CRISM Summary Parameter Calculation Reference

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1 Introduction

This document provides the specific mathematical formulas and algorithms used to compute spectral summary parameters within the CRISM Analysis Toolkit (CAT). These algorithms were used to calculate spectral parameter values derived from CRISM spectral data as delivered to the PDS. Most formulations are also available in Viviano et al. (2014) and reproduced in Table 3-12 of the CRISM Software Interface Specification, although there have been minor adjustments to the parameter formulations since the publication of that manuscript.

1.1 References and Further Reading

- Viviano et al., 2014. Revised CRISM spectral parameters and summary products based on the currently detected mineral diversity on Mars. *JGR: Planets*. `https://doi.org/10.1002/2014JE004627`
- CRISM Software Interface Specification

  `https://pds-geosciences.wustl.edu/mro/mro-m-crism-3-rdr-targeted-v1/mrocr_2104/document/crism_dpsis.pdf`
- NASA PDS Geosciences Node, CRISM Portal

  `https://pds-geosciences.wustl.edu/missions/mro/crism.htm`

2 Basic Operations and Notation

2.1 Reflectance Extraction (R_λ)

CRISM summary parameters are derived from specific reflectance values extracted at specific wavelengths. Depending on the data product, these reflectances are extracted using either a "multispectral" or "hyperspectral" formulation.

Multispectral Formulation: The reflectance R_λ is the data value from the single spectral band whose center wavelength is closest to the target λ.

Hyperspectral Formulation: To account for spectral noise in hyperspectral products, R_λ is calculated using a spectral window with a fixed width called the kernel (k). Unless otherwise specified, this is a 5-band window ($k = 5$). The procedure is as follows:

1. Identify the target band whose center wavelength is closest to λ.
2. Select a spectral window consisting of the target band and its immediately adjacent neighboring bands with a width equal to the kernel (e.g. for $k = 5$, select the 2 closest bands below and the 2 closest bands above the target band).

- If an even kernel is specified, the odd number immediately above it is treated as the kernel width, instead.
- If the spectral window were to extend beyond the edge of the detector, it is instead truncated at the edge of the detector. For example, with $k = 5$, a spectral window centered at the very first band (index 0) would shrink to include only bands 0, 1, and 2, as the rest of the window would be beyond the edge of the detector.

3. Calculate R_λ as the **median** value of the reflectances in this spectral window.

   - If the spectral window has an even number of values (such as near the edge of the detector), the mean of the two middle values is returned, instead.
   - CRISM data uses `65535.0` as an invalid data flag. Any bands within the spectral window with reflectances of `65535.0` should be ignored.

2.2 Wavelength Extraction (W_λ)

Many CRISM summary parameters depend on the specific wavelengths of the spectral data. The notation W_λ is used to denote the actual wavelength of the CRISM band with the wavelength closest to the target wavelength λ.

Within the CAT formulations, W_λ is typically expressed in nanometers. In practice, any unit can be used for calculations involving W_λ so long as the same unit is used consistently.

2.3 Continuum Interpolation (RC_λ)

Continuum interpolated reflectances are intended to indicate the "expected reflectance" if a particular absorption feature were not present in the spectrum. They are calculated by fitting a straight line between two "anchor" wavelengths elsewhere in the spectrum, and interpolating the reflectance on that line at a target wavelength. Algorithmically, given low and high anchor wavelengths λ_L and λ_H and target central wavelength λ_C, RC_{λ_C} is calculated as follows:

1. Extract the wavelengths W_L, W_C, and W_H of the bands closest to the target wavelengths
2. Extract the reflectances R_L and R_H at the anchor wavelengths
3. Calculate the interpolation coefficients:

$$a = \frac{W_C - W_L}{W_H - W_L}$$
$$b = 1.0 - a$$

4. Calculate the interpolated continuum

$$RC_{\lambda_C} = b \times R_L + a \times R_H$$

2.4 Simple Band Depth (RB_λ)

Many parameters are defined in terms of a "simple band depth", which evaluates the depth of an absorption feature relative to an interpolated continuum. Simple band depths are defined as:

$$RB_\lambda = 1.0 - \left(\frac{R_\lambda}{RC_\lambda}\right)$$

Simple band depths used in parameter formulations always have their anchor wavelengths λ_L and λ_H and the kernels k_L, k_C, and k_H of all reflectances specified.

3 Parameter Definitions

Unless otherwise specified, for each parameter all interpolated continua RC_λ and simple band depths RB_λ used to define that parameter share the same anchor wavelengths λ_L and λ_H. All wavelengths are specified in nanometers.

3.1 VNIR Parameters

Parameter	Multi-/Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
R770	R_{770}	-	$k_{770} = 5$
RBR	$\frac{R_{770}}{R_{440}}$	-	$k_{440} = 5$ $k_{770} = 5$
BD530_2	RB_{530}	$\lambda_L = 440$ $\lambda_H = 614$	$k_{440} = 5$ $k_{530} = 5$ $k_{614} = 5$
SH600_2	$1.0 - \left(\frac{RC_{600}}{R_{600}}\right)$	$\lambda_L = 533$ $\lambda_H = 716$	$k_{533} = 5$ $k_{600} = 5$ $k_{716} = 3$
SH770	$1.0 - \left(\frac{RC_{775}}{R_{775}}\right)$	$\lambda_L = 716$ $\lambda_H = 860$	$k_{716} = 3$ $k_{775} = 5$ $k_{860} = 5$
BD640_2	RB_{624}	$\lambda_L = 600$ $\lambda_H = 760$	$k_{600} = 5$ $k_{624} = 3$ $k_{760} = 5$
BD860_2	RB_{860}	$\lambda_L = 755$ $\lambda_H = 977$	$k_{755} = 5$ $k_{860} = 5$ $k_{977} = 5$
BD920_2	RB_{920}	$\lambda_L = 807$ $\lambda_H = 984$	$k_{807} = 5$ $k_{920} = 5$ $k_{984} = 5$
RPEAK1	*see below*	-	-
BDI1000VIS	*see below*	-	-

3.2 IR Parameters

Parameter	Multispectral Formulation	Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
BDI1000IR	*see below*		-	-
R1330	R_{1330}		-	$k_{1330} = 11$
BD1300	RB_{1320}		$\lambda_L = 1080$ $\lambda_H = 1750$	$k_{1080} = 5$ $k_{1320} = 15$ $k_{1750} = 5$
OLINDEX3	$RB_{1210} \times 0.1 + RB_{1250} \times 0.1 +$ $RB_{1263} \times 0.2 + RB_{1276} \times 0.2 +$ $RB_{1330} \times 0.4$ *OLINDEX3 band depth continua are extrapolated from two anchors at higher wavelength*		$\lambda_L = 1750$ $\lambda_H = 1862$	$k_\lambda = 7 \quad \forall\lambda$
LCPINDEX2	$RB_{1690} \times 0.2 + RB_{1750} \times 0.2 +$ $RB_{1810} \times 0.3 + RB_{1870} \times 0.3$		$\lambda_L = 1560$ $\lambda_H = 2450$	$k_\lambda = 7 \quad \forall\lambda$
HCPINDEX2	$RB_{2120} \times 0.1 + RB_{2140} \times 0.2 +$ $RB_{2230} \times 0.15 + RB_{2250} \times 0.3 +$ $RB_{2430} \times 0.2 + RB_{2460} \times 0.15$		$\lambda_L = 1690$ $\lambda_H = 2530$	$k_{2120} = 5$ $k_\lambda = 7$ otherwise
VAR	*see below*		-	-
ISLOPE1	$\dfrac{R_{1815} - R_{2530}}{W_{2530} - W_{1815}}$ *ISLOPE1 is typically expressed as (reflectance / μm)*		-	$k_{1815} = 5$ $k_{2530} = 5$
BD1400	RB_{1395}		$\lambda_L = 1330$ $\lambda_H = 1467$	$k_{1330} = 5$ $k_{1395} = 3$ $k_{1467} = 5$
BD1435	RB_{1434}		$\lambda_L = 1370$ $\lambda_H = 1470$	$k_{1370} = 3$ $k_{1434} = 1$ $k_{1470} = 3$

<table>
<tr><th>Parameter</th><th>Multispectral Formulation</th><th>Hyperspectral Formulation</th><th>Continuum Anchors</th><th>Hyperspectral Kernels</th></tr>
<tr><td>BD1500_2</td><td>$0.5 \times RB_{1505} + 0.5 \times RB_{1558}$</td><td>$RB_{1525}$</td><td>$\lambda_L = 1367$
$\lambda_H = 1808$</td><td>$k_{1367} = 5$
$k_{1525} = 11$
$k_{1808} = 5$</td></tr>
<tr><td>ICER1_2</td><td colspan="2">$1.0 - \left(\frac{1.0 - BD1435}{1.0 - BD1500\_2}\right)$
ICER1_2 is defined in terms of the BD1435 and BD1500_2 parameters</td><td>-</td><td>-</td></tr>
<tr><td>BD1750_2</td><td colspan="2">RB_{1750}</td><td>$\lambda_L = 1690$
$\lambda_H = 1815$</td><td>$k_{1690} = 5$
$k_{1750} = 3$
$k_{1815} = 5$</td></tr>
<tr><td>BD1900_2</td><td>$0.5 \times RB_{1930} + 0.5 \times RB_{1985}$</td><td>$RB_{1930}$</td><td>$\lambda_L = 1850$
$\lambda_H = 2067$</td><td>$k_{1850} = 5$
$k_{1930} = 5$
$k_{2067} = 5$</td></tr>
<tr><td>BD1900r2</td><td>$1.0 - \left(\frac{2 \times \frac{R_{1928}}{RC_{1928}}}{\frac{R_{1875}}{RC_{1875}} + \frac{R_{2112}}{RC_{2112}}}\right)$</td><td>$1.0 - \left(\frac{\sum_{\mu \in M} \frac{R_\mu}{RC_\mu}}{\sum_{\nu \in N} \frac{R_\nu}{RC_\nu}}\right)$
$M = \{1908, 1914, 1921, 1928, 1934, 1941\}$
$N = \{1862, 1869, 1875, 2112, 2120, 2126\}$</td><td>$\lambda_L = 1815$
$\lambda_H = 2132$</td><td>$k_{1815} = 5$
$k_{2132} = 5$
$k_\lambda = 1$ otherwise</td></tr>
<tr><td>BDI2000</td><td colspan="2">see below</td><td>-</td><td>-</td></tr>
</table>

Parameter	Multispectral Formulation	Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
BD2100_2	$1.0 - \left(\frac{R_C^*}{b \times R_L^* + a \times R_{2250}}\right)$ $W_L^* = 0.5 \times (W_{1862} + W_{1930})$ $R_L^* = 0.5 \times (R_{1862} + R_{1930})$ $W_C^* = 0.5 \times (W_{2120} + W_{2130})$ $R_C^* = 0.5 \times (R_{2120} + R_{2130})$ $a = \frac{W_C^* - W_L^*}{W_{2250} - W_L^*}$ $b = 1.0 - a$	RB_{2132}	$\lambda_L = 1930$ $\lambda_H = 2250$	$k_{1930} = 3$ $k_{2132} = 5$ $k_{2250} = 3$
BD2165	RB_{2165}		$\lambda_L = 2120$ $\lambda_H = 2230$	$k_{2120} = 5$ $k_{2165} = 3$ $k_{2230} = 3$
BD2190	RB_{2185}		$\lambda_L = 2120$ $\lambda_H = 2250$	$k_{2120} = 5$ $k_{2185} = 3$ $k_{2250} = 3$
MIN2200	$\mathbf{min}\left[RB_{2165}, RB_{2210}\right]$		$\lambda_L = 2120$ $\lambda_H = 2350$	$k_{2120} = 5$ $k_{2165} = 3$ $k_{2210} = 3$ $k_{2350} = 5$
BD2210_2	RB_{2210}		$\lambda_L = 2165$ $\lambda_H = 2290$	$k_{2165} = 5$ $k_{2210} = 5$ $k_{2290} = 5$

Parameter	Multispectral Formulation	Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
D2200	$1.0 - \left(\frac{\frac{R_{2210}}{RC_{2210}} + \frac{R_{2230}}{RC_{2230}}}{2 \times \frac{R_{2165}}{RC_{2165}}} \right)$		$\lambda_L = 1815$ $\lambda_H = 2430$	$k_{1815} = 7$ $k_{2165} = 5$ $k_{2210} = 7$ $k_{2230} = 7$ $k_{2430} = 7$
BD2230	RB_{2235}		$\lambda_L = 2210$ $\lambda_H = 2252$	$k_{2210} = 3$ $k_{2235} = 3$ $k_{2252} = 3$
BD2250	RB_{2245}		$\lambda_L = 2120$ $\lambda_H = 2340$	$k_{2120} = 5$ $k_{2245} = 7$ $k_{2340} = 3$
MIN2250	$\mathbf{min}\left[RB_{2210}, RB_{2265}\right]$		$\lambda_L = 2165$ $\lambda_H = 2350$	$k_{2165} = 5$ $k_{2210} = 3$ $k_{2265} = 3$ $k_{2350} = 5$
BD2265	RB_{2265}		$\lambda_L = 2120$ $\lambda_H = 2340$	$k_{2120} = 5$ $k_{2265} = 3$ $k_{2340} = 5$
BD2290	RB_{2290}		$\lambda_L = 2250$ $\lambda_H = 2350$	$k_{2250} = 5$ $k_{2290} = 5$ $k_{2350} = 5$
D2300	$1.0 - \frac{\frac{R_{2290}}{RC_{2290}} + \frac{R_{2320}}{RC_{2320}} + \frac{R_{2330}}{RC_{2330}}}{\frac{R_{2120}}{RC_{2120}} + \frac{R_{2170}}{RC_{2170}} + \frac{R_{2210}}{RC_{2210}}}$		$\lambda_L = 1815$ $\lambda_H = 2530$	$k_{2290} = 3$ $k_{2320} = 3$ $k_{2330} = 3$ $k_\lambda = 5$ otherwise
BD2355	RB_{2355}		$\lambda_L = 2300$ $\lambda_H = 2450$	$k_{2300} = 5$ $k_{2355} = 5$ $k_{2450} = 5$

Parameter	Multispectral Formulation	Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
SINDEX2	$1.0 - \left(\frac{RC_{2290}}{R_{2290}}\right)$		$\lambda_L = 2120$ $\lambda_H = 2400$	$k_{2120} = 5$ $k_{2290} = 7$ $k_{2400} = 3$
ICER2_2	RB_{2600}		$\lambda_L = 2456$ $\lambda_H = 2530$	$k_{2456} = 5$ $k_{2530} = 5$ $k_{2600} = 5$
MIN2295_2480	$\mathbf{min}\left[RB_{2295}, RB_{2480}\right]$		RB_{2295} $\lambda_L = 2165$ $\lambda_H = 2364$ RB_{2480} $\lambda_L = 2364$ $\lambda_H = 2570$	$k_{2165} = 5$ $k_{2295} = 5$ $k_{2364} = 5$ $k_{2480} = 5$ $k_{2570} = 5$
MIN2345_2537	$\mathbf{min}\left[RB_{2345}, RB_{2537}\right]$		RB_{2345} $\lambda_L = 2250$ $\lambda_H = 2430$ RB_{2537} $\lambda_L = 2430$ $\lambda_H = 2602$	$k_{2250} = 5$ $k_{2345} = 5$ $k_{2430} = 5$ $k_{2537} = 5$ $k_{2602} = 5$
BD2500_2	RB_{2480}		$\lambda_L = 2364$ $\lambda_H = 2570$	$k_{2364} = 5$ $k_{2480} = 5$ $k_{2570} = 5$

Parameter	Multispectral Formulation	Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
BD3000	$1.0 - \left(\frac{R_{3000} \times R_{2210}}{R_{2530} \times R_{2530}}\right)$		-	$k_{2210} = 5$ $k_{2530} = 5$ $k_{3000} = 5$
BD3100	RB_{3120}		$\lambda_L = 3000$ $\lambda_H = 3250$	$k_{3000} = 5$ $k_{3120} = 5$ $k_{3250} = 5$
BD3200	RB_{3320}		$\lambda_L = 3250$ $\lambda_H = 3390$	$k_{3250} = 5$ $k_{3320} = 5$ $k_{3390} = 5$
BD3400_2	$1.0 - \left(\frac{R_C^*}{b \times R_{3250} + a \times R_{3630}}\right)$ $W_C^* = 0.5 \times (W_{3390} + W_{3500})$ $R_C^* = 0.5 \times (R_{3390} + R_{3500})$ $a = \frac{W_C^* - W_{3250}}{W_{3630} - W_{3250}}$ $b = 1.0 - a$	RB_{3420}	$\lambda_L = 3250$ $\lambda_H = 3630$	$k_{3250} = 10$ $k_{3420} = 15$ $k_{3630} = 10$
CINDEX2	$1.0 - \left(\frac{RC_{3610}}{R_{3610}}\right)$		$\lambda_L = 3450$ $\lambda_H = 3875$	$k_{3450} = 9$ $k_{3610} = 11$ $k_{3875} = 7$

3.3 Atmospheric Parameters and Browse Product Components

Parameter	Multi-/Hyperspectral Formulation	Continuum Anchors	Hyperspectral Kernels
R440	R_{440}	-	$k_{440} = 5$
R530	R_{530}	-	$k_{530} = 5$
R600	R_{600}	-	$k_{600} = 5$
IRR1	$\frac{R_{800}}{R_{997}}$	-	$k_{800} = 5$ $k_{997} = 5$
R1080	R_{1080}	-	$k_{1080} = 5$
R1506	R_{1506}	-	$k_{1506} = 5$
R2529	R_{2529}	-	$k_{2529} = 5$
BD2600	RB_{2600}	$\lambda_L = 2530$ $\lambda_H = 2630$	$k_{2530} = 5$ $k_{2600} = 5$ $k_{2530} = 5$
IRR2	$\frac{R_{2530}}{R_{2210}}$	-	$k_{2210} = 5$ $k_{2530} = 5$
IRR3	$\frac{R_{3500}}{R_{3390}}$	-	$k_{3390} = 7$ $k_{3500} = 7$

3.4 RPEAK1

The RPEAK1 parameter is formally defined as “the wavelength where the 1st derivative is 0 of a 5th-order polynomial fit to reflectances at all valid VNIR wavelengths”. The algorithms used are described here; users are referred to CAT for implementation details.

Related to RPEAK1 is the “RPEAK1 modeled reflectance”, the interpolatead reflectance of the best-fit polynomial at the RPEAK1 wavelength. This modeled reflectance is not a formal spectral parameter, but is used as an intermediate value while calculating the BDI1000VIS parameter.

Note: both the multispectral and hyperspectral formulations implemented in CAT are slightly different from this definition. The CAT multispectral formulation identifies the wavelength that maximizes a 4th-degree polynomial and returns the value of that 4th-degree polynomial as the modeled reflectance. The CAT hyperspectral formulation identifies the wavelength that maximizes a 5th-degree polynomial and returns the value of that 5th-degree polynomial as the modeled reflectance. The formulations presented here are intended to allow reproduction of the CAT implementations.

Multispectral Formulation: For each spatial pixel:

1. Extract reflectances from bands with wavelengths $415 \leq \lambda \leq 644$ or $700 \leq \lambda \leq 940$ (11 bands total).

2. Fit a 4th-degree polynomial to those reflectances using a least-squares fit.

3. Find and return the wavelength in the range $442 \leq \lambda \leq 925$ which maximizes that polynomial.
4. The RPEAK1 modeled reflectance is the value of the 4th-degree polynomial fit when evaluated at the maximizing wavelength.

Hyperspectral Formulation: For each spatial pixel:

1. Extract reflectances from bands with wavelengths $410 \leq \lambda \leq 644$ or $684 \leq \lambda \leq 1023$.
2. Fit a 5th-degree polynomial to those reflectances using a least-squares fit.
3. Find the wavelength which maximizes that polynomial. If that wavelength is less than 900 nm, return it.
4. Otherwise, calculate numeric first and second derivatives of that 5th-degree polynomial. Identify and return the smallest wavelength where the first derivative is 0 and the second derivative is negative.
5. The RPEAK1 modeled reflectance is the value of the 5th-degree polynomial fit when evaluated at the returned wavelength.

3.5 BDI1000VIS

The BDI1000VIS parameter is formally defined as "the 1-µm integrated band depth over VNIR wavelengths". For each spatial pixel, it is calculated as follows:

1. Calculate the RPEAK1 modeled reflectance. Call the modeled reflectance R^*.
2. Extract reflectances from bands with wavelengths $833 \leq \lambda \leq 1023$. Call these reflectances R_λ.
3. Compute the following via numeric integration:

$$BDI1000VIS = \int_{833}^{1023} \left(1 - \frac{R_\lambda}{R^*}\right) d\lambda$$

3.6 BDI1000IR

The BDI1000IR parameter is formally defined as "the 1-µm integrated band depth over IR wavelengths". For each spatial pixel, it is calculated as follows:

1. Extract reflectances from bands with wavelengths $1020 < \lambda \leq 1255$. Call these reflectances R_λ.
2. Calculate BDICONT at all wavelengths.
3. Compute the following via numeric integration:

$$BDI1000IR = \int_{1020}^{1255} \left(1 - \frac{R_\lambda}{BDICONT(\lambda)}\right) d\lambda$$

Note: the multispectral formulation as defined in CAT omits $\lambda = 1180$. By the parameter definition, this band should be included in the calculation, but it should be omitted in scenarios where reproducing CAT output exactly is required.

3.7 VAR

The VAR parameter is formally defined as “fit a line from 1-2.3 microns and find variance of observed values from fit values by summing in quadrature over the intervening wavelengths”. For each spatial pxiel, it is calculated as follows:

1. Identify the lower anchor as the band closest to $\lambda = 1014$. Define W_L as its wavelength and R_L as its reflectance.
2. Identify the higher anchor as the band closest to $\lambda = 2287$. Define W_H as its wavelength and R_H as its reflectance.
3. Extract wavelengths W_λ and reflectances R_λ from bands with wavelengths $1021 \leq \lambda \leq 2253$
4. Compute interpolated reflectances RC_λ at all wavelengths as follows:

$$RC_\lambda = \left(\frac{R_H - R_L}{W_H - W_L}\right) \times (W_\lambda - W_L) + R_L$$

5. Compute the sum of squared errors across all wavelengths:

$$VAR = \sum_\lambda (R_\lambda - RC_\lambda)^2$$

3.8 BDI2000

The BDI2000 parameter is formally defined as “the 2-µm integrated band depth”. For each spatial pixel, it is calculated as follws:

1. Extract reflectances from bands with wavelengths $\lambda_L \leq \lambda \leq \lambda_H$. Call these reflectances R_λ.
   - Multispectral: $\lambda_L = 1660$ $\quad\lambda_H = 2455$
   - Hyperspectral: $\lambda_L = 1660$ $\quad\lambda_H = 2390$
2. Calculate BDICONT at all wavelengths.
3. Compute the following via numeric integration:

$$BDI2000 = \int_{\lambda_L}^{\lambda_H} \left(1 - \frac{R_\lambda}{BDICONT(\lambda)}\right) d\lambda$$

3.9 BDICONT

BDICONT is not an official spectral parameter. Instead, it is a continuum model interpolated over IR wavelengths used in the calculation of other parameters (BDI1000IR, BDI2000). It is defined as follows:

- Lower Anchor
  - Identify the bands with wavelengths $1330 \leq \lambda_L \leq 1875$.
  - The lower anchor wavelength W_L is the median of the wavelengths of those bands.
  - The lower anchor reflectance R_L is the 75th percentile of the reflectances of those bands.

- Higher Anchor
  - Identify the bands with wavelengths $2430 \leq \lambda_H \leq 2600$.
  - The higher anchor wavelength W_H is the median of the wavelengths of those bands.
  - The higher anchor reflectance R_H is the median of the reflectances of those bands.

BDICONT is then generated by fitting a straight line through both anchors. It can be expressed as a function of wavelength as follows:

$$BDICONT(\lambda) = \left(\frac{R_H - R_L}{W_H - W_L}\right) \times (\lambda - W_L) + R_L$$