The **S**pectral **A**nalysis **R**outine for **A**steroids, SARA[☆]: v01,[☆☆] User's Guide.

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Abstract

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1. Introduction

The purpose of this document is to describe a new visible and near-infrared (NIR, 0.5 - 2.5 μm) spectral band parameter analysis code called the Spectral Analysis Routine for Asteroids (SARA). The code is developed for IDL, and it aims to act as a generalized band parameter analysis program that is simple to use and freely available to the community. The benefit of a generalized and easily deployable code is that it offers the potential for a band parameter analysis standard in the field. Widespread use of SARA would lead to band parameter analyses that can be directly compared between research groups.

The SARA package you have includes the main SARA program and four post-SARA band analysis routines designed to collate SARA outputs as well as perform mineralogy calculations, identify meteorite analogs, and determine S-subtypes. The main algorithm should be run first on an entire data set of NIR asteroid spectra. If the user has not already created a directory [home]/SARA/, the initial execution of SARA will create this directory for the user as well as the subdirectory [home]/SARA/spectra. For SARA to run appropriately, the user needs to place their spectral data files in this subdirectory. For naming and formatting of the spectra data files see §3.

A generalized description of the SARA algorithm is introduced here and explained further in the proceeding sections. The SARA algorithm reads in 0.5

[☆] Use of the SARA Algorithm should be referenced with Lindsay et al. (2014). **Composition, Mineralogy, and Porosity of Multiple Asteroid Systems from Visible and Near-infrared Spectral Data**. *Icarus*, in review.

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- 2.5 μm NIR (and visible if available) spectral data for S- and V-type asteroids and returns frequently used band parameters for the 1- and 2-μm features due to olivine and pyroxene. The returned parameters with estimated uncertainties are: 1) Band I and II centers, areas, and depths; 2) Band I slope; 3) the Band Area Ratio, or BAR = [Band II Area]/[Band I Area]. The algorithm then proceeds in the following sequence with plotting to band assignments and parameters plotted to the user's screen[1]:

1. Adaptively build Band I and II boundaries to isolate the bands.
2. Fit linear continua for Bands I and II and divide each band by its continuum[2].
3. Pass the now isolated Bands I and II to the subroutine *band_ parameters*[3], which measures the centers and areas, as well as estimating those parameters' uncertainties using Monte Carlo simulations (subroutines: *band_ center_ montecarlo, band_ area_ montecarlo).*.
4. Collate band parameters into data structures and print the results to screen; to text files [ID_ Name_ bandanalysis_ X.txt], where X is 3, 4, or 5 and represents the polynomial order used to find band centers; and to binary files (.sav) with the average of the band_ parameters for the three polynomial saved in a structure *band_ analysis_ avg* and the individual band parameters for each polynomial order in a structure *band_ analysis*.

For a full introduction to the SARA algorithm with application to asteroid data sets, please refer to Lindsay et al. (2014).

The SARA algorithm is designed for minimal manual organization on the part of the user. Once the programs are copied to your computer, they are ready to run with no additional effort on the part of the user. The packaged SARA programs include:

- SARA_v01.pro
- SARA_post1_master.pro
- SARA_post2_mineralogy.pro
- SARA_post3_analogs.pro
- SARA_post4_ssubtypes.pro

The only program required for calculating band parameters is SARA_v01.pro. However, the first post-SARA program SARA_ post1_ master.pro collates the

[1]SARA also generates low resolution JPGs for the Band I and II calculations/fits plots, as well as the entire spectral range with band continua definitions over plotted.

[2]At this point, SARA also computes Band I slopes and uses a Montecarlo simulation to estimate slope uncertainties using the subroutine *band_slope_montecarlo*

[3]This subroutine also computes the band depths and uses the observational uncertainties to estimate the depth uncertainties

output of all the asteroid spectra analyzed into a consolidated files ([home]/output/master_ output/band_ parameter_ master.txt and band_ parameter_ master_ averages.txt for individual polynomial calculations and the averages of the polynomial calculations, respectively). Please note that post-SARA programs 1 - 4 require the user to follow the naming conventions described in §3. For this reason, it is highly recommended that the user follows the spectral data file naming conventions.

For SARA and the post-analysis programs to run, the IDL Astronomy Library must be installed. Post-analysis programs 3-4 also require the IDL Coyote Library. These libraries with installation instructions can be found online[4][5]. Please refer to the websites instructions for download and installation.

2. Setting up and running SARA on your machine

SARA is designed for ease on the part of the user. The initial setup only requires you to place the SARA codes on you computer. Once the programs are obtained, the program is ready to run and can be done so from any directory. The user has the option of creating the directories [home]/SARA/ and [home]/SARA/spectra/ prio to the initial execution of SARA. Here [home] refers to the machine's home directory path. This step is not necessary, but it will allow for a successful execution of SARA on the first run if the data files have been placed in [home]/SARA/spectra/. **If the user wishes, SARA_ v01.pro initially can be compiled and ran to create these two directories**. However, in this case, the program will exit and ask you to place your asteroid spectral data files into the newly created directory [home]/SARA/spectra. After placing the spectral data into this directory, SARA is ready to run, and it will automatically create the following directories:

- [home]/SARA/output/ with subdirectories: /band_ images/, /band_ definitions, /band_ master_ output, /ast_ temps, and /mineralogy/. These directories are for SARA outputs.
  - */band_images/*: Directory for the generated JPG files. Useful for user review in case of anomalous band parameter results.
  - */band_defintions/*: Directory for storing wavelength values for anchor points (i), (ii), (iii), and (iv) (See §5).
  - */band_master_output/*: Directory for the file master output file generated by SARA_ post1_ master.pro (See §4.1).
  - */ast_temps/*: Optional directory for a file containing asteroid temperatures (See §4.2).
  - */mineralogy/*: Directory for mineralogy output (See §4.2).

[4]IDL Astronomy Library: http://idlastro.gsfc.nasa.gov/
[5]IDL Coyote Library: http://www.idlcoyote.com/

- [home]/plots/. This directory stores the Encapsulated Postscript (EPS) files created by post processing programs 3 and 4. See §4.3 and 4.4 for details.

2.1. Running SARA

When SARA is run, the user will be prompted with "Enter object name [ID_ Name]:". SARA will then automatically search the [home]/SARA/spectra/ directory to find the matching file. While the user only needs to input a string so that SARA can uniquely identify the filename, it is strongly recommended that the input be in the ID_ Name format for the internal formatting purposes of SARA. Once the ID_ Name is input, SARA will locate the file and perform its band parameter analysis.

SARA contains two keywords which instruct the algorithm how to perform the band parameter analysis for S- versus V-type asteroids. This demands that SARA is run from the command prompt. The two keywords *v_type* and *s_type*, and are implemented while running SARA by

[*prompt*]> SARA_ v01, \v_type

These two keywords configure the algorithm for S- and V-types as well as instructing the suite of programs as to the asteroid type, which is used in the later post-analysis programs. If neither the S-type or V-type keywords are used, SARA assigns a default string value of 'U' for the asteroid type. This designation will prevent the mineralogy post-SARA program from performing an appropriate calculation. For details on the specific differences between S-type and V-type mode, see §5.

SARA is designed to perform a band parameter analysis for the sample that is placed in the user's spectra subdirectory. It is recommended that all the outputs are moved their own directories between analyzing each sample of asteroids. For example, given two data sets that require separate band parameter analyses for, SARA should first be run on each asteroid in Sample 1. After every asteroid spectra has been processed by SARA, the post-SARA analysis programs should be run in sequence. Once this process is completed, the output should then be moved to their own directories. The entire process of band parameter analyses via SARA and then post-SARA analyses should then be performed for Sample 2. After which, the outputs of Sample 2 should be placed in their own directories.

3. Input data naming conventions and formatting

The author strongly suggests that the user follows the naming conventions described here. Doing so is required for post-analysis programs 1 – 4 to run without the user manually editing the code. The file formatting for the spectral data is required for the algorithm to work, but the formatting is standard and should not require any special care on the part of the user.

3.1. Naming conventions

The asteroid spectra files should have filenames following an ID#_ Name.txt convention. The rational behind this is SARA will automatically separate the ID number and asteroid name into separate string variables that are useful for the program outputs and plotting purposes. The user may also append additional information with a subsequent _ , i.e., ID#_ Name_ [more info]. In this case, the user should still enter ID#_ Name when SARA prompts them for the post-analysis programs to run appropriately.

3.2. File formatting

The asteroid spectral files need to have three data columns: Wavelength, Reflectance, and Uncertainty. Note that SARA will not reduce your data. That process is left to the user and their preferred reduction methods. The data columns need to be either space or tab delimited. Any number of header lines are acceptable, and left to the user's preference.

If the user desires a version of SARA that works with data without uncertainties, as many RELAB (Pieters and Hiroi, 2004) meteorite spectra do not include uncertainties, then please email Sean Lindsay at Sean.Lindsay@physics.ox.ac.uk for a version of the code designed for RELAB data.

4. Post-analysis program descriptions

This section describes the purpose of the four post-SARA analysis programs. These programs are not necessary for the band parameter calculations, but rather are designed to make use of SARA's calculated band parameters to perform a battery of useful calculations and analysis techniques. **These programs should be run after you have completed running SARA on your entire sample of asteroids**. Post-SARA 1 collates the band parameter analysis outputs for whatever sample of objects you have run into files useful to the user and the rest of the post-analysis programs. Post-SARA 2 performs a mineralogical analysis including relative and modal abundances using the band parameters calculated by SARA. Post-SARA 3 overplots the band parameter analysis in Band I Center vs. BAR space onto meteorite analog zones identified in the literature. Post-SARA 4 overplots the band parameter analysis in Band I Center vs. BAR space onto the S-subtype zones defined in Gaffey et al. (1993).

4.1. SARA_ post1_ master.pro

The first post-SARA program collates the SARA band parameter analysis output files into two master output files. The output for this program is contained in [home]/SARA/output/master_ output. The first file, *band_ parameter _ master.txt*, contains the band parameters calculated for the $3^{rd}, 4^{th},$ and 5^{th} polynomial order fits used to calculate band centers for all of the asteroids that SARA has already processed. The second file, *band_ parameter_ master_ averages.txt* contains only the band parameters averaged over the three polynomial orders.

4.2. SARA_ post2_ mineralogy.pro

The second post-SARA program uses the average master output file to calculate relative and modal abundances for olivine and pyroxene (where applicable). The program is designed to use the designation of asteroid type that was set in the main SARA program with the S-type and V-type keywords. For S-types, the mineralogy equations derived in Dunn et al. (2010b,a,c) are applied. Note that these equations have been derived for S(IV) asteroids, so mineralogical results for other S-subtypes should be taken at the user's caution. These equations give the mol% Fa in olivine, mol% Fs in pyroxene, and the olivine ratio defined as amount of olivine/(olivine + pyroxene). Columns where the calculations do not apply are filled with a place-holding value of 999.

For V-types, the calibration equations of Burbine et al. (2007, 2009) are applied. These equations give the mol% Fs and Wo in pyroxene. Columns where the calculations do not apply are filled with a place-holding value of 999.

For S- and V-types, the iterative mineralogy equations described in Gaffey et al. (2002) are applied. These equations apply broadly to nearly every S- and V-type, but have many caveats that can compromise the accuracy of the mineralogy calculations. They should be used only after reading Gaffey (2007) and should be quoted with caution. Note that the previously mentioned calibrations were carefully done by calibrating laboratory measured mineralogy and spectral band parameter measurements, and are therefore the more robust mineralogy calculations.

This program also prompts the user for the input of a file called ast_ temps.txt. This file is used for temperature corrections to certain band parameters. SARA uses the equations described in (Sanchez et al., 2012) for band parameter temperature corrections (See §5.2). The user can opt to skip temperature corrections by entering 999. If this is done, the user is responsible for reporting that their band parameters have not been temperature corrected, which can have significant consequences on their mineralogical calculations and identification of meteorite analogs and S-subtypes. **The ast_ temp.txt file should be placed in [home]/SARA/output/ast_ temps/ , and it should contain a single column of the asteroid temperatures of the sample in the order that they appear in band parameters average master file**. The user is responsible for determining the heliocentric distance of the asteroid at the time of observation and then estimating the temperature.

4.3. SARA_ post3_ analogs.pro

The third post-SARA program uses the average master output file to overplot the asteroids in Band I Center vs. BAR space onto meteorite analog zones defined in the literature. These zones include the olivine meteorites, ordinary chondrites (OCs), and basaltic achondrites (BAs) defined by Gaffey et al. (1993); the primitive achondritic Lodranites and Acapulcoites defined by Burbine et al. (2001); and the anomalous meteorite group, the Ureilites, defined by Cloutis et al. (2010). Of these meteorite analog zones, the OCs and BAs have the strongest link between asteroid spectra and meteorite spectra. The other analog

zones should not be taken to be absolute and should be appropriately discussed by the user if the zones are used in an article. An example of SARA_ post3_ analogs.pro output is shown in Fig. 1.

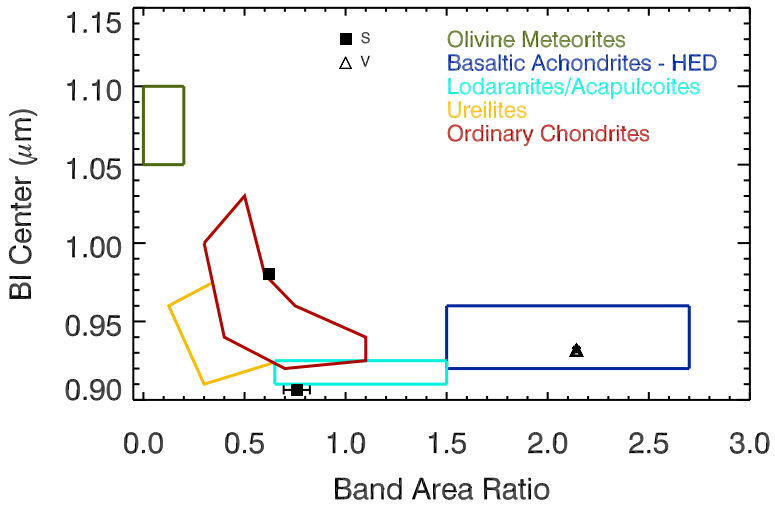

Figure 1: The Band I Center versus BAR spectral parameters of 2 S-type (*solid squares*) and 1 V-type (*open triangle*) MASs over-plotted on regions of potential meteorite analogs. The olivine, ordinary chondrite, and basaltic achondrite regions are from Gaffey et al. (1993); the primitive achondrite region (lodranites/acapulcoites) is from Burbine et al. (2001); and the ureilite region is from Cloutis et al. (2010). The 1σ uncertainties for Band I Center and BAR are plotted for each object.

4.4. SARA_ post4_ ssubtypes.pro

The fourth post-SARA program uses the average master output file to over-plot the asteroids in Band I Center vs. BAR space onto the S-subtype zones defined by Gaffey et al. (1993). These seven zones, S(I) - S(VII), roughly trace the mineralogy such that S(I)s are nearly mono-mineralic olivine and the S(VII) are nearly mono-mineralic orthopyroxene. The solid line tracing through and around the subtype zones is the olivine-orthopyroxene mixing line (Cloutis et al., 1986). For further reading on S-subtypes please refer to Gaffey et al. (1993). An example of SARA_ post3_ analogs.pro output is shown in Fig. 2.

5. SARA methods

The following sections are an adaptation from Lindsay et al. (2014), and they describe the specifics behind how the SARA algorithm performs its band parameter calculations.

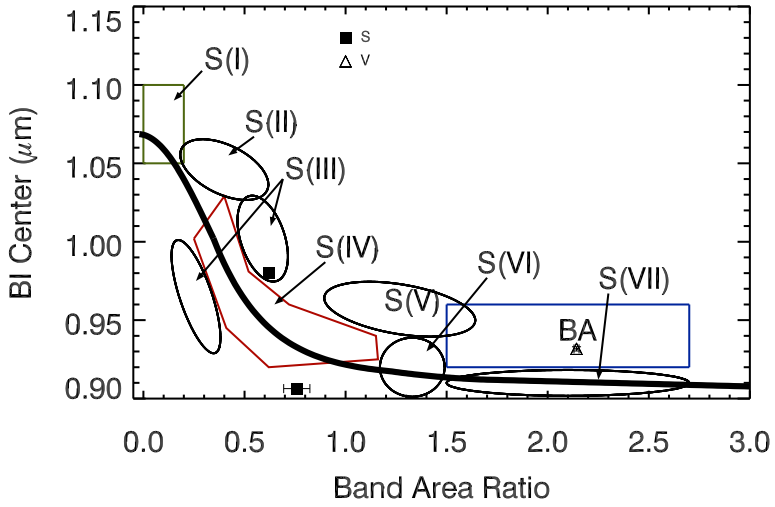

Figure 2: The Band I Center versus BAR spectral parameters of 2 S-type (*solid squares*) and 1 V-type (*open triangle*) MASs over-plotted on the S(I) - S(VII) regions plus basaltic achondrite region defined in Gaffey et al. (1993). The solid curve is the oliviine-orthopyroxene mixing line defined in Cloutis et al. (1986), and the qualitative relative abundance of each zone is listed for each zone. The 1σ uncertainties for Band I Center and BAR are plotted for each object.

SARA's first step is to isolate Bands I and II located near 1- and 2-μm, respectively. In order to accomplish this, the algorithm must identify four critical points that will define the boundaries of the two bands. Figure 3a indicates the four points (i, ii, iii, and iv) for this determination, where the point pairs (i, ii) and (iii, iv) define the boundaries of Band I and Band II, respectively. Points (i) and (iii) are defined by the two reflectance maxima near 0.75 and 1.4 μm, respectively. SARA fits 5^{th} order polynomials to reflectance data range defined by ± 0.3 μm of the data maxima near 0.75 and 1.4 μm. The maxima of these fits are then defined to be points (i) and (iii). Fifth order polynomials are chosen to maximize the accuracy and generality of the algorithm. These regions can exhibit complicated structure due to Band I being a composite of three olivine absorptions and one pyroxene absorption as well as (potentially) poor telluric corrections to the spectral data near 1.35 and 1.9 μm. Trial and error testing demonstrated that lower order polynomials are insufficient in replicating this structure in a repeatable manner. Point (ii) is defined as the point where a line extending from point (i) lies tangent to the polynomial fit of the

1.4 μm region. By using the tangent point instead of the point (iii) maximum, the band analysis algorithm ensures the continuum does not undercut reflectance values. As such, it more accurately measures the Band I and Band II areas by avoiding band reflectance points that lie above the continuum.

The quality of the IRTF SpeX data decreases significantly longward of 2.45 μm, and for typical IRTF SpeX data the signal-to-noise drops precipitously at this point. To guarantee an accurate representation of reflectance values, the red-edge of Band II, point (iv), is set to the reflectance value at 2.44 μm of a 5^{th} order polynomial fit to the entirety of Band II[6]. With the boundaries of Band I and II defined, linear continua are generated connecting points (i)-(ii) and (iii)-(iv). The slope of Band I is recorded as the slope of the Band I continuum, and the algorithm divides each band by its respective continuum.

The band centers are measured by computing a 3^{rd}, 4^{th} and 5^{th} order polynomial fit to the bottom of the continuum-divided band (indicated as red points in Fig. 3b and c). Here, the procedure for V-types and S-complex asteroids diverge. For both S-complex and V-type asteroids, the Band I center is measured by computing polynomial fits to the bottom half of the band. For S-types, with shallower Band IIs that are more sensitive to the effects of observational uncertainties and telluric contamination near 1.9 μm, the center is measured by computing the polynomial fits to the entirety of Band II. However, for V-types, with deeper Band IIs that are less sensitive to the effects of observational uncertainties, the center is measured by computing polynomial fits to the bottom half of Band II. Recall that SARA is run in S- or V-type mode by using the keywords s_type and v_type. The band depth is taken to be one minus a ten-point boxcar smooth of the reflectance at the wavelength position of the band center. The band center and depth are then defined as the average of the measured center and depths over the three polynomial fits. The band areas are calculated as the area between flat continuum and the continuum divided band reflectance data. The BAR is computed as (Band II Area) / (Band I Area).

A graphical example of SARA's assignment of points (i - iv) and the linear continua fits is provided in Fig. 3. Figs. 3b and 3c show the continuum divided Bands I and II with the polynomial fits to determine the band centers.

[6]To avoid tracing extremely noisy data longward of $\sim$2.4 μm, certain asteroid spectra required the use of a 3^{rd} order polynomial fit to characterize point (iv). This requires manual manipulation of the SARA code at line 353. For this, the user need to change the value of red_edge_po from 5 to 3.

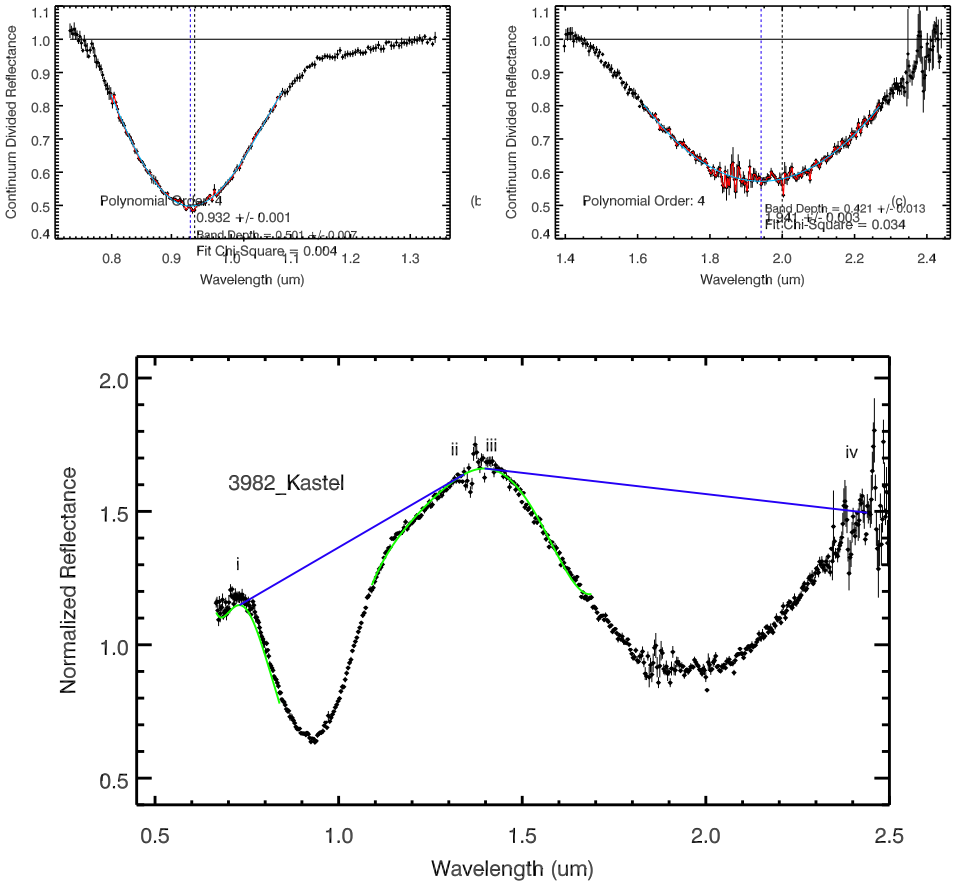

Figure 3: *(a)* The near-infrared reflectance spectrum of V-type asteroid 3982 Kastel overlain with the band definitions and linear continua (*blue*) for Band I and Band II. The vertical dashed lines are the minimum of a ten-point boxcar smoothing of Band I (*black*) and the band center (*blue*)determined by an n = 3, 4, or 5 n^{th} order polynomial fit to bottom half of Band I (polynomial fit in *cyan* and reflectance data fit is applied to in *red*). *(c)* Same as (b) but for Band II. For Band II the n^{th} order polynomial fit is applied to the entire band for S-complex asteroids and the bottom half for V-type asteroids. See text for the definitions of points (i - iv).

5.1. Band Parameter Errors

SARA assesses the 1σ error bars using Monte Carlo simulations. Using Monte Carlo simulations to estimate errors is particularly important for band center errors because the error is in the wavelength direction, but the observational uncertainties are along the reflectance axis. For Band I and II, gaussian noise set to the level of the measured signal-to-noise is added to the measured reflectance values. This gives a new set

of band reflectance points that are consistent with the observational uncertainties. New 3^{rd}, 4^{th} and 5^{th} order polynomials are fit to the simulated reflectance values and the band centers, depths, and areas are re-measured. For each polynomial order, this process is iterated 20,000 times to give $3 \times 20,000$ measurements for band center and depth. For each polynomial order, the band center and depth error is taken to be the standard deviation of the 20,000 measurements, and the final 1σ center and depth errors are assigned to be the average of the three error measurements. The measured band area is independent of the polynomial fits, and the 1σ band area error is taken as the standard deviation of the 20,000 measured areas.

SARA also computes Band I slope errors. This error is also assessed using an iteration of 20,000 Monte Carlo simulations, but here the Monte Carlo simulation is applied to the reflectance values used to define points (i, ii, and iii). Using simulated reflectance values, new 5^{th} order polynomials are fit to identify points (i) and (iii), which in turn defines the tangent point (ii). The value of the slope is recorded for each simulation, and the final error is taken to be the standard deviation of the 20,000 measured slopes.

5.2. Band Parameter Temperature Corrections

For the temperature corrections to be made to the band parameter dataset, the user needs to generate the file ast_ temps.txt. This file contains a single column of the asteroid temperatures in the order that they appear in band parameter master file.

The temperature of the asteroid surfaces influences the band center positions and widths of the 1- and 2-μm bands (Singer and Roush, 1985; Schade and Wäsch, 1999; Moroz et al., 2000; Hinrichs and Lucey, 2002; Sanchez et al., 2012). Laboratory measurements of band parameters are typically obtained at near room temperature (∼300 K), and will therefore have slightly different band parameters than asteroid surfaces. Hence, corrections to the band parameters at asteroidal temperatures are required when comparisons or calibrations based on laboratory measurements are made. Sanchez et al. (2012) found that Band II is the most effected by temperature effects and derived the following equations to correct for these effects with respect to room temperature:

$$\Delta BIIC(\mu m) = 0.06 - 0.0002 \times T(\mathrm{K}) \quad (1)$$

$$\Delta BAR = 0.00075 \times T(\mathrm{K}) - 0.23. \quad (2)$$

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