



*National Aeronautics and Space Administration
Goddard Earth Science
Data Information and Services Center (GES DISC)*

README for the Version 3 Atmospheric Trace Molecule Spectroscopy Experiment (ATMOS) Data Products

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Overview

The Atmospheric Trace Molecule Spectroscopy Experiment (ATMOS) was funded by the [NASA Earth Science Enterprise](#). It was designed to study the composition of the atmosphere from space, carried on board the Space Shuttle.

Version 3 retrievals of the ATMOS spectral data extends the data set to new molecules and lower altitudes. Rather than using the "onion-peeling" algorithms in Version 2, this version uses a global fit algorithm for more reliable and robust retrievals at tropospheric altitudes.

A description of Version 3 retrieval methods, along with selected results, may be found in *Irion et al.*, "Atmospheric Trace Molecule Spectroscopy (ATMOS) Experiment Version 3 data retrievals," *Applied Optics*, Vol. 41, No. 33, 6968–6979, 20 November 2002.

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General Information

ATMOS is an infrared spectrometer (a Fourier transform interferometer) that is designed to study the chemical composition of the atmosphere.

Since the molecules of interest to the ATMOS investigation must be measured remotely (i.e., from outside the atmosphere itself), solar spectroscopy was the method of choice for making the measurements, using those periods during each orbit of the spacecraft when the atmosphere is between the Sun and the instrument (i. e., at sunrise and sunset as seen from the spacecraft). During sunset, for example, the tangent point of the ray path to the instrument penetrates deeper and deeper into the atmosphere until it is blocked by the surface of the Earth (or clouds); as seen from a typical shuttle orbit, the height of the tangent point changes at about 2 kilometers per second so that, to be able to distinguish changes in the composition with altitude, successive measurements of the spectrum must be made very rapidly. By analyzing the absorptions due to a given molecule in each successive spectrum, the variations in its concentration with altitude can be determined.

The rapidity at which the measurements must be made precludes the use of conventional scanning spectrometers which record the spectrum wavelength by wavelength, requiring minutes or even hours to cover relatively modest wavelength intervals. Furthermore, such instruments by their nature are limited to collecting radiation through very narrow entrance apertures. Thus, only a small amount of light enters the instrument, and only a very small fraction of that light is measured at any given time.

A technique which overcomes these limitations is based on the interference properties of light waves, and was first used in an analytical instrument by Albert Michelson almost a century ago. This technique, called interferometry, does not involve dispersion of the radiation being analyzed, and hence it can be admitted to the system through much larger apertures than the slits required for scanning instruments. Once inside, the radiation is split into two beams which travel separate paths through the instrument and are then recombined. If the length of one path is varied with respect to the other, the various wavelengths of light contained in the recombined beam will go in and out of phase as a function of the wavelengths themselves and the path difference. If the recombined beam is then focussed on a detector and sampled at the proper intervals, a signal called an interferogram is produced which is extremely complex but can be transformed to yield the amount of radiation contained in the original beam as a function of wavelength. Since information about all wavelengths of light in the beam is contained in every

sample recorded, the technique is not subject to the second limitation of scanning spectrometers mentioned above.

Although the concepts involved in interferometry are straightforward, the instrument itself must work in the realm of fractions of wavelengths of the light being measured and thus severe demands are placed on the fidelity of the optics and the precision and accuracy of the sampling intervals. But for the advent of high stability single-frequency lasers, ultra-fast electronic components, and modern optical polishing techniques, the ATMOS sensor could not have been built. The instrument uses optical components polished flat to within a twentieth of the shortest wavelength of the light being measured, and generates an interferogram containing 400,000 sample points (the intervals between which are precisely controlled using a reference laser) every second! The corresponding rate at which the data are transmitted to the ground is 16 million bits per second.

Instrument

Background

The current ATMOS instrument represents the outgrowth of an atmospheric measurement program begun at the Jet Propulsion Laboratory (JPL) in 1972 using a flight model High Speed Interferometer (HSI) designed and built by the Laboratory for use on aircraft and balloon borne platforms. The original instrument, designated the Mark I, covered the wavelength region from 1.8 to 5.2 *micrometers* with an *unapodized* resolution of 0.125 *wavenumbers*. This instrument, which was flown on a wide variety of aircraft and balloon borne platforms, gathered information on the mixing ratios of atmospheric minor and trace species from ground level to a height of 40 km. Among these measurements were several stratospheric "firsts," including the first spectroscopic detection of NO, the first NO/NO₂ ratio, the first spectroscopic detection of HCl, the first HF/HCl ratio, and the first profile for HF in the 20 to 40 km region of the atmosphere.

During the 1976-1977 time period, a Shuttle Definition Study was conducted both to determine the feasibility of acquiring infrared interferometric data from the Space Shuttle and to provide a conceptual design for an instrument capable of making the measurements. This study culminated with the award of a contract to Honeywell ElectroOptics Center (HEOC) in January 1978 to design and build the ATMOS sensor. The following paragraphs describe the design and development of the ATMOS instrument by HEOC.

Instrument Overview

Radiation enters the instrument via a suntracker and a foreoptics subsystem, with the latter defining the *FOV* and the size of the beam. The energy rejected by the *field stop* is reflected to a video camera and is recorded as an image of the Sun with the position of the FOV of the instrument superimposed. The wave front passing through the field stop is divided by the *beamsplitter* and modulated by the moving elements in the interferometer. The modulated radiation leaving the beamsplitter passes through one of the eight selectable bandpass filters and is focused on a Mercury Cadmium Telluride (HgCdTe) detector cooled to 77 K.

The signal produced at the detector is conditioned and digitized by the Signal Handling Subsystem (SHSS). The digitized signal is then formatted by the Data Handling Subsystem (DHSS) into a Pulse Code Modulated (PCM) data stream. This signal is then output to the instrument Ground Support Equipment (GSE) or, during a flight, directly to the Shuttle High Rate Multiplexer (HRM). Additional engineering and housekeeping data is processed by the Engineering Data Handling Subsystem (EDHSS) and is output as a part of the high rate data stream as well as in a separate low rate engineering stream. All command and control functions for the instrument are performed by the Command and Control Interface Subsystem (CCISS).

Instrument Description

For purposes of discussion the instrument can be divided into two sections: (1) the optical sensor, composed of all the optical subsystems and the scan servo control unit, and (2) the electronic assemblies, including the compressor for the detector cooler. All the elements of the optical sensor are mounted to an aluminum baseplate that in turn is mounted via vibration isolators to a substructure assembly. This assembly attaches to, but is thermally isolated from, a platform located in the payload cargo bay of the Shuttle. An aluminum cover, which also mounts to the baseplate, encloses all but the suntracker and camera. The internal pressure of the sensor is maintained at ambient through a vent that is fitted with a desiccant filter assembly designed to provide a clean, dry environment under all conditions.

The electronics section is mounted on a secondary support platform that is mechanically isolated from the main support structure through vibration isolators. The electronics are physically separated into two units, one chassis containing the SHSS, DHSS, EDHSS, and CCISS and the other containing the power supply subsystem. A thermal control plate mounts to the underside of the secondary platform and provides a nominal thermal operating range of +5 degrees C to +45 degrees C under pallet conditions ranging from -150 degrees C to +120 degrees C.

Suntracker and Foreoptics

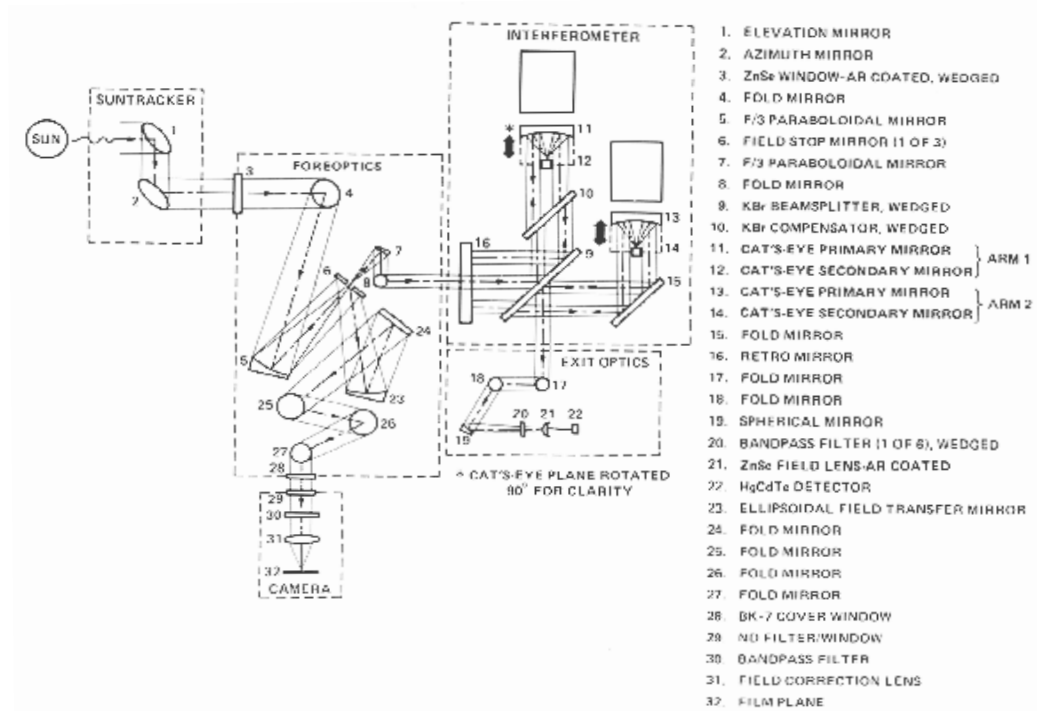


Figure 1: The optical layout for the suntracker and foreoptics, including the frame camera optics.

The two axis servo controlled suntracker tracks the Sun to an accuracy of 0.4 mr with a stability of 0.06 mr. Sun detection and positive feedback are provided by a silicon quadrant array with an acceptance cone angle of 20 deg. In the tracking mode, the sensor's FOV is centered on the solar disk; however, commands can be sent to offset the tracker null position in 1 mr steps to avoid or seek out sunspot activity. The tracker can be prepositioned to intercept the Sun at the appropriate time for a subsequent sunset or sunrise encounter by a commandable pointing capability that provides near hemispheric coverage.

Energy reflected by the suntracker passes through a Zinc Selenide (ZnSe) window and enters the instrument foreoptics. The cover window is anti reflective (AR) coated for improved efficiency in the 2 to 16 micron region without significant loss at the camera wavelength of 0.575 microns. The foreoptics telescope has a 7.5 cm diameter collecting aperture and consists of two confocal f/3 off axis paraboloids with a selectable field stop located at their common focus. Field stops corresponding to instrument FOVs of 1, 1.4, 2, and 2.8 mr can be selected. Energy passing through the stop is *recollimated* by the telescope secondary and transferred to the interferometer. Angular magnification is restricted to 2.6 because of *obliquity* limitations within the interferometer. The rejected energy is reflected by an ellipsoidal mirror to a camera which records one solar image at the end of each scan.

Interferometer

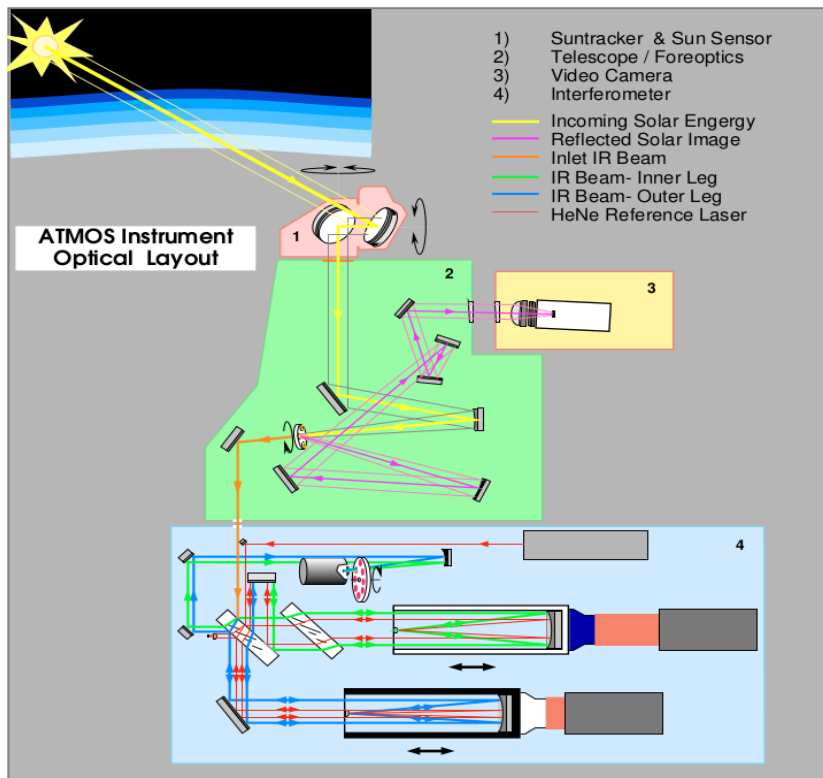


Figure 2: A block diagram of the optical layout of the interferometer.

The optical system is a modified version of the classical Michelson interferometer that uses cat's eye retroreflectors in place of plane mirrors and double passing techniques for maximum alignment stability. This relaxes component alignment tolerances from a few arc seconds to several arc minutes, rendering the instrument insensitive to mechanically or thermally induced misalignments.

Energy enters the interferometer through an aperture in the common retro mirror and impinges on the beamsplitter at an angle of 45 deg. The beamsplitter substrate is Potassium Bromide (KBr) with a Ge/KRS-5 coating designed for optimum efficiency over the 2 to 16 micron region. Radiation reflected from the beamsplitter passes through a KBr compensator plate and goes to the cat's eye retroreflector, which consists of an f/2.7 paraboloid primary and a slightly convex secondary. The radiation exits the cat's eye displaced, travels through the compensator, and is reflected off a gold coated area on the beamsplitter substrate that directs the energy to the retro mirror. The reflected beam then retraces its path back to the beamsplitter surface. The radiation transmitted by the beamsplitter follows a similar path but uses the beamsplitter substrate in transmission rather than in reflection. The Optical Path Difference (OPD) is varied continuously from +50 cm to -50 cm at a rate of 50 cm/second by moving both cat's eyes equal distances but

in opposite directions. This has two advantages over a single moving element system: first, it decreases the mechanical scan rate to 6.25 cm/second, half its former value; and second, by scanning the cat's eyes in opposite directions, it rejects common mode forces, thus providing for a first order velocity correction. Requirements for high spectral data quality dictate precision control of the OPD scan to a velocity uniformity of 0.1% peak to peak. This level of performance is achieved through the use of a frequency stabilized HeNe laser for OPD velocity feedback. The reference laser used in the ATMOS interferometer is a modified Hewlett Packard HP5501A Zeeman split actively stabilized laser providing single mode, single frequency output at 0.6330 microns. The laser energy passes through the interferometer parallel to the infrared beam.

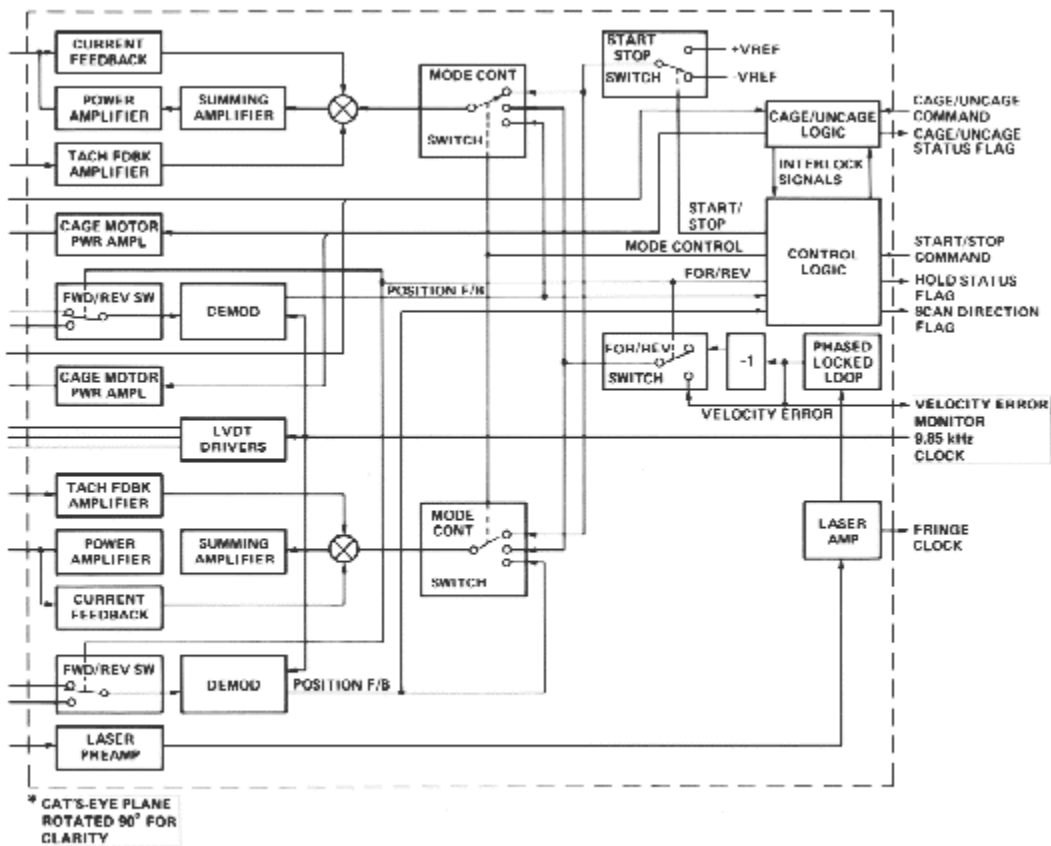


Figure 3: The key elements of the scan servo subsystem.

The velocity servo is implemented with two control levels: (1) an outer control that uses a phase locked loop to convert laser feedback to an error signal and provides the precise velocity control; and (2) two inner control loops, one for each slide, that use moving coil tachometers for velocity feedback. The function of the inner loops is to force both slides to operate at approximately the same velocity. As each slide reaches the end of its travel, control is switched to position feedback with the loop closed around Linear Variable Differential Transformer (LVDT)

position sensors; the return scan is initiated after both sliding assemblies are brought to a halt in their hold positions. To maximize the duty cycle, scan control is provided in both directions with turnaround times of 150 ms at each end.

The output from the interferometer passes through one of the eight selectable bandpass filters and is focused by an AR coated ZnSe lens onto a photoconductive HgCdTe detector, where a pupil image is formed. The detector is a single element, 27 mils on a side; the size of the chip was chosen on the basis of both sensitivity and linearity requirements under high signal flux conditions. It is AR coated to improve quantum efficiency and uses a constant bias voltage to improve linearity. The element is packaged in a sealed glass vacuum dewar and cooled to 77 K using a split Stirling cycle mechanical cooler with a 1.6 watt cooling capacity.

Electronics Description

The output from the detector is transferred to the SHSS, where it is amplified, filtered, and digitized for insertion into the DHSS.

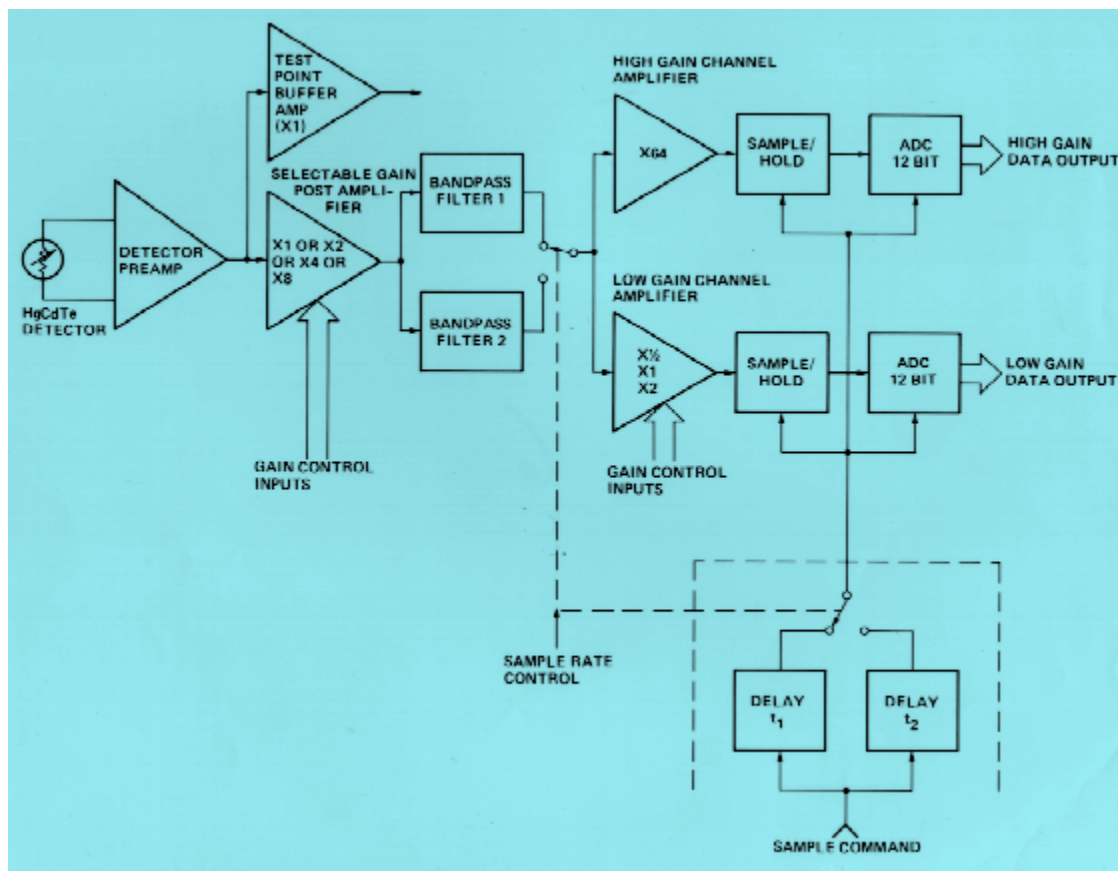


Figure 4: Schematic of the Signal Handling Subsystem (SHSS).

The SHSS has been designed to preserve source noise limited performance while accommodating an expected dynamic range of 18 bits with minimum phase and amplitude distortion. The 18 bit dynamic range, high data rate operation is obtained through the use of two 12 bit parallel data channels offset in gain by 5, 6, or 7 bits, selectable by command. Both outputs are included in the PCM data stream. During ground processing, valid data from each channel is interleaved to reconstruct an effective 18 bit signal that preserves peak signal precision and maintains source noise limited performance at high spectral resolution. Sampling of the analog interferogram in both channels is based on delayed reference laser fringe sampling at every second (395 kHz) or third (263 kHz) laser fringe, selectable by command. Electronic distortion has been minimized through proper delay of the sampling waveform as well as through use of multipole compensated Butterworth filters for noise bandlimiting.

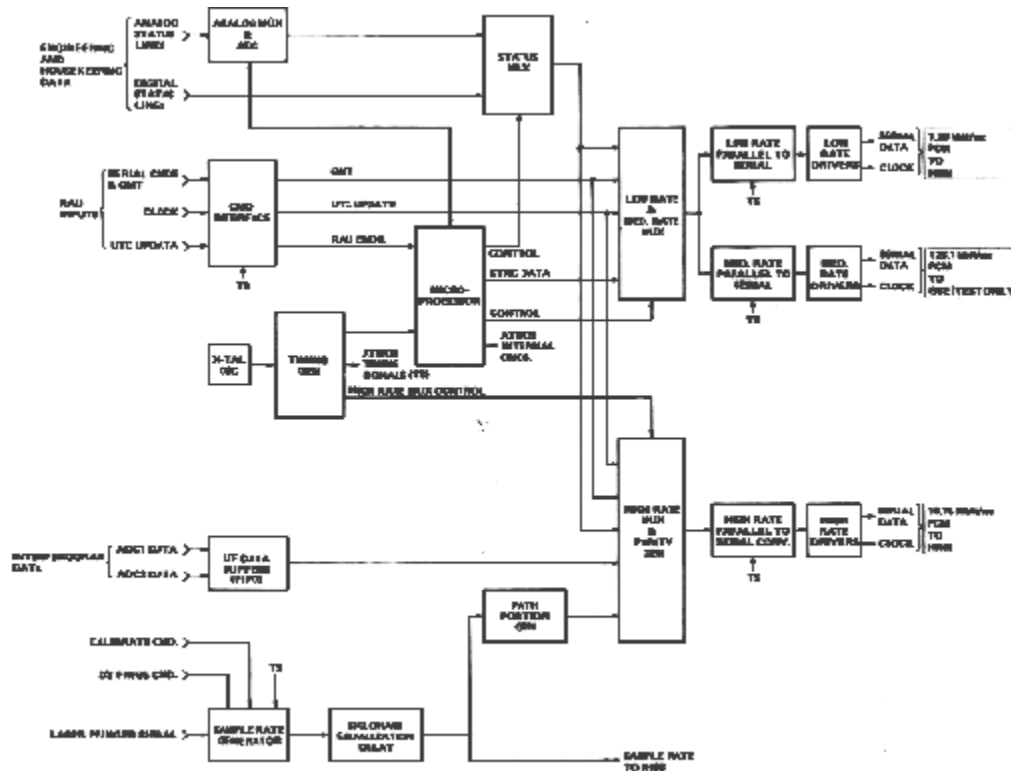


Figure 5: The remaining elements of the ATMOS electronics.

The DHSS accepts the digitized high and low gain interferometric data to be buffered and formatted into a Shuttle compatible Non Return to Zero Logic (NRZ L) serial 15.76 Mbit/s PCM data stream. The formatting section is a hard wired design with formatting accomplished by a digital multiplexer. The high rate data format includes the engineering and housekeeping data and both time and optical path position references. Also shown in the block diagram are the main elements of the EDHSS and CCISS. A common feature of these subsystems is a Motorola MC6802 microprocessor that formats the system engineering and housekeeping data as well as

decoding and implementing the instrument commands received through the Shuttle interface. In addition to the high rate PCM data channel, the ATMOS instrument provides a 1.28 kbit/s low rate PCM output containing engineering and housekeeping data only.

Platform

The ATMOS instrument has flown four times on the Space Shuttle from 1985 to 1993. The predecessor to ATMOS, flown on aircraft and high altitude balloon platforms, was born in the early 1970s out of concern for the effects of Super Sonic Transport exhaust products on the ozone layer. The experiment was redesigned for the Space Shuttle when the potential for ozone destruction by man-made chlorofluorocarbons was discovered and the need for global measurements became crucial. The investigation is conducted by JPL under the sponsorship of the Upper Atmospheric Office at NASA.

Spacelab 3



The STS-51B/Spacelab 3 mission was launched on April 30, 1985 from the Kennedy Space Center. The set of high-resolution infrared solar observations made with the ATMOS - Fourier transform spectrometer (30 April - 1 May 1985) has been used to evaluate the total budgets of the odd chlorine and fluorine chemical families in the stratosphere. There were 4 measurements taken at orbital sunrise between 77 south and 79 south latitude, and 11 measurements between 25 north and 35 north latitude. After a week in orbit, the shuttle landed at Edwards Air Force Base on May 6.

ATLAS 1



The STS-45/ATLAS 1 mission was launched on March 24, 1992 from the Kennedy Space Center. During 8 days of operation, the ATMOS instrument made a total of 98 observations, spanning a substantial portion of the globe. The 53 measurements taken at orbital sunrise covered the mid-latitude and equatorial regions of the earth from 30 degrees south to 30 degrees north. The 41 sunset observations were made at 25 south to 55 south. ATMOS was only able to monitor the atmosphere down to a height of about 20 km, due to a recent eruption of Mount Pinatubo, which clouded the region below that with dust and aerosols. The shuttle landed on Runway 33 at KSC on April 2.

ATLAS 2



The STS-56/ATLAS 2 mission was launched on April 8, 1993 from the Kennedy Space Center. During 9 days of operation, the ATMOS instrument made a total of 104 observations, 65 at sunrise in the north polar region around 65 degrees north, and 39 at sunset between 10 and 50 degrees south. The Arctic polar vortex, the airmass over the north pole where the processes leading to ozone depletion occur, was still partially intact even at this late date in the springtime; ATMOS took measurements both inside and out of this air. The shuttle landed on Runway 33 at KSC on April 17.

ATLAS 3



The STS-66/ATLAS 3 mission was launched on November 3, 1994 from the Kennedy Space Center. During nearly 11 days of operation, the ATMOS instrument made a total of 228 observations, 105 over the northern hemisphere at sunset, and 94 over the south polar region (Antarctica) at sunrise. ATMOS took measurements both inside and outside of the Antarctic ozone hole, which was still present even at this late date in the southern springtime. The shuttle landed at Edwards Air Force Base in California on November 14.

Outstanding Issues

- Diurnal corrections for NO and NO2 for many occultations have not been done yet.
- HDO retrieval procedures are currently being revised. HDO should not be considered reliable below about 15 km.
- Retrieval procedures for the water isotopomers H2-17O and H2-18O are currently being defined, and these molecules will be included in future updates.
- Due to an ephemeris bug, the spacecraft longitudes of the AT3SS85 occultation were in gross error for the spectra r941110182635, r941110182637, and r941110182639. This has also resulted in a lat/long error in the retrieval around 16.5 km. We do not expect that this has caused an appreciable error in the gas retrievals themselves since the tangent altitudes are calculated using an assumed CO2 profile, and there are no unexpected "jumps" in retrieved tropospheric CH4 and N2O.

We suggest using the following interpolated spacecraft longitudes (deg E) for these spectra:

r941110182635 359.913
r941110182637 0.004
r941110182639 0.096

and the following fitted latitudes and longitudes for the retrievals

Alt(km) Lat(deg N) Long (deg E)

13.5	21.8163	-17.8208
14.5	21.9073	-17.8477
15.5	21.9984	-17.8745
16.5	22.0894	-17.9014
17.5	22.1805	-17.9282
18.5	22.2715	-17.9551
19.5	22.3626	-17.9819

File Formats

L2 Profile Results

File naming convention is occultation.filter.product.suffix

Where

- occultation = mission (sl3 = Spacelab-3, at1 = ATLAS-1, at2 = ATLAS-2 or at3 = ATLAS-3) + type (sr = sunrise or ss = sunset) + number (01-105),
- filter_number = F1-F12,
- product = oca (altitude gridded), ocp (pressure gridded) or ocpt (potential temperature gridded) for tab-delimited files. Fixed field files have an 'f' appended, i.e. ocaf, ocpf, ocptf.
- suffix = externally compressed using gzip (.gz)

Example: at3sr64.F9.oca.gz

There are three griddings for the ATMOS Version 3 results: altitude, pressure, and potential temperature. In addition, each of these gridding formats are available in either a fixed field format (useful for Fortran programs) and tab-delimited (useful for spreadsheets). Thus there are six different file types for these data. Some sample Fortran code is provided below.

In all types of files, the first line in a file contains the field names. Field order is the same for tab delimited and fixed-field formats (see table below). For the tab-delimited files, field names are separated by tabs. For the fixed field files, field names are each left justified beginning at the first column and at every 15th column (e.g., 1, 15, 30, 45, 60, etc.).

Data are separated by tabs in the tab-delimited files, and where no data are available, "NaN" is used.

For fixed field files, most data are in the first 9 characters of the field. Where there are no data in the fixed-field files, a field of 9's (e.g. 999.999) is used. For exponential numbers, 9.99e+33 is written. See table below.

"Reserved" fields are for physical parameters that are not analyzed but may be added later into the database. Additional gases will be tacked on as new columns at the end (i.e. to the right of CH3D_ERR).

Altitude gridding

.oca suffix: gridded by altitude and formatted by tab-delimits.

.ocaf suffix: same as .oca except in a fixed-field format.

Levels (in km) are 0.5, 1.5, 2.5, 3.5, ..., 99.5 km. (100 records per occultation).

Pressure gridding

.ocp suffix: gridded by pressure and formatted by tab-delimits.

.ocpf suffix: same as .ocp except in a fixed-field format

There are 12 pressure levels (in atmospheres) per decade: 1.00000, 0.82540, 0.68129, 0.56234, 0.46416, 0.38312, 0.31623, 0.26102, 0.21544, 0.17783, 0.14678, 0.12115, ...and so forth using lower powers of ten down to 1E-7 atm. (85 records per occultation)

Potential temperature gridding

.ocpt suffix: gridded by potential temperature and formatted by tab-delimits.

.ocptf suffix: same as .ocpt except in a fixed-field format.

Levels (in K) are 280, 290, 300, 310, 320, 330, 340, 350, 360, 375, 395, 420, 445, 470, 495, 525, 555, 590, 630, 670, 710, 750, 800, 850, 900, 970, 1050, 1150, 1250, 1350, 1450, 1550, 1650, 1750, 1850, 1950, 2050, 2150, 2250, 2350, 2450, 2550, 2650, 2750, 2850, 2950, 3050, 3200, 3350, 3500, 3650, 3800, 3950. (53 records per occultation)

Field position and ordering for fixed-field files

Field#	Column	Field	Format	If no data	Notes
1	1	occultation	A9	Not applicable	9 character field right justified. Currently only 7 or 8 characters used.
2	15	update	I9	Not applicable	Date file created in YYYYMMDD
3	30	filter	I9	Not applicable	ATMOS spectral filter number
4	45	yydoy	I9	Not applicable	Date of occultation in YYDayOfYear, e.g., Feb 1, 1992 would be 92032
5	60	ut	F9.3	99999.999	Greenwich time of occultation
6	75	density	E9.3	1.00E+34	Molecular density (molecules cm ⁻³)
7	90	theta	F9.3	99999.999	Potential temperature (K)
8	105	longitude	F9.3	99999.999	Longitude (deg.)
9	120	latitude	F9.3	99999.999	Latitude (deg.)
10	135	altitude	F9.3	99999.999	Altitude (km)
11	150	pressure	E9.3	1.00E+34	Pressure (atmospheres)
12	165	temperature	F9.3	99999.999	Temperature (K)
13	180	is_data	A1	F	Field showing whether ATMOS data is available at that level: 'T' if gas data available, 'F' if not.
14	195	pv	E10.3	1.00E+34	Potential vorticity (10 ⁻⁴ K m ²) / (kg s)

15	210	spv	E10.3	1.00E+34	Scaled potential vorticity (in units of 10 ⁻⁴ s ⁻¹)
16	225	uarsday	I9	99999	UARS day
17	240	uarssec	I9	99999	UARS time (same as field #5)
18	255	reserved1	I9	99999	Reserved field 1
19	270	reserved2	I9	99999	Reserved field 2
20	285	reserved3	I9	99999	Reserved field 3
21	300	H2O	E9.2	9.99E+33	Gas 1 volume mixing ratio
22	315	H2O_ERR	"	"	Gas 1 volume mixing ratio error
23	330	CO2	"	"	Gas 2
24	345	CO2_ERR	"	"	
25	360	O3	"	"	Gas 3
26	375	O3_ERR	"	"	
27	390	N2O	"	"	Gas 4
28	405	N2O_ERR	"	"	
29	420	CO	"	"	Gas 5
30	435	CO_ERR	"	"	
31	450	CH4	"	"	Gas 6
32	465	CH4_ERR	"	"	
33	480	NO	"	"	Gas 7 - not diurnally corrected
34	495	NO_ERR	"	"	
35	510	NO2	"	"	Gas 8 - not diurnally corrected

36	525	NO2_ERR	"	"	
37	540	HNO3	"	"	Gas 9
38	555	HNO3_ERR	"	"	
39	570	HF	"	"	Gas 10
40	585	HF_ERR	"	"	
41	600	HCL	"	"	Gas 11
42	615	HCL_ERR	"	"	
43	630	OCS	"	"	Gas 12
44	645	OCS_ERR	"	"	
45	660	H2CO	"	"	Gas 13
46	675	H2CO_ERR	"	"	
47	690	HOCL	"	"	Gas 14
48	705	HOCL_ERR	"	"	
49	720	H2O2	"	"	Gas 15
50	735	H2O2_ERR	"	"	
51	750	HO2NO2	"	"	Gas 16
52	765	HO2NO2_ERR	"	"	
53	780	N2O5	"	"	Gas 17
54	795	N2O5_ERR	"	"	
55	810	CLONO2	"	"	Gas 18
56	825	CLONO2_ERR	"	"	
57	840	HCN	"	"	Gas 19

58	855	HCN_ERR	"	"	
59	870	CH3F	"	"	Gas 20
60	885	CH3F_ERR	"	"	
61	900	CH3CL	"	"	Gas 21
62	915	CH3CL_ERR	"	"	
63	930	CF4	"	"	Gas 22
64	945	CF4_ERR	"	"	
65	960	CCL2F2	"	"	Gas 23
66	975	CCI2F2_ERR	"	"	
67	990	CCL3F	"	"	Gas 24
68	1005	CCL3F_ERR	"	"	
69	1020	CCL4	"	"	Gas 25
70	1035	CCL4_ERR	"	"	
71	1050	COF2	"	"	Gas 26
72	1065	COF2_ERR	"	"	
73	1080	C2H6	"	"	Gas 27
74	1095	C2H6_ERR	"	"	
75	1110	C2H2	"	"	Gas 28
76	1125	C2H2_ERR	"	"	
77	1140	N2	"	"	Gas 29
78	1155	N2_ERR	"	"	
79	1170	CHF2CL	"	"	Gas 30

80	1185	CHF2CL_ERR	"	"	
81	1200	HCOOH	"	"	Gas 31
82	1215	HCOOH_ERR	"	"	
83	1230	HDO	"	"	Gas 32
84	1245	HDO_ERR	"	"	
85	1260	SF6	"	"	Gas 33
86	1275	SF6_ERR	"	"	
87	1290	NO_DC	"	"	Gas 34: NO diurnally corrected
88	1305	NO_DC_ERR	"	"	
89	1320	NO2_DC	"	"	Gas 35: NO2 diurnally corrected
90	1335	NO2_DC_ERR	"	"	
91	1350	CH3D	"	"	Gas 36
92	1365	CH3D_ERR "	"	"	

Sample Code

This is a sample program that reads in the data and writes a subset to a file:

```

PROGRAM FORMTEST
C
C This program reads in data in the fixed field format and writes
C the gas volume mixing ratios (but not errors) for altitudes for
C which IS_DATA = "T". It contains a general read statement that
C can be quickly modified to use in other Fortran programs.
C
      INTEGER*4 I, J
      CHARACTER*9 GASNAME(36)
      CHARACTER*8 OCCULTN
      INTEGER*4 UPDATE, FILTER, YYDOY

```

```

REAL*4 UT(100), DENSITY(100), THETA(100)
REAL*4 LONGITUDE(100), LATITUDE(100)
REAL*4 ALTITUDE(100), PRESSURE(100), TEMPERATURE(100)
CHARACTER*1 IS_DATA(100)
REAL*4 PV(100), SPV(100)
INTEGER*4 UARSDAY, UARSSEC(100)
REAL*4 VMR(36,100), VMRERR(36,100)

OPEN(UNIT=25,FILE='input.ocptf',STATUS='OLD')
OPEN(UNIT=27,FILE='output.ocptf',STATUS='NEW')
READ(25,100) (GASNAME(I), I = 1, 36)
100 FORMAT(T300, 36(A9, 21X))
WRITE(27, 140) "ALT", (GASNAME(I), I = 1, 36)
140  FORMAT(T4, A3, T12, 36(A6,5X))

DO 200 J = 1, 100 READ(25, FMT = 110, END=300) OCCULTN, UPDATE,
FILTER, YYDOY,
& UT(J), DENSITY(J), THETA(J), LONGITUDE(J), LATITUDE(J),
& ALTITUDE(J), PRESSURE(J), TEMPERATURE(J), IS_DATA(J),
& PV(J), SPV(J), UARSDAY, UARSSEC(J),
& (VMR(I,J), VMRERR(I,J), I = 1, 36)
110  FORMAT(T1, A9, T15, I9, T30, I9, T45, I9, T60, F9.3, T75,
& E9.3, T90, F9.3, T105, F9.3, T120, F9.3, T135, F9.3,
& T150, E9.3, T165, F9.3, T180, A1, T195, E10.3, T210,
& E10.3, T225, I9, T240, I9, T300, 36(E9.2, 6X, E9.2, 6X))

IF (IS_DATA(J) .EQ. "T") THEN
WRITE(27,170,ERR=300) ALTITUDE(J), (VMR(I,J), I = 1, 36)
ENDIF
170  FORMAT(T4, F6.2, 2X, 36(E10.3, 1X))
200  CONTINUE
300  CLOSE(25)
CLOSE(27)
END

```


L1 Spectra and Runlogs

File naming convention = mission (sl3, at1, at2, at3) + run number (r + integer) + suffix (.nc.gz = netCDF externally compressed using gzip), example: at3sr84.nc.gz

Spectra and runlog (i.e., associated metadata) information are combined into a single file, one per occultation. Files are in netCDF format and gzipped (.nc.gz). Information on the netCDF format, and source code for software interfaces, can be found at Unidata's [netCDF](#) site. Also, interfaces to netCDF are available in Python, IDL and MATLAB.

Transmission spectra are given (that is, spectra ratioed from ATMOS high sun observations, on a scale of 0 to 1). These are the same data used for the Version 3 processing.

The spectra are stored as a short (2 byte) integer array to conserve space. The spectral points can be rescaled to their original values by multiplying by scaleFactor.

The frequency (in wavenumbers) of any point can be calculated as

$\text{Freq} = (N + \text{ifirst} - 1) * \text{delta_nu}$ where N = index of point (counted from 0)

Below is a sample header from an occultation file (using the ncdump command line tool).

```
dimensions:
    spectralPoint = 240274 ;
    spectrumNameSize = 15 ;
    apodizFnNameSize = 4 ;
    spectrumNumber = UNLIMITED ; // (34 currently)

variables:
    char spectrumName(spectrumNumber, spectrumNameSize) ;
    int notUsedFlag(spectrumNumber) ;
        notUsedFlag:description = "notUsedFlag is set to 1 if spectrum NOT
used in ATMOS Vers 3 processing." ;
    int year(spectrumNumber) ;
        year:description = "Year of measurement" ;
    int day(spectrumNumber) ;
        day:description = "Day of measurement. Jan 1 = 1, Feb 1 = 32, etc." ;
    float hour(spectrumNumber) ;
        hour:description = "Hour (incl minutes as fraction of hour) of
measurement (GMT)" ;
    float latitude(spectrumNumber) ;
        latitude:description = "Latitude of observing instrument" ;
        latitude:units = "degrees_east" ;
    float longitude(spectrumNumber) ;
        longitude:description = "Longitude of observing instrument" ;
        longitude:units = "degrees_north" ;
```

```

float altitude(spectrumNumber) ;
    altitude:description = "Altitude of observing instrument" ;
    altitude:units = "km" ;
float asza(spectrumNumber) ;
    asza:long_name = "initial_zenith_angle" ;
    asza:description = "Initial guess for zenith angle of observation,
measured from vertical" ;
    asza:units = "degrees" ;
float poff(spectrumNumber) ;
    poff:long_name = "zenith_angle_correction" ;
    poff:description = "Correction to zenith angle (add to asza to get
zenith angle)" ;
    poff:units = "degrees" ;
float opd(spectrumNumber) ;
    opd:long_name = "optical_path_difference" ;
    opd:description = "Maximum path difference in interferometer" ;
    opd:units = "cm" ;
float fovi(spectrumNumber) ;
    fovi:long_name = "internal_field_of_view" ;
    fovi:units = "rad" ;
float fovo(spectrumNumber) ;
    fovo:long_name = "external_field_of_view" ;
    fovo:units = "rad" ;
float amal(spectrumNumber) ;
    amal:long_name = "misalignment_angle" ;
    amal:description = "Interferometer misalignment angle" ;
    amal:units = "rad" ;
int ifirst(spectrumNumber) ;
    ifirst:long_name = "index_of_first_point" ;
    ifirst:description = "Index of first point saved, counted from 1 (not
0)" ;
int ilast(spectrumNumber) ;
    ilast:long_name = "index_of_last_point" ;
    ilast:description = "Index of last point saved, counted from 1 (not
0)" ;
double delta_nu(spectrumNumber) ;
    delta_nu:long_name = "frequency_interval" ;
    delta_nu:description = "Frequency interval between successive points"
;
    delta_nu:units = "/cm" ;
int pointer(spectrumNumber) ;
    pointer:long_name = "data_offset" ;
    pointer:description = "Position of first data point from beginning of
file." ;
    pointer:units = "bytes" ;
int bpw(spectrumNumber) ;
    bpw:long_name = "bytes_per_word" ;
    bpw:description = "Number of bytes per data word. 2 = 2 byte int, 4 =
4 byte real" ;
float zoff(spectrumNumber) ;
    zoff:long_name = "zero_level_offset" ;

```

```

        zoff:description = "Spectrum zero level offset, as fraction of
continuum level (dimensionless)" ;
        float zerr(spectrumNumber) ;
        zerr:long_name = "zero_level_offset_err" ;
        zerr:description = "Uncertainty in spectrum zero level offset
(dimensionless)" ;
        float snr(spectrumNumber) ;
        snr:long_name = "signal_to_noise" ;
        snr:description = "Signal to noise ratio" ;
        float scaleFactor(spectrumNumber) ;
        scaleFactor:long_name = "scale_factor" ;
        scaleFactor:description = "Rescaling factor to convert integer
spectral values to real" ;
        char ApodizFnNam(spectrumNumber, apodizFnNameSize) ;
        ApodizFnNam:long_name = "apodization_function" ;
        ApodizFnNam:description = "Apodization function for spectra. BX =
boxcar (no apodization)" ;
        float t_obs(spectrumNumber) ;
        t_obs:long_name = "observation_temperature" ;
        t_obs:description = "Ambient temperature at observing instrument" ;
        t_obs:units = "degrees_K" ;
        float p_obs(spectrumNumber) ;
        p_obs:long_name = "observation_pressure" ;
        p_obs:description = "Ambient pressure at observing instrument" ;
        p_obs:units = "atm" ;
        float h_obs(spectrumNumber) ;
        h_obs:long_name = "relative_humidity" ;
        h_obs:description = "Ambient relative humidity at observing
instrument" ;
        h_obs:units = "percent" ;
        short specVal(spectrumNumber, spectralPoint) ;
        specVal:long_name = "spectra_data" ;
        specVal:description = "Spectral data. Multiply by scaleFactor for true
values." ;

// global attributes:
        :title = "ATMOS version 3 spectra and runlog for sl3ss13" ;
        :fileCreationDate = "Jun 19 2002 23:31 GMT" ;

```

Data Services

GES DISC Search

The GES DISC provides keyword, spatial, temporal and advanced (event) search and subset services through its online User Interface. Searches will display content items such as Data Collections as well as Documentation, FAQs, Glossary, How-To, and News.

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Appendix

Version 3 CO₂ Spectral Microwindows

These CO₂ windows were used for determining tangent altitudes.

Key for CO₂ isotopomers: CO₂ = (626)CO₂, CO₂-2 = (636)CO₂, CO₂-3 = (628)CO₂, CO₂-4 = (627)CO₂, CO₂-5 = (638)CO₂, CO₂-6 = (637)CO₂, CO₂-7 = (828)CO₂, CO₂-8 = (728)CO₂

Window Center (cm ⁻¹)	Window Width (cm ⁻¹)	Upper Height (km)	Lower Height (km)	Other gases fitted
Filter 1 (600 - 1200 cm ⁻¹)				
686	12	90	60	O ₃
723	26	75	40	H ₂ O O ₃ N ₂ O HCN CO ₂ -3 CO ₂ -4 CO ₂ -5
805	12	50	0	H ₂ O O ₃ CCL ₄ CO ₂ -3 CO ₂ -4 CO ₂ -5
959	24	50	0	H ₂ O O ₃ N ₂ O CO ₂ -3 CO ₂ -4 CO ₂ -5
Filter 12 (600 - 1400 cm ⁻¹)				
686	12	90	60	O ₃
723	26	75	40	H ₂ O O ₃ N ₂ O HCN CO ₂ -3 CO ₂ -4 CO ₂ -5
805	12	50	20	H ₂ O O ₃ CCL ₄ CO ₂ -3 CO ₂ -4 CO ₂ -5
804.9	12	10	0	H ₂ O O ₃ CCL ₄ CO ₂ -3 CO ₂ -4 CO ₂ -5
959	24	50	20	H ₂ O O ₃ N ₂ O CO ₂ -3 CO ₂ -4 CO ₂ -5
958.9	24	10	0	H ₂ O O ₃ N ₂ O CO ₂ -3 CO ₂ -4 CO ₂ -5
1241.5	11	35	0	H ₂ O N ₂ O CH ₄
1257	6	35	0	N ₂ O CH ₄
1273.39	0.5	35	0	N ₂ O CH ₄
1279.24	0.18	35	0	N ₂ O CH ₄

Filter 9 (625 - 2450 cm ⁻¹)				
1241.5	11	35	0	H2O N2O CH4
1257	6	35	0	N2O CH4
1273.39	0.5	35	0	N2O CH4
1279.24	0.18	35	0	N2O CH4
1348.5	11	30	0	H2O N2O CH4 HNO3
1912.5	17	60	25	H2O O3 N2O NO COF2 CO2-3 CO2-5
1944.25	0.3	30	0	H2O
1947.48	0.5	25	0	H2O
1955.5	15	30	0	H2O O3 N2O
2055.5	16	70	35	H2O O3 CO OCS CO2-3 CO2-4 CO2-5
2327.5	11	99	70	H2O CO2-4 CO2-5
2366.5	11	99	70	H2O CO2-4 CO2-5
Filter 2 (1100 - 2000 cm ⁻¹)				
1241.5	11	35	0	H2O N2O CH4
1257	6	35	0	N2O CH4
1273.39	0.5	35	0	N2O CH4
1279.24	0.18	35	0	N2O CH4
1348.5	11	30	0	H2O N2O CH4 HNO3
1912.5	17	90	25	H2O O3 N2O NO COF2 CO2-3 CO2-5
Filter 3 (1580 - 3400 cm ⁻¹)				
1912.5	17	60	25	H2O O3 N2O NO COF2 CO2-3 CO2-5
1944.25	0.3	30	0	H2O
1947.48	0.5	25	0	H2O

1955.5	15	30	0	H2O O3 N2O
2055.5	16	70	35	H2O O3 CO OCS CO2-3 CO2-4 CO2-5
2327.5	11	99	70	H2O CO2-4 CO2-5
2366.5	11	99	70	H2O CO2-4 CO2-5
3158.74	0.5	35	0	H2O O3 CH4
3160.21	0.5	35	0	H2O O3
3161.69	0.5	35	0	H2O O3 CH4 HDO
3194.97	0.5	35	0	H2O O3
3206.25	4.5	38	0	H2O N2O CH4
3318	15	45	15	H2O O3 N2O CH4 HCN C2H2
3339.73	0.9	45	15	H2O N2O HCN C2H2
3349.6	7	60	18	H2O N2O HCN C2H2
3360.5	8	60	18	H2O N2O HCN
Filter 4 (3100 - 4700 cm ⁻¹)				
3158.74	0.5	35	0	H2O O3 CH4
3160.21	0.5	35	0	H2O O3
3161.69	0.5	35	0	H2O O3 CH4 HDO
3194.97	0.5	35	0	H2O O3
3206.25	4.5	38	0	H2O N2O CH4
3318	15	45	15	H2O O3 N2O CH4 HCN C2H2
3339.73	0.9	45	15	H2O N2O HCN C2H2
3349.6	7	60	18	H2O N2O HCN C2H2
3360.5	8	60	18	H2O N2O HCN
3632.5	9.9	99	55	H2O CO2-3 CO2-4

Version 3 Gas Spectral Microwindows

Key for CO₂ isotopomers: CO₂ = (626)CO₂, CO₂-2 = (636)CO₂, CO₂-3 = (628)CO₂, CO₂-4 = (627)CO₂, CO₂-5 = (638)CO₂, CO₂-6 = (637)CO₂, CO₂-7 = (828)CO₂, CO₂-8 = (728)CO₂

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Center (cm ⁻¹)	Width (cm ⁻¹)	Upper Height (km)	Lower Height (km)	Other fitted gases
H2O				
808.26	0.4	40	13	CO ₂ O ₃
825.17	2	30	0	CO ₂ O ₃ CH ₄ HNO ₃ C ₂ H ₆
841.9	1	20	0	CO ₂ O ₃ C ₂ H ₆
881.08	1	10	0	HNO ₃
887.22	0.5	35	10	HNO ₃
1244.14	0.5	65	15	N ₂ O CH ₄ CO ₂ -4 CO ₂ -5
1260.34	0.5	70	25	N ₂ O CH ₄ HDO CO ₂ -4 CO ₂ -5
1271.79	0.5	70	25	N ₂ O CH ₄ CO ₂ -4
1320.06	0.5	70	25	N ₂ O CH ₄ HNO ₃ CO ₂ -4
1333.49	0.5	37	15	N ₂ O CH ₄ HNO ₃ HDO CO ₂ -6
1349.38	0.5	70	27	CH ₄ HNO ₃ HDO CO ₂ -4
1362.6	0.5	70	27	CH ₄ HDO CO ₂ -4
1368.63	0.5	70	30	CH ₄ HDO CO ₂ -4

1373.77	0.4	70	30	CH4 HDO CO2-4
1375.09	0.5	70	35	CH4 SO2 CO2-4
1379.88	0.45	70	35	CH4 SO2 CO2-4 CO2-5
1388.48	0.5	40	13	CH4 SO2 HDO CO2-4 CO2-5
1606.8	0.4	65	25	
1635.65	0.7	80	46	
1637.6	0.8	80	35	
1647.4	0.3	80	35	NO2
1653.3	0.6	85	45	
1669.3	0.6	85	43	
1675.35	0.7	85	43	
1684.83	0.5	85	45	
1695.7	1	85	45	O3 HNO3
1700.65	0.7	80	40	O3 HNO3
1701.15	0.5	80	35	O3 HNO3
1704.45	0.7	80	40	O3 HNO3
1715.15	0.5	80	40	O3 HNO3
1717.4	0.5	80	43	O3 HNO3
1718.5	0.4	80	43	O3 HNO3
1745.78	0.4	73	30	O3
1748.65	0.6	80	40	O3
1770.85	0.3	67	27	O3

1805.14	0.25	67	27	O3
1810.62	0.5	80	35	O3
1829.12	0.4	80	36	O3
1830.12	0.4	80	40	O3
1835.9	0.5	55	20	
1844.3	0.7	80	40	O3
1854.1	0.5	40	10	CO2 O3
1868	0.6	75	33	
1884.56	0.4	70	35	CO2 O3
1904.36	0.4	64	24	O3
1925.1	0.3	33	10	CO2
1926.73	0.5	21	0	CO2 CO2-3 CO2-4
1946.36	0.5	70	27	
1951.13	0.5	35	10	
1959.63	0.5	25	10	
1976.15	0.4	55	15	O3
1983.03	0.7	15	0	CO2 O3 OCS CO2-3
1987.34	0.5	30	10	O3
1999.95	0.7	25	0	CO2 O3 CO OCS
2020.53	0.5	15	0	CO2 O3 OCS CO2-3 CO2-4
2136.67	0.5	10	0	O3 N2O CO CH4
2819.4	0.4	20	0	HCL

2830.01	0.5	20	0	CH4
2879.71	0.5	33	0	CH4 HDO
2936.97	0.5	33	15	CH4 HDO
2984.21	0.5	46	10	O3 CH4 HDO
3029.83	0.35	35	0	O3 CH4 HCL
3064.4	0.5	70	30	O3
3077.95	0.5	70	27	O3 CH4
3079.6	0.6	65	25	O3 CH4
3101.15	0.5	70	30	O3 CH4
3107.33	0.5	60	20	O3 CH4
3110.63	0.45	40	10	O3 CH4
3151.35	0.5	40	15	CO2 CH4
3155.38	0.45	15	0	O3 CH4
3163.83	0.5	33	10	CO2 O3 N2O
3164.2	0.2	20	0	O3 CH4
3174.94	0.33	40	10	CO2 O3 CH4
3182.5	0.5	33	10	CO2 O3 CH4
3197.85	0.5	75	28	O3
3207.32	0.5	25	0	CH4
3210.72	0.5	33	10	CH4
3219.4	0.4	70	30	
3220.01	0.5	30	0	

3222.05	0.4	65	25	CH4
3223.33	0.56	15	0	CO2 CH4 C2H2
3227.46	0.6	65	25	
3231.36	0.5	15	0	
3233.02	0.5	68	21	
3234.62	0.5	27	10	CH4
3237.95	0.5	35	10	CH4
3240.1	0.4	65	25	
3242.6	0.6	27	10	
3244.9	2	70	33	C2H2
3253.95	0.5	70	35	
3254.62	0.25	30	10	
3257.22	0.5	65	25	
3260.43	0.6	65	25	C2H2
3263.8	0.6	20	0	C2H2
3267.24	0.5	20	0	
3272.6	0.9	25	7	CO2 CH3CL
3275.83	0.5	15	0	C2H2
3276.4	1	65	25	
3278.46	0.25	15	0	
3281	1.2	35	0	CO2 HCN C2H2
3285.73	0.5	15	0	CO2

3288.7	1	61	21	CO2 O3 C2H2
3293.7	0.6	15	0	CO2 CO2-4
3307.5	0.9	40	12	CO2 N2O C2H2 CO2-3
3311.1	0.8	15	0	CO2 CH3CL
3317.8	0.6	25	0	CO2 N2O CH3CL
3362.86	0.43	45	10	HDO CO2-3
3363.86	0.6	35	10	CH4 HCN HDO
O3				
770.75	14.5	55	0	H2O CO2
1054.00	16	80	35	CO2
1109.00	16	50	0	H2O
1148.00	16	50	0	H2O N2O
1806.25	0.6	40	0	H2O
1836.4	0.5	40	0	H2O
1840.8	0.5	40	0	H2O
2054.05	0.14	50	0	CO2 OCS
2095.2	0.4	63	30	CO2
2100	1	63	30	CO2
2101.97	0.9	60	30	CO2
2104.5	1	60	30	CO2
2120.55	0.5	65	30	CO2
2123.25	0.55	65	35	

2166.8	0.4	45	0	N2O
2167.8	0.3	45	0	N2O
3172	4	40	0	H2O CO2 N2O CH4
N2O				
1150.00	10	45	0	H2O O3 CH4
1160.00	10	40	0	H2O O3 CH4
1170.00	10	40	0	H2O O3 CH4
1180.00	10	45	0	H2O O3 CH4
1190.00	10	45	0	H2O O3 CH4
1243.76	0.25	40	20	CO2 CH4
1248.67	0.25	45	24	CH4
1251.6	0.25	45	25	CH4
1255.4	0.4	47	27	
1257.35	0.2	47	27	HDO
1258.26	0.14	50	30	
1259.2	0.2	47	27	
1260.15	0.28	47	27	
1262.85	0.3	50	30	CH4
1264.75	0.3	50	30	
1266.57	0.25	50	30	H2O
1270.2	0.4	50	30	
1272.85	0.3	50	30	

1273.73	0.45	50	30	HDO
1278.08	0.35	50	30	
1300.92	0.3	50	30	CH4
1857.49	0.25	27	0	H2O CO2 O3 CO2-3
1861.12	0.25	27	0	H2O O3
1862.02	0.25	27	0	H2O O3 CO2-3
1865.6	0.25	27	0	H2O O3 CO2-3
1871.75	0.25	27	0	H2O CO2 O3 CO2-3
1873.46	0.25	27	0	H2O CO2 O3 CO2-4
1874.33	0.25	27	0	CO2 O3 CO2-4
1886.85	0.25	25	0	H2O CO2 O3 CH4 CO2-5
1888.48	0.5	25	0	H2O CO2 O3 CO2-3 CO2-4 CO2-5
1890.88	0.5	27	0	H2O CO2 O3 CH4 CO2-4 CO2-5
1891.67	0.5	27	0	H2O CO2 O3 HDO CO2-4
1894.03	0.22	27	0	H2O CO2 O3 CO2-4
1896.39	0.25	27	0	H2O CO2 CO2-3 CO2-5
2198.65	0.3	55	35	O3
2199.74	0.2	55	30	
2203.6	0.7	55	30	O3
2204.72	0.3	55	30	O3
2205.72	0.25	55	30	O3
2207.62	0.3	55	30	CO2

2208.57	0.3	55	30	CO2
2242.28	0.5	55	30	CO2
2444.9	0.2	35	20	
2452.68	0.2	35	20	
2481.95	1.5	40	20	CO2 CH4
2535.26	1	40	20	
2542.36	1	40	20	
2543.34	1	40	20	
2544.32	1	45	22	
2575.09	1	45	22	CH4
2576.54	1	45	22	CO2 CH4
2577.26	1	45	22	CH4
2579.36	0.25	45	22	CH4
2581.4	0.25	42	22	CH4
2584.03	0.35	42	22	CO2 CH4
2775.44	0.32	30	0	O3 CH4 HDO CO2-4
2778.34	0.32	36	0	H2O CO2 O3 CH4 H2CO HDO CO2-4
2779.3	0.23	36	0	O3 CH4 HDO CO2-4
2780.25	0.4	30	0	O3 CH4 CO2-4
2782.22	0.4	35	0	O3 CH4 H2CO CO2-4
2793.17	0.28	30	0	O3 CH4 H2CO CO2-4
2806.31	0.5	33	0	CH4 H2CO

2819.15	0.4	30	0	CH4 HDO
3337.65	0.5	35	0	H2O CO2 C2H2
3338.62	0.5	35	0	H2O
3344.4	0.5	35	8	H2O
3347.2	0.5	35	8	H2O
3373.25	1.1	35	15	H2O CO2
3382.3	1.2	35	12	H2O CO2
3388.8	4.8	31	0	H2O CO2
3456.3	6.8	46	12	H2O CO2 HDO
CO				
2045.78	1	40	10	H2O CO2
2111.54	0.8	99	30	CO2 O3
2135.54	0.7	99	20	O3
2139.43	1	99	20	H2O CO2 O3 N2O
2144.03	1	30	0	H2O CO2 O3 CH4
2147.08	0.8	99	20	H2O O3
2156.51	1	20	0	H2O CO2 O3
2158.3	1	99	20	O3 N2O
2183.2	0.4	99	20	O3 N2O
2186.64	0.4	99	20	O3 N2O
2189.9	0.4	99	20	O3 N2O
4180.28	0.26	25	0	H2O HDO

4190.24	0.16	25	0	H2O CH4 HDO
4199.93	0.5	50	0	H2O CH4
4231.68	0.5	99	0	H2O CH4 HDO
4236	0.5	85	0	H2O CH4 HDO
4248.32	0.5	90	0	H2O CH4 HDO
4274.74	0.35	80	0	CH4 HDO
4285.01	0.22	90	0	CH4
4300.66	0.35	85	0	CH4
CH4				
1177.74	0.5	35	0	O3 N2O
1185.06	0.5	35	0	O3 N2O
1190.63	0.65	45	0	O3 N2O HDO
1203.6	0.7	45	0	O3 N2O
1208.7	0.5	35	0	O3 N2O HDO
1221.38	0.5	40	0	O3 N2O HDO
1228.1	1	40	0	CO2 O3 N2O HDO
1231.77	0.5	40	0	CO2 N2O
1233.35	0.4	50	25	
1245.2	0.4	60	30	N2O
1253.3	0.35	60	30	N2O
1255	0.4	60	30	CO2
1256.65	0.3	60	30	CO2 N2O

1259.7	0.7	60	30	N2O
1261.65	0.4	60	30	H2O CO2 N2O
1262.2	0.3	60	30	N2O
1268.98	0.45	65	35	CO2 N2O
1270.78	0.4	65	30	N2O
1271.5	0.4	65	30	H2O N2O HDO
1277.47	0.35	65	30	N2O
1282.6	0.3	70	35	N2O
1287.85	0.2	65	30	
1299.9	0.3	65	30	N2O
1300.2	0.36	65	35	N2O
1303	1	65	30	N2O
1304.98	0.5	65	35	N2O
1306	1	70	35	H2O N2O
1337.3	1	65	30	H2O HNO3 HDO
1341.7	0.8	65	35	H2O HDO
1342.8	0.8	65	30	H2O CO2 HDO
1346.7	1	65	30	H2O CO2
1348	0.6	65	30	
1351.77	0.25	60	30	H2O CO2
1356.3	1	60	30	H2O CO2 CO2-4
2494.35	0.2	43	16	N2O

2525.08	0.35	27	0	N2O CO2-4
2535.96	0.5	30	0	H2O N2O HDO CO2-4 CO2-5
2538.7	0.5	30	0	N2O CO2-4 CO2-5
2553.4	0.5	30	0	N2O HDO
2557.6	0.25	35	0	N2O HDO
2560.24	0.25	35	0	N2O
2561.3	0.45	35	0	N2O HDO
2596.66	0.15	35	0	N2O HDO CO2-4
2605.00	10	40	0	N2O HDO CO2-4 CO2-6
2623.25	0.3	35	0	HDO CO2-4 CO2-5
2631.1	0.2	35	0	H2O HDO CO2-4
2633.6	1	35	0	H2O HDO CO2-4
2639.5	1	40	0	H2O HDO CO2-4 CO2-5
2644.7	0.45	35	0	H2O HDO CO2-4
2650.73	0.25	30	0	HDO CO2-4 CO2-5
2658.6	0.4	33	0	HDO
2657.95	0.9	40	10	CO2 HDO
2662.07	0.5	35	0	HDO CO2-5
2666.8	1	40	10	HDO
2671.4	1	40	0	HDO
2672.14	0.32	35	0	HDO
2675.8	0.8	35	0	HDO

2691.4	1	40	18	HDO
2708.75	0.25	35	0	HDO
2711.6	2	45	18	HDO
2750.9	0.25	30	0	O3 N2O HDO CO2-4
2753.7	0.25	35	0	O3 N2O HDO CO2-4
2808.95	0.6	50	21	HDO
2820.58	0.85	50	18	HDO
2822.5	0.8	55	21	N2O HDO
2835.00	10	50	0	H2O N2O HDO
2858.1	0.9	50	18	
2869.47	0.5	35	0	H2CO HDO
2903.87	0.3	50	18	
2932	1	55	20	
2937.55	1	70	35	H2O
3111.29	0.5	35	0	H2O O3
3123.63	0.14	30	0	H2O O3 HDO
3124.41	0.4	30	0	H2O O3
3130.32	0.4	35	0	H2O O3
3137.67	0.35	35	0	CO2 O3
3141.68	0.35	35	0	H2O
3146.87	0.45	35	0	H2O O3
3153.08	0.5	35	0	H2O CO2 O3

3159.1	0.3	35	0	H2O O3
3168.25	0.25	35	0	H2O CO2 O3
3170.53	0.25	35	0	H2O CO2 O3
3171.5	0.5	35	0	H2O O3
4041	0.8	37	0	H2O HDO
4050	4	35	0	H2O N2O HDO
4174	3	46	12	H2O CO HDO
4184.2	2	55	18	H2O CO HDO
4195	4	50	12	H2O CO HDO
4211.3	2	50	9	H2O HDO
4224	2	53	0	H2O CO
4229.1	3	55	12	H2O CO HDO
4305	4	44	9	H2O CO HDO
4308.5	1.4	50	9	CO
4315	4	55	17	H2O CO
NO				
1842.98	0.6	99	10	H2O O3
1846.6	0.6	99	0	CO2 O3
1849.23	0.2	50	0	
1850.2	0.5	70	11	H2O CO2 O3
1853.74	0.4	99	8	H2O CO2 O3 N2O CO2-3
1856.55	0.6	99	0	H2O O3 N2O

1857.29	0.14	99	0	
1860.77	0.17	99	0	H2O
1863.68	0.4	50	10	H2O CO2 O3 N2O CO2-3
1887.58	0.26	99	0	O3 N2O
1890.71	0.25	99	11	H2O CO2 N2O CO2-3 CO2-4
1893.86	0.5	99	0	H2O CO2 O3 N2O CO2-3
1894.2	0.25	99	0	H2O CO2 O3 N2O HDO CO2-4 CO2-5
1897.03	0.25	99	0	H2O CO2 N2O OCS CO2-3
1887.58	0.26	99	0	O3 N2O
1903.08	0.6	99	0	CO2 O3
1906.72	0.6	99	0	CO2
1909.07	0.6	99	0	CO2
1912.05	0.6	99	0	H2O CO2
1915	0.6	99	0	H2O CO2 O3
1920.72	0.6	99	0	H2O CO2
1924.45	0.2	99	0	
NO2				
1584.25	2.5	99	0	H2O
1589.7	2.4	99	0	H2O CH4
1592.51	0.58	99	0	H2O
1593.35	0.7	99	0	
1595.3	0.4	99	0	

1597.1	0.6	99	0	
1598.01	0.8	99	0	CH4
1599	0.6	99	0	H2O CH4
1602.38	0.4	99	0	H2O
1604.4	0.7	99	0	
1605.82	0.98	99	0	
1606.38	0.24	99	0	
1607.99	0.47	99	0	
1632.00	10	99	0	H2O CH4
2891.14	4.6	99	0	H2O CH4 HDO
2913.1	3.4	99	0	H2O O3 CH4 OCS H2CO HDO
2914.66	0.23	99	0	CH4
2923	6	99	0	H2O O3 CH4 HCL OCS H2CO HDO
HNO3				
868.1	2.2	40	0	OCS
872.9	2.2	40	0	OCS
878.5	2.96	40	0	
1698.44	0.38	40	0	H2O
1701.85	0.7	40	0	H2O O3
1703.11	0.62	40	0	H2O
1705.4	0.8	40	0	H2O
1728.6	0.6	40	0	O3

HF				
3788.1	0.5	60	0	H2O CO2 N2O HDO
3833.66	0.25	70	0	H2O CO2 N2O CH4 HDO
3877.9	0.5	70	0	H2O N2O
3920.31	0.5	65	15	H2O CH4
4000.95	0.45	70	0	H2O CO2 O3 CH4
4038.96	0.5	70	0	H2O CO2 O3 CH4
4109.94	0.5	65	0	H2O CH4 HDO
4142.82	0.2	65	0	H2O CH4
HCl				
2727.85	0.24	99	0	O3
2775.78	0.24	99	0	O3
2819.57	0.14	99	0	
2821.59	0.2	99	0	CH4
2843.66	0.28	99	0	CH4
2904.12	0.36	99	0	O3 CH4
2925.9	0.24	99	0	CH4
2944.9	0.24	99	0	CH4
2963.3	0.78	99	0	CH4
OCS				
2038.96	0.24	30	0	H2O O3 CO2-3 CO2-4 CO2-5
2045.08	0.3	30	0	CO2 O3 CO2-4 CO2-5

2048.02	0.4	30	0	H2O O3 CO2-3 CO2-4 CO2-5
2049.85	1.5	30	0	H2O CO2 O3 CO CO2-4 CO2-5
2052.77	0.3	30	0	H2O O3 CO2-4 CO2-5
H2CO				
2806.95	0.5	15	0	N2O CH4
2831.64	0.25	15	0	N2O CH4 HDO
HOCl				
1221.21	0.46	40	0	O3 CH4 HNO3 COF2 HDO
1227.5	2.25	40	0	N2O CH4 COF2
1232.03	2.54	40	0	CO2 O3 N2O CH4 COF2
1234.66	2.16	40	0	CO2 O3 N2O CH4 COF2
H2O2				
1241.38	0.68	20	0	N2O
1243.59	0.2	20	0	CH4
1247.12	0.43	20	0	N2O CH4
1248.91	0.3	20	0	N2O CH4
1256.05	0.48	20	0	N2O CH4
1261.48	0.11	20	0	
1265.11	0.31	20	0	N2O CH4
1276.66	0.14	20	0	CH4
HNO4				
802.89	2.08	40	0	H2O CO2 O3

N2O5				
1240.006	60	45	20	CO2 O3 N2O CH4 HNO3
ClNO3				
780.2	1.05	40	0	CO2 O3 CO2-3
HCN				
744.45	0.25	25	0	H2O CO2 CH3CL CO2-3 CO2-4
753.3	0.13	25	0	H2O CO2 CO2-5
765.06	0.25	25	0	H2O CO2 C2H2 CO2-3
1423.39	0.25	20	0	H2O CH4 HDO
1426.42	0.18	25	0	H2O CH4 HDO
1429.46	0.18	30	0	H2O CH4 HDO
1432.52	0.18	30	0	H2O CH4 HDO
1438.67	0.2	25	0	H2O CH4
1444.86	0.3	30	0	H2O CH4
1454.19	0.1	20	0	H2O CH4 HDO
3255.13	0.46	30	0	H2O O3 C2H2
3258.44	0.26	30	0	H2O C2H2
3261.7	0.68	30	0	H2O O3 CO2-3
3268.26	0.98	35	0	H2O O3 C2H2 CO2-3
3271.41	0.5	30	0	H2O O3
3274.6	0.3	30	0	H2O CO2 O3 C2H2
3277.7	0.6	35	0	H2O CO2 C2H2

3284.15	0.36	40	0	H2O
3287.2	0.28	35	0	H2O CO2 C2H2
3293.45	0.5	37	0	H2O CO2 C2H2
3302.55	0.3	35	0	H2O C2H2
3331.61	0.71	37	0	H2O CO2 N2O C2H2 CO2-4
3334.3	0.3	35	0	H2O
3337.15	0.3	35	0	H2O N2O
3342.65	0.2	35	0	H2O N2O
3350.6	0.4	37	0	H2O CO2 N2O
3353.23	0.44	40	0	H2O CO2 N2O
3358.47	0.22	35	0	H2O CO2 N2O
3361.09	0.28	30	0	H2O CO2 N2O
CH3Cl				
2966.95	1.5	28	0	H2O O3 CH4 HDO
CF4				
1283.7	3	60	0	N2O CH4 HNO3 ClONO2 C2H2 HDO CO2-4
CCl2F2 (Freon 12)				
921.8	3.6	50	0	H2O CO2 CHF2Cl
1161	3.5	50	0	O3 N2O CH4
CCl3F (Freon 11)				
845.903	1.5	50	0	H2O CO2 HNO3 OCS C2H6
CCl4				

799.4	7	28	0	H2O CO2 O3 HCN
COF2				
773.95	1.9	40	10	CO2 O3
1938	4	40	10	H2O CO2
1951.7	5.8	40	10	H2O CO2
C2H6				
809	2	25	0	H2O CO2 O3 CCL4 CO2-3 CO2-4 CO2-5
822	2	20	0	H2O CO2 O3
2976.85	0.5	20	0	O3 CH4 HDO
2986.69	0.48	20	0	H2O O3 CH4 HDO
C2H2				
766.75	0.36	15	0	H2O CO2 O3
776.09	0.5	15	0	CO2 O3
3250.63	0.53	20	0	O3 CH4
3268.49	0.25	20	0	O3 HCN
3278.18	0.42	20	0	H2O O3 HCN
3295.8	0.4	20	0	H2O CO2 O3 CO2-4
3304.15	0.3	20	0	H2O O3 HDO
3305.05	0.53	20	0	H2O CO2 O3
N2				
2395.96	0.8	40	10	N2O CH4
2403.57	0.8	45	10	CO2 N2O

2411.13	0.8	35	10	CO2 N2O CH4
2418.65	0.8	55	10	N2O
CHCIF2 (Freon 22)				
829.05	0.5	32	0	CO2 O3
HDO				
1344.8	0.8	40	0	CO2 CH4 C2H2 CO2-4
1350.2	0.5	35	0	H2O CO2 CH4 SO2 CO2-4 CO2-6
1354.58	0.25	35	0	CH4 SO2
1358.46	0.25	39	0	H2O CH4 CO2-4
1360.89	0.18	30	0	H2O SO2 CO2-5
1367.57	1	35	0	H2O CO2 CH4 SO2 CO2-4 CO2-5 CO2-6
1369.05	0.15	30	0	H2O CH4 SO2 C2H2
1370.97	0.25	35	0	H2O CO2 CH4 SO2 CO2-4 CO2-5
1372.01	0.5	35	0	H2O CO2 CH4 SO2 CO2-4 CO2-5
1377.17	0.25	30	10	H2O CH4 SO2
1378.35	0.4	15	0	H2O CO2 CH4 SO2 CO2-4 CO2-5
1383.65	0.4	40	0	H2O CO2 CH4 CO2-5
1402.8	0.5	35	0	H2O CO2 CH4 CO2-4 CO2-5
1408.39	0.5	30	0	H2O CO2 CO2-4
1413.64	0.5	30	0	CO2 O3 CH4 CO2-4
1421.65	0.4	35	0	H2O O3 CH4
1422.03	0.5	30	0	O3 CH4

1426.06	0.28	35	0	H2O CH4
1435.25	0.5	35	0	H2O CH4 HCN
1439.7	0.9	30	0	H2O CH4
1447.47	0.5	35	10	H2O CH4
1451.2	0.5	35	0	H2O CH4 HCN
1469.3	0.9	40	0	H2O CH4
1474.11	0.2	30	10	H2O CH4
1475.62	0.31	35	0	H2O CH4
1477.2	0.9	30	10	H2O CH4
1479.96	0.42	30	0	CH4
1484.11	0.25	40	0	H2O CH4
1488.1	0.5	35	10	H2O CH4
1491.2	0.25	35	15	H2O CH4
1494.86	0.29	30	0	H2O CH4
1497.88	0.28	35	12	H2O CH4
1510.95	0.5	35	10	H2O CH4
1512.8	1	35	10	H2O CH4
3761.15	0.5	35	0	H2O CO2 N2O
3764.25	0.4	30	0	H2O CO2 N2O
3767.75	0.25	35	0	H2O N2O CH4
3772.31	0.5	35	0	H2O N2O CH4
3775.66	0.5	25	0	H2O N2O

3776.5	1	25	0	H2O N2O
3778.65	0.25	30	0	H2O CO2 N2O CH4
3787.51	0.5	35	0	H2O CH4
3799.52	0.5	35	0	H2O CO2 N2O CH4
SF6				
948.5	7	35	0	H2O O3
CH3D				
2951.0	1.1	40	0	H2O O3 CH4
2960.43	0.78	40	0	H2O O3 CH4
3061.46	0.68	40	0	H2O O3 CH4
3065.06	0.81	40	0	H2O O3 CH4
3070.80	0.64	40	0	H2O O3 CH4
3072.65	0.72	40	0	O3 CH4
3078.40	0.42	40	0	H2O O3 CH4
3089.53	0.35	40	0	O3 CH4
3091.30	0.73	40	0	H2O O3 CH4
3100.30	0.79	40	0	H2O O3 CH4
3106.41	0.98	40	0	H2O O3 CH4

Median random errors

Median random errors in these files are estimated combined pointing, temperature, signal-to-noise and fitting error given as a fraction. Files are tab-delimited text and organized by spectral filter. Read "F12sr_N2O5_err" as Filter 12 sunrise N2O5 random error, "F12ss_N2O5_err" as Filter 12 sunset N2O5 random error, etc.

Filter 1

Filter 2

Filter 3

Filter 4

Filter 9

Filter 12