The Smithsonian Astrophysical Observatory Database SAO92

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ABSTRACT

The Smithsonian Astrophysical Observatory (SAO) maintains a molecular line database (the SAO line database) for the analysis of atmospheric spectra in the far infrared and longer-wave mid infrared, from 10-800 cm^{-1}. This database combines the best currently available line parameters, including the HITRAN[1,2] molecular database, the JPL submillimeter, millimeter, and microwave spectral line catalog[3] (JPLSMM), and other available measurements and calculations. The current version of the database contains 154,895 lines from H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2 (including the $^1\Delta$ state), NO, SO_2, NO_2, NH_3, HNO_3, OH, HF, HCl, HBr, HI, ClO, OCS, H_2CO, HOCl, HCN, H_2O_2, $O(^3P)$, and HO_2. The database is available in both HITRAN-type 80 character (SAO92) and 100 character (SAO92A) formats.

INTRODUCTION

Far infrared techniques have now been successfully used in thermal emission from balloon-borne stratospheric spectrometers to measure atmospheric OH, HO_2, H_2O_2, H_2O (including a number of hot bands and minor isotopic species), $O(^3P)$ atoms (in the mesosphere and thermosphere), O_2, O_3 (including a number of hot bands and minor isotopic species), HCl, HOCl, HF, NO_2, HCN, HNO_3, and a significant upper limit for HBr. The SAO FIRS-2 balloon-borne spectrometer, which is configured to take spectra in the far infrared from 80-210 cm^{-1}, has made measurements of most of these species. FIRS-2 also has a measurement channel in the longer-wave mid infrared from 350-700 cm^{-1}, where CO_2, HNO_3, N_2O, and H_2O have been measured. The analysis of flight spectra obtained with this instrument is the prime motivation for maintaining the SAO database. Our concern has been to perform the best possible quantitative analyses of the flight spectra to obtain atmospheric measurements, including a rigorous consideration of the effects of line parameters and their uncertainties on the analysis. This consideration has led in some cases to laboratory measurements and calculations specifically aimed at the improvement of line parameters in order to support the analysis of flight spectra.[4−10]

Our experience in analyzing flight spectra in the FIRS-2 spectral range has been that the traditional databases, HITRAN and JPLSMM, have often proved inadequate for accurate analysis and that, in any case, it has been necessary to review the original literature in order to assess uncertainties. The SAO database is the natural outcome of this process. It is the result of an ongoing review of published data and the inclusion of more recent laboratory measurements and calculations. As such, the working database is in a continual state of change. The version described here is current as of November, 1993. The SAO database does not include uncertainties in the molecular parameters except for those that are included in transitions taken from HITRAN. In the analysis of FIRS-2 flight spectra, our standard practice is to use molecular parameter uncertainties taken from the original literature whenever possible. Since the effects of line parameter errors are usually systematic, the uncertainties from parameters are usually added to the other uncertainties at the end of retrieval analysis. Thus we do not find it necessary to explicitly include them on the database at this time. A summary of the typical spectroscopic parameter errors for most molecules retrieved by the FIRS-2 instrument, and the resulting effect on the retrievals, is given in Table 1.

Table 1: Summary of SAO92 Line Parameter Uncertainties For Species Measured by FIRS-2

Mol.	ΔStrength (%)	$\Delta\gamma$ (%)	ΔMixing Ratio (%)
H_2O	1-2	10-20	3-10
CO_2	1-2	5-10	5
O_3	1-2	10-20	3-10
N_2O	1	10	8
HNO_3	10	30[a]	10
H_2O_2	2	30[a]	2
HO_2	2	30[a]	3
OH	1	2-10	2-8
O_2	2	10-30	5-30
HCl	1	10	7
HF	1	10	7
HBr	1	30[a]	2
HOCl	2	30[a]	2

[a] pressure broadening coefficients unknown; estimates may be good to 30%. Retrievals are insensitive to these numbers as may be seen from the ΔMixing Ratio column.

Table 2 is a summary of the database, including the sources of parameters for each species. The molecule numbering follows the HITRAN convention for molecules 1-28, with additional molecules defined as 29-36. Number 35 is used as a dummy molecule, for instances where unidentified lines must be added on a temporary basis during the investigation and fitting of spectra. Unless otherwise noted, isotope ratios are adopted from HITRAN. In several cases (notably H_2O and O_3) minor isotopic and hot band lines are assigned separate molecule numbers because of possible changes in isotope ratios as a function of altitude and considerations of non-local thermodynamic equilibrium. As in HITRAN (but not JPLSMM), isotopic abundances are included in the cataloged intensities. Changes in line positions necessitated by observations and fitting of atmospheric spectra are noted in the discussion below. The position changes included to date are by no means exhaustive, but are what have been discovered during the fitting of atmospheric spectra from the SAO FIRS-2 FTS instrument. For some molecules (CO_2, CH_4, SO_2, NH_3, HNO_3, H_2CO, and HO_2) we have implemented intensity cutoffs, indicated in Table 2, in order to control the size of the database. In each case we have carefully chosen the cutoff so that the lines eliminated are at least an order of magnitude smaller in the atmosphere than our current instrument noise limit. This size criterion is based either on SAO stratospheric measurements of the species or (in the cases where we are unable to measure the species, such as SO_2 or NH_3) upon calculations using modeled concentrations.

We maintain both random-access and sequential-access versions of the 80-character and 100-character databases, as well as files for the individual molecules. The sequential access versions are what are normally distributed to interested users. The sequential access files are SAO92*n*.DAT and SAO92A*n*.DAT, n = 1-8. The lines are in 100 cm^{-1} bins, where $100 \times n$ is the upper limit, in cm^{-1}, for each file.

Table 2: Summary of SAO92 Molecular Line Database

Mol.	Number	Source	Notes
H_2O	1	HITRAN92	161 isotopic species only. See text for line position changes.
CO_2	2	HITRAN92	Intensity (296 K) $\geq 10^{-25}$.
O_3	3	HITRAN92	666 isotopic species, vibrational ground state
N_2O	4	HITRAN92, SAO	Intensities for ν_2 fundamental transitions from J. W. C. Johns, private communication, 1993; everything else from HITRAN92.
CO	5	SAO, HITRAN92	Positions for $^{12}C^{16}O$ fundamental from TuFIR work;[12] everything else from HITRAN92.
CH_4	6	HITRAN92	Intensity (296 K) $\geq 10^{-27}$.
O_2	7	HITRAN92, JPLSMM	All intensities and positions are from JPLSMM where available; all others are from HITRAN92; all pressure-broadening are from HITRAN92. See text for more detail.
NO	8	HITRAN92	HITRAN92 only goes to 100 cm^{-1}.
SO_2	9	HITRAN92	Intensity (296 K) $\geq 10^{-21}$.
NO_2	10	HITRAN92, JPLSMM	Strengths and intensities are from JPLSMM where available. All other strengths and intensities, as well as all pressure-broadening are from HITRAN92. Intensity (296 K) $\geq 10^{-23}$.
NH_3	11	HITRAN92	Intensity (296 K) $\geq 10^{-20}$.
HNO_3	12	HITRAN92	Intensity (296 K) $\geq 10^{-22}$.
OH	13	JPLSMM, SAO	All widths are from the TuFIR measured 118.455 cm^{-1} measurement (including temperature dependence).[7] Positions and strengths are from JPLSMM except for the 118.455 cm^{-1} line.
HF	14	HITRAN92, SAO	TuFIR positions are used where available,[4] all others are from HITRAN92. Intensities are from SAO calculations and widths are calculated from the Pine and Looney measurements.[16] See text for more details. All hot band parameters are from HITRAN92.
HCl	15	SAO, HITRAN92	TuFIR positions and SAO calculated intensities are used up to $R(11)$ (these include quadrupole splittings)[4], HITRAN92 values are used everywhere else. Widths are calculated from Pine and Looney measurements[16] up to $R(10)$; HITRAN92 values are used everywhere else. See text for more detail. Chlorine isotope ratio = .7576/.2423.
HBr	16	SAO, HITRAN92	Positions for fundamental below 200 cm^{-1} are from TuFIR measurements;[18] all other positions are from HITRAN92. Intensities for the rotational fundamental are from SAO dipole moment calculation; hot band values are from HITRAN92. All widths are from HITRAN92.

Mol.	Number	Source	Notes
HI	17	HITRAN92	
ClO	18	HITRAN92	
OCS	19	HITRAN92	
H_2CO	20	HITRAN92	Intensity (296 K) $\geq 10^{-22}$.
HOCl	21	SAO, HITRAN92	Positions for most (i.e., the strongest) lines are calculated from constants in Ref. 20; the rest are from HITRAN92. All intensities and widths are from HITRAN92.
N_2	22	HITRAN92	No SAO92 lines; included for completeness.
HCN	23	HITRAN92	
CH_3Cl	24	HITRAN92	No SAO92 lines; included for completeness.
H_2O_2	25	SAO	Only the $^RQ_4$ (94 cm^{-1}) and $^RQ_5$ (112 cm^{-1}) sub bands are listed. These positions are calculated from measured rotational constants[21], intensities are calculated from the dipole moment[22], and widths are arbitrarily set to 0.1. Note that far infrared positions in HITRAN92 are demonstrably incorrect and that these Q branches are not included.
C_2H_2	26	HITRAN92	No SAO92 lines; included for completeness.
C_2H_6	27	HITRAN92	No SAO92 lines; included for completeness.
PH_3	28	HITRAN92	No SAO92 lines; included for completeness.
O_3ISO	29	HITRAN92, JPLSMM	The 668 and 686 listings are from HITRAN92. The 667 and 676 listings are from JPLSMM (676 only goes to 139 cm^{-1}); widths for 667 and 676 are set to 0.07; isotopic abundance for 667 is 0.00074; isotopic abundance for 676 is 0.00037.
$HOTO_3$	30	HITRAN92	$HOTO_3$ @ 112.1909 → 112.1900 $HOTO_3$ @ 112.3404 → 112.3402 $HOTO_3$ @ 112.3611 → 112.3606 $HOTO_3$ @ 112.3930 → 112.3924
O^3P	31	SAO	Corrected positions[23]
HO_2	32	SAO, JPLSMM	Where available, TuFIR-measured line positions are used. These include all of FIRS-2 measured atmospheric lines. All other positions, and all intensities, are calculated from JPL Hamiltonian (H. M. Pickett, private communication). Intensity (296 K) $\geq 10^{-24}$.
H_2OIS	33	HITRAN92	Minor H_2O isotopomers other than HDO.
$O_2\,^1D$	34	JPLSMM	O_2 ($^1\Delta$)
DUMMY	35		Used to make dummy lines (see text).
HDO	36	HITRAN92, HITRAN82	Lines above the one at 100.4901 are from HITRAN82 (they are left out of HITRAN92 and HITRAN86). HDO @ 112.299 → 112.298

Following are brief descriptions of the parameter listings for each molecule having significantly different parameters than those of HITRAN92.

H_2O

The entries for the main isotopomer of H_2O are essentially the same as HITRAN except for four transitions, including two from the (010) hot band, which fall in the FIRS-2 fitting regions for transitions of other molecules. These four lines are found to have frequencies which are significantly different from the HITRAN listing, which causes problems in the nonlinear least-squares fitting of stratospheric spectra in these regions. We have adjusted the frequencies of these lines to match their positions in the FIRS-2 data. Based on our ability to calibrate atmospheric spectra, and comparisons with lines whose positions are know to extremely high accuracy (e.g., HF and HCl), the uncertainties in the SAO positions are estimated to be 1-2×10^{-4} cm^{-1}, except at the highest wavenumber region where the signal to noise ratios obtainable in the spectra limits the determination to ca. 10^{-3} cm^{-1}. These changes can also be justified by comparing the adjusted frequencies with the results of obtained from differences in the H_2O energy levels published by Toth.[11] A systematic exercise of recalculating the H_2O rotational positions from these energy levels should remedy many of these frequency differences and should be done in the near future. To date, the changes are as follows:

Transition				HITRAN92	SAO92	Toth
v'	Q'	v''	Q''			
(010)	$5_{2,4}$	(010)	$5_{1,5}$	101.3197	101.3236	101.32363
(010)	$3_{3,1}$	(010)	$2_{2,0}$	163.9602	163.9650	163.96507
(000)	$10_{7,3}$	(000)	$10_{6,4}$	178.9045	178.9071	178.90699
(000)	$13_{2,11}$	(000)	$13_{1,12}$	204.5760	204.5750	204.57432

Due to uncertainties in the pressure broadening coefficients, only weak transitions of H_2O are used for atmospheric retrievals with the FIRS-2 data.

N_2O

Recent laboratory measurements (J.W.C. Johns, private communication, 1993) revealed a significant error in intensities for the ν_2 fundamental band of N_2O in HITRAN. The HITRAN intensities are systematically too high (by a few percent) and do not include Herman-Wallis factors, which are significant for N_2O. The differences between the HITRAN and Johns intensities are as great as 30% in some cases. The estimated errors in the Johns intensities are about 1%. Since most of the transitions used for retrievals from data of the FIRS-2 instrument are in the P-branch of the ν_2 fundamental band, where the Herman-Wallis factors decrease the relative intensities, use of the Johns intensities increases retrieved FIRS-2 N_2O mixing ratios by about 10%, which is greater than the sum of all errors from FIRS-2 N_2O retrievals excluding line parameter errors. For the hot bands, intensities are left at the HITRAN values; they are too weak to be observed in the atmosphere at present, and were not measured by Johns. Because of the high sensitivity of the FIRS-2 instrument to atmospheric N_2O and the dependence on pressure-broadening, as shown in Table 1, laboratory measurement of more accurate pressure broadening coefficients for the ν_2 band would be of great value.

CO

Highly accurate TuFIR measurements of the frequency positions exist for rotational transitions in the vibrational ground state of CO.[12] The uncertainties for these lines are less than 10^{-6} cm^{-1} for the most intense lines and 10^{-5} cm^{-1} in the worst case for the lines included here. These are not currently included in HITRAN, but are added to SAO92 because they are the best values available. These transitions are too weak to be observed by the FIRS-2 instrument in the atmosphere. Vibrational hot band line positions and all intensities and pressure broadening coefficients are taken from HITRAN92.

O_2

The intensities and frequencies for $^{16}O^{16}O$ have recently been recalculated for the JPL catalog. The intensities in HITRAN were found to be in error by as much as 10%. We therefore incorporate the values from the JPL catalog. For those transitions not listed in the JPL catalog, including the other isotopomers, HITRAN values are used. In all cases, the pressure broadening parameters from HITRAN are used. Accurate broadening coefficients for O_2 are available for only a few lines.[6] A systematic study of these coefficients would be valuable since O_2 lines can be used for validation of the retrieval algorithms for both the FIRS-2 instrument and the IROE instrument.[13,14]

NO_2

JPLSMM is used for NO_2 lines below 200 cm^{-1} for mostly historical reasons. Before the release of HITRAN92, only transitions below 100 cm^{-1} were included in HITRAN. We therefore have relied on the JPL listing for NO_2 transitions. Higher frequency NO_2 transitions which agree well in position and strength with the JPL listing are now included in HITRAN (HITRAN92). All SAO92 transitions above 580 cm^{-1} are from HITRAN92. The pressure broadening coefficients are set to 0.067 cm^{-1} atm^{-1} as listed in HITRAN92. This value has little effect on atmospheric retrievals due to the weakness of the atmospheric transitions.

OH

The JPLSMM positions and strengths are used for OH (except for the lines at 118.455 cm^{-1}) since they are more accurate than HITRAN (2×10^{-5} cm^{-1} or better for the strong lines) and are in better agreement with atmospheric spectra. The TuFIR measured positions for the 118.455 cm^{-1} lines are included because they are the best available measurements, with uncertainties of 1×10^{-6} cm^{-1}.[7] The pressure broadening coefficient has been measured accurately for only the 118.455 cm^{-1} transition.[7] This value is used for all the other lines since no other data exists. Measurements of pressure broadening parameters for the other transitions would be of great value for the FIRS-2 data since many lines are used in the retrieval of atmospheric OH, all of which show some degree of saturation.

HF

The positions for the rotational lines up to R(4) come from high accuracy TuFIR measurements.[4] Additional, lower accuracy, positions come from HITRAN. Line intensities are calculated directly from the dipole moment,[15] with a small correction so that temperature correction of the intensities which approximates the rotational partition function as proportional to T will give the exact value at 230 K, which is an average mid-stratospheric temperature. The pressure broadening parameters are calculated to be consistent with the measured values of Pine and Looney[16] for the vibrational fundamental band: for the 80 character version of the database, where the line dependent temperature coefficient, n, is not included, n is assumed to be 0.67 and $\gamma(296)$ is set to give the correct width at 230 K (the average stratospheric temperature); for the 100 character, n and γ are exactly the values from the Pine and Looney measurements. Lines not measured by Pine and Looney retain the HITRAN pressure broadening values. The HITRAN92 pressure broadening coefficients are not updated from the values used in HITRAN86.

HCl

HCl is treated in a fashion similar to HF. Here TuFIR measured positions up to R(11) are included (these include quadrupole splittings).[4] Intensities are calculated directly from dipole moment measurements[17] and include a correction factor for partition sums as for HF. Pressure broadening coefficients are treated exactly the same as for HF, where the Pine and Looney measurements[16] are used when applicable.

HBr

Line positions below 200 cm^{-1} are calculated directly from TuFIR measured rotational constants[18] and intensities are calculated from the dipole moment.[19] All other transitions, as well as all pressure broadening coefficients, are from HITRAN92.

HOCl

Positions for most lines are calculated from constants obtained from recent measurements[20] which have yet to be included in HITRAN. Strengths and pressure broadening widths are from HITRAN92. Positions from all other lines ($J \geq 50$, $K_a \geq 6$, a-type Q-branch, and $\Delta K_a = 3$ transitions) are from HITRAN92. These latter transitions are too weak to be observed in the atmosphere with existing instruments.

H_2O_2

We have included only the $^{R}Q_4$ (94 cm^{-1}) and $^{R}Q_5$ (112 cm^{-1}) bands which have recently been measured (Ref. 21 and J.-M. Flaud, private communication, 1991). The intensities are calculated directly from dipole moment measurements.[22] All the other transitions are too weak to be observable by any current atmospheric technique. It should be noted that the H_2O_2 transitions currently listed in HITRAN92 do not correspond at all with this listing, and should be corrected in the next HITRAN release.

O_3 minor isotopomers (referred to as O3ISO in database)

These are separated from the main isotopomer to account for possible altitude dependence of the isotopomer ratio in the stratosphere. The isotopomers containing one ^{18}O are extracted the HITRAN92 listings. The isotopomers containing one ^{17}O are extracted from JPLSMM since they are not included in HITRAN92. For these isotopomers, the pressure broadening coefficients are set to 0.07 cm^{-1} atm^{-1} (a typical value for the main isotope of O_3). This value has little effect of atmospheric retrievals since the atmospheric lines are generally very weak. The isotopic abundance for the 667 and 676 species are set to 0.00074 and 0.00037, respectively, from the JPLSMM choice for relative isotopic abundances.[3]

O_3 hot bands (referred to as HOTO3 in database)

These are separated from the fundamental transitions to account for any possible effect from non local thermodynamic equilibrium. The listings are essentially the same as HITRAN92 with the exception that the positions of a few lines have been shifted to agree with their observed positions in the FIRS-2 atmospheric spectra (as with H_2O, the FIRS-2 positions are accurate to $1\text{-}2\times10^{-4}$ cm^{-1}). The discrepancies are now very small due to many improvements in the O_3 listings between the HITRAN86 and HITRAN92 releases. The changes are as follows:

Transition				HITRAN92	SAO92
v'	Q'	v''	Q''		
(010)	$41_{13,29}$	(010)	$40_{12,28}$	112.1909	112.1900
(010)	$34_{14,20}$	(010)	$33_{13,21}$	112.3404	112.3402
(010)	$20_{16,4}$	(010)	$19_{15,5}$	112.3611	112.3606
(010)	$27_{15,13}$	(010)	$26_{14,12}$	112.3930	112.3924

O^3P

As this is not a HITRAN molecule, the listing included here comes completely from the literature.[23] Since these transitions are weak, the pressure broadening coefficients are not significant, and a typical value is used, 0.05 cm^{-1} atm^{-1}.

HO_2

This molecule is not in HITRAN92. Positions and strengths are obtained from calculations using the JPL Hamiltonian (H.M. Pickett, private communication), and positions are substituted with TuFIR measurements where they exist (K. Chance, unpublished data; this includes all the lines currently used for atmospheric retrievals with the FIRS-2 data).

H_2O isotopomers containing ^{17}O and ^{18}O (referred to as H2OIS in database)
These listings are the HITRAN92 values, but have given a separate molecule number to account for possible altitude dependence of the isotopomer ratios. As with the main isotopomer of H_2O, a systematic recalculation of the transition frequencies from the energy levels of Toth[24] would improve the positions for this listing.

O_2 $^1\Delta$ (referred to as O21D in database)
This is not in HITRAN92 and therefore is obtained from JPLSMM. Pressure broadening coefficients are arbitrarily set to 0.04 cm^{-1} atm^{-1}, a typical O_2 value.

HDO
HITRAN92 only contains HDO transitions up to 100.4901 cm^{-1}. All of the rotational HDO transitions above this are missing from every HITRAN release since HITRAN82. Therefore, we appended the values from this older HITRAN release above 100.5 cm^{-1} to our HDO listing. The position of one transition has been shifted to correspond with its position observed in the FIRS-2 data:

	Transition			HITRAN92	SAO92
v′	Q′	v″	Q″		
(000)	$7_{3,4}$	(000)	$6_{3,3}$	112.299	112.298

DATABASE FORMATS

80 Character Database. Line positions are now all in the F10.6 format, to keep increased accuracy above 100 cm^{-1}. The format is an “old AFGL” one (see Ref. 1 for details on quantum numbers):

`F10.6`	`1PE10.3`	`F5.3`	`F10.3`	`2A8`	`2A9`	`4X`	`I4`	`I3`
`a`	`b`	`c`	`d`	`e`	`f`		`g`	`h`

a. Position (cm^{-1})
b. Intensity (cm, at 296 K)
c. Air pressure-broadening coefficient (HWHM, cm^{-1} atm^{-1})
d. Lower state energy (cm^{-1})
e. Vibrational quantum numbers
f. Rotational, electronic, and hyperfine quantum numbers
g. HITRAN isotope code
h. Molecule number

Note that portions of e-g are missing for some non-HITRAN transitions.

100 Character Database. This is in the current HITRAN format (see Refs. 1 and 2 for details on quantum numbers and indices):

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I2 I1 F12.6 E10.3 E10.3 F5.4 F5.4 F10.4 F4.2 F8.5 I3 I3 A9 A9 3I1 3I2
a  b  c     d     e     f    g    h     i    j    k  l  m  n  o   p
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a. Molecule number
b. Isotope number (1 = most abundant, etc.)
c. Position (cm^{-1})
d. Intensity (cm, at 296 K)
e. Transition probability ($Debye^2$)
f. Air pressure-broadening coefficient (HWHM, cm^{-1} atm^{-1})
g. Self pressure-broadening coefficient (HWHM, cm^{-1} atm^{-1})
h. Lower state energy (cm^{-1})
i. Coefficient of temperature dependence, n, for air-broadened HWHM ($\gamma = \gamma_0 \times (296/T)^n$)
j. Either the pressure shift (cm^{-1} atm^{-1}) or line-coupling coefficients
k. Upper state global quanta index
l. Lower state global quanta index
m. Upper state local quanta
n. Lower state local quanta
o. Accuracy indices
p. Indices for lookup of references

We use only fields a-j in our “100 character”-style files.

AVAILABILITY OF SAO92

The SAO92 database is available using ftp, upon request to K. Chance or K. W. Jucks. Magnetic tapes (9 track or Exabyte cartridges) can be furnished under special circumstances.

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