Mars Global Surveyor
Thermal Emission Spectrometer

Data Processing User's Guide

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1.0 OVERVIEW

INSTRUMENT DESCRIPTION

The Thermal Emission Spectrometer (TES) investigation is designed to study the surface and atmosphere of Mars using thermal infrared (IR) spectroscopy, together with broadband thermal and solar reflectance radiometry. The specific objectives of the TES experiment are: (i) to determine and map the composition of surface minerals, rocks, and ices; (ii) to study the composition, particle size, and spatial and temporal distribution of atmospheric dust; (iii) to locate water-ice and CO_2 condensate clouds and determine their temperature, height, and condensate abundance; (iv) to study the growth, retreat, and total energy balance of the polar cap deposits; (v) to measure the thermophysical properties of the martian surface materials; and (vi) to characterize the thermal structure and dynamics of the atmosphere. A complete description of the TES instrument is given in (*Christensen et al.*, 1992).

The TES instrument consists of three sub-sections, the primary one being a Michelson interferometer that produces spectra from 1700 to 200 cm^{-1} (~6 to 50 μm), at a spectral sampling of either ~5 or ~10 cm^{-1}. The instrument cycle time, including collection of the interferogram, mirror flyback, and electronic reset, is 2 sec for 10 cm^{-1} ("single scan") operation, and 4 sec for 5 cm^{-1} ("double scan") operation.   The interferometer includes a visible interferometer with a monochromatic source that is used to generate fringes which control the linear drive servo and determine position in the interferogram. This system uses two redundant neon lamps that produce an emission line at 703.2 nm for fringe generation and a continuum that is used for a quasi-white-light source for determination of zero path difference.

The TES instrument returns 143 points in single-scan or 286 points in double-scan mode. The starting spectral sample point can be determined by ground command. In single-scan mode the default PROM sequence for Detector 2 begins at 148.6 cm^{-1} and ends at 1655.9 cm^{-1}. This spectral range was used throughout the aerobraking and Science Phasing Orbits. However, the first five spectra samples in single-scan mode (first 10 in double-scan mode) have very low instrument response and a very low signal-to-noise ratio. Therefore, beginning with the mapping orbits the starting sample in single-scan mode will be changed to 201.6 cm^{-1} (Det. 2), with an ending sample of 1708.9 cm^{-1}. The single-scan data are stored in a 148-point array beginning at 148.6 cm^{-1}

(Det. 2), in which either the first five (mapping phase) or last five (aerobraking phase) samples are set to zero or null. The double-scan data are stored in a 296-point array with corresponding offsets and null values. The wavenumber positions for each detector from sample 1 to 148 (single scan) or sample 1 to 296 (double scan) are given in Table A1.

The finite size and off-axis position of the six detectors results in self-apodization and a spectral shift that is a function of both distance from the axis and optical frequency. The resulting full-width half-maximum (FWHM) value is ~12.5 cm^{-1} for 10 cm^{-1} sampling at 200 cm^{-1} and 15.4 cm^{-1} at 1650 cm^{-1}. For the corner detectors and at the highest frequency (shortest wavelength) there is a significant departure from the ideal line width, giving a worst-case degradation of a FWHM of ~24 cm^{-1}. Because all of the response functions have the same area there is no loss in signal when viewing a smooth continuum scene like Mars. However, there will be a slight loss in contrast of narrow spectral features due to broadening of the spectral width. Because the self-apodization is considerable, the data are used without further apodization. Separate fast fourier transform (FFT) algorithms are used for the center and edge detectors in order to partially compensate for the different spectral shifts introduced into these detectors. These offsets are discussed in Section 2.4.

A pointing mirror capable of rotating 360° provides views to space, both limbs, and to internal, full-aperture thermal and visible calibration targets, as well as image motion compensation. In addition to the spectrometer, the instrument has bore sighted bolometric thermal radiance (4.5 to ~100 μm) and solar reflectance (0.3 to 2.7 μm) channels. Each instrument sub-section has six instantaneous fields of view (IFOV) of ~8.5 mrad that provide a contiguous strip three elements wide with a spatial resolution designed to be 3 km from the final MGS mapping orbit altitude of 350 km. The outputs from all TES channels are digitized at 16 bits, processed, and formatted before being sent to the spacecraft Payload Data Subsystem (PDS). The outputs of the interferometer receive the following processing within the instrument before transfer to the PDS: 1) selectable apodization; 2) Fast Fourier Transformation (FFT) of data from all six interferometer channels; 3) correction for gain and offsets; 4) data editing and aggregation; 5) data compression; and 6) formatting for the PDS.

A separate 1.5 cm diameter reflecting telescope, collimated with the main telescope and using the same pointing mirror, is used for the thermal and visible bolometer channels. These channels have similar 3x2 arrays of detectors, that are bore sighted with the spectrometer array. The optical system consists of a single off-axis

paraboloidal mirror operating at f/8. A reflecting resonant fork chopper operating at 30 Hz is used to separate the solar reflectance and thermal emission bands.

2.0 SPECTROMETER CALIBRATION

2.1 SPECTROMETER ALGORITHM OVERVIEW

The measured spectra can be characterized at each wavenumber by the equation:

$$Vt = (Rt - Ri) * IRF$$

where,

  Vt is the voltage generated by the TES looking at a target
  Rt is the radiance of the target
  Ri is the radiance of the instrument
  IRF is the instrument response function

The radiance of the target can be determined from the above equation once the instrument radiance and the response function are known. These parameters are determined using observations of space and the internal reference surface at planned time intervals. These observations give two equations of the form:

$$Vr = (Rr - Ri) * IRF$$
$$Vs = (Rs - Ri) * IRF$$

where Vr and Vs are the measured voltages viewing space and reference respectively, Rr is derived from the measured temperature of the reference surface, and Rs is the radiance of space ($\sim$0 W cm^{-2} str^{-1} /cm^{-1}). These equations can be solved for the two unknown values, Ri and IRF, giving:

  $$Ri = (Vs*Rr - Vr*Rs) / (Vs - Vr)$$

  $$IRF = Vr / (Rr - Ri)$$

  Or the equivalent:

  $$IRF = Vs / (Rs - Ri)$$

These computed values are then used to compute the radiance of the planet using:

   Rp = (Vp / IRF) + Ri

2.2 SPECTROMETER ALGORITHM VERSION (V.002D)

The simultaneous determination of IRF and Ri requires Space (S) and Reference surface (R) observations spaced closely in time. Typically these are acquired as consecutive or interleaved observations that are termed "SR-pairs". The IRF is assumed to vary slowly, whereas Ri can vary throughout the orbit. Thus, the SR-pairs are only acquired several times per orbit to determine IRF, whereas Space observations are acquired approximately every 3-5 minutes to determine Ri.

It is necessary for the calibration that the required subsets of all the parameters are also available. For example, the spectral values for the planet acquired from detector 5 can only be calibrated if all other parameters are also available for detector 5. Similarly, single-scan planet observations are calibrated using single-scan S and R observations, and double-scan planet observations require double-scan S and R observations.

During the aerobraking and Science Phasing Orbits the thermal state of the TES was not stable. For example, during each spacecraft roll the Sun could directly illuminate the reference surface. Therefore, it was not possible to use long-term averages of IRF and Ri to reduce the noise level present in a single determination of these parameters. In this version of the algorithm the bounding values of IRF and Ri are simply interpolated to determine Rp. The instrument response was not averaged over multiple SR-pairs, nor was the Ri term smoothed to reduce noise.

The following sequence of operations was carried out for spectral calibration:

1) Read the data associated with all the observations under consideration.
2) Find all of the single and double scan SR-pairs and Space observations (S) in the given set of observations.
3) At each SR-pair, compute the radiance of the instrument (Ri), the IRF, and the temperature of the instrument (Ti) (for reference only). For each detector:
   a)   Average the voltage of all the Space observations having the same scan length. This is Vs.

b)   Average the voltage of all the reference observations having the same scan length. This is Vr. Average the reference surface thermistor temperatures (aux_temp[1-3]) to find the average temperature of the reference surface for this SR-pair. This is Tr.

c)   Compute the radiance of the reference surface (Rr) at temperature Tr using the Planck blackbody radiance function.

d)   Compute the radiance of space (Rs) at the temperature of space (3K), using the Planck radiance function.

e)   Compute the radiance of the instrument by substituting the calculated values in the equation:

$$Ri = (Vs*Rr - Vr*Rs) / (Vs - Vr)$$

f)   Compute the instrument brightness temperature (Ti) at each spectral sample by inverting the blackbody radiance function with radiance Ri.

g)   Take the average of the instrument brightness temperatures from spectral samples 50 through 90 (single scan; samples 100-180 double scan), to determine a single best-fit value of Ti.   This is the temperature of this particular detector and is used for information only.

h)   Compute IRF using the equation:

$$IRF = Vs / (Rs - Ri)$$

If IRF equals zero or ∞ for a particular spectral sample, then average the two neighboring spectral samples to compute an IRF value for that spectral sample.

i)   In order to calibrate spectrally masked planet data it is necessary to compute a spectrally averaged Ri and IRF. To do this Vr and Vs are averaged over the spectral range averaged on-board by the TES instrument. Rr and Rs are computed over this spectral range and used with the averaged Vr and Vs to compute an averaged Ri and IRF for each spectral mask. These values are stored separately for use in the planet data calibration.

4) Store the computed values of IRF, Ri, and Ti into one packet, tag it as an SR-pair with its starting sclk_time and pool it among other similar packets for SR-pairs and Space observations in ascending order of their sclk_time. This pool is called the IRF-pool.

5) Replicate the first SR-pair as an additional SR-pair in the beginning of the given set of observations.

6) Replicate the last SR-pair as an additional SR-pair at the end of the given set of observations.

7) At each Space observation, compute Ri. For each detector:
   a) Average the voltage of all the Space spectra in a given set of consecutive spectra having the same scan length. This is Vs.
   b) Compute radiance of space (Rs) at temperature of space (3K) using the Planck radiance function.
   c) Search in the IRF-pool to find the closest SR-pair in each direction. Interpolate over sclk_time between the two bounding SR-pairs to compute the IRF of this Space observation.
   d) Compute the radiance of the instrument using the value of IRF in the equation:

   $$Ri = Rs - (Vs / IRF)$$

   e) Compute the instrument brightness temperature (Ti) at each spectral sample by inverting the blackbody radiance function with radiance Ri.
   f) Take the average of the instrument brightness temperatures from spectral samples 50 through 90 (single scan; samples 100 to 180 double scan) to determine a value of Ti (used for information only).
   g) Store the computed values of Ti and Ri for this Space observation into one packet. Tag this packet as an S with its starting sclk_time and pool it in the IRF-pool in ascending order of its sclk_time.
   h) For spectrally-masked planet data, a spectrally averaged Ri is computed using the interpolated values of the spectrally averaged IRF computed and stored for the bounding S,R pairs.

8) At each planet observation, determine IRF and Ri and compute Rp. For each detector:
   a) Interpolate over sclk_time between the IRF values of the two bounding SR observations to determine the IRF at this planet observation.
   b) Interpolate over sclk_time between the Ri values of the two bounding SR or S points to determine Ri at this planet observation.
   c) If this observation had a spectral mask other than full spectral resolution, average the Ri and IRF corresponding to the mask.
   d) Use IRF and Ri to compute Rp using the equation:

   $$Rp = (Vp / IRF) + Ri.$$

e)   Spectrally masked planet data are calibrated using the appropriate spectrally averaged IRF and Ri. For spectral masks that averaged only two spectral samples the calculated calibrated radiance is stored for both spectral samples. For spectral masks that averaged more than two samples the calibrated radiance is stored at the sample closest to the mid-point of the spectral mask and the calibrated radiance of all other samples in the mask are set to zero.

In Version 002D the data collected using spectral masks that include spectral samples 144-148 (single scan) (~1655-1709 cm^{-1}; Table A2) have not been calibrated and the calibrated radiance is not stored in the TES database. Subsequent versions will include these calibrated data.

9)   Write the calibrated spectra to the database.

2.3 PRECISION AND ACCURACY

The TES spectrometer has a noise equivalent spectral radiance near 1.2 x10^{-8} W cm^{-2} str^{-1} /cm^{-1}. This corresponds to a signal-to-noise ratio (SNR) of 490 at 1000 cm^{-1} (10 μm) viewing a 270K scene. Absolute radiometric accuracy was estimated from pre-launch data to be better than 4 x 10^{-8} W cm^{-2} str^{-1} /cm^{-1}. In flight deviations are discussed in Section 6.

2.4 WAVENUMBER SAMPLE POSITION AND SPECTRAL LINE SHAPE

In an ideal interferometer with an on-axis point detector, the spectral samples are uniformly distributed in wavenumber, and the full-width, half maximum (FWHM) of each sample is simply determined by the optical displacement of the Michelson mirror. The TES uses a neon bulb with a line at 0.7032 μm in the visible interferometer to sample the IR interferometer. The ideal sample spacing of the interferometer is given by:

$$\text{Sample spacing} = \frac{1}{(0.7032 \times 10^{-4} \text{ cm}) * \text{Npts}}$$ (2.1)

where Npts is the number of points in the FFT.

For a large detector, the two beams of the interferometer are not in phase over the entire areal extent of the detector, producing "self-apodization", or widening of the instrument line shape. In addition, the path length of the rays traveling to the off-axis portion of each detector is decreased relative to the optical axis rays by a factor of cos ø, where ø is the angle of the off-axis ray. As a result, the mirror must move farther to produce interference of the off-axis rays, producing a shift of the center frequency of

each spectral sample to a higher apparent wavelength (lower wavenumber) than its true spectral position. All six detectors are offset from the optical axis, producing separate shifts in the spectral line position, shape, and modulation efficiency of each detector.

The TES flight software processes the interferogram data with prime factors FFTs that use a different number of points for the center and edge detectors respectively. These FFT's were selected to produce a slightly different spacing that partially compensates for the different spectral offsets due to self-apodization between the edge and center detectors. The number of points and sample spacing is given in Table 2-1.

Table 2-1.

	Edge Detectors (1,3,4,6)		Center Detectors (2,5)	
	Single Scan	Double Scan	Single Scan	Double Scan
Npts in FFT	1350	2700	1344	2688
Sample Spacing	10.53 cm^{-1}	5.267 cm^{-1}	10.58 cm^{-1}	5.290 cm^{-1}
Sample 1 Position (ideal)	147.47 cm^{-1}	147.47 cm^{-1}	148.13 cm^{-1}	148.13 cm^{-1}
Sample 148 (single; 296 double) Position (ideal)	1695.95 cm^{-1}	1701.22 cm^{-1}	1703.52 cm^{-1}	1708.81 cm^{-1}

 (Note: the sample spacing used to compute the sample position of the archived data is computed in full digital precision using 0.7032 μm in Eq. 2.1.)

A numerical model has been developed by Co-Investigator Stillman Chase to model the self-apodization effects and to determine the true spectral position, FWHM, and spectral line shape of each sample. Interferogram data of Mars were collected immediately after Mars orbit insertion, and the atmospheric CO_2 data were used to verify Chase's model of line shape and position. Because the focal plane is symmetric in the cross-track direction (e.g. detectors 1 and 3 are symmetrically located relative to the optical axis), the position and FWHM are identical for detector pairs 1 and 3 and detector pairs 4 and 6. The sample position offset was calculated for each detector, taking into account the actual prime factor FFT used for each detector. Examples of the offset and the actual sample position calculated with this offset and the actual prime factors FFT used for the double-scan samples 1 and 296 are given in Table 2-2. The full set of sample positions for each detector are tabulated in Table A1 in the Appendix. The sample positions are identical for single and double scans. The modeled full-width half-

maximum values for double scan observations are tabulated in Table A2. The full-width half-maximum values for single scan data are twice the double scan values.

Table 2-2. Double Scan Self-Apodization

	Edge Detectors (1,3)	Center Detector (2)
Sample 1 Self-Apodization Offset	1.19 cm^{-1}	0.44 cm^{-1}
Sample 296 Self-Apodization Offset	14.00 cm^{-1}	5.45 cm^{-1}
Sample 1 (actual)	148.66 cm^{-1}	148.57 cm^{-1}
Sample 296 (actual)	1715.22 cm^{-1}	1714.26 cm^{-1}

3.0 VISIBLE BOLOMETER CALIBRATION

3.1 VISIBLE BOLOMETER ALGORITHM OVERVIEW

The in-flight calibration of the TES visible bolometer is performed for each detector in the following stages.

1) Use observations of the internal TES reference calibration lamp and space to determine the instrument response function (IRF) and the zero-level radiance (background).

2) Convert each target observation to calibrated radiance using the IRF and background.

3) Compute the Lambert albedo using the calibrated radiance, the Sun-Mars distance, and the incidence angle.

3.2 VISIBLE BOLOMETER ALGORITHM VERSION V004.A

1) Read the data associated with all the observations to be calibrated. For each observation this includes:

sclk_time	Spacecraft Clock Time
pnt_view	Pointing Angle View
det_mask	Detector mask

scan_len	Scan length
solar_distance	Solar distance
aux_temps[1-3]	Temperature of the reference surface
temps[1]	Temperature of the detector array
detector	Detector Number
vbol	Raw voltages from visible bolometer
incidence	Solar incidence angle at the target
latitude	Latitude of the target

2) Separate the data into single and double scan modes. Each mode is calibrated separately.

3) Sort the data on ascending sclk_time.

4) Find all distinct groups of space observations (S) in the given set of observations.

   Between each set of bounding calibration lamp observations (collected at ~two day intervals) for each detector:

   a) Find the mode value of all Space observations in this set. This is called the background. This method eliminates erroneously high visible bolometer observations due to scattering off of the TES pointing mirror when the Space view was pointing within 20-40 degrees of the Sun.

   b) Store the background value with the beginning sclk_time of this set in one packet.

5) Find all distinct groups of consecutive visible bolometer reference observations (REFAn) within the given set of observations, where n refers to the calibration lamp number 1 or 2.

   At each REFAn for each detector:

   a) Compute the IRF for each internal lamp observation:

      i) Average the vbol for all consecutive observations within this set of lamp observations.

      ii) Correct vbol for the background signal by subtracting the background from the nearest Space observation to give the lamp_voltage.

iii) Average the temperature of the detector array (temps[1]) to yield detector temperature (det_temp) in °C.

iv) Average the three reference surface temperatures (aux_temps[1-3]) to yield lamp temperature (lamp_temp).

v) Choose the lamp absolute radiance at 28.2 °C (lamp_absolute) for this lamp and scan length (single or double) using the values in the TES Calibration Report.

vi) Select the $\partial R_L/\partial T$ from the for the lamp that was observed.

vii) Compute the actual lamp radiance $(R_L)(T_L)_{cal}$ for each detector at the lamp temperature using lamp_absolute, the variation in lamp radiance (R_L) with temperature $(\partial R_L/\partial T_L,)$ from the TES Calibration Report, and the difference (ΔT_L) between lamp_temp and the internal lamp absolute calibration temperature (28.2°). The lamp radiance equation is:

lamp_radiance = lamp_absolute + ($\partial R_L/\partial T$ * (lamp_temp -28.2)))

vii) Compute IRF using the equation:

IRF = lamp_voltage / lamp_radiance

b) Store the IRF, the background voltage, and the detector temperature in one packet. Tag it as a REFAn packet and pool it among other REFAn packets in ascending order of their beginning sclk_time.

6) Replicate the first REFAn as an additional REFAn in the beginning of the given set.

7) Replicate the last REFAn as an additional REFAn at the end of the given set.

8) At each target (planet) observation, compute the calibrated visible bolometer radiance (cal_vbol). The visible bolometer response function must be corrected at each planet observation to account for changes in the detector temperature between the lamp and planet observations. In order to avoid discrete jumps at each lamp observation, it is necessary to interpolate IRF and the detector temperature between successive lamp views. This baseline IRF is then corrected to the actual IRF at each planet observation using $\partial f/\partial T_D$, and $\partial^2 f/\partial T_D^2$, along with the coefficients in the TES Calibration Report and the detector temperature difference between the baseline lamp observations and the planet observations. This is done by:

a) Search the pool of REFAn observations to find the two bounding observations.

For each detector:

i) Interpolate linearly on sclk_time between this observation and two bounding REFAn times to compute the baseline IRF.

ii) Interpolate linearly on sclk_time between this observation and two bounding REFAn times to get the baseline detector.

iii) Determine $\partial IRF/\partial T$ and $\partial^2 IRF/\partial T^2$ using the calibration coefficients determined pre-launch and the equations:

$\partial IRF/\partial T = 3*af*(detector\_temp)^2 + 2*bf*detector\_temp + cf$

$\partial^2 IRF/\partial T^2 = 6*af*detector\_temp + 2*bf$

where,

af = 'alpha' of the visual bolometer from the TES Calibration Report.

bf = 'beta' of the visual bolometer from the TES Calibration Report.

cf = 'chi' of the visual bolometer from the TES Calibration Report.

iii) Get the actual detector temperature (temps[1]) for this observation.

iv) Calculate ΔT by subtracting the baseline detector temperature value from the actual value.

v) Correct IRF for this detector temperature value by the equation:

Corr_IRF = IRF + $\partial IRF/\partial T *\Delta T + \partial^2 IRF/\partial T^2 * \Delta T^2 / 2!$

vi) Compute cal_vbol using the equation:

cal_vbol = (vbol - background) / Corr_IRF

9) Compute Lambert albedo.

a) Extract incidence angle and solar distance from the database.   Convert solar_distance to Astronomical Units.

b) Compute albedo using the equation:

lambert_alb = cal_vbol / ((Sun_absolute / solar_distance^2) *cos(incidence_angle))

where Sun_absolute is the solar radiance at 1 A.U. integrated over the TES visible bolometer relative spectral response, and is equal to 1.666×10^{-2} W cm^{-2} str^{-1}

Note: The cos(incidence_angle) in the denominator can lead to division by small numbers (including zero), generating highly inaccurate values for the albedo. To avoid this problem, the Lambert albedo is not computed for incidence angles >88°.

10) Write cal_vbol and lambert_alb to the database.

3.3 PRECISION AND ACCURACY

The precision, zero-level offset, and absolute accuracy of the in-flight calibration was determined using data from cruise (test tes_c2a and tes_c9a) and orbits P3 through P460.

The in-flight precision (noise level) of the calibrated radiance measurements was determined using observations of deep space acquired away from Mars during spacecraft rolls prior to and after periapsis.. The internal lamp was not used because its temperature increases if left on for an extended period of time, which changes its brightness level. The data used were acquired on orbits P95 through P100 (no data were available for orbit P99) at a Mars-Sun distance of $2.068*10^8$ km (1.382 A.U.). Only observations well away from Mars, selected by constraining the height of the tangent point of the observation to be >2000 km above the martian surface, were included. The sigma values of the calibrated radiance of the space observations are given in Table 3-1.

Table 3-1

Detector	Sigma (Radiance) $(x10^{-6}$ W cm^{-2} str$^{-1})$	Mean Zero-level Radiance $(x10^{-6}$ W cm^{-2} str$^{-1})$
1	3.62	0.914
2	3.74	1.03
3	3.77	1.07
4	3.73	0.676
5	3.67	0.942
6	3.59	1.00

The 1σ variation in the zero-level radiance is ~3.75 $x10^{-6}$ W cm^{-2} str^{-1} for all six detectors. This value is consistent with the variation in the internal lamp brightness measured pre-flight (1-6 $x10^{-6}$ W cm^{-2} str^{-1}; Table 4-6). A Lambertian surface with a reflectivity of 1.0 would have a radiance of 8.718 $x10^{-3}$ W cm^{-2} str^{-1} at the Mars-Sun distance of these observations, measured at normal incidence angle. The 1σ precision of the visible bolometer calibrated radiance corresponds to a noise-equivalent delta reflectivity (NEΔR) of 0.0004, and is equivalent to an SNR of 2100 for a surface with unit reflectivity.

The zero-level radiance as a function of time is determined by the calibration algorithm using periodic observations of space and the internal lamps to correct for detector response and offset drifts. Table 3-1 gives the mean zero-level radiance of the space observations. This radiance is a factor of nearly four lower than the 1σ variation of the data, indicating that there are no measurable systematic biases introduced into the data by incorrectly removing the variations in detector response and lamp brightness with time and temperature. In addition, no systematic offsets, trends, or discrete changes in value at space or lamp observations were observed in the calibrated radiance of space. From these data it is concluded that the calibration algorithm is accurately accounting for variations in detector response and lamp brightness with time and temperature at the noise level of the instrument. The 3σ accuracy of the zero-level radiance is approximately $\pm 1*10^{-5}$ W cm^{-2} str^{-1} for all six detectors, consistent with the values in Table 3-1.

The data given in Table 3-1 were acquired of a black target (space) with zero signal and therefore do not provide a measure of the true absolute calibration for bright surfaces. This can only be determined by observations of a bright source with known radiance. No surfaces of known brightness exist on Mars to verify the absolute radiance. In addition, because the internal calibration lamps are used in the calibration, they do not provide an independent test of the absolute radiance. However, it is possible to estimate changes in the lamp output with time by comparing the measured lamp voltage, corrected for background, with the pre-flight measurements as a function of lamp and detector temperature.

The pre-flight thermal vacuum tests (albm tests) and the in-flight data from cruise (tests tes_c2 and tes_c9, and orbits 12, 15, 95-98, 100, 222, and 460) indicate a 0-~3% increase in the measured signal for detector temperatures of ~10-15°C, and an increase of ~3-6% near 0°C relative to the pre-flight measurements. This change can be due to a combination of: 1) a change in the alignment of the lamp relative to the detectors; 2) an increase in lamp 1 brightness; 3) a change in the chopper alignment or timing; or 4) an increase in detector response. Of these, a change in alignment is least likely because no decrease in lamp signal was observed for any detector. A possible change in lamp 1 brightness was investigated using the ratio of lamp 1 to lamp 2 for pre-flight and in-flight data. Lamp 2 was observed once during cruise (test tes_c9) and once in orbit early in the mission (orbit P59). The lamp ratio, adjusted for lamp temperature, is unchanged for detectors 3 and 6, is ~1% higher for detectors 1, 4, and 5, and is ~1% lower for detector 2. The change in lamp 1 relative to lamp 2, averaged for all detectors, is ~0.7%, and is essentially constant with temperature. Based on experience at SBRS on the Galileo PPR

instrument, the stability of these lamps is estimated to be ±0.5% on a long-term (years) basis and ±0.15% on a short term (hours) basis.   The ratio of the two TES lamps is consistent with these stability values. Furthermore, both lamps would have to have increased in brightness to account for changes in the lamp 1 signal levels. It is therefore concluded that the changes in lamp 1 signal level are not associated with changes in lamp output.

It is more likely that either the detector response with temperature has varied in flight, which would account for both the variations between detectors and the relatively large changes over temperature, or that the chopper alignment or timing has changed slightly. Neither of these cases will affect the absolute calibration because the detector views both Mars and the lamps with the same chopper and detector characteristics. Indeed, the on-board calibration lamps are specifically intended to remove these effects. It is concluded that the absolute calibration is most likely ~1% relative to the pre-flight calibration of the internal lamps. The relative accuracy from orbit P15 to P460 is ~0.5%.

4.0 THERMAL BOLOMETER CALIBRATION

4.1 THERMAL BOLOMETER ALGORITH OVERVIEW

The measured integrated radiance can be characterized by the following equation:

$$Vt = (Rt - Ri) * IRF$$

where,

   Vt is the voltage generated by the TES looking at a target
   Rt is the integrated radiance of the target
   Ri is the integrated radiance of the instrument
   IRF is the instrument response function

The integrated radiance of the target is determined from the above equation once the instrument radiance and the response function are known. These parameters are determined using observations of space and the internal reference surface at planned time intervals. These observations give two equations of the form:

$$Vr = (Rr - Ri) * IRF$$

$Vs = (Rs - Ri) * IRF$

where Vr and Vs are the measured voltages viewing space and reference respectively, Rr is derived from the measured temperature of the reference surface, and Rs is the integrated radiance of space (~0 W cm-2 str-1). These equations can be solved for the two unknown values, Ri and IRF, giving:

$Ri = (Vs*Rr - Vr*Rs) / (Vs - Vr)$

$IRF = Vr / (Rr - Ri)$
Or:
$IRF = Vs / (Rs - Ri)$

These computed values then are used to compute the radiance of the planet:

$Rp = (Vp / IRF) + Ri$

4.2 THERMAL BOLOMTER ALGORITHM VERSION V001.A

The simultaneous determination of IRF and Ri requires space (S) and reference surface (R) observations spaced closely in time. Typically these are acquired as consecutive or interleaved observations that are termed "SR-pairs". The IRF is assumed to vary slowly, whereas Ri can vary throughout the orbit. Thus, the SR-pairs are only acquired several times per orbit to determine IRF, whereas Space observations are acquired approximately every 3-5 minutes to determine Ri.

Prior to calibration, the weighted integrated radiance as a function of scene temperature is computed by convolving the instrument relative spectral response with the blackbody radiance at each wavenumber from 0 through 2500 with a step of 2 wavenumbers. The relative spectral response of the TES thermal bolometer was determined pre-launch and is given in the TES Calibration Report. The integrated radiance is computed for temperature values from 60K through 400K with a step of 0.01 degrees. A look-up table consisting of two columns: temperature and weighted integrated radiance, is stored in a separate file, and is used to convert brightness temperature (TB) to radiance and radiance to TB.

The following sequence of operations is carried out for spectral calibration:

1)   Read the data associated with all the observations under consideration.

2) Find all of the single and double scan SR-pairs and Space observations (S) in the given set of observations.

3) At each SR-pair, compute the temperature of the instrument (Ti) and IRF. For each detector:

a) Average the voltage of all the Space observations having the same scan length. This is Vs.

b) Average the voltage of all the reference observations having the same scan length. This is Vr. Average the reference surface thermistor temperatures (aux_temp[1-3]) to find the average temperature of the reference surface for this SR-pair. This is Tr.

c) Compute the radiance of the reference surface (Rr) at temperature Tr using the TB-to-radiance look-up table.

d) Assume the radiance of space (Rs) to be equal to zero.

e) Compute IRF using the equation:

$$IRF = Vs / (Rs - Ri)$$

f) Compute the integrated radiance of the instrument by substituting the calculated values in the equation:

$$Ri = (Vs*Rr - Vr*Rs) / (Vs - Vr)$$

g) Compute the instrument brightness temperature of the instrument (Ti) from the radiance Ri using the radiance-to-brightness temperature look-up table.

4) Store the computed values of IRF and Ti into one packet, tag it as an SR-pair with its starting sclk_time and pool it among other similar packets for SR-pairs and Space observations in ascending order of their sclk_time. This pool is called the IRF-pool.

5) Replicate the first SR-pair as an additional SR-pair in the beginning of the given set of observations.

6) Replicate the last SR-pair as an additional SR-pair at the end of the given set of observations.

7) At each set of Space observations, compute Vs. Vs is used to compute the radiance of the instrument (Ri) in the planet caibration using the equation:

$$Ri = Rs - (Vs / IRF)$$

For each detector:

a)   Average the voltage of all the Space observations in a given set of consecutive observations having the same scan length. This is Vs.

b)   Store the value of Vs for this Space observation into one packet, tag this packet as an S with its starting sclk_time, and pool it in ascending order of its sclk_time.

8) At each planet observation compute Rp. For each detector:

a)   Interpolate linearly over sclk_time between the IRF values at the two bounding SR or S observations to determine the IRF at this planet observation.

b)   Interpolate linearly over sclk_time between the Vs values at the two bounding SR or S observations to compute Vs at this planet observation.

c)   Compute Rp from IRF and Vs using:

$$Rp = (\, Vp \, / \, IRF \,) + Ri.$$

Replacing Ri in this equation with $Ri = Rs - (\, Vs \, / \, IRF \,)$ gives:

$$Rp = Rs + (\, Vp - Vs \,) \, / \, IRF$$

d)   Convert Rp to the brightness temperature of the planet (Tp) using the radiance-to-brightness temperature look-up table.

9) Write the brightness temperature to the database.

5.0 SURFACE TEMPERATURE DETERMINATION

A simple algorithm was performed on each TES spectrum in order to estimate the effective surface kinetic temperature using the TES spectrometer data. The primary use of this temperature is for emissivity determination where only a first-order estimate of the surface temperature is required. No attempt is made to model mixtures of surface materials at different kinetic temperatures, nor to remove atmospheric effects.

This algorithm is based on the desire to use the entire spectrum to locate the region with the highest emissivity, where the brightness temperature will provide the closest approximation to the surface kinetic temperature. In practice, both in laboratory measurements and in TES data, the short-wavelength region (<8 μm) often has the highest emissivity. Unfortunately, at low temperatures (<~225 K), the short-wavelength

region of the spectrum has significant noise and measurements in this spectral region are unreliable. Thus, it is necessary to have a flexible algorithm that uses the best available data to estimate surface temperature.

1) Convert the calibrated radiance to brightness temperature at each wavenumber assuming that: a) the emissivity is unity (temp. = TB); and b) the emissivity is 0.97 and dividing the calibrated radiance by this value before determining the brightness temperature (temp. = TB'). Filter the brightness temperatures using a unity-weight filter 7 samples wide to reduce noise effects.

2) Find the maximum brightness temperature over the sample ranges from:

   a) 300 to 1350 cm^{-1}, excluding the region from 500 cm^{-1} to 800 cm^{-1} where atmospheric CO_2 has strong absorptions. This range was selected to include both the long and short wavelength portions of the spectrum, and to include the wavenumber typically with the highest brightness temperature (~1300 cm^{-1}) as determined by both the Mariner 9 IRIS and the preliminary TES data.

   b) 300 to 500 cm^{-1} only. This range covers only the long wavelength portion of the spectrum.

3) If TB is $\geq$ T2 (225 K), set $T_{surface}$ to TB; If TB' is $\leq$ T1 (215 K) set $T_{surface}$ to TB'. Otherwise, provide a smooth transition between these to cases by setting $T_{surface}$ to weighted average of TB and TB'. Weighting is determined by:

   Weight1 = 1 - ((T2-TB) / (T2-T1))

   Weight2 = 1 - ((TB'-T1) / (T2-T1))

   If Weight1 or Weight2 < 0, then they are set to 0.

4) Finally:

   Tsurface = ((TB*Weight1) + (TB'*Weight2)) / (Weight1 + Weight2)

6.0 THERMAL INERTIA DETERMINATION

A method to derive thermal inertia values of the Martian surface from the TES temperature observations has been developed and is fully described in *Mellon, et al.* [2000]. The approach is to match TES temperature observations against thermal model predictions of the surface temperature and brightness temperature, which are functions of thermal inertia and several other factors. Two fields of thermal inertia values are available in the TES dataset: "spectral_thermal_inertia" is derived using the surface kinetic temperature estimated from TES spectral radiance measurements in the 20 micron spectral region; "bolometric_thermal_inertia" is derived using the planetary brightness temperature measured by the thermal bolometer. A general summary of the model is provided below, however, users should obtain the reference mentioned above for full details and discussion of this derivation method.

The numerical thermal model used is similar to that of *Haberle and Jakosky,* [1991], with several enhancements to account for seasonal effects and most of the factors affecting surface temperature variability (e.g. solar heating, thermal radiation to space, carbon dioxide condensation, atmospheric thermal re-radiation, etc.). This model is used to predict surface kinetic and planetary brightness temperatures as a function of seven parameters: local time of day, season, latitude, thermal inertia, albedo, surface pressure, and atmospheric dust opacity. Using Mars appropriate ranges for each parameter, model results are precomputed and stored in a lookup table to be matched with the TES observed temperatures and correlated parameters. The lookup table presents each possible combination of the latter four parameters (thermal inertia, albedo, dust opacity, and surface pressure) binned per every 5 degrees of latitude and accessed through the diurnal and seasonal surface temperatures. During processing, any necessary interpolating between lookup table values employs the fit (quadratic, cubic spline, linear, or log) most appropriate for each parameter.

Each thermal inertia value is determined by matching observed values for the remaining six thermal model parameters and surface temperature to the lookup tables. TES observed surface temperatures and the correlating time and position parameters are available directly from the TES dataset, while the remaining three parameter values are determined from other sources. Albedo values are obtained from published maps with 1/4 degree resolution and 65% surface coverage, based on TES observations [*Christensen*, 1999]. Surface pressure is estimated from 1 degree resolution elevation maps published by MGS-MOLA [*Smith et al.*, 1999], and from a seasonal pressure model

[*Tillman*, 1993].   Dust opacity is estimated to be 0.1 at infrared wavelengths normalized to 6.1 mb.

Three major sources of uncertainty have been recognized: instrument noise, the thermal model, and lookup-table interpolation. Each has been quantitatively evaluated for a representative nighttime surface at 180 K to establish that the maximum total uncertainty from all three sources is 6.0% and 16.9% for the bolometric and spectral thermal inertia, respectively [*Mellon, et al.,* 2000]. The first, uncertainty due to instrument noise in TES measured temperature values, is the primary contribution to the above estimates. A rough estimate of this uncertainty has been used to assign a quality rating for each thermal inertia value available (see DOCUMENT/QUALITY.TXT for more information). The second, uncertainty due to the thermal model performance, has been evaluated through comparison of model results with analytical solutions. The third, uncertainty due to interpolation error, is determined by comparison of direct calculation results with interpolated results. Thermal model performance and interpolation error contribute <2% each to the total uncertainty. Additional uncertainty from the remaining input values, (e.g. dust opacity, albedo, etc.), may contribute to the total uncertainty, but this has not been quantified nor accounted for here.

7.0 ATMOSPHERIC PRODUCT DETERMINATION

7.1 ATMOSPHERIC TEMPERATURE

A method to derive Martian atmospheric temperature profiles from the TES spectra has been developed and is fully described in *Conrath, et al.* [2000]. The approach uses known CO_2 transmittances to find the atmospheric temperature profile that best fits the observed thermal emission measurements of the CO_2 absorption band complex, centered at 667 cm^{-1} (15µm). Results, sampled at 38 pressure levels, are in the "nadir_temperature_profile" field of the ATM table, along with the other ancillary parameters discussed here. A general summary of the algorithm used to generate the profile is provided below, however, users should obtain *Conrath, et al*. [2000] for a full mathematical description and discussion of this method.

As on previous Mars missions, the nadir-view TES CO_2 absorption band measurements are useful for the retrieval of atmospheric thermal structure because of the variation of opacity across the band. Near the band center (667 cm^{-1}), the atmosphere is most opaque and measurements at these frequencies provide information about the upper

atmospheric levels. In the band wings (~624 and ~708 cm^{-1}), the atmosphere is nearly transparent and measurements at these frequencies provide information about the near-surface levels. In this algorithm it is assumed that there is no scattering and that local thermodynamic equilibrium exists at all atmospheric levels. TES (nadir) measured spectral radiance is the sum of the atmosphere attenuated surface emission plus the emission from the integrated atmospheric column. Therefore, by accounting for the surface component with boundary conditions, a temperature profile can be quantitatively derived from the atmospheric component. The temperature profile is obtained by inverting the atmospheric spectrum using an algorithm that includes filtering to reduce the inherent sensitivity to instrument noise.

The TES spectral data used in this analysis are averages of spectra from all six detectors collected while the instrument was nadir looking (i.e. <82 degree emission angle), and are limited to measurements taken between 625.32 and 710.14 cm^{-1}. Values for three boundary conditions are required to model the surface emission component: surface emissivity, surface pressure, and effective surface temperature. Surface emissivity is assumed to be unity for the CO_2 absorption band wavelengths. Surface pressure is calculated using the hydrostatic law (assuming 10 km scale height) and surface elevations from the MGS-MOLA 1/4 degree resolution topographic maps (averaged over the entire 6-detector footprint of TES). Surface pressure adjustments are made for the seasonal CO_2 cycle, but not for local time of day. An effective surface temperature is calculated by defining a continuum for the 667 cm^{-1} CO_2 band as the interpolated average brightness temperature between the two spectral bands: 507.89 - 529.05 cm^{-1} and 804 - 825.31 cm^{-1}. Surface pressure and mean continuum temperature values used in each atmospheric temperature retrieval are available in the fields "surface_pressure" and "co2_continuum_temp" respectively.

Four sources of uncertainty contribute to the total error associated with this algorithm: instrument noise, uncertainty in surface temperature and pressure, assumption of a unit surface emissivity and omission of aerosol opacity, and uncertainty in CO_2 absorption coefficients. Propagation of instrument noise, estimated at about 2.0x10^{-8} W cm^{-2} str^{-1} /cm^{-1}, results in retrieved temperature errors of 2-4 K. Errors from estimates of surface pressure and temperature will affect the lower atmospheric levels, but are negligible above one-pressure scale height. Errors resulting from the assumption of unit surface emissivity and neglect of aerosol opacity are partially compensated by use of the calculated effective surface temperature continuum. Uncertainties in the calculated CO_2 absorption coefficients may contribute systematic atmospheric temperature errors of up to 2 K. Two fields in the ATM table are useful for monitoring the quality of each

atmospheric temperature profile: the "temperature_profile_residual" gives the RMS difference between the final calculated and observed radiance values; the "quality:temperature_profile_rating" gives a qualitative rating for the temperature profile as described in INDEX/QUALITY.TXT.

7.2 ATMOSPHERIC OPACITIES

A method to derive Martian atmospheric aerosol opacity observed in the TES spectra has been developed and is fully described in *Smith, et al.* [2000a]. The approach is to match TES spectral observations against atmospheric radiative transfer models that account for contributions from aerosol opacity, surface temperature, and atmospheric temperature to get an equivalent column-integrated total atmospheric opacity. This opacity is then separated into dust, water-ice, and "surface" components using spectral shape fitting techniques. The resulting contribution to the atmospheric opacity from each component is stored in the ATM table array field "nadir_opacity", and the spectral shapes used in the retrieval calculation are available in DATA/STDSHAPE.TAB. A general summary of the algorithm used to extract atmospheric opacities is provided below, however, users should obtain *Smith, et al.* [2000a] for a full mathematical description and discussion of this method.

Dust and water-ice aerosol opacity can be extracted from TES nadir observations because each spectrum has contributions from the surface emissivity, the aerosol opacity, the surface temperature, and the atmospheric temperature. Two assumptions are made: the only sources of atmospheric opacity are well mixed with the CO_2 gas, and atmospheric aerosols are non-scattering. The method applied here to derive the dust and water-ice opacity involves two steps: first, determine the total atmospheric opacity as a function of wavenumber; second, extract the atmospheric dust and water-ice components from the total opacity calculated in the first step. TES measured radiances are matched against a series of radiative transfer solutions which combine the effects of the opacity range of pure aerosol absorbers, the corresponding atmospheric temperature profile ("nadir_temperature_profile", retrieved as described in the previous section), and the TES measured surface temperature ("brightness_temperature" at ~1300 cm^{-1}). Once model solutions bracket the TES observation, a final total atmospheric opacity value is determined by standard root-finding techniques.

Using the solution from the first step as the "dust opacity" could significantly overestimate the amount of atmospheric dust, since this calculated opacity potentially includes contributions from several sources. Thus, a second step is required to extract the

dust and water-ice components from the total opacity measurement by applying a method of least-square-fitting with selected spectral shapes. Four spectral shapes are fit as a function of wavenumber against the total opacity solution: dust, water-ice, CO_2 hot and isotope bands, and a typical basaltic, non-unit emissivity "surface" spectrum. Final solutions ("nadir_opacity") are restricted to include only those with real physical meaning and low fitting residuals ("nadir_opacity_residual").

Each spectral shape used was carefully chosen to be globally representative of Martian conditions (*Smith, et al.* [2000b], *Bandfield, et. al.* [2000]). However, the water-ice spectral shape employed assumes uniform mixing; this becomes invalid whenever water-ice clouds are stratified. For typical daytime conditions this could result in an overestimate of the water-ice cloud opacity by 20-50%.

Three major sources of uncertainty contribute error to the solutions derived by this method: instrument noise, derived surface and atmospheric temperatures, and the assumption of fixed spectral endmember shapes. The first two sources can each add uncertainties of 0.02 in aerosol opacity for spectra with a typical daytime atmospheric-surface thermal contrast of 20-40 K. The uncertainty due to instrument noise is measured per spectral channel, and thus is minimized in this method by fitting aerosol opacities and spectral shapes over the full range of frequencies measured by TES. The uncertainty due to temperature estimates can be further minimized by restricting the use of aerosol opacities to only those with high thermal contrast (users should select on "co2_continuum_temp" > 220K). Besides the problems inherent with water-ice clouds, the uncertainty due to the chosen spectral shapes is estimated to be 0.03 in aerosol opacity. Including all sources, the total uncertainty for any one aerosol opacity retrieval is estimated to be no greater than 0.05; overall quality of each aerosol opacity retrieved is available in the "quality:atmospheric_opacity_rating" field (see INDEX/QUALITY.TXT).

7.3 DOWNWELLING FLUX

Downwelling flux is calculated using the same radiative transfer algorithms employed in the temperature and aerosol opacity retrievals. Computation of the total downwelling flux as seen from a point on the surface involves integration over height, angle, and frequency. The integration over height is performed from the top of the atmosphere down to the surface. The angular integration is performed over all solid angles in the "upward" hemisphere as viewed from the surface. The integration over frequency is performed over the TES spectral range. Results are provided divided into

two parts: 1) the contribution from the CO_2 gas alone ("co2_downwelling_flux") is available for all TES measurements for which the atmospheric temperature retrieval is successful; 2) the total downwelling flux ("total_downwelling_flux") is evaluated for those cases where the aerosol retrieval is also successful, and therefore, is restricted to daytime observations only. The total downwelling flux includes contributions from both CO_2 gas and aerosols, with the former typically accounting for an estimated 60-80% of the total calculated flux.

8.0 DATA QUALITY/ANOMALIES

8.1 SPECTRAL RINGING

The TES spectra occasionally exhibit a high frequency "ringing" in which the amplitude of the spectrum oscillates from one spectral point to the next. This ringing has been found to occur when there is a large change in scene temperature from one observation to the next. These large temperature variations frequently occur during observations of Mars acquired at large distances where there is a significant change in position on the planet between successive observations. The TES analog electronics are designed to keep the DC (base) level of interferogram centered at zero volts. However, when the radiance of the scene changes, the base level of the interferogram changes and there is a finite time required for the electronics to compensate. The frequency of the TES interferogram information band is 10-100 Hz, so the electronics are designed to pass all information within this band to avoid filtering out signal information. Therefore, the base correction electronics are designed to have a time constant >0.1 seconds to avoid altering the true interferogram spectral information. There are only 0.2 seconds between the end of one interferogram and the start of the next, so if the scene changes temperature rapidly between observations, then the electronics will not have sufficient time to fully recenter the base level of the interferogram before the start of the next scan. In this case the interferogram will still be settling (or rising) toward the base level during the first ~0.1-0.2 seconds of the interferogram scan. This settling results in a discontinuity at the beginning of the scan due to the fact that the first point is significantly greater (or less) than zero. Because this spike occurs at the beginning of the scan, it always produces a sine wave at the highest possible frequency in the transformed spectrum. As a result, a sine wave with a point-to-point variation is superimposed on the data. The interferogram base level can be increasing or decreasing if the temperature of the current scan is higher or lower respectively than the previous scan. Therefore, the phase of the superimposed sine wave can vary by 180°.

An algorithm has been developed to artificially remove the spectral ringing by transforming the spectral data back to frequency and removing the end points of the interferogram. However, this approximation lowers the spectral resolution of the data, and has not been applied to the calibrated spectra on the TES CD-ROMS in this release. A more sophisticated approach is being developed using the measured time constant of the TES electronics to model the settling of the interferogram toward the base level. This correction will be applied in later releases of the TES data.

Up to 80% of the low resolution data acquired away from periapsis can show significant ringing. Even data that do not exhibit a visible ringing can have higher than expected power in the highest frequency, suggesting that some "ringing" is present. The ringing effect should be significantly reduced when the TES is operated in the planned mode during mapping.

8.2 SPECTROMETER NON-ZERO BACKGROUND CALIBRATED RADIANCE

In-flight observations indicate that a small, systematic calibration offset with a magnitude of $\sim 1 \times 10^{-7}$ W cm^{-2} str^{-1} /cm^{-1} is present in the TES data presented on this CD-ROM. This error is primarily due to slight variations in the instrument background energy between observations taken of space at an angle of $-90°$ aft ($0° =$ nadir) for calibration and those viewing the planet at angle other than $-90°$. This error is not significant for surface observations at temperatures above ~ 240 K. However, for observations of the polar caps and the atmosphere above the limbs, where the radiance is low, this error can be significant.

Observations have been collected to characterize the variation in the calibration offset with pointing mirror angle and instrument temperatures. Models are being developed to account for this effect. This correction will be applied in later releases of the TES data.

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APPENDIX

Table A1. Spectrometer Wavenumber Position

Sample Number		Det. 1	Det. 2	Det. 3	Det. 4	Det. 5	Det. 6
Single Scan	Double Scan						
1	1	148.66	148.57	148.66	148.36	148.45	148.36
	2	153.99	153.89	153.99	153.66	153.74	153.66
2	3	159.31	159.21	159.31	158.95	159.06	158.95
	4	164.61	164.50	164.61	164.25	164.35	164.25
3	5	169.94	169.82	169.94	169.58	169.64	169.58
	6	175.23	175.11	175.23	174.87	174.96	174.87
4	7	180.56	180.43	180.56	180.17	180.25	180.17
	8	185.86	185.75	185.86	185.47	185.57	185.47
5	9	191.19	191.04	191.19	190.77	190.86	190.77
	10	196.51	196.36	196.51	196.06	196.15	196.06
6	11	201.81	201.65	201.81	201.36	201.47	201.36
	12	207.14	206.97	207.14	206.69	206.76	206.69
7	13	212.43	212.29	212.43	211.98	212.08	211.98
	14	217.76	217.58	217.76	217.28	217.37	217.28
8	15	223.06	222.90	223.06	222.58	222.66	222.58
	16	228.38	228.19	228.38	227.87	227.98	227.87
9	17	233.68	233.52	233.68	233.17	233.28	233.17
	18	239.01	238.81	239.01	238.50	238.60	238.50
10	19	244.31	244.13	244.31	243.79	243.89	243.79
	20	249.60	249.45	249.60	249.09	249.18	249.09
11	21	254.93	254.74	254.93	254.39	254.50	254.39
	22	260.23	260.06	260.23	259.69	259.79	259.69
12	23	265.55	265.35	265.55	264.98	265.11	264.98
	24	270.85	270.67	270.85	270.28	270.40	270.28
13	25	276.18	275.99	276.18	275.58	275.69	275.58
	26	281.47	281.28	281.47	280.90	281.01	280.90
14	27	286.80	286.60	286.80	286.20	286.30	286.20
	28	292.10	291.89	292.10	291.50	291.62	291.50

15	29	297.42	297.21	297.42	296.79	296.91	296.79
	30	302.72	302.50	302.72	302.09	302.20	302.09
16	31	308.02	307.82	308.02	307.39	307.52	307.39
	32	313.35	313.14	313.35	312.69	312.81	312.69
17	33	318.64	318.43	318.64	317.98	318.13	317.98
	34	323.97	323.75	323.97	323.28	323.42	323.28
18	35	329.27	329.04	329.27	328.58	328.71	328.58
	36	334.59	334.36	334.59	333.87	334.03	333.87
19	37	339.89	339.65	339.89	339.20	339.32	339.20
	38	345.19	344.97	345.19	344.50	344.64	344.50
20	39	350.51	350.30	350.51	349.79	349.93	349.79
	40	355.81	355.59	355.81	355.09	355.23	355.09
21	41	361.14	360.91	361.14	360.39	360.55	360.39
	42	366.44	366.20	366.44	365.68	365.84	365.68
22	43	371.73	371.52	371.73	370.98	371.16	370.98
	44	377.06	376.81	377.06	376.28	376.45	376.28
23	45	382.36	382.13	382.36	381.58	381.74	381.58
	46	387.68	387.45	387.68	386.87	387.06	386.87
24	47	392.98	392.74	392.98	392.17	392.35	392.17
	48	398.28	398.06	398.28	397.47	397.67	397.47
25	49	403.60	403.35	403.60	402.76	402.96	402.76
	50	408.90	408.67	408.90	408.09	408.25	408.09
26	51	414.23	413.96	414.23	413.39	413.57	413.39
	52	419.52	419.28	419.52	418.68	418.86	418.68
27	53	424.85	424.60	424.85	423.98	424.18	423.98
	54	430.15	429.89	430.15	429.28	429.47	429.28
28	55	435.45	435.21	435.45	434.57	434.76	434.57
	56	440.77	440.50	440.77	439.87	440.08	439.87
29	57	446.07	445.82	446.07	445.17	445.37	445.17
	58	451.40	451.14	451.40	450.47	450.69	450.47
30	59	456.69	456.43	456.69	455.76	455.98	455.76
	60	462.02	461.75	462.02	461.06	461.27	461.06
31	61	467.32	467.05	467.32	466.36	466.59	466.36
	62	472.64	472.37	472.64	471.65	471.89	471.65
32	63	477.94	477.66	477.94	476.95	477.21	476.95
	64	483.24	482.98	483.24	482.25	482.50	482.25

33	65	488.56	488.30	488.56	487.54	487.79	487.54
	66	493.86	493.59	493.86	492.84	493.11	492.84
34	67	499.19	498.91	499.19	498.17	498.40	498.17
	68	504.49	504.20	504.49	503.47	503.69	503.47
35	69	509.81	509.52	509.81	508.76	509.01	508.76
	70	515.11	514.84	515.11	514.06	514.30	514.06
36	71	520.41	520.13	520.41	519.36	519.62	519.36
	72	525.73	525.45	525.73	524.65	524.91	524.65
37	73	531.03	530.74	531.03	529.95	530.20	529.95
	74	536.36	536.06	536.36	535.25	535.52	535.25
38	75	541.65	541.35	541.65	540.54	540.81	540.54
	76	546.98	546.67	546.98	545.84	546.13	545.84
39	77	552.28	551.99	552.28	551.14	551.42	551.14
	78	557.61	557.28	557.61	556.43	556.71	556.43
40	79	562.90	562.60	562.90	561.73	562.03	561.73
	80	568.23	567.89	568.23	567.03	567.32	567.03
41	81	573.53	573.21	573.53	572.36	572.64	572.36
	82	578.85	578.50	578.85	577.65	577.93	577.65
42	83	584.15	583.82	584.15	582.95	583.22	582.95
	84	589.48	589.15	589.48	588.25	588.55	588.25
43	85	594.77	594.44	594.77	593.54	593.84	593.54
	86	600.07	599.76	600.07	598.84	599.16	598.84
44	87	605.40	605.05	605.40	604.14	604.45	604.14
	88	610.69	610.37	610.69	609.43	609.74	609.43
45	89	616.02	615.66	616.02	614.73	615.06	614.73
	90	621.32	620.98	621.32	620.03	620.35	620.03
46	91	626.65	626.30	626.65	625.32	625.67	625.32
	92	631.94	631.59	631.94	630.65	630.96	630.65
47	93	637.27	636.91	637.27	635.95	636.25	635.95
	94	642.57	642.20	642.57	641.25	641.57	641.25
48	95	647.86	647.52	647.86	646.54	646.86	646.54
	96	653.19	652.81	653.19	651.84	652.18	651.84
49	97	658.49	658.13	658.49	657.14	657.47	657.14
	98	663.81	663.42	663.81	662.43	662.76	662.43
50	99	669.11	668.74	669.11	667.73	668.08	667.73
	100	674.44	674.06	674.44	673.03	673.37	673.03

51	101	679.74	679.35	679.74	678.32	678.69	678.32
	102	685.06	684.67	685.06	683.62	683.98	683.62
52	103	690.36	689.96	690.36	688.95	689.27	688.95
	104	695.66	695.28	695.66	694.25	694.59	694.25
53	105	700.98	700.57	700.98	699.54	699.88	699.54
	106	706.28	705.90	706.28	704.84	705.20	704.84
54	107	711.61	711.22	711.61	710.14	710.50	710.14
	108	716.90	716.51	716.90	715.43	715.79	715.43
55	109	722.23	721.83	722.23	720.73	721.11	720.73
	110	727.53	727.12	727.53	726.03	726.40	726.03
56	111	732.82	732.44	732.82	731.32	731.72	731.32
	112	738.15	737.76	738.15	736.62	737.01	736.62
57	113	743.45	743.05	743.45	741.95	742.30	741.95
	114	748.78	748.37	748.78	747.24	747.62	747.24
58	115	754.07	753.66	754.07	752.54	752.91	752.54
	116	759.37	758.98	759.37	757.84	758.23	757.84
59	117	764.70	764.27	764.70	763.14	763.52	763.14
	118	769.99	769.59	769.99	768.43	768.81	768.43
60	119	775.32	774.91	775.32	773.73	774.13	773.73
	120	780.62	780.20	780.62	779.03	779.42	779.03
61	121	785.94	785.52	785.94	784.32	784.74	784.32
	122	791.24	790.81	791.24	789.62	790.03	789.62
62	123	796.54	796.13	796.54	794.92	795.32	794.92
	124	801.86	801.42	801.86	800.24	800.64	800.24
63	125	807.16	806.74	807.16	805.54	805.93	805.54
	126	812.49	812.06	812.49	810.84	811.25	810.84
64	127	817.79	817.35	817.79	816.13	816.54	816.13
	128	823.11	822.68	823.11	821.43	821.83	821.43
65	129	828.41	827.97	828.41	826.73	827.16	826.73
	130	833.71	833.29	833.71	832.03	832.45	832.03
66	131	839.03	838.58	839.03	837.32	837.77	837.32
	132	844.33	843.90	844.33	842.62	843.06	842.62
67	133	849.66	849.22	849.66	847.92	848.35	847.92
	134	854.95	854.51	854.95	853.21	853.67	853.21
68	135	860.25	859.83	860.25	858.51	858.96	858.51
	136	865.58	865.12	865.58	863.81	864.28	863.81

69	137	870.88	870.44	870.88	869.10	869.57	869.10
	138	876.20	875.73	876.20	874.43	874.86	874.43
70	139	881.50	881.05	881.50	879.73	880.18	879.73
	140	886.80	886.37	886.80	885.03	885.47	885.03
71	141	892.12	891.66	892.12	890.32	890.79	890.32
	142	897.42	896.98	897.42	895.62	896.08	895.62
72	143	902.75	902.27	902.75	900.92	901.37	900.92
	144	908.04	907.59	908.04	906.21	906.69	906.21
73	145	913.37	912.88	913.37	911.51	911.98	911.51
	146	918.67	918.20	918.67	916.81	917.27	916.81
74	147	923.96	923.49	923.96	922.10	922.59	922.10
	148	929.29	928.81	929.29	927.40	927.88	927.40
75	149	934.59	934.13	934.59	932.70	933.20	932.70
	150	939.92	939.43	939.92	937.99	938.49	937.99
76	151	945.21	944.75	945.21	943.32	943.79	943.32
	152	950.51	950.04	950.51	948.62	949.11	948.62
77	153	955.84	955.36	955.84	953.92	954.40	953.92
	154	961.13	960.65	961.13	959.21	959.72	959.21
78	155	966.46	965.97	966.46	964.51	965.01	964.51
	156	971.76	971.26	971.76	969.81	970.30	969.81
79	157	977.08	976.58	977.08	975.10	975.62	975.10
	158	982.38	981.90	982.38	980.40	980.91	980.40
80	159	987.68	987.19	987.68	985.70	986.23	985.70
	160	993.01	992.51	993.01	990.99	991.52	990.99
81	161	998.30	997.80	998.30	996.29	996.81	996.29
	162	1003.63	1003.12	1003.63	1001.59	1002.13	1001.59
82	163	1008.93	1008.41	1008.93	1006.88	1007.42	1006.88
	164	1014.22	1013.73	1014.22	1012.18	1012.74	1012.18
83	165	1019.55	1019.05	1019.55	1017.48	1018.03	1017.48
	166	1024.85	1024.34	1024.85	1022.78	1023.32	1022.78
84	167	1030.17	1029.66	1030.17	1028.10	1028.64	1028.10
	168	1035.47	1034.95	1035.47	1033.40	1033.93	1033.40
85	169	1040.77	1040.27	1040.77	1038.70	1039.25	1038.70
	170	1046.09	1045.56	1046.09	1043.99	1044.54	1043.99
86	171	1051.39	1050.88	1051.39	1049.29	1049.83	1049.29
	172	1056.72	1056.17	1056.72	1054.59	1055.15	1054.59

87	173	1062.01	1061.49	1062.01	1059.88	1060.44	1059.88
	174	1067.34	1066.82	1067.34	1065.18	1065.76	1065.18
88	175	1072.64	1072.11	1072.64	1070.48	1071.06	1070.48
	176	1077.94	1077.43	1077.94	1075.77	1076.35	1075.77
89	177	1083.26	1082.72	1083.26	1081.07	1081.67	1081.07
	178	1088.56	1088.04	1088.56	1086.37	1086.96	1086.37
90	179	1093.89	1093.33	1093.89	1091.67	1092.25	1091.67
	180	1099.18	1098.65	1099.18	1096.99	1097.57	1096.99
91	181	1104.48	1103.97	1104.48	1102.29	1102.86	1102.29
	182	1109.81	1109.26	1109.81	1107.59	1108.18	1107.59
92	183	1115.10	1114.58	1115.10	1112.88	1113.47	1112.88
	184	1120.40	1119.87	1120.40	1118.18	1118.76	1118.18
93	185	1125.73	1125.19	1125.73	1123.48	1124.08	1123.48
	186	1131.03	1130.48	1131.03	1128.77	1129.37	1128.77
94	187	1136.35	1135.80	1136.35	1134.07	1134.69	1134.07
	188	1141.65	1141.12	1141.65	1139.37	1139.98	1139.37
95	189	1146.95	1146.41	1146.95	1144.66	1145.27	1144.66
	190	1152.27	1151.73	1152.27	1149.96	1150.59	1149.96
96	191	1157.57	1157.02	1157.57	1155.26	1155.88	1155.26
	192	1162.90	1162.34	1162.90	1160.56	1161.20	1160.56
97	193	1168.19	1167.63	1168.19	1165.85	1166.49	1165.85
	194	1173.49	1172.95	1173.49	1171.15	1171.78	1171.15
98	195	1178.82	1178.24	1178.82	1176.48	1177.10	1176.48
	196	1184.11	1183.57	1184.11	1181.77	1182.39	1181.77
99	197	1189.44	1188.89	1189.44	1187.07	1187.72	1187.07
	198	1194.74	1194.18	1194.74	1192.37	1193.01	1192.37
100	199	1200.04	1199.50	1200.04	1197.66	1198.30	1197.66
	200	1205.36	1204.79	1205.36	1202.96	1203.62	1202.96
101	201	1210.66	1210.11	1210.66	1208.26	1208.91	1208.26
	202	1215.99	1215.40	1215.99	1213.56	1214.23	1213.56
102	203	1221.28	1220.72	1221.28	1218.85	1219.52	1218.85
	204	1226.58	1226.01	1226.58	1224.15	1224.81	1224.15
103	205	1231.91	1231.33	1231.91	1229.45	1230.13	1229.45
	206	1237.20	1236.65	1237.20	1234.74	1235.42	1234.74
104	207	1242.53	1241.94	1242.53	1240.04	1240.74	1240.04
	208	1247.83	1247.26	1247.83	1245.34	1246.03	1245.34

105	209	1253.13	1252.55	1253.13	1250.66	1251.32	1250.66
	210	1258.45	1257.87	1258.45	1255.96	1256.64	1255.96
106	211	1263.75	1263.16	1263.75	1261.26	1261.93	1261.26
	212	1269.08	1268.48	1269.08	1266.55	1267.25	1266.55
107	213	1274.37	1273.77	1274.37	1271.85	1272.54	1271.85
	214	1279.67	1279.09	1279.67	1277.15	1277.83	1277.15
108	215	1285.00	1284.38	1285.00	1282.45	1283.15	1282.45
	216	1290.29	1289.70	1290.29	1287.74	1288.44	1287.74
109	217	1295.62	1295.02	1295.62	1293.04	1293.76	1293.04
	218	1300.92	1300.32	1300.92	1298.34	1299.05	1298.34
110	219	1306.21	1305.64	1306.21	1303.63	1304.34	1303.63
	220	1311.54	1310.93	1311.54	1308.93	1309.67	1308.93
111	221	1316.84	1316.25	1316.84	1314.23	1314.96	1314.23
	222	1322.17	1321.54	1322.17	1319.52	1320.25	1319.52
112	223	1327.46	1326.86	1327.46	1324.82	1325.57	1324.82
	224	1332.76	1332.15	1332.76	1330.12	1330.86	1330.12
113	225	1338.09	1337.47	1338.09	1335.41	1336.18	1335.41
	226	1343.38	1342.79	1343.38	1340.71	1341.47	1340.71
114	227	1348.71	1348.08	1348.71	1346.01	1346.76	1346.01
	228	1354.01	1353.40	1354.01	1351.31	1352.08	1351.31
115	229	1359.30	1358.69	1359.30	1356.63	1357.37	1356.63
	230	1364.63	1364.01	1364.63	1361.93	1362.69	1361.93
116	231	1369.93	1369.30	1369.93	1367.23	1367.98	1367.23
	232	1375.25	1374.62	1375.25	1372.52	1373.27	1372.52
117	233	1380.55	1379.91	1380.55	1377.82	1378.59	1377.82
	234	1385.88	1385.23	1385.88	1383.12	1383.88	1383.12
118	235	1391.18	1390.55	1391.18	1388.41	1389.17	1388.41
	236	1396.47	1395.84	1396.47	1393.71	1394.49	1393.71
119	237	1401.80	1401.16	1401.80	1399.01	1399.78	1399.01
	238	1407.10	1406.45	1407.10	1404.31	1405.10	1404.31
120	239	1412.42	1411.77	1412.42	1409.60	1410.39	1409.60
	240	1417.72	1417.06	1417.72	1414.90	1415.68	1414.90
121	241	1423.05	1422.39	1423.05	1420.20	1421.00	1420.20
	242	1428.34	1427.68	1428.34	1425.49	1426.30	1425.49
122	243	1433.64	1433.00	1433.64	1430.79	1431.62	1430.79
	244	1438.97	1438.32	1438.97	1436.09	1436.91	1436.09

123	245	1444.27	1443.61	1444.27	1441.38	1442.20	1441.38
	246	1449.59	1448.93	1449.59	1446.68	1447.52	1446.68
124	247	1454.89	1454.22	1454.89	1451.98	1452.81	1451.98
	248	1460.22	1459.54	1460.22	1457.27	1458.13	1457.27
125	249	1465.51	1464.83	1465.51	1462.57	1463.42	1462.57
	250	1470.81	1470.15	1470.81	1467.87	1468.71	1467.87
126	251	1476.14	1475.44	1476.14	1473.17	1474.03	1473.17
	252	1481.43	1480.76	1481.43	1478.49	1479.32	1478.49
127	253	1486.76	1486.05	1486.76	1483.79	1484.61	1483.79
	254	1492.06	1491.37	1492.06	1489.09	1489.93	1489.09
128	255	1497.38	1496.69	1497.38	1494.38	1495.22	1494.38
	256	1502.68	1501.98	1502.68	1499.68	1500.54	1499.68
129	257	1508.01	1507.30	1508.01	1504.98	1505.83	1504.98
	258	1513.31	1512.59	1513.31	1510.27	1511.12	1510.27
130	259	1518.63	1517.91	1518.63	1515.57	1516.44	1515.57
	260	1523.93	1523.20	1523.93	1520.87	1521.73	1520.87
131	261	1529.26	1528.52	1529.26	1526.16	1527.05	1526.16
	262	1534.55	1533.81	1534.55	1531.46	1532.34	1531.46
132	263	1539.88	1539.14	1539.88	1536.76	1537.63	1536.76
	264	1545.18	1544.43	1545.18	1542.06	1542.96	1542.06
133	265	1550.50	1549.75	1550.50	1547.35	1548.25	1547.35
	266	1555.80	1555.07	1555.80	1552.65	1553.57	1552.65
134	267	1561.13	1560.36	1561.13	1557.95	1558.86	1557.95
	268	1566.43	1565.68	1566.43	1563.24	1564.15	1563.24
135	269	1571.75	1570.97	1571.75	1568.54	1569.47	1568.54
	270	1577.05	1576.29	1577.05	1573.84	1574.76	1573.84
136	271	1582.38	1581.58	1582.38	1579.13	1580.08	1579.13
	272	1587.67	1586.90	1587.67	1584.43	1585.37	1584.43
137	273	1593.00	1592.19	1593.00	1589.73	1590.66	1589.73
	274	1598.30	1597.51	1598.30	1595.03	1595.98	1595.03
138	275	1603.62	1602.80	1603.62	1600.32	1601.27	1600.32
	276	1608.92	1608.12	1608.92	1605.62	1606.59	1605.62
139	277	1614.25	1613.41	1614.25	1610.92	1611.88	1610.92
	278	1619.54	1618.73	1619.54	1616.21	1617.17	1616.21
140	279	1624.87	1624.05	1624.87	1621.51	1622.49	1621.51
	280	1630.17	1629.34	1630.17	1626.81	1627.78	1626.81

141	281	1635.50	1634.66	1635.50	1632.10	1633.07	1632.10
	282	1640.82	1639.95	1640.82	1637.40	1638.39	1637.40
142	283	1646.12	1645.27	1646.12	1642.70	1643.68	1642.70
	284	1651.45	1650.56	1651.45	1647.99	1649.00	1647.99
143	285	1656.74	1655.89	1656.74	1653.29	1654.29	1653.29
	286	1662.07	1661.18	1662.07	1658.59	1659.58	1658.59
144	287	1667.40	1666.50	1667.40	1663.89	1664.91	1663.89
	288	1672.69	1671.79	1672.69	1669.15	1670.20	1669.15
145	289	1678.02	1677.11	1678.02	1674.45	1675.52	1674.45
	290	1683.32	1682.40	1683.32	1679.75	1680.81	1679.75
146	291	1688.64	1687.72	1688.64	1685.04	1686.10	1685.04
	292	1693.97	1693.04	1693.97	1690.34	1691.42	1690.34
147	293	1699.27	1698.33	1699.27	1695.64	1696.71	1695.64
	294	1704.60	1703.65	1704.60	1700.93	1702.03	1700.93
148	295	1709.92	1708.94	1709.92	1706.23	1707.32	1706.23
	296	1715.22	1714.26	1715.22	1711.53	1712.61	1711.53

Table A2. Spectrometer Line Shape. Full-width Half-maximum. Double Scan.

Note: Single scan full-width half-maximum values can be estimated by doubling the corresponding double scan value. Use the first and second columns of Table A1 to determine the correspondence between single and double scans.

Example: single scan, channel 100, Detector 2 FWHM ≈ [6.93 * 2]

Sample Number Double Scan	Det. 1	Det. 2	Det. 3	Det. 4	Det. 5	Det. 6
1	6.33	6.24	6.33	6.30	6.24	6.30
2	6.33	6.24	6.33	6.30	6.21	6.30
3	6.33	6.24	6.33	6.33	6.24	6.33
4	6.33	6.27	6.33	6.33	6.24	6.33
5	6.36	6.24	6.36	6.33	6.21	6.33
6	6.33	6.27	6.33	6.33	6.24	6.33
7	6.36	6.27	6.36	6.33	6.24	6.33
8	6.36	6.27	6.36	6.33	6.24	6.33
9	6.36	6.27	6.36	6.33	6.24	6.33
10	6.39	6.27	6.39	6.33	6.27	6.33
11	6.36	6.27	6.36	6.33	6.24	6.33
12	6.39	6.27	6.39	6.36	6.27	6.36
13	6.36	6.27	6.36	6.36	6.27	6.36
14	6.39	6.27	6.39	6.36	6.27	6.36
15	6.36	6.30	6.36	6.36	6.27	6.36
16	6.39	6.27	6.39	6.36	6.27	6.36
17	6.39	6.30	6.39	6.39	6.27	6.39
18	6.39	6.30	6.39	6.39	6.27	6.39
19	6.39	6.30	6.39	6.39	6.27	6.39
20	6.39	6.30	6.39	6.39	6.27	6.39
21	6.39	6.30	6.39	6.36	6.30	6.36
22	6.39	6.30	6.39	6.36	6.27	6.36
23	6.39	6.33	6.39	6.39	6.30	6.39
24	6.42	6.30	6.42	6.39	6.30	6.39
25	6.42	6.33	6.42	6.39	6.27	6.39
26	6.42	6.33	6.42	6.39	6.30	6.39

27	6.42	6.33	6.42	6.39	6.30	6.39
28	6.42	6.33	6.42	6.39	6.30	6.39
29	6.45	6.33	6.45	6.39	6.30	6.39
30	6.42	6.33	6.42	6.42	6.30	6.42
31	6.45	6.33	6.45	6.42	6.30	6.42
32	6.45	6.33	6.45	6.42	6.30	6.42
33	6.45	6.33	6.45	6.42	6.30	6.42
34	6.45	6.36	6.45	6.42	6.30	6.42
35	6.48	6.33	6.48	6.42	6.33	6.42
36	6.45	6.36	6.45	6.42	6.30	6.42
37	6.48	6.33	6.48	6.45	6.33	6.45
38	6.48	6.36	6.48	6.45	6.33	6.45
39	6.48	6.36	6.48	6.45	6.30	6.45
40	6.48	6.36	6.48	6.45	6.33	6.45
41	6.51	6.36	6.51	6.42	6.30	6.42
42	6.48	6.36	6.48	6.42	6.33	6.42
43	6.51	6.36	6.51	6.42	6.33	6.42
44	6.51	6.36	6.51	6.42	6.33	6.42
45	6.51	6.36	6.51	6.45	6.33	6.45
46	6.51	6.36	6.51	6.45	6.33	6.45
47	6.54	6.39	6.54	6.45	6.33	6.45
48	6.51	6.36	6.51	6.45	6.33	6.45
49	6.54	6.39	6.54	6.45	6.33	6.45
50	6.57	6.36	6.57	6.45	6.33	6.45
51	6.54	6.39	6.54	6.45	6.33	6.45
52	6.57	6.39	6.57	6.48	6.33	6.48
53	6.57	6.39	6.57	6.48	6.33	6.48
54	6.60	6.39	6.60	6.48	6.36	6.48
55	6.57	6.39	6.57	6.48	6.33	6.48
56	6.60	6.39	6.60	6.51	6.36	6.51
57	6.63	6.42	6.63	6.51	6.33	6.51
58	6.60	6.39	6.60	6.51	6.33	6.51
59	6.63	6.39	6.63	6.54	6.36	6.54
60	6.63	6.42	6.63	6.54	6.33	6.54
61	6.66	6.39	6.66	6.54	6.36	6.54
62	6.66	6.42	6.66	6.54	6.36	6.54

63	6.66	6.39	6.66	6.54	6.33	6.54
64	6.69	6.42	6.69	6.54	6.36	6.54
65	6.66	6.42	6.66	6.57	6.33	6.57
66	6.69	6.42	6.69	6.57	6.36	6.57
67	6.72	6.42	6.72	6.57	6.36	6.57
68	6.72	6.42	6.72	6.57	6.36	6.57
69	6.72	6.42	6.72	6.57	6.36	6.57
70	6.72	6.45	6.72	6.60	6.33	6.60
71	6.75	6.42	6.75	6.60	6.36	6.60
72	6.75	6.45	6.75	6.60	6.36	6.60
73	6.75	6.42	6.75	6.60	6.36	6.60
74	6.78	6.42	6.78	6.60	6.36	6.60
75	6.81	6.45	6.81	6.63	6.36	6.63
76	6.78	6.42	6.78	6.63	6.36	6.63
77	6.81	6.45	6.81	6.63	6.36	6.63
78	6.84	6.45	6.84	6.63	6.36	6.63
79	6.84	6.45	6.84	6.63	6.36	6.63
80	6.84	6.45	6.84	6.66	6.39	6.66
81	6.84	6.45	6.84	6.66	6.36	6.66
82	6.87	6.45	6.87	6.69	6.36	6.69
83	6.90	6.48	6.90	6.69	6.39	6.69
84	6.87	6.45	6.87	6.69	6.36	6.69
85	6.90	6.48	6.90	6.72	6.39	6.72
86	6.93	6.48	6.93	6.72	6.36	6.72
87	6.90	6.48	6.90	6.72	6.36	6.72
88	6.93	6.48	6.93	6.72	6.39	6.72
89	6.96	6.45	6.96	6.75	6.36	6.75
90	6.96	6.48	6.96	6.75	6.39	6.75
91	6.96	6.48	6.96	6.75	6.39	6.75
92	6.99	6.48	6.99	6.75	6.39	6.75
93	6.99	6.48	6.99	6.78	6.39	6.78
94	7.02	6.48	7.02	6.78	6.36	6.78
95	6.99	6.48	6.99	6.78	6.39	6.78
96	7.02	6.51	7.02	6.78	6.39	6.78
97	7.05	6.48	7.05	6.78	6.39	6.78
98	7.05	6.51	7.05	6.81	6.39	6.81

99	7.08	6.51	7.08	6.81	6.39	6.81
100	7.08	6.51	7.08	6.84	6.39	6.84
101	7.08	6.51	7.08	6.84	6.39	6.84
102	7.11	6.51	7.11	6.87	6.39	6.87
103	7.14	6.51	7.14	6.87	6.39	6.87
104	7.11	6.54	7.11	6.87	6.39	6.87
105	7.14	6.51	7.14	6.87	6.39	6.87
106	7.17	6.54	7.17	6.90	6.39	6.90
107	7.17	6.54	7.17	6.90	6.42	6.90
108	7.20	6.54	7.20	6.90	6.39	6.90
109	7.20	6.54	7.20	6.93	6.42	6.93
110	7.20	6.54	7.20	6.93	6.39	6.93
111	7.23	6.54	7.23	6.93	6.39	6.93
112	7.26	6.54	7.26	6.93	6.42	6.93
113	7.26	6.54	7.26	6.96	6.39	6.96
114	7.29	6.54	7.29	6.99	6.42	6.99
115	7.29	6.54	7.29	6.99	6.42	6.99
116	7.32	6.54	7.32	6.99	6.39	6.99
117	7.32	6.57	7.32	7.02	6.42	7.02
118	7.35	6.54	7.35	7.02	6.39	7.02
119	7.38	6.57	7.38	7.02	6.42	7.02
120	7.38	6.57	7.38	7.02	6.42	7.02
121	7.38	6.57	7.38	7.05	6.42	7.05
122	7.41	6.57	7.41	7.05	6.42	7.05
123	7.41	6.57	7.41	7.05	6.42	7.05
124	7.44	6.57	7.44	7.08	6.42	7.08
125	7.47	6.60	7.47	7.11	6.42	7.11
126	7.50	6.57	7.50	7.11	6.42	7.11
127	7.50	6.60	7.50	7.11	6.42	7.11
128	7.53	6.60	7.53	7.14	6.42	7.14
129	7.53	6.60	7.53	7.14	6.42	7.14
130	7.56	6.60	7.56	7.14	6.42	7.14
131	7.56	6.63	7.56	7.14	6.45	7.14
132	7.59	6.60	7.59	7.17	6.42	7.17
133	7.62	6.63	7.62	7.20	6.45	7.20
134	7.65	6.60	7.65	7.20	6.42	7.20

135	7.65	6.63	7.65	7.23	6.42	7.23
136	7.68	6.63	7.68	7.23	6.45	7.23
137	7.71	6.63	7.71	7.23	6.42	7.23
138	7.74	6.63	7.74	7.23	6.45	7.23
139	7.74	6.66	7.74	7.26	6.45	7.26
140	7.77	6.63	7.77	7.29	6.42	7.29
141	7.77	6.66	7.77	7.29	6.45	7.29
142	7.80	6.63	7.80	7.32	6.42	7.32
143	7.83	6.66	7.83	7.32	6.45	7.32
144	7.83	6.66	7.83	7.32	6.45	7.32
145	7.86	6.66	7.86	7.35	6.45	7.35
146	7.89	6.66	7.89	7.38	6.45	7.38
147	7.92	6.69	7.92	7.38	6.45	7.38
148	7.95	6.66	7.95	7.41	6.45	7.41
149	7.98	6.69	7.98	7.41	6.45	7.41
150	7.98	6.69	7.98	7.41	6.45	7.41
151	8.01	6.69	8.01	7.44	6.45	7.44
152	8.04	6.69	8.04	7.47	6.45	7.47
153	8.07	6.69	8.07	7.47	6.45	7.47
154	8.10	6.69	8.10	7.50	6.45	7.50
155	8.13	6.72	8.13	7.50	6.48	7.50
156	8.13	6.69	8.13	7.50	6.45	7.50
157	8.16	6.72	8.16	7.56	6.48	7.56
158	8.19	6.72	8.19	7.56	6.45	7.56
159	8.22	6.72	8.22	7.56	6.45	7.56
160	8.25	6.72	8.25	7.59	6.48	7.59
161	8.28	6.75	8.28	7.62	6.45	7.62
162	8.31	6.72	8.31	7.65	6.48	7.65
163	8.31	6.75	8.31	7.65	6.48	7.65
164	8.34	6.72	8.34	7.65	6.48	7.65
165	8.37	6.75	8.37	7.68	6.48	7.68
166	8.40	6.75	8.40	7.71	6.48	7.71
167	8.43	6.75	8.43	7.74	6.48	7.74
168	8.46	6.75	8.46	7.74	6.48	7.74
169	8.49	6.78	8.49	7.74	6.48	7.74
170	8.52	6.78	8.52	7.80	6.48	7.80

171	8.55	6.78	8.55	7.80	6.48	7.80
172	8.55	6.81	8.55	7.83	6.48	7.83
173	8.58	6.78	8.58	7.86	6.48	7.86
174	8.61	6.81	8.61	7.86	6.51	7.86
175	8.67	6.81	8.67	7.89	6.48	7.89
176	8.70	6.81	8.70	7.89	6.51	7.89
177	8.73	6.81	8.73	7.95	6.48	7.95
178	8.76	6.81	8.76	7.95	6.48	7.95
179	8.79	6.81	8.79	7.98	6.51	7.98
180	8.82	6.84	8.82	8.01	6.48	8.01
181	8.85	6.81	8.85	8.01	6.51	8.01
182	8.88	6.84	8.88	8.04	6.51	8.04
183	8.91	6.84	8.91	8.04	6.48	8.04
184	8.94	6.84	8.94	8.10	6.51	8.10
185	9.00	6.84	9.00	8.10	6.51	8.10
186	9.03	6.87	9.03	8.13	6.51	8.13
187	9.06	6.84	9.06	8.16	6.51	8.16
188	9.09	6.87	9.09	8.19	6.51	8.19
189	9.12	6.90	9.12	8.19	6.51	8.19
190	9.15	6.87	9.15	8.25	6.51	8.25
191	9.18	6.90	9.18	8.25	6.51	8.25
192	9.21	6.90	9.21	8.28	6.51	8.28
193	9.27	6.90	9.27	8.31	6.54	8.31
194	9.30	6.90	9.30	8.34	6.51	8.34
195	9.33	6.93	9.33	8.34	6.54	8.34
196	9.36	6.90	9.36	8.40	6.54	8.40
197	9.39	6.93	9.39	8.40	6.51	8.40
198	9.42	6.93	9.42	8.46	6.54	8.46
199	9.48	6.93	9.48	8.46	6.51	8.46
200	9.51	6.93	9.51	8.49	6.54	8.49
201	9.54	6.96	9.54	8.52	6.54	8.52
202	9.57	6.96	9.57	8.55	6.51	8.55
203	9.60	6.96	9.60	8.61	6.54	8.61
204	9.66	6.99	9.66	8.61	6.54	8.61
205	9.69	6.96	9.69	8.64	6.54	8.64
206	9.72	6.99	9.72	8.67	6.54	8.67

207	9.75	6.99	9.75	8.70	6.57	8.70
208	9.78	6.99	9.78	8.73	6.54	8.73
209	9.84	6.99	9.84	8.76	6.54	8.76
210	9.87	7.02	9.87	8.82	6.54	8.82
211	9.93	6.99	9.93	8.82	6.54	8.82
212	9.96	7.02	9.96	8.85	6.57	8.85
213	10.00	7.05	10.00	8.88	6.54	8.88
214	10.06	7.02	10.06	8.91	6.57	8.91
215	10.09	7.05	10.09	8.97	6.57	8.97
216	10.12	7.05	10.12	8.97	6.54	8.97
217	10.15	7.05	10.15	9.03	6.57	9.03
218	10.21	7.05	10.21	9.06	6.57	9.06
219	10.24	7.08	10.24	9.09	6.57	9.09
220	10.30	7.08	10.30	9.12	6.57	9.12
221	10.33	7.08	10.33	9.18	6.57	9.18
222	10.39	7.11	10.39	9.18	6.57	9.18
223	10.42	7.08	10.42	9.24	6.57	9.24
224	10.45	7.11	10.45	9.27	6.57	9.27
225	10.48	7.11	10.48	9.30	6.57	9.30
226	10.54	7.11	10.54	9.33	6.60	9.33
227	10.60	7.11	10.60	9.39	6.57	9.39
228	10.63	7.14	10.63	9.42	6.60	9.42
229	10.69	7.14	10.69	9.45	6.60	9.45
230	10.72	7.14	10.72	9.51	6.57	9.51
231	10.75	7.17	10.75	9.54	6.60	9.54
232	10.78	7.14	10.78	9.57	6.60	9.57
233	10.84	7.17	10.84	9.60	6.60	9.60
234	10.90	7.20	10.90	9.66	6.60	9.66
235	10.93	7.20	10.93	9.72	6.57	9.72
236	10.96	7.20	10.96	9.72	6.60	9.72
237	11.02	7.20	11.02	9.78	6.60	9.78
238	11.05	7.23	11.05	9.84	6.60	9.84
239	11.11	7.20	11.11	9.87	6.60	9.87
240	11.17	7.23	11.17	9.93	6.63	9.93
241	11.20	7.26	11.20	9.93	6.60	9.93
242	11.23	7.23	11.23	10.00	6.60	10.00

243	11.29	7.26	11.29	10.06	6.63	10.06
244	11.32	7.26	11.32	10.09	6.60	10.09
245	11.38	7.26	11.38	10.15	6.63	10.15
246	11.41	7.29	11.41	10.18	6.63	10.18
247	11.47	7.29	11.47	10.21	6.63	10.21
248	11.50	7.32	11.50	10.27	6.63	10.27
249	11.53	7.29	11.53	10.33	6.60	10.33
250	11.62	7.32	11.62	10.39	6.63	10.39
251	11.65	7.35	11.65	10.42	6.63	10.42
252	11.68	7.32	11.68	10.48	6.63	10.48
253	11.74	7.35	11.74	10.54	6.63	10.54
254	11.77	7.35	11.77	10.54	6.66	10.54
255	11.80	7.38	11.80	10.60	6.63	10.60
256	11.89	7.38	11.89	10.66	6.63	10.66
257	11.92	7.38	11.92	10.72	6.66	10.72
258	11.95	7.41	11.95	10.75	6.63	10.75
259	12.01	7.38	12.01	10.81	6.66	10.81
260	12.04	7.41	12.04	10.87	6.66	10.87
261	12.10	7.44	12.10	10.93	6.66	10.93
262	12.13	7.41	12.13	10.99	6.66	10.99
263	12.19	7.44	12.19	11.02	6.66	11.02
264	12.22	7.44	12.22	11.08	6.66	11.08
265	12.25	7.47	12.25	11.14	6.66	11.14
266	12.31	7.47	12.31	11.20	6.69	11.20
267	12.37	7.47	12.37	11.23	6.66	11.23
268	12.40	7.50	12.40	11.29	6.69	11.29
269	12.46	7.53	12.46	11.35	6.66	11.35
270	12.49	7.50	12.49	11.41	6.66	11.41
271	12.52	7.53	12.52	11.47	6.69	11.47
272	12.58	7.53	12.58	11.53	6.66	11.53
273	12.64	7.53	12.64	11.56	6.69	11.56
274	12.67	7.56	12.67	11.62	6.69	11.62
275	12.73	7.56	12.73	11.68	6.69	11.68
276	12.76	7.59	12.76	11.74	6.69	11.74
277	12.79	7.59	12.79	11.80	6.69	11.80
278	12.85	7.59	12.85	11.86	6.69	11.86

279	12.88	7.62	12.88	11.89	6.69	11.89
280	12.94	7.62	12.94	11.95	6.72	11.95
281	13.00	7.62	13.00	12.01	6.69	12.01
282	13.03	7.65	13.03	12.07	6.72	12.07
283	13.06	7.65	13.06	12.13	6.72	12.13
284	13.12	7.68	13.12	12.19	6.72	12.19
285	13.15	7.68	13.15	12.25	6.72	12.25
286	13.18	7.68	13.18	12.28	6.72	12.28
287	13.27	7.71	13.27	12.37	6.72	12.37
288	13.30	7.74	13.30	12.43	6.72	12.43
289	13.33	7.71	13.33	12.49	6.75	12.49
290	13.39	7.74	13.39	12.55	6.72	12.55
291	13.42	7.77	13.42	12.61	6.75	12.61
292	13.45	7.77	13.45	12.67	6.72	12.67
293	13.51	7.77	13.51	12.70	6.72	12.70
294	13.54	7.80	13.54	12.76	6.75	12.76
295	13.57	7.80	13.57	12.82	6.72	12.82
296	13.63	7.83	13.63	12.88	6.75	12.88