>3</sub> linelist for MASTER includes numerous transitions which involve an extended set of rotational transitions an empirical model was designed down to characterize the rotational dependence of the air-broadening coefficients for this molecule. Finally it is clear that the data on air line shifts are still rather sparse in the literature but that its effect is likely to be negligible in the investigated frequency range for most of the molecules studied here.

### Acknowledgments

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### Appendix: Partition Function for $^{79}\text{BrO}$ and $^{81}\text{BrO}$ in the 150–320 K Temperature Range

As for other halogen monoxides, BrO has a single vacancy in the  $p\pi$  anti-bonding orbital. This gives rise to an inverted doublet  $\Pi$  ground electronic state. More explicitly the  $X_1^2\Pi_{1/2}$  (with  $J \geq 1/2$ ) doublet component is located at  $\sim 970\text{ cm}^{-1}$  above the lower  $X_1^2\Pi_{3/2}$  (with  $J \geq 3/2$ ) component. The vibrational frequencies are  $\omega_0 = 723.41420\text{ cm}^{-1}$  and  $\omega_0 = 721.92715\text{ cm}^{-1}$  for the  $^{79}\text{BrO}$  and  $^{81}\text{BrO}$  species, respectively.

Therefore, for BrO the partition function takes the general form

$$Z_{\text{Tot}}(T) = Z_{\text{Vib}}(T)[Z_{\text{Rot}}^{3/2}(T) + Z_{\text{Rot}}^{1/2}(T)] \quad (\text{A1})$$

where  $Z_{\text{Vib}}(T)$  is the vibrational partition function (see Equation (2)), and  $Z_{\text{Rot}}^{3/2}(T)$  and  $Z_{\text{Rot}}^{1/2}(T)$  are the individual contribution of the rotational partition function for the  $^2\Pi_{3/2}$  and  $^2\Pi_{1/2}$  spin components respectively.

To reproduce the rotational energy levels, one has to account for the various hyperfine effects. More explicitly, because the nuclear spin of  $^{79}\text{Br}$  and  $^{81}\text{Br}$  is equal to  $I = 3/2$ , each rotational component (with a given  $J$  value) is split in general into four  $F$  components corresponding to  $|F - J| = 3/2$  or  $1/2$ . Also it is necessary to account for the  $\Lambda$  doubling which is quoted either by the “ $\pm$ ” in Equations (A.2) and (A.3).

One has

$$Z_{\text{Rot}}^{3/2}(T) = \sum_{J \geq 3/2} \sum_F \sum_{\pm} (2F + 1) \exp(-E_{J,F,\pm}^{3/2,\text{Rot}}/kT) \quad (\text{A2})$$

$$Z_{\text{Rot}}^{1/2}(T) = \sum_{J \geq 1/2} \sum_F \sum_{\pm} (2F + 1) \exp(-E_{J,F,\pm}^{1/2,\text{Rot}}/kT) \quad (\text{A3})$$

In Equations (A.1) and (A.2) the summation is performed starting from  $J \geq 3/2$  and  $J \geq 1/2$  for  $Z_{\text{Rot}}^{3/2}(T)$  and  $Z_{\text{Rot}}^{1/2}(T)$ , respectively, up to maximum  $J$  values of  $J_{\text{Max}} = 85.5$  and  $J_{\text{Max}} = 65.5$  for the  $X_1^2\Pi_{3/2}$  and  $X_1^2\Pi_{1/2}$  system, respectively (since preliminary tests have shown that the convergence of the summation was already achieved). This calculation was performed using the rotational levels for  $X_1^2\Pi_{3/2}$  and  $X_1^2\Pi_{1/2}$  which are quoted in the JPL catalog. The results of the calculations are presented in Tables (A.I) and (A.II) for the  $^{79}\text{BrO}$  and  $^{81}\text{BrO}$  isotopic

Table A.I. Partition function for  $^{79}\text{BrO}$ 

$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$	$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$
150	1965.33	0.184	1.001	1967.42	236	3085.08	8.501	1.0123	3131.63
151	1978.34	0.197	1.001	1980.55	237	3098.1	8.752	1.0125	3145.8
152	1991.36	0.21	1.0011	1993.69	238	3111.13	9.008	1.0128	3159.98
153	2004.38	0.225	1.0011	2006.83	239	3124.15	9.27	1.013	3174.19
154	2017.39	0.24	1.0012	2019.98	240	3137.18	9.538	1.0133	3188.42
155	2030.41	0.256	1.0012	2033.13	241	3150.21	9.811	1.0135	3202.66
156	2043.42	0.273	1.0013	2046.29	242	3163.23	10.089	1.0137	3216.93
157	2056.44	0.291	1.0013	2059.45	243	3176.26	10.374	1.014	3231.21
158	2069.45	0.31	1.0014	2072.62	244	3189.28	10.664	1.0142	3245.52
159	2082.47	0.329	1.0014	2085.79	245	3202.31	10.96	1.0145	3259.85
160	2095.49	0.35	1.0015	2098.98	246	3215.34	11.261	1.0148	3274.2
161	2108.5	0.372	1.0016	2112.16	247	3228.36	11.569	1.015	3288.57
162	2121.52	0.395	1.0016	2125.36	248	3241.39	11.883	1.0153	3302.96
163	2134.54	0.418	1.0017	2138.56	249	3254.42	12.203	1.0155	3317.37
164	2147.55	0.444	1.0018	2151.77	250	3267.44	12.529	1.0158	3331.8
165	2160.57	0.47	1.0018	2164.98	251	3280.47	12.861	1.0161	3346.26
166	2173.59	0.497	1.0019	2178.21	252	3293.5	13.2	1.0163	3360.73
167	2186.6	0.526	1.002	2191.44	253	3306.53	13.545	1.0166	3375.23
168	2199.62	0.556	1.002	2204.67	254	3319.55	13.896	1.0169	3389.75
169	2212.64	0.588	1.0021	2217.92	255	3332.58	14.254	1.0172	3404.29
170	2225.66	0.62	1.0022	2231.17	256	3345.61	14.618	1.0174	3418.86
171	2238.67	0.655	1.0023	2244.43	257	3358.64	14.989	1.0177	3433.45
172	2251.69	0.69	1.0024	2257.7	258	3371.66	15.366	1.018	3448.06
173	2264.71	0.728	1.0024	2270.97	259	3384.69	15.751	1.0183	3462.69
174	2277.73	0.766	1.0025	2284.26	260	3397.72	16.142	1.0186	3477.35
175	2290.75	0.807	1.0026	2297.55	261	3410.75	16.54	1.0189	3492.03
176	2303.76	0.849	1.0027	2310.86	262	3423.78	16.944	1.0192	3506.73
177	2316.78	0.893	1.0028	2324.17	263	3436.81	17.356	1.0195	3521.46
178	2329.8	0.938	1.0029	2337.49	264	3449.84	17.775	1.0198	3536.21
179	2342.82	0.986	1.003	2350.82	265	3462.86	18.201	1.0201	3550.98
180	2355.84	1.035	1.0031	2364.16	266	3475.89	18.634	1.0204	3565.78
181	2368.86	1.086	1.0032	2377.51	267	3488.92	19.074	1.0207	3580.6
182	2381.88	1.139	1.0033	2390.87	268	3501.95	19.522	1.021	3595.45
183	2394.9	1.195	1.0034	2404.23	269	3514.98	19.976	1.0213	3610.32
184	2407.91	1.252	1.0035	2417.61	270	3528.01	20.439	1.0216	3625.21
185	2420.93	1.311	1.0036	2431	271	3541.04	20.908	1.0219	3640.13
186	2433.95	1.373	1.0037	2444.4	272	3554.07	21.385	1.0223	3655.07
187	2446.97	1.436	1.0038	2457.81	273	3567.1	21.87	1.0226	3670.04
188	2459.99	1.502	1.004	2471.23	274	3580.13	22.363	1.0229	3685.04
189	2473.01	1.571	1.0041	2484.67	275	3593.16	22.863	1.0232	3700.06
190	2486.03	1.641	1.0042	2498.11	276	3606.19	23.371	1.0236	3715.1
191	2499.05	1.714	1.0043	2511.56	277	3619.22	23.886	1.0239	3730.17

(Continued on next page)

Table A.1. (Continued)

$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$	$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$
192	2512.07	1.79	1.0044	2525.03	278	3632.25	24.41	1.0242	3745.27
193	2525.09	1.868	1.0046	2538.51	279	3645.28	24.941	1.0246	3760.39
194	2538.11	1.949	1.0047	2552	280	3658.31	25.48	1.0249	3775.54
195	2551.13	2.033	1.0048	2565.5	281	3671.34	26.028	1.0252	3790.71
196	2564.15	2.119	1.005	2579.01	282	3684.37	26.583	1.0256	3805.91
197	2577.17	2.208	1.0051	2592.54	283	3697.4	27.147	1.0259	3821.13
198	2590.2	2.3	1.0052	2606.08	284	3710.43	27.719	1.0263	3836.39
199	2603.22	2.394	1.0054	2619.63	285	3723.46	28.299	1.0266	3851.67
200	2616.24	2.492	1.0055	2633.2	286	3736.49	28.887	1.027	3866.97
201	2629.26	2.593	1.0057	2646.77	287	3749.53	29.484	1.0273	3882.3
202	2642.28	2.696	1.0058	2660.36	288	3762.56	30.089	1.0277	3897.66
203	2655.3	2.803	1.006	2673.97	289	3775.59	30.703	1.028	3913.05
204	2668.32	2.913	1.0061	2687.59	290	3788.62	31.325	1.0284	3928.46
205	2681.35	3.027	1.0063	2701.22	291	3801.65	31.956	1.0288	3943.9
206	2694.37	3.143	1.0064	2714.87	292	3814.68	32.595	1.0291	3959.37
207	2707.39	3.263	1.0066	2728.53	293	3827.72	33.244	1.0295	3974.87
208	2720.41	3.387	1.0068	2742.2	294	3840.75	33.9	1.0299	3990.39
209	2733.43	3.514	1.0069	2755.89	295	3853.78	34.566	1.0302	4005.94
210	2746.46	3.645	1.0071	2769.59	296	3866.81	35.241	1.0306	4021.52
211	2759.48	3.779	1.0073	2783.31	297	3879.84	35.924	1.031	4037.13
212	2772.5	3.917	1.0074	2797.05	298	3892.88	36.616	1.0314	4052.77
213	2785.52	4.058	1.0076	2810.8	299	3905.91	37.318	1.0318	4068.43
214	2798.55	4.204	1.0078	2824.56	300	3918.94	38.028	1.0321	4084.13
215	2811.57	4.353	1.008	2838.34	301	3931.98	38.747	1.0325	4099.85
216	2824.59	4.506	1.0081	2852.14	302	3945.01	39.476	1.0329	4115.6
217	2837.61	4.664	1.0083	2865.95	303	3958.04	40.214	1.0333	4131.38
218	2850.64	4.825	1.0085	2879.78	304	3971.08	40.961	1.0337	4147.18
219	2863.66	4.991	1.0087	2893.62	305	3984.11	41.717	1.0341	4163.02
220	2876.68	5.16	1.0089	2907.48	306	3997.14	42.483	1.0345	4178.89
221	2889.71	5.334	1.0091	2921.36	307	4010.18	43.258	1.0349	4194.78
222	2902.73	5.513	1.0093	2935.25	308	4023.21	44.043	1.0353	4210.71
223	2915.76	5.695	1.0095	2949.16	309	4036.24	44.836	1.0357	4226.66
224	2928.78	5.883	1.0097	2963.09	310	4049.28	45.64	1.0361	4242.65
225	2941.8	6.074	1.0099	2977.04	311	4062.31	46.453	1.0365	4258.66
226	2954.83	6.271	1.0101	2991	312	4075.34	47.276	1.0369	4274.71
227	2967.85	6.472	1.0103	3004.98	313	4088.38	48.108	1.0373	4290.78
228	2980.88	6.677	1.0105	3018.98	314	4101.41	48.95	1.0377	4306.89
229	2993.9	6.888	1.0107	3033	315	4114.45	49.802	1.0381	4323.02
230	3006.93	7.103	1.0109	3047.03	316	4127.48	50.664	1.0385	4339.19
231	3019.95	7.323	1.0112	3061.08	317	4140.52	51.535	1.039	4355.38
232	3032.98	7.549	1.0114	3075.16	318	4153.55	52.417	1.0394	4371.61
233	3046	7.779	1.0116	3089.25	319	4166.59	53.308	1.0398	4387.86
234	3059.03	8.014	1.0118	3103.35	320	4179.62	54.209	1.0402	4404.15
235	3072.05	8.255	1.0121	3117.48	321	4192.66	55.121	1.0407	4420.47

Table A.II. Partition function for  $^{81}\text{BrO}$ 

$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$	$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$
150	1973.4	0.18	1.001	1975.5	236	3097.82	8.53	1.0123	3144.56
151	1986.47	0.2	1.001	1988.69	237	3110.9	8.79	1.0125	3158.79
152	1999.54	0.21	1.0011	2001.88	238	3123.98	9.04	1.0128	3173.04
153	2012.61	0.23	1.0011	2015.08	239	3137.06	9.31	1.013	3187.3
154	2025.68	0.24	1.0012	2028.28	240	3150.14	9.58	1.0133	3201.59
155	2038.75	0.26	1.0012	2041.48	241	3163.22	9.85	1.0135	3215.89
156	2051.82	0.27	1.0013	2054.7	242	3176.3	10.13	1.0137	3230.22
157	2064.89	0.29	1.0013	2067.92	243	3189.38	10.42	1.014	3244.56
158	2077.96	0.31	1.0014	2081.14	244	3202.46	10.71	1.0142	3258.93
159	2091.03	0.33	1.0014	2094.37	245	3215.54	11	1.0145	3273.32
160	2104.1	0.35	1.0015	2107.61	246	3228.62	11.31	1.0148	3287.72
161	2117.17	0.37	1.0016	2120.85	247	3241.7	11.62	1.015	3302.15
162	2130.25	0.4	1.0016	2134.1	248	3254.78	11.93	1.0153	3316.6
163	2143.32	0.42	1.0017	2147.36	249	3267.87	12.25	1.0155	3331.07
164	2156.39	0.45	1.0018	2160.62	250	3280.95	12.58	1.0158	3345.57
165	2169.46	0.47	1.0018	2173.89	251	3294.03	12.91	1.0161	3360.08
166	2182.53	0.5	1.0019	2187.17	252	3307.11	13.25	1.0163	3374.62
167	2195.6	0.53	1.002	2200.45	253	3320.19	13.6	1.0166	3389.18
168	2208.67	0.56	1.002	2213.74	254	3333.27	13.95	1.0169	3403.76
169	2221.74	0.59	1.0021	2227.04	255	3346.36	14.31	1.0172	3418.36
170	2234.82	0.62	1.0022	2240.35	256	3359.44	14.68	1.0174	3432.99
171	2247.89	0.66	1.0023	2253.67	257	3372.52	15.05	1.0177	3447.64
172	2260.96	0.69	1.0024	2266.99	258	3385.6	15.43	1.018	3462.31
173	2274.03	0.73	1.0024	2280.32	259	3398.68	15.81	1.0183	3477
174	2287.1	0.77	1.0025	2293.66	260	3411.77	16.21	1.0186	3491.72
175	2300.18	0.81	1.0026	2307.01	261	3424.85	16.61	1.0189	3506.46
176	2313.25	0.85	1.0027	2320.37	262	3437.93	17.01	1.0192	3521.23
177	2326.32	0.9	1.0028	2333.74	263	3451.02	17.43	1.0195	3536.01
178	2339.39	0.94	1.0029	2347.11	264	3464.1	17.85	1.0198	3550.83
179	2352.47	0.99	1.003	2360.5	265	3477.18	18.27	1.0201	3565.66
180	2365.54	1.04	1.0031	2373.89	266	3490.27	18.71	1.0204	3580.52
181	2378.61	1.09	1.0032	2387.3	267	3503.35	19.15	1.0207	3595.4
182	2391.69	1.14	1.0033	2400.71	268	3516.43	19.6	1.021	3610.31
183	2404.76	1.2	1.0034	2414.14	269	3529.52	20.06	1.0213	3625.24
184	2417.83	1.26	1.0035	2427.57	270	3542.6	20.52	1.0216	3640.2
185	2430.91	1.32	1.0036	2441.02	271	3555.68	20.99	1.0219	3655.18
186	2443.98	1.38	1.0037	2454.47	272	3568.77	21.47	1.0223	3670.19
187	2457.05	1.44	1.0038	2467.94	273	3581.85	21.96	1.0226	3685.22
188	2470.13	1.51	1.004	2481.42	274	3594.94	22.45	1.0229	3700.28
189	2483.2	1.58	1.0041	2494.9	275	3608.02	22.96	1.0232	3715.36
190	2496.28	1.65	1.0042	2508.4	276	3621.1	23.47	1.0236	3730.47
191	2509.35	1.72	1.0043	2521.91	277	3634.19	23.98	1.0239	3745.6
192	2522.43	1.8	1.0044	2535.44	278	3647.27	24.51	1.0242	3760.76

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Table A.II. (Continued)

$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$	$T(K)$	$Z_{\text{Rot}}^{3/2}(T)$	$Z_{\text{Rot}}^{1/2}(T)$	$Z_{\text{Vib}}(T)$	$Z_{\text{Tot}}(T)$
193	2535.5	1.88	1.0046	2548.97	279	3660.36	25.04	1.0246	3775.94
194	2548.57	1.96	1.0047	2562.52	280	3673.44	25.58	1.0249	3791.15
195	2561.65	2.04	1.0048	2576.07	281	3686.53	26.13	1.0252	3806.39
196	2574.72	2.13	1.005	2589.64	282	3699.61	26.69	1.0256	3821.65
197	2587.8	2.22	1.0051	2603.23	283	3712.7	27.26	1.0259	3836.94
198	2600.87	2.31	1.0052	2616.82	284	3725.78	27.83	1.0263	3852.26
199	2613.95	2.4	1.0054	2630.43	285	3738.87	28.41	1.0266	3867.6
200	2627.03	2.5	1.0055	2644.05	286	3751.96	29	1.027	3882.97
201	2640.1	2.6	1.0057	2657.69	287	3765.04	29.6	1.0273	3898.37
202	2653.18	2.71	1.0058	2671.33	288	3778.13	30.21	1.0277	3913.79
203	2666.25	2.81	1.006	2685	289	3791.21	30.83	1.028	3929.24
204	2679.33	2.93	1.0061	2698.67	290	3804.3	31.45	1.0284	3944.72
205	2692.4	3.04	1.0063	2712.36	291	3817.39	32.09	1.0288	3960.22
206	2705.48	3.16	1.0064	2726.06	292	3830.47	32.73	1.0291	3975.76
207	2718.56	3.28	1.0066	2739.78	293	3843.56	33.38	1.0295	3991.32
208	2731.63	3.4	1.0068	2753.51	294	3856.64	34.04	1.0299	4006.91
209	2744.71	3.53	1.0069	2767.26	295	3869.73	34.71	1.0302	4022.52
210	2757.79	3.66	1.0071	2781.02	296	3882.82	35.38	1.0306	4038.17
211	2770.86	3.79	1.0073	2794.79	297	3895.91	36.07	1.031	4053.84
212	2783.94	3.93	1.0074	2808.59	298	3908.99	36.77	1.0314	4069.54
213	2797.02	4.07	1.0076	2822.39	299	3922.08	37.47	1.0318	4085.27
214	2810.09	4.22	1.0078	2836.21	300	3935.17	38.18	1.0321	4101.03
215	2823.17	4.37	1.008	2850.05	301	3948.25	38.91	1.0325	4116.82
216	2836.25	4.52	1.0081	2863.91	302	3961.34	39.64	1.0329	4132.63
217	2849.33	4.68	1.0083	2877.77	303	3974.43	40.38	1.0333	4148.48
218	2862.4	4.84	1.0085	2891.66	304	3987.52	41.13	1.0337	4164.35
219	2875.48	5.01	1.0087	2905.56	305	4000.61	41.89	1.0341	4180.26
220	2888.56	5.18	1.0089	2919.48	306	4013.69	42.66	1.0345	4196.19
221	2901.64	5.36	1.0091	2933.42	307	4026.78	43.43	1.0349	4212.15
222	2914.71	5.53	1.0093	2947.37	308	4039.87	44.22	1.0353	4228.14
223	2927.79	5.72	1.0095	2961.34	309	4052.96	45.02	1.0357	4244.16
224	2940.87	5.91	1.0097	2975.32	310	4066.05	45.83	1.0361	4260.22
225	2953.95	6.1	1.0099	2989.33	311	4079.13	46.64	1.0365	4276.3
226	2967.03	6.3	1.0101	3003.35	312	4092.22	47.47	1.0369	4292.41
227	2980.11	6.5	1.0103	3017.39	313	4105.31	48.3	1.0373	4308.55
228	2993.18	6.7	1.0105	3031.44	314	4118.4	49.15	1.0377	4324.72
229	3006.26	6.92	1.0107	3045.52	315	4131.49	50	1.0381	4340.92
230	3019.34	7.13	1.0109	3059.61	316	4144.58	50.87	1.0385	4357.16
231	3032.42	7.35	1.0112	3073.72	317	4157.67	51.75	1.039	4373.42
232	3045.5	7.58	1.0114	3087.85	318	4170.76	52.63	1.0394	4389.71
233	3058.58	7.81	1.0116	3102	319	4183.85	53.53	1.0398	4406.04
234	3071.66	8.05	1.0118	3116.17	320	4196.94	54.43	1.0402	4422.39
235	3084.74	8.29	1.0121	3130.36					

species respectively. In these Tables are detailed the rotational contribution due to the  $X_1^2\Pi_{3/2}$  and  $X_1^2\Pi_{1/2}$  spin components ( $Z_{\text{Rot}}^{3/2}(T)$  and  $Z_{\text{Rot}}^{1/2}(T)$ , respectively) the vibrational contribution  $Z_{\text{Vib}}(T)$  together with the final result  $Z_{\text{Tot}}(T)$ .

## Notes

<sup>1</sup> In the following, each molecule is identified by a number which is actually the molecule code number used in HITRAN. The exception is BrO which is absent in HITRAN and for which the number 40 was associated.

<sup>2</sup> It is worth stressing that for oxygen the broadening coefficients given in the MASTER database are the N<sub>2</sub>- and O<sub>2</sub>-broadening coefficients and *not* the air and self broadening coefficients which are given for all other molecular species.

<sup>3</sup> In Equation (8) the decimals, which have no real physical meaning are given in order to reproduce the list of line broadening coefficients quoted in MASTER.

<sup>4</sup> The <sup>79</sup>BrO and <sup>81</sup>BrO partition functions for the 150–320 K temperatures range have been deposited as supplementary material at the Journal library.

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