**Appendices:**

Appendices are provided below that illustrate example labels from an actual CheMin analysis, the first Mary Anning drill sample, which was collected overnight on Mars during nights beginning on sols 2842, 2846, and 2853 (with corresponding files downlinked on sols 2842, 2847, and 2854). These files represent the three key data formats in a CheMin analysis: RE1 X-ray fluorescence, RDA X-ray diffraction, and the MIN file developed by analysis of the RDA file. Each appendix has two part (A= the PDS3 file, B= the PDS4 XML label).

Comparison of the two label formats provides traceability of product information (sourcde and product file identifications, start times, data file formats, descriptions, etc.) between the PDS3 and PDS4 versions.

1A: Example of PDS3 label for a CheMin RE1 product

1B: Corresponding PDS4 label for the CheMin RE1 product

2A: Example of PDS3 label for a CheMin RDA product

2B: Corresponding PDS4 label for the CheMin RDA product

3A: Example of PDS3 label for a CheMin MIN product

3B: Corresponding PDS4 label for the CheMin MIN product

Appendix 1A: Example of PDS3 label for a CheMin RE1 product

PDS\_VERSION\_ID = PDS3

RECORD\_TYPE = STREAM

RECORD\_BYTES = 24549

FILE\_RECORDS = 1451

^HEADER = ("CMB\_649856935RE128420822176CH00111P1.CSV",1)

^SPREADSHEET = ("CMB\_649856935RE128420822176CH00111P1.CSV",2)

DATA\_SET\_ID = "MSL-M-CHEMIN-4-RDR-V1.0"

PRODUCT\_ID = "CMB\_649856935RE128420822176CH00111P1"

PRODUCT\_VERSION\_ID = "V1.0"

RELEASE\_ID = "0026"

SOURCE\_PRODUCT\_ID = {"CMB\_649856935EE128420822176CH00111M1",

"CMB\_649857305EE128420822176CH00111M1",

"CMB\_649857674EE128420822176CH00111M1",

"CMB\_649858044EE128420822176CH00111M1",

"CMB\_649858414EE128420822176CH00111M1",

"CMB\_649858785EE128420822176CH00111M1",

"CMB\_649859156EE128420822176CH00111M1",

"CMB\_649859526EE128420822176CH00111M1",

"CMB\_649859898EE128420822176CH00111M1",

"CMB\_649860267EE128420822176CH00111M1",

"CMB\_649860637EE128420822176CH00111M1",

"CMB\_649861007EE128420822176CH00111M1",

"CMB\_649861377EE128420822176CH00111M1",

"CMB\_650300807EE128470822176CH00111M1",

"CMB\_650301177EE128470822176CH00111M1",

"CMB\_650301546EE128470822176CH00111M1",

"CMB\_650301916EE128470822176CH00111M1",

"CMB\_650302285EE128470822176CH00111M1",

"CMB\_650302656EE128470822176CH00111M1",

"CMB\_650303025EE128470822176CH00111M1",

"CMB\_650303395EE128470822176CH00111M1",

"CMB\_650303764EE128470822176CH00111M1",

"CMB\_650304134EE128470822176CH00111M1",

"CMB\_650304503EE128470822176CH00111M1",

"CMB\_650304873EE128470822176CH00111M1",

"CMB\_650305242EE128470822176CH00111M1",

"CMB\_650922339EE128540822176CH00111M1",

"CMB\_650922709EE128540822176CH00111M1",

"CMB\_650923078EE128540822176CH00111M1",

"CMB\_650923448EE128540822176CH00111M1",

"CMB\_650923818EE128540822176CH00111M1",

"CMB\_650924188EE128540822176CH00111M1",

"CMB\_650924558EE128540822176CH00111M1",

"CMB\_650924929EE128540822176CH00111M1",

"CMB\_650925299EE128540822176CH00111M1",

"CMB\_650925668EE128540822176CH00111M1",

"CMB\_650926038EE128540822176CH00111M1",

"CMB\_650926408EE128540822176CH00111M1",

"CMB\_650926778EE128540822176CH00111M1"}

PRODUCT\_TYPE = "CHEMIN\_RE1"

INSTRUMENT\_HOST\_ID = "MSL"

INSTRUMENT\_HOST\_NAME = "MARS SCIENCE LABORATORY"

INSTRUMENT\_ID = "CHEMIN"

TARGET\_NAME = "MARS"

MSL:CALIBRATION\_STANDARD\_NAME = "N/A"

MISSION\_PHASE\_NAME = "PRIMARY SURFACE MISSION"

PRODUCT\_CREATION\_TIME = 2021-01-22T19:57:30

START\_TIME = 2020-08-05T00:30:48.438

STOP\_TIME = UNK

SPACECRAFT\_CLOCK\_START\_COUNT = "649856935.562"

SPACECRAFT\_CLOCK\_STOP\_COUNT = "UNK"

OBJECT = HEADER

BYTES = 15

HEADER\_TYPE = TEXT

DESCRIPTION = "This header record contains column headings

for the following table."

END\_OBJECT = HEADER

OBJECT = SPREADSHEET

ROWS = 1450

ROW\_BYTES = 24534

FIELDS = 2

FIELD\_DELIMITER = "COMMA"

^STRUCTURE = "CHEMIN\_EDH.FMT"

DESCRIPTION = "This table contains energy-single

fluorescence data for the first Mary Anning drill sample, in CheMin cell

number 7a (Mylar window), which had previously held the scoop samples

Rocknest (fifth scoop) and Gobabeb. The 39 minor frames of best data

quality from sol 2842 to sol 2854 were selected and averaged, including

7020 individual 10-second frames in the 39 minor frames of 180 10-second

frames each. A threshold of 50 DN was used. CCD temperatures during data

collection were ~-50 degrees centigrade. Column 1 of the table shows energy

in keV converted from digital number (DN) using a conversion factor of

128.9063 DN/keV, based on position of the 6.400 keV Fe K-alpha peak at DN

825. Results are listed from DN 51 to 1500 (0.39564 to 11.63636 keV), 1450

entries. Column 2 lists the log-scale intensity for each value of keV in

column 1."

END\_OBJECT = SPREADSHEET

END

Appendix 1B: Corresponding PDS4 label for the CheMin RE1 product

<?xml version="1.0" encoding="UTF-8" standalone="no"?>

<?xml-model href="https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.sch" schematypens="http://purl.oclc.org/dsdl/schematron"?>

<?xml-model href="http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.sch"

schematypens="http://purl.oclc.org/dsdl/schematron"?>

<Product\_Observational xmlns="http://pds.nasa.gov/pds4/pds/v1"

xmlns:msn="http://pds.nasa.gov/pds4/msn/v1"

xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"

xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1 https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.xsd http://pds.nasa.gov/pds4/msn/v1 http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.xsd">

<Identification\_Area>

<logical\_identifier>urn:nasa:pds:msl\_chemin\_derived:chemin\_re:cmb\_649856935re128420822176ch00111p1</logical\_identifier>

<version\_id>1.0</version\_id>

<title>MSL CheMin Energy-single fluorescence Table</title>

<information\_model\_version>1.16.0.0</information\_model\_version>

<product\_class>Product\_Observational</product\_class>

<Modification\_History>

<Modification\_Detail>

<modification\_date>2022-10-01</modification\_date>

<version\_id>1.0</version\_id>

<description>Initial PDS4 version of this product.</description>

</Modification\_Detail>

</Modification\_History>

</Identification\_Area>

<Observation\_Area>

<Time\_Coordinates>

<start\_date\_time>2020-08-05T00:30:48.438Z</start\_date\_time>

<stop\_date\_time nilReason="unknown" xsi:nil="true"/>

</Time\_Coordinates>

<Primary\_Result\_Summary>

<purpose>Science</purpose>

<processing\_level>Derived</processing\_level>

<description>Data from the MSL CheMin Instrument.</description>

</Primary\_Result\_Summary>

<Investigation\_Area>

<name>MARS SCIENCE LABORATORY</name>

<type>Mission</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:investigation:mission.mars\_science\_laboratory</lid\_reference>

<reference\_type>data\_to\_investigation</reference\_type>

</Internal\_Reference>

</Investigation\_Area>

<Observing\_System>

<name>MARS SCIENCE LABORATORY</name>

<Observing\_System\_Component>

<name>MARS SCIENCE LABORATORY</name>

<type>Host</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:instrument\_host:spacecraft.msl</lid\_reference>

<reference\_type>is\_instrument\_host</reference\_type>

</Internal\_Reference>

</Observing\_System\_Component>

<Observing\_System\_Component>

<name>CHEMISTRY AND MINERALOGY INSTRUMENT</name>

<type>Instrument</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:instrument:chemin.msl</lid\_reference>

<reference\_type>is\_instrument</reference\_type>

</Internal\_Reference>

</Observing\_System\_Component>

</Observing\_System>

<Target\_Identification>

<name>Mars</name>

<type>Planet</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:target:planet.mars</lid\_reference>

<reference\_type>data\_to\_target</reference\_type>

</Internal\_Reference>

</Target\_Identification>

<Discipline\_Area>

<msn:Mission\_Information>

<msn:mission\_phase\_name>SURFACE MISSION</msn:mission\_phase\_name>

<msn:product\_type\_name>CHEMIN</msn:product\_type\_name>

<msn:spacecraft\_clock\_start>649856935.562</msn:spacecraft\_clock\_start>

<msn:spacecraft\_clock\_stop nilReason="unknown" xsi:nil="true"/>

</msn:Mission\_Information>

</Discipline\_Area>

</Observation\_Area>

<Reference\_List>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:msl\_chemin\_calibrated:document:chemin\_rdrsis</lid\_reference>

<reference\_type>data\_to\_document</reference\_type>

</Internal\_Reference>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:msl\_chemin\_calibrated:document:chemin\_basics</lid\_reference>

<reference\_type>data\_to\_document</reference\_type>

</Internal\_Reference>

<Source\_Product\_Internal> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649856935ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649857305ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649857674ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649858044ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649858414ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649858785ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649859156ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649859526ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649859898ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649860267ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649860637ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649861007ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_649861377ee128420822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650300807ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650301177ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650301546ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650301916ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650302285ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650302656ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650303025ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650303395ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650303764ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650304134ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650304503ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650304873ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650305242ee128470822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650922339ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650922709ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650923078ee128540822176ch00111m1::1.0</lidvid\_reference>

<lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650923448ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650923818ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650924188ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650924558ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650924929ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650925299ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650925668ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650926038ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650926408ee128540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650926778ee128540822176ch00111m1::1.0</lidvid\_reference>

<reference\_type>data\_to\_derived\_source\_product</reference\_type>

<comment>This is a reference to a data file corresponding to this data.</comment>

</Source\_Product\_Internal>

</Reference\_List>

<File\_Area\_Observational>

<File>

<file\_name>cmb\_649856935re128420822176ch00111p1.csv</file\_name>

</File>

<Header>

<offset unit="byte">0</offset>

<object\_length unit="byte">15</object\_length>

<parsing\_standard\_id>7-Bit ASCII Text</parsing\_standard\_id>

<description>Column headings</description>

</Header>

<Table\_Delimited>

<offset unit="byte">15</offset>

<parsing\_standard\_id>PDS DSV 1</parsing\_standard\_id>

<description>This table contains energy-single fluorescence data for the first Mary Anning drill sample, in CheMin cell number 7a (Mylar window), which had previously held the scoop samples Rocknest (fifth scoop) and Gobabeb. The 39 minor frames of best data quality from sol 2842 to sol 2854 were selected and averaged, including 7020 individual 10-second frames in the 39 minor frames of 180 10-second frames each. A threshold of 50 DN was used. CCD temperatures during data collection were ~-50 degrees centigrade. Column 1 of the table shows energy in keV converted from digital number (DN) using a conversion factor of 128.9063 DN/keV, based on position of the 6.400 keV Fe K-alpha peak at DN 825. Results are listed from DN 51 to 1500 (0.39564 to 11.63636 keV), 1450 entries. Column 2 lists the log-scale intensity for each value of keV in column 1.</description>

<records>1450</records>

<record\_delimiter>Carriage-Return Line-Feed</record\_delimiter>

<field\_delimiter>Comma</field\_delimiter>

<Record\_Delimited>

<fields>2</fields>

<groups>0</groups>

<Field\_Delimited>

<name>ENERGY</name>

<field\_number>1</field\_number>

<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">8</maximum\_field\_length>

<unit>kev</unit>

<description>Energy in keV converted from digital number (DN)</description>

</Field\_Delimited>

<Field\_Delimited>

<name>INTENSITY</name>

<field\_number>2</field\_number>

<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">8</maximum\_field\_length>

<unit>counts</unit>

<description>The log-scale intensity for each value of keV in column 1</description>

</Field\_Delimited>

</Record\_Delimited>

</Table\_Delimited>

</File\_Area\_Observational>

</Product\_Observational>

Appendix 2A: Example of PDS3 label for a CheMin RDA product

PDS\_VERSION\_ID = PDS3

RECORD\_TYPE = STREAM

RECORD\_BYTES = 10481

FILE\_RECORDS = 1002

^HEADER = ("CMB\_649856565RDA28420822176CH00111P1.CSV",1)

^SPREADSHEET = ("CMB\_649856565RDA28420822176CH00111P1.CSV",2)

DATA\_SET\_ID = "MSL-M-CHEMIN-4-RDR-V1.0"

PRODUCT\_ID = "CMB\_649856565RDA28420822176CH00111P1"

PRODUCT\_VERSION\_ID = "V1.0"

RELEASE\_ID = "0026"

SOURCE\_PRODUCT\_ID = {"CMB\_649856565EDA28420822176CH00111M1",

"CMB\_649856935EDA28420822176CH00111M1",

"CMB\_649857304EDA28420822176CH00111M1",

"CMB\_649857674EDA28420822176CH00111M1",

"CMB\_649858043EDA28420822176CH00111M1",

"CMB\_649858413EDA28420822176CH00111M1",

"CMB\_649858784EDA28420822176CH00111M1",

"CMB\_649859156EDA28420822176CH00111M1",

"CMB\_649859526EDA28420822176CH00111M1",

"CMB\_649859897EDA28420822176CH00111M1",

"CMB\_649860267EDA28420822176CH00111M1",

"CMB\_649860636EDA28420822176CH00111M1",

"CMB\_649861006EDA28420822176CH00111M1",

"CMB\_649861376EDA28420822176CH00111M1",

"CMB\_649861741EDA28420822176CH00111M1",

"CMB\_650300437EDA28470822176CH00111M1",

"CMB\_650300807EDA28470822176CH00111M1",

"CMB\_650301176EDA28470822176CH00111M1",

"CMB\_650301546EDA28470822176CH00111M1",

"CMB\_650301915EDA28470822176CH00111M1",

"CMB\_650302285EDA28470822176CH00111M1",

"CMB\_650302655EDA28470822176CH00111M1",

"CMB\_650303024EDA28470822176CH00111M1",

"CMB\_650303394EDA28470822176CH00111M1",

"CMB\_650303764EDA28470822176CH00111M1",

"CMB\_650304133EDA28470822176CH00111M1",

"CMB\_650304502EDA28470822176CH00111M1",

"CMB\_650304872EDA28470822176CH00111M1",

"CMB\_650305241EDA28470822176CH00111M1",

"CMB\_650305606EDA28470822176CH00111M1",

"CMB\_650921969EDA28540822176CH00111M1",

"CMB\_650922339EDA28540822176CH00111M1",

"CMB\_650922708EDA28540822176CH00111M1",

"CMB\_650923078EDA28540822176CH00111M1",

"CMB\_650923448EDA28540822176CH00111M1",

"CMB\_650923817EDA28540822176CH00111M1",

"CMB\_650924188EDA28540822176CH00111M1",

"CMB\_650924557EDA28540822176CH00111M1",

"CMB\_650924928EDA28540822176CH00111M1",

"CMB\_650925298EDA28540822176CH00111M1",

"CMB\_650925668EDA28540822176CH00111M1",

"CMB\_650926038EDA28540822176CH00111M1",

"CMB\_650926407EDA28540822176CH00111M1",

"CMB\_650926777EDA28540822176CH00111M1",

"CMB\_650927142EDA28540822176CH00111M1"}

PRODUCT\_TYPE = "CHEMIN\_RDA"

INSTRUMENT\_HOST\_ID = "MSL"

INSTRUMENT\_HOST\_NAME = "MARS SCIENCE LABORATORY"

INSTRUMENT\_ID = "CHEMIN"

TARGET\_NAME = "MARS"

MSL:CALIBRATION\_STANDARD\_NAME = "N/A"

MISSION\_PHASE\_NAME = "PRIMARY SURFACE MISSION"

PRODUCT\_CREATION\_TIME = 2021-01-27T18:27:10

START\_TIME = 2020-08-05T00:24:38.101

STOP\_TIME = "UNK"

SPACECRAFT\_CLOCK\_START\_COUNT = "649856565.343"

SPACECRAFT\_CLOCK\_STOP\_COUNT = "UNK"

OBJECT = HEADER

BYTES = 19

HEADER\_TYPE = TEXT

DESCRIPTION = "This header record contains column headings

for the following table."

END\_OBJECT = HEADER

OBJECT = SPREADSHEET

ROWS = 1001

ROW\_BYTES = 10462

FIELDS = 2

FIELD\_DELIMITER = "COMMA"

^STRUCTURE = "CHEMIN\_XRD.FMT"

DESCRIPTION = "This table contains diffraction-all K-alpha

diffraction data for the first Mary Anning drill sample, analyzed in CheMin

cell number 7a (Mylar window), which had previously held the scoop samples

Rocknest (fifth scoop) and Gobabeb. The table represents results from

sequences uploaded from sol 2842 to sol 2853, including 45 minor frames

that represent a total of 22.5 hours of analysis. Refined plagioclase c and

gamma cell parameters were used to make a minor adjustment in the sample to

detector distance, reducing this by 86 um. CCD temperatures during data

collection were ~-50 degrees centigrade. Column 1 of the table lists 2-

theta from 2.00 to 52.00 degrees cobalt K-alpha, in increments of 0.05

degrees (1001 entries). Column 2 lists the intensity of the diffraction for

each 2-theta value in column 1."

END\_OBJECT = SPREADSHEET

END

Appendix 2B: Corresponding PDS4 label for the CheMin RDA product

<?xml version="1.0" encoding="UTF-8" standalone="no"?>

<?xml-model href="https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.sch" schematypens="http://purl.oclc.org/dsdl/schematron"?>

<?xml-model href="http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.sch"

schematypens="http://purl.oclc.org/dsdl/schematron"?>

<Product\_Observational xmlns="http://pds.nasa.gov/pds4/pds/v1"

xmlns:msn="http://pds.nasa.gov/pds4/msn/v1"

xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"

xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1 https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.xsd http://pds.nasa.gov/pds4/msn/v1 http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.xsd">

<Identification\_Area>

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<version\_id>1.0</version\_id>

<title>MSL CheMin diffraction-all K-alpha

diffraction data </title>

<information\_model\_version>1.16.0.0</information\_model\_version>

<product\_class>Product\_Observational</product\_class>

<Modification\_History>

<Modification\_Detail>

<modification\_date>2022-10-01</modification\_date>

<version\_id>1.0</version\_id>

<description>Initial PDS4 version of this product.</description>

</Modification\_Detail>

</Modification\_History>

</Identification\_Area>

<Observation\_Area>

<Time\_Coordinates>

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</Time\_Coordinates>

<Primary\_Result\_Summary>

<purpose>Science</purpose>

<processing\_level>Derived</processing\_level>

<description>Data from the MSL CheMin Instrument.</description>

</Primary\_Result\_Summary>

<Investigation\_Area>

<name>MARS SCIENCE LABORATORY</name>

<type>Mission</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:investigation:mission.mars\_science\_laboratory</lid\_reference>

<reference\_type>data\_to\_investigation</reference\_type>

</Internal\_Reference>

</Investigation\_Area>

<Observing\_System>

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<Observing\_System\_Component>

<name>MARS SCIENCE LABORATORY</name>

<type>Host</type>

<Internal\_Reference>

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<reference\_type>is\_instrument\_host</reference\_type>

</Internal\_Reference>

</Observing\_System\_Component>

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<name>CHEMISTRY AND MINERALOGY INSTRUMENT</name>

<type>Instrument</type>

<Internal\_Reference>

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</Internal\_Reference>

</Observing\_System\_Component>

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<Target\_Identification>

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<type>Planet</type>

<Internal\_Reference>

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</Internal\_Reference>

</Target\_Identification>

<Discipline\_Area>

<msn:Mission\_Information>

<msn:mission\_phase\_name>SURFACE MISSION</msn:mission\_phase\_name>

<msn:product\_type\_name>CHEMIN</msn:product\_type\_name>

<msn:spacecraft\_clock\_start>649856565.343</msn:spacecraft\_clock\_start>

<msn:spacecraft\_clock\_stop nilReason="unknown" xsi:nil="true"/>

</msn:Mission\_Information>

</Discipline\_Area>

</Observation\_Area>

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</Internal\_Reference>

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<lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650926777eda28540822176ch00111m1::1.0</lidvid\_reference> <lidvid\_reference>urn:nasa:pds:msl\_chemin\_edr:cmb\_650927142eda28540822176ch00111m1::1.0</lidvid\_reference>

<reference\_type>data\_to\_derived\_source\_product</reference\_type>

<comment>This is a reference to a data file corresponding to this data.</comment>

</Source\_Product\_Internal>

</Reference\_List>

<File\_Area\_Observational>

<File>

<file\_name>cmb\_649856565rda28420822176ch00111p1.csv</file\_name>

</File>

<Header>

<offset unit="byte">0</offset>

<object\_length unit="byte">19</object\_length>

<parsing\_standard\_id>7-Bit ASCII Text</parsing\_standard\_id>

<description>Column headings</description>

</Header>

<Table\_Delimited>

<offset unit="byte">19</offset>

<parsing\_standard\_id>PDS DSV 1</parsing\_standard\_id>

<description>This table contains diffraction-all K-alpha diffraction data for the first Mary Anning drill sample, analyzed in CheMin cell number 7a (Mylar window), which had previously held the scoop samples Rocknest (fifth scoop) and Gobabeb. The table represents results from sequences uploaded from sol 2842 to sol 2853, including 45 minor frames that represent a total of 22.5 hours of analysis. Refined plagioclase c and gamma cell parameters were used to make a minor adjustment in the sample to detector distance, reducing this by 86 um. CCD temperatures during data collection were ~-50 degrees centigrade. Column 1 of the table lists theta from 2.00 to 52.00 degrees cobalt K-alpha, in increments of 0.05 degrees (1001 entries). Column 2 lists the intensity of the diffraction for each 2-theta value in column 1.</description>

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<Record\_Delimited>

<fields>2</fields>

<groups>0</groups>

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<field\_number>1</field\_number>

<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">6</maximum\_field\_length>

<unit>degrees</unit>

<description>2-theta</description>

</Field\_Delimited>

<Field\_Delimited>

<name>INTENSITY</name>

<field\_number>2</field\_number>

<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">7</maximum\_field\_length>

<unit>counts</unit>

<description>The intensity of the diffraction for each 2-theta value in column 1</description>

</Field\_Delimited>

</Record\_Delimited>

</Table\_Delimited>

</File\_Area\_Observational>

</Product\_Observational>

Appendix 3A: Example of PDS3 label for a CheMin MIN product

PDS\_VERSION\_ID = PDS3

RECORD\_TYPE = STREAM

RECORD\_BYTES = 157

FILE\_RECORDS = 8

^HEADER = ("CMB\_649856565MIN28420822176CH00111P1.CSV",1)

^SPREADSHEET = ("CMB\_649856565MIN28420822176CH00111P1.CSV",2)

DATA\_SET\_ID = "MSL-M-CHEMIN-5-RDR-V1.0"

PRODUCT\_ID = "CMB\_649856565MIN28420822176CH00111P1"

PRODUCT\_VERSION\_ID = "V1.0"

RELEASE\_ID = "0026"

SOURCE\_PRODUCT\_ID = "CMB\_649856565RDA28420822176CH00111P1"

PRODUCT\_TYPE = "CHEMIN\_MIN"

INSTRUMENT\_HOST\_ID = "MSL"

INSTRUMENT\_HOST\_NAME = "MARS SCIENCE LABORATORY"

INSTRUMENT\_ID = "CHEMIN"

TARGET\_NAME = "MARS"

MSL:CALIBRATION\_STANDARD\_NAME = "N/A"

MISSION\_PHASE\_NAME = "PRIMARY SURFACE MISSION"

PRODUCT\_CREATION\_TIME = 2021-02-07T16:36:00

START\_TIME = 2020-08-05T00:24:38.101

STOP\_TIME = "UNK"

SPACECRAFT\_CLOCK\_START\_COUNT = "649856565.343"

SPACECRAFT\_CLOCK\_STOP\_COUNT = "UNK"

OBJECT = HEADER

BYTES = 23

HEADER\_TYPE = TEXT

DESCRIPTION = "This header record contains column headings

for the following table."

END\_OBJECT = HEADER

OBJECT = SPREADSHEET

ROWS = 7

ROW\_BYTES = 134

FIELDS = 3

FIELD\_DELIMITER = "COMMA"

^STRUCTURE = "CHEMIN\_MIN.FMT"

DESCRIPTION = "This table contains mineral abundances and

analytical errors derived from diffraction-all K-alpha diffraction data for

the first Mary Anning drill sample, analyzed in CheMin cell number 7a (Mylar

window). The analysis is based on RDA file

CMB\_649856565RDA28420822176CH00111P1. Mineral identifications, abundances

and analytical errors for crystalline phases, other than clay minerals,

were determined using the program JADE. Mineral identification as

Fe-carbonate may include siderite and/or ankerite. In addition to these

crystalline phases, the program FULLPAT was used to estimate the abundance

of poorly crystalline clay minerals at ~28 +/- 10 weight% of the total

sample. High intensity in the low 2-theta region and a broad amorphous hump

are modeled using FULLPAT to indicate that ~27 +/- 20 weight% of the total

sample consists of X-ray amorphous materials. Column 1 of the table lists

mineral identifications, column 2 lists the mineral abundances in weight

percent, and column 3 indicates the estimated 2-sigma analytical errors."

END\_OBJECT = SPREADSHEET

END

Appendix 3B: Corresponding PDS4 label for the CheMin MIN product

<?xml version="1.0" encoding="UTF-8" standalone="no"?>

<?xml-model href="https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.sch" schematypens="http://purl.oclc.org/dsdl/schematron"?>

<?xml-model href="http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.sch"

schematypens="http://purl.oclc.org/dsdl/schematron"?>

<Product\_Observational xmlns="http://pds.nasa.gov/pds4/pds/v1"

xmlns:msn="http://pds.nasa.gov/pds4/msn/v1"

xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"

xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1 https://pds.nasa.gov/pds4/pds/v1/PDS4\_PDS\_1G00.xsd http://pds.nasa.gov/pds4/msn/v1 http://pds.nasa.gov/pds4/msn/v1/PDS4\_MSN\_1G00\_1300.xsd">

<Identification\_Area>

<logical\_identifier>urn:nasa:pds:msl\_chemin\_derived:chemin\_min:cmb\_649856565min28420822176ch00111p1</logical\_identifier>

<version\_id>1.0</version\_id>

<title>MSL CheMin Mineral Abundances Table</title>

<information\_model\_version>1.16.0.0</information\_model\_version>

<product\_class>Product\_Observational</product\_class>

<Modification\_History>

<Modification\_Detail>

<modification\_date>2022-10-01</modification\_date>

<version\_id>1.0</version\_id>

<description>Initial PDS4 version of this product.</description>

</Modification\_Detail>

</Modification\_History>

</Identification\_Area>

<Observation\_Area>

<Time\_Coordinates>

<start\_date\_time>2020-08-05T00:24:38.101Z</start\_date\_time>

<stop\_date\_time nilReason="unknown" xsi:nil="true"/>

</Time\_Coordinates>

<Primary\_Result\_Summary>

<purpose>Science</purpose>

<processing\_level>Derived</processing\_level>

<description>Data from the MSL CheMin Instrument.</description>

</Primary\_Result\_Summary>

<Investigation\_Area>

<name>MARS SCIENCE LABORATORY</name>

<type>Mission</type>

<Internal\_Reference>

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<reference\_type>data\_to\_investigation</reference\_type>

</Internal\_Reference>

</Investigation\_Area>

<Observing\_System>

<name>MARS SCIENCE LABORATORY</name>

<Observing\_System\_Component>

<name>MARS SCIENCE LABORATORY</name>

<type>Host</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:instrument\_host:spacecraft.msl</lid\_reference>

<reference\_type>is\_instrument\_host</reference\_type>

</Internal\_Reference>

</Observing\_System\_Component>

<Observing\_System\_Component>

<name>CHEMISTRY AND MINERALOGY INSTRUMENT</name>

<type>Instrument</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:instrument:chemin.msl</lid\_reference>

<reference\_type>is\_instrument</reference\_type>

</Internal\_Reference>

</Observing\_System\_Component>

</Observing\_System>

<Target\_Identification>

<name>Mars</name>

<type>Planet</type>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:context:target:planet.mars</lid\_reference>

<reference\_type>data\_to\_target</reference\_type>

</Internal\_Reference>

</Target\_Identification>

<Discipline\_Area>

<msn:Mission\_Information>

<msn:mission\_phase\_name>SURFACE MISSION</msn:mission\_phase\_name>

<msn:product\_type\_name>CHEMIN</msn:product\_type\_name>

<msn:spacecraft\_clock\_start>649856565.343</msn:spacecraft\_clock\_start>

<msn:spacecraft\_clock\_stop nilReason="unknown" xsi:nil="true"/>

</msn:Mission\_Information>

</Discipline\_Area>

</Observation\_Area>

<Reference\_List>

<Internal\_Reference>

<lid\_reference>urn:nasa:pds:msl\_chemin\_calibrated:document:chemin\_rdrsis</lid\_reference>

<reference\_type>data\_to\_document</reference\_type>

</Internal\_Reference>

<Internal\_Reference>

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<reference\_type>data\_to\_document</reference\_type>

</Internal\_Reference>

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</Source\_Product\_Internal>

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</File>

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<offset unit="byte">23</offset>

<parsing\_standard\_id>PDS DSV 1</parsing\_standard\_id>

<description>This table contains mineral abundances and analytical errors derived from diffraction-all K-alpha diffraction data for the first Mary Anning drill sample, analyzed in CheMin cell number 7a (Mylar window). The analysis is based on RDA file CMB\_649856565RDA28420822176CH00111P1. Mineral identifications, abundances and analytical errors for crystalline phases, other than clay minerals, were determined using the program JADE. Mineral identification as Fe-carbonate may include siderite and/or ankerite. In addition to these crystalline phases, the program FULLPAT was used to estimate the abundance of poorly crystalline clay minerals at ~28 +/- 10 weight% of the total sample. High intensity in the low 2-theta region and a broad amorphous hump were modeled using FULLPAT to indicate that ~27 +/- 20 weight% of the total sample consists of X-ray amorphous materials. Column 1 of the table lists mineral identifications, column 2 lists the mineral abundances in weight percent, and column 3 indicates the estimated 2-sigma analytical errors.</description>

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<groups>0</groups>

<Field\_Delimited>

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<field\_number>1</field\_number>

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<maximum\_field\_length unit="byte">16</maximum\_field\_length>

<description>Mineral identification</description>

</Field\_Delimited>

<Field\_Delimited>

<name>PERCENT</name>

<field\_number>2</field\_number>

<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">9</maximum\_field\_length>

<unit>wt%</unit>

<description>The mineral abundances in weight percent</description>

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<data\_type>ASCII\_Real</data\_type>

<maximum\_field\_length unit="byte">7</maximum\_field\_length>

<unit>estimated\_error</unit>

<description>The estimated 2-sigma analytical errors</description>

</Field\_Delimited>

</Record\_Delimited>

</Table\_Delimited>

</File\_Area\_Observational>

</Product\_Observational>