

Infrared spectroscopic line lists

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This document contains a listing of all the atomic and molecular spectroscopic data as used in Decin (2000). A summary of all the spectroscopic line lists is given in Sect. 1 – 6, while a comparison between some line lists is made in Sect. 7. This document should be referred to as “Decin, L., 2000, PhD thesis ‘Synthetic spectra of cool stars observed with the Short-Wavelength Spectrometer: improving the models and the calibration of the instrument’, University of Leuven”.

1 Atomic data

1. Hirata and Horaguchi (1995):

This compilation is aimed at providing a general catalog of atomic lines for comparatively low-ionized species in the wavelength range from 1.4 to 10000 nm. All ionization stages for atoms with atomic number $Z \leq 8$ are given, ionization stage I to VI for $Z = 9 - 30$, I to II or V for $Z = 31 - 92$. The total number of lines is 629771. The database lists the wavelength in nm (vacuum wavelength below and air wavelength above 200 nm), the oscillator strength, the quality of the oscillator strength, the laboratory intensity, the lower and upper energy level (cm^{-1}), the lower and upper term. The catalog can be queried from: <http://vizier.u-strasbg.fr/cgi-bin/VizieR?-source=VI/69>.

2. Reader et al. (1980):

This catalog contains wavelength information for 99 different atomic species in the wavelength range from 40 to 40000 Å. The wavelength in Å, relative intensity, chemical element and ionization stage for about 46610 spectral lines of neutral to quadruply ionized atoms are tabulated. The catalog can be queried from: <http://vizier.u-strasbg.fr/cgi-bin/VizieR?-source=VI/16>.

3. Fuhr et al. (1988a,b):

Atomic transition probabilities for scandium ($Z = 21$) through nickel ($Z=28$) for about 18300 spectral lines are critically compiled, based on all available literature sources at that moment. The atomic element, stage of ionization, transition type (allowed or forbidden), lower and upper energy level configuration, lower and upper energy level term, the statistical weight g for the lower and upper level and the oscillator strength are tabulated. The catalog can be queried from: <http://vizier.u-strasbg.fr/cgi-bin/VizieR?-source=VI/72>

4. NIST Atomic Spectra Database:

The Atomic Spectra Database (ASD) contains data for radiative transitions and energy levels in atoms and atomic ions. Data are included for observed transitions of 99 elements and energy levels of 52 elements. ASD contains data on about 900 spectra from about 1 Å to 200 μm , with about 70000 energy levels and 91000 lines, 40000 of which have transition probabilities listed. The most current NIST-evaluated data associated with each transition are integrated under a single listing.

Energy level data are included for most spectra of H - Kr ($Z = 1 - 36$), Mo ($Z = 42$), plus up to the first five spectra of the lanthanide rare earths ($Z = 57 - 71$). Classified lines with transition probabilities are included for most spectra of H - Ni ($Z = 1 - 28$), including new extensive transition probabilities for C, N, and O; output for these can be ordered by either multiplet (for a given spectrum) or wavelength. Also, prominent lines (unclassified) with wavelengths and relative intensities are included for up to the first five spectra of H - Es ($Z = 1 - 99$). Some transition probabilities are listed for selected lines of Cu - Es ($Z = 29 - 99$). Comprehensive wavelength lists of observed lines with relative intensities are incorporated for all spectra of Mg, Al, S, Sc, plus Be I, O II, and Ne I. The NIST compilation is limited as far as the number of lines is concerned, but the collected data is critically compiled.

The NIST Atomic Spectra Database can be queried from:
http://physics.nist.gov/cgi-bin/AtData/main_asd.

5. Atomic spectral line database by Kurucz and Bell (1995):

The atomic spectral line database at <http://www.pmp.uni-hannover.de/projekte/kurucz/sekur.html> is built from CD-ROM 23 of Kurucz and Bell (1995). This line list is a replacement for the Kurucz-Peytremann line list. The database contains all 534910 lines of the file 'gfall.dat' with the following items for each line: wavelength (nm); $\log gf$; element code; lower level: energy in cm^{-1} , J , configuration; upper level: energy in cm^{-1} , J , configuration; the damping constants for the radiation damping, Stark broadening and van der Waals broadening and the reference code. The original line database at CD-ROM 23 of Kurucz and Bell (1995) is, however, not complete. There are no references after 1988. For light elements there are no references after 1979. One new development was the inclusion of hyperfine splitting for the iron group elements using hyperfine data from the literature through 1993. The data are very incomplete. Data for isotopic splitting were not yet included. These atomic data are of variable quality, especially the calculated gf -values can be much in error.

6. Infrared atomic line list by van Hoof (1998):

The infrared atomic line list of van Hoof (1998) is a compilation of approximately 136000 allowed and forbidden atomic transitions with wavelengths in the range from 1 to 1000 μm . Its primary intention is to allow the identification of observed infrared absorption or emission features. The wavelengths in this list are all calculated from the difference between the energy of the upper and lower level of the transition. No attempt has been made to include observed wavelengths. Almost all of the atomic energy level data has been taken from the Atomic Spectroscopic database provided by the National Institute of Standards and Technology (NIST). One may obtain parts of the line list at <http://www.pa.uky.edu/~peter/atomic/>, containing the wavelength in μm , the transition type, the electronic configuration of the lower and upper level, the spectroscopic term of the lower and upper level, the quantum number J for the lower and upper level and the energy of the lower and upper level in cm^{-1} .

7. Vienna Atomic Line Database: VALD

The Vienna Atomic Line Database (VALD) (Piskunov et al., 1995; Ryabchikova et al., 1997; Kupka et al., 1999) is a collection of atomic line parameters of astronomical interest and pro-

vides tools for selecting subsets of lines for typical astrophysical applications: line identification, chemical composition and radial velocity measurements, model atmosphere calculations etc. Lot of line parameters may be found, such as the element and ionization stage, central wavelength in Å, excitation in eV, $\log(gf)$, three damping constants (radiative, quadratic Stark and van der Waals) in logarithm per second and per perturber at 10000 K (in the case of Stark and van der Waals constants), and the mean Lande factor. A reference label to the used catalog is also given. Links to the WWW interfaces of VALD (at both Vienna and Uppsala) can be found at <http://www.astro.univie.ac.at/~vald/> and <http://www.astro.uu.se/~vald/>.

2 Molecular data

1. CO line list by [Goorvitch and Chackerian \(1994\)](#):

A complete line list with improved accuracy for all the rotation-vibration transitions of the fundamental, first and second overtone bands up to $v = 20$ and $J = 149$ of the ground state $X^1\Sigma^+$ of the seven CO isotopes - $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{18}\text{O}$, $^{14}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{17}\text{O}$ - is made available to the astronomical community. A line list of the pure rotational transitions up to $v = 5$ and $J = 60$ is also made available for these seven isotopes. This line list contains the transition frequency (cm^{-1}), the lower state energy in cm^{-1} , the Einstein A -value in s^{-1} , the gf -value, the transition strength in cm mol^{-1} at 3000 K or 1000 K for the pure rotational transitions, the expectation value of the effective dipole moment operator in Debye², the upper and lower state vibrational quantum number (v' and v''), the transition type (R or P), the lower state angular momentum number (J'') and the isotopic designation. Each overtone band for each isotope consists of 6279 lines. A line list containing 2562 lines is available for the pure rotational transitions. This line list is available using an anonymous ftp transfer from <ftp.aas.org>, in computer-readable form on the AAS CD-ROM Series, Vol. 3 or by sending an e-mail to the internet address co@cma.arc.nasa.gov.

2. SiO line list by [Langhoff and Bauschlicher \(1993\)](#):

[Langhoff and Bauschlicher \(1993\)](#) have computed an accurate electric dipole moment function for the SiO molecule which not only reproduces accurate dipole moments, but also line strengths for vibrational-rotational transitions within the ground-state manifold. The resulting line list contains 22301 lines for ^{28}SiO , 22375 lines for ^{29}SiO and 22456 lines for ^{30}SiO in the wavelength range of our research (2.38 – 12.0 μm). J_{max} is very high (250), but v_{max} is limited to 15.

3. SiO line list by [Drira et al. \(1997\)](#):

Spectroscopic properties of SiO have been calculated from highly correlated wave functions. The computed dipole moments for $v = 0 - 3$ agree well with experimental data. Only ^{28}SiO is considered here, with J_{max} limited to 100 and v_{max} to 40. For each transition, the upper and lower state vibrational quantum number (v' and v''), the upper and lower state angular momentum quantum number (J' and J''), the wavenumber in cm^{-1} , the transition probability R (in Debye), the Einstein A coefficient in s^{-1} and the absorption ($= f \cdot S_J/g''$, with g'' the statistical weight or degeneracy for the lower state) are given. They estimate that the resulting

theoretical line strengths should be accurate to 20 % for the fundamental band. Infrared data are available at the Centre de Données de Strasbourg (<http://cdsarc.u-strasbg.fr/>).

4. **SiO linelist by Tipping and Chackerian (1981):**

Tipping and Chackerian (1981) reported transition probabilities for a large number of transitions based on a dipole moment which was chosen to reproduce the accurate experimental dipole moments for $v = 0 - 3$, to have the proper united and separated atom limits, and to have the correct long-range dependence on internuclear separation. They suggested that the accuracy of their results is approximately 10 %.

5. **CN line list by Plez (*priv. comm.*)**

This CN line list of Plez was prepared in the same way as his TiO line list (Plez, 1998). In the absence of an up-to-date line list for the violet system, he has compiled one using the available molecular constants (Prasad et al., 1992; Prasad and Bernath, 1992; Rehfuß et al., 1992; Kotlar et al., 1980; Ito et al., 1988). The red system was also recomputed to try to remedy unexplained discrepancies of the gf -values of Jørgensen and Larsson (1990). The line positions were calculated using molecular constants for all isotopic combinations of C and N. The gf -values for both systems were computed using the transition moments of Bauschlicher et al. (1988). Following Costes et al. (1990), the dissociation energy adopted for CN is 7.76 eV.

6. **OH database by Schwenke:**

The OH data bank of Schwenke contains 38068 ^{16}OH lines (main and satellite branches). The isotope code, transition frequency (in cm^{-1}), gf -value, square of dipole matrix element in Debye², initial state energy (in cm^{-1}) and final and initial state total angular momentum quantum number are given. The energy levels and wave functions are determined from calculations including the X and A states. The dipole moment is from the ab initio calculations of Langhoff and Bauschlicher (1989). The agreement with experimental energy levels is not very good. The gf -values may be too large by a factor of two.

The database may be obtained at

<http://george.arc.nasa.gov/~dschwenke>.

7. **OH line list by Goldman et al. (1998):**

New spectral line parameters have been generated for the OH $X^2\Pi-X^2\Pi$ transitions for $\Delta v = 0, \dots, 6$, with $v' = 0, \dots, 10$ and $J_{\text{max}} = 49.5$. Hitran type line parameter sets with low intensity cut-offs are provided at 296 K and 6000 K. Recent improvements in line intensities and line positions have been incorporated into the calculations. The absolute intensities and line positions of the high v , high J transitions are expected to have large uncertainties. The EDMF (Electric Dipole Moment Function) of Nelson et al. (1990) is used.

8. **H₂O line list by Partridge and Schwenke (1997):**

Partridge and Schwenke (1997) reported on the determination of a high quality ab initio potential energy surface and dipole moment function for water. Comparison with the observed H₂O lines in Hitran indicates that about 3 % of the tabulated line positions appear to be incorrect (more than 0.1 cm^{-1} inaccuracy). The intensities summed over vibrational bands are usually in good agreement between the calculations and the tabulated results, but individual

line strengths can differ greatly. A high-temperature list consisting of nearly 400 million lines is generated for H_2^{16}O , with J up to 55. The line frequency (in cm^{-1}), energy level and line strength are tabulated. So far, this line list is the most complete H_2O line list.

The database may be obtained at
<http://george.arc.nasa.gov/~dschwenke>.

9. **H_2O line list by Viti et al. (1997):**

This H_2O line list of transition frequencies and intensities greatly has improved the accuracy of the energy levels and the transition frequencies over existing hot water line lists. Although it does not cover many high vibrational states of the molecule, it does include all the rotational levels up to $J = 38$. In total, 230000 lines in the wavelength range from 0 to 903 cm^{-1} are given. The accuracy of the line list should be enough to assign laboratory line transitions at high temperature and to provide water transitions that could be observed in other hot molecular environments including magnetohydrodynamic shocks, circumstellar outflows and active galactic nuclei. This line list is however not sufficient for modeling cool star atmospheres: the weak transitions of the - not included - higher vibrational states will still make an important contribution to the opacity.

10. **Line lists by Sauval (*priv. comm.*):**

Several line databases compiled by J. Sauval were used for this research. Each of them contains the same quantities: for each line the wavenumber (cm^{-1}), the excitation energy (cm^{-1}), the individual oscillator strength f , the dimensionless Hönl-London factor S_J (also called the rotational intensity factor or rotational line strength) and the molecular line designation are given.

The OH line database (Mélen et al., 1995) includes about 2610 lines (main branches) in the spectral range $800\text{--}4200 \text{ cm}^{-1}$, with 300 pure rotation lines (0-0, 1-1, 2-2, 3-3, 4-4) and 2310 vibration-rotation lines (1-0, 2-2, 3-2, 4-3 bands for the P, R and Q branch; 5-4 band for the P branch; 2-0, 3-1, 4-2 bands for the P, R and Q branch; 5-3 band for the P branch). The line positions are very accurate. Due to the fact that there was a lack of theoretical transition moments for all individual lines based on the same electric dipole moment function (EDMF), the individual line oscillator strengths were taken from Langhoff et al. (1989); Werner et al. (1983); Turnbull and Lowe (1988) besides Nelson et al. (1990). The last result was finally adopted for most of the branches/bands due to a better fit with the solar P line intensities. Although OH is a diatomic molecule, it is difficult to calculate the oscillator strength due to strong well-known vibration-rotation interactions. For R-branches the dependence $f(J)$ is rather strange, a rapid decrease which is followed by a strong increase up to high J -values. For Q-branches, there is always a strong decrease of S_J with J , which means that only low J -values are present.

In the framework of this research, J. Sauval has prepared two NO databases. The first one includes the most intense lines of the fundamental bands (~ 6400 lines) with calculated gf -values from Hitran (Rothman et al., 1998). A selection is made from the 15154 lines listed by Hitran (13776 lines belong to the most abundant species $^{14}\text{N}^{16}\text{O}$ and 1378 lines belong to other less abundant isotopic species). Out of these 13776 lines, there are 42 pure rotation lines, 10658 vibration-rotation lines of the fundamental bands and 2496 vibration-rotation lines of

the first-overtone bands. Since the Hönl-London factor is not included in the Hitran database, this factor has to be included for each line adopting different normalization for specific lines. The gf -values calculated from the transition moments listed by Hitran are generally higher than these based on other intensity data. A systematic error by a factor 2 or 3 in the gf -values for any NO line is not impossible due to the absence of detailed information about the adopted normalization of Hitran. A second NO database was based on the intensity data of Goldman (1998, *priv. comm.*), which was generated at $T = 3000$ K. The conversion to gf -values - with appropriate normalization - resulted in a database of 23808 lines in the wavelength range from 800-2400 cm^{-1} , with $J_{\text{max}} = 125$ and including the 1-0 up to 14-13 bands. This database should be more accurate than the one based on Hitran.

The CH data bank (Mélen et al., 1989) has about 1900 lines containing pure rotation lines (0-0, 1-1, 2-2, 3-3, 4-4) and vibration-rotation lines of the fundamental bands (1-0, 2-1, 3-2, 4-3 bands for the R, P and Q branch). The EDMF was based on Follmeg et al. (1987).

The NH database (Grevesse et al., 1990; Geller et al., 1991) includes 892 vibration-rotation lines of the 1-0, 2-1, 3-2, 4-3 and 5-4 bands (R and P branches) and 553 pure rotation lines for $v = 0, 1, 2, 3, 4$ and 5. The term values were derived from analytical expressions given by Boudjaadar et al. (1986). The EDMF for the pure rotation lines was taken from Meyer and Rosmus (1975) and for the vibration-rotation lines from Bauschlicher and Langhoff (1987) and Chackerian et al. (1989).

The HF database contains about 1000 lines: 710 vibration-rotation lines of the 1-0 up to 9-8 bands and 280 pure rotation lines of the 0-0 up to 7-7 bands. Line positions are very accurate and the - at that moment - best available intensity values were adopted. The positions were based on Le Roy (1999) and the EDMF on Ogilvie et al. (1980) and Arunan et al. (1992).

About 250 Fe I high-excitation lines (5g-6h transitions around 1350 cm^{-1} , 4f-5g transitions around 2565 cm^{-1} and 4f-6g transitions around 3900 cm^{-1}) are included as well (Johansson et al., 1994; Schoenfeld et al., 1995). Two additional columns, which give calculated values to be adopted for the Stark broadening, are added. Broadening due to collisions with electrons is computed with the formalism developed by Chang and Schoenfeld (1991).

The HCl data bank has 550 vibration-rotation lines of the 1-0 up to 7-6 bands and 180 pure rotation lines of the 0-0 up to 5-5 bands. The positions were taken from Rank et al. (1965) and the EDMF was based on Arunan et al. (1992); Ogilvie et al. (1980); Tipping and Ogilvie (1982).

11. Scan database:

The scan database (Jørgensen, 1994a) contains 70 million molecular lines from CN (Jørgensen and Larsson, 1990), TiO (Jørgensen, 1994b), CH (Jørgensen et al., 1996), HCN (Jørgensen, 1990), C_2H_2 (Eriksson et al., 1984), C_3 (Jørgensen et al., 1989) and H_2O (Jørgensen and Jensen, 1993).. The identification of the electronic transition, the vibrational quantum numbers v' and v'' at the upper and lower vibrational level respectively, the rotational quantum number J'' of the lower level, the branch identification, the dimensionless gf -values, the wavenumber in cm^{-1} , the excitation energy above the ground level (in cm^{-1}) and the isotopic shift (in cm^{-1}) are listed. The complete database is available via anonymous ftp to stella.nbi.dk.

The vibrational transitions of the water molecule in its electronic ground state is calculated by [Jørgensen and Jensen \(1993\)](#). They have located 412 vibrational energy levels below 30000 cm^{-1} and have computed the transition moments for all of the 80000 transitions between these states. More than 99 % of the partition function is represented by these computed energy levels for temperatures up to 5000 K. Depending on the threshold level introduced, typically on the order of 10 million rotation-vibration lines could routinely be calculated from the 80000 transition moments.

12. JPL catalog:

The JPL molecular catalog ([Poynter and Pickett, 1985](#)) tabulates the frequency of the lines in MHz, the integrated intensity in units of $\text{nm}^2\text{ MHz}$ at 300K, the degrees of freedom in the rotational partition function, the lower state energy in cm^{-1} relative to the ground state, the upper state degeneracy and the quantum numbers for both upper and lower state. This is given for 323 molecules, resulting in 1906883 entries in total. This catalog is currently available at <http://spec.jpl.nasa.gov>.

3 Atmospheric molecular data

1. Hitran:

A good source for both intensities and frequencies is the high-resolution transmission molecular absorption database, also known as the Hitran database ([Rothman et al., 1987, 1992, 1998](#)). Hitran contains many transitions for 32 molecules and their isotopomers, mostly of atmospheric importance, especially in the lowest vibrational bands. The first edition of the Hitran database contained already 348043 entries between 0 and 17900 cm^{-1} . The information of the database originates from different sources in the literature. The database lists the molecule number, the isotope number, the frequency of the transition in cm^{-1} , the intensity in $\text{cm}^{-1}/(\text{molec} \cdot \text{cm}^{-2})$ at 296 K, the transition probability in Debye squared ($1\text{ Debye} = 10^{-18}\text{ esu cm}$) and often the spectroscopic notation of both upper and lower level. Conversion formulae to the oscillator strength may be found in Helmich (1996). The allowed temperature extrapolation range is 70 to 3000 K, although large errors from the extrapolation may occur near the ends of this range.

2. The SAO molecular database:

This database is maintained at the Smithsonian Astrophysical Observatory for the analysis of atmospheric measurements with the FIRS-2 spectrometer system ([Chance et al., 1994](#)). FIRS-2 currently measures OH, HO₂, H₂O, O, O₂, O₃, HF, HCl, HOCl, ClNO₃, HBr, HOBr, NO₂, N₂O, HNO₃, CO₂, CO and HCN. The SAO database combines the best currently available line parameters from 10 - 800 cm^{-1} , including the Hitran listing, the JPL listing and other available measurements and calculations. The database is available at <http://firs-www.harvard.edu/www/sao92.html>. It lists the molecule number, the isotope number, the wavelength (cm^{-1}), the intensity (cm) at 296 K, the transition probability (Debye^2), the lower state energy and the spectroscopic notation of both upper and lower energy level.

3. Geisa database:

Another large database is GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: [Husson et al., 1992](#)), which involves 40 molecules (86 isotopic species) and

contains 731206 entries, between 0 and 22656 cm^{-1} , of atmospheric interest. The wavenumbers (cm^{-1}), the intensity of the line (cm molec^{-1} at 296 K), the energy of the lower level (cm^{-1}), the transition quantum identifications for the lower and upper levels of the transition, the identification of the isotope and molecule and the transition probability (Debye) are given. Geisa lists individual lines, but its software is specially tailored to atmospheric applications, prohibiting its use in this work. More information may be found at <http://www.ara.polytechnique.fr/geisan.html>.

4 Stellar spectral data

1. Infrared atlas of the Arcturus spectrum, 0.9 - 5.3 microns:

A spectral atlas of the infrared spectrum of the bright K2 giant Arcturus (α Boo) has been completed using the 4m Mayall telescope and the Fourier Transform Spectrometer (FTS) at Kitt Peak (Hinkle et al., 1995). The 0.9 - 5.3 μm spectrum of Arcturus was observed at high signal-to-noise with a resolving power of 100000. They have attempted to identify lines with central depths stronger than a few percent. The atlas is available either on an AAS CD-ROM series Vol. 5 or on hard-copy. The hard-copy is useful for the line identification of the atoms and molecules.

2. High-resolution spectra of ordinary cool stars in the K band:

An atlas of high-resolution ($R \geq 45000$) spectra in the wavelength range from 2.02 to 2.41 μm of twelve representative stars is presented by (Wallace and Hinkle, 1996). The molecular lines of the CO first-overtone, HF fundamental, and several bands of H_2O as well as the CN red system are identified. The atomic features include H, C, Na, Mg, Al, Si, S, Ca, Sc, Ti, V and Fe. Spectra and line lists are available on the AAS CD-ROM series Vol. 7.

3. Atlas of infrared spectra by Ridgway et al. (1984):

This short atlas of infrared spectra for the wavelength range $2400\text{-}2778\text{ cm}^{-1}$ includes K, M, C and S stars. Molecular identifications are given for OH, CH, NH, SiO, CS and HCl. Positions are given for 174 probable atomic lines from the spectra of α Ori and α Tau. Seventy two lines of Na, Mg, Al, Si, K, Ca, Fe, Ti and Cr have been identified in this list.

5 Solar spectral data

1. Infrared spectral atlases of the sun from NOAO:

Wallace et al. (1996) have prepared a series of four solar spectral atlases. The atlases illustrate the disk center photospheric spectrum from 0.7 to 22 μm and the sunspot umbral spectrum from 1.2 to 21 μm . The spectra were observed at high resolution (~ 300000) with the Fourier Transform Spectrometer (FTS) at Kitt Peak. The solar lines have been identified by searching the literature on atomic and molecular laboratory spectroscopy and when necessary by additional laboratory spectroscopy. It was for the first time that H_2O lines have been identified in the spectra of two sunspot umbrae (Wallace et al., 1995). These atlases are available at <ftp.aas.org> or at AAS CD-ROM series, Vol. 7 and are meant to be used in conjunction with the original hard-copy version.

2. **Atomic data bank by Sauval (2000, *priv. comm.*):**

J. Sauval has empirically determined the gf -values for infrared atomic lines from the high-resolution solar ATMOS spectra. Therefore, the computer file generated by Toon (1998, *unpublished results*) was used. This computer file contains a total of 16145 lines and is an updated version (computer file) of the printed 'Table of line identifications' by Geller (1992) (Geller (1995) and Geller (1998, *unpublished results*)). New line identifications of solar lines based on the ATMOS 1994 solar spectra were also performed. This line list is currently still in test-phase.

6 Other databases

1. **Constants for molecules of astrophysical interest in the gas phase: photodissociation, microwave and infrared spectra (Crovisier, 1997):**

This is a compilation of references for molecular data relevant to radio and infrared observations of molecules, radicals and ions of astrophysical interest. It contains 229 species, representing all (or almost all) molecules detected at the present time in the interstellar medium, in comets and in planetary atmospheres (except the Earth), as well as several other molecules, not yet detected, but which are believed to be of astrophysical importance. Isotopic species are not systematically included. This compilation is given without warranty. It has not been cautiously proofread. The compilation is freely available by anonymous ftp to <ftp.obspm.fr/transit/CROVISIER/> molecule. It gives the formula, official designation, other names, electronic state of the ground state and symmetry, photodissociation rates (at the Solar system at 1 AU from the Sun and in the interstellar medium), the fundamental vibrational modes (numbering, symmetry species, fundamental frequency, band strength measured in the laboratory (generally in units of $\text{cm}^{-2} \text{atm}^{-1}$ at STP ($T=273 \text{ K}$, pressure $P=1 \text{ atmosphere}$)), the Einstein A -coefficient of the band, excitation rate (g -factor) of the band by the Sun at 1 AU, mode assignation, references to vibrational data), electronic bands (optional, when such bands occur in the infrared with the frequency cut-off fixed around 10000 cm^{-1}), rotational structure and constants (A , B and C constants, dipolar moments and references to rotational structure) and astrophysical detections. A very useful list, tabulating by increasing band transition wavelength of the different molecules, is also included. A disadvantage is that no individual lines are given.

2. **RadEn database:**

The RadEn database is designed to accumulate published information on radiative and energy parameters of 91 diatomic molecules as well as to analyze it and recommend the more reliable values. It contains information on the potential curves, the dipole moments, the radiative lifetimes, the transition dipole moments, the Franck-Condon factors, the oscillator strengths for the vibrational and vibronic transitions, the Einstein coefficients for the vibrational and vibronic transitions and the vibronic transition strengths. More information may be found at <http://www.chem.msu.su/eng/raden/>.

7 Comparison between some infrared spectroscopic line lists

1. Comparison between the OH line list of Schwenke, [Goldman et al. \(1998\)](#), and Sauval

The line positions in the OH database of Schwenke are good for opacity and low-resolution spectra, but are only moderately accurate for very high-resolution spectra. The spectral region is from 0.00656 to 28363 cm^{-1} . The maximum of the (integral) rotational quantum number N_{max} and the maximum vibrational quantum number v_{max} are respectively 30 and 10, and both the main and satellite branches are given.

The OH line list of [Goldman et al. \(1998\)](#) extend the spectral region from 0.0046 to 19300 cm^{-1} and contains main and satellite branches. The line positions are very accurate even for high-resolution spectra. $N_{\text{max}} = 45$ and $v_{\text{max}} = 10$.

The OH line list of Sauval is limited to the 12 main branches, with $v_{\text{max}} = 4$ and $N_{\text{max}} = 46$ (with a somewhat lower value for the weakest bands). The line positions, based on solar observations, are very accurate.

The differences in $\log gf$ -values for the main branches are small: smaller than 0.01 between [Goldman et al. \(1998\)](#) and Sauval and somewhat larger (< 0.05) between Schwenke and Sauval. For the satellite branches, the differences appear to be generally larger: 0.1 up to about 1 in the worst cases in $\log gf$. This (large) difference occurs even for low-excitation lines, which are important in circumstellar envelopes. The adopted EDMF is responsible for such differences. Generally gf increases with J for main branches, whereas gf tends to decrease with J for satellite branches (with sometimes an increase thereafter). Therefore the intensity of low-excitation circumstellar lines could change from one data file to another. Because Schwenke and [Goldman et al. \(1998\)](#) adopted the same EDMF for the whole database (the one of [Langhoff et al. \(1989\)](#) and [Nelson et al. \(1990\)](#) respectively), their data bank is more consistent than the one of Sauval. The OH line list to recommend is therefore the one of [Goldman et al. \(1998\)](#).

2. Comparison between the SiO line list by [Langhoff and Bauschlicher \(1993\)](#), [Drira et al. \(1997\)](#), and [Tipping and Chackerian \(1981\)](#):

[Langhoff and Bauschlicher \(1993\)](#) have computed an accurate electric dipole moment function for the SiO molecule which not only reproduces accurate dipole moments, but also line strengths for vibrational-rotational transitions within the ground state manifold. This theoretical result differs significantly from the results of [Tipping and Chackerian \(1981\)](#). An extensive theoretical study [Drira et al. \(1997\)](#) and comparisons with observations ([Langhoff and Bauschlicher, 1993](#); [Decin et al., 1997](#); [Tsuji et al., 1994](#)) revealed that the Einstein coefficients based on the results of Tipping and Chackerian are about a factor two larger for the 2-0 overtone band than the currently accepted value. A disadvantage for the SiO line list by [Drira et al. \(1997\)](#) is that only the parameters for ^{28}SiO are calculated. In our research, we therefore have used the SiO line list by [Langhoff and Bauschlicher \(1993\)](#).

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