Mars Science Laboratory (MSL) Software Interface Specification

SAM Reduced Data Record (RDR)

Version 2.0
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CHANGE LOG

DATE	SECTIONS CHANGED	REASON FOR CHANGE	REVISION
4/3/12	1.2, 1.3, Table 2-8, 2.4.8, 3.2.2, 4.1, 4.2, Appx A	Minor edits	S. Slavney / PDS
4/3/12	Table 2.5	Suggested data set ID revisions	S. Slavney / PDS
4/3/12	2.3.2	Comment about adding calibration and processing information	S. Slavney / PDS
4/3/12	Appx A	Comment about completing definitions for SAM-specific keywords to be added to the MSL Data Dictionary	S. Slavney / PDS
4/3/12	2.3.4, Appx C	File names must be case-insensitive	S. Slavney / PDS
5/9/12	Appx A, Appx B, Appx C	Updated SAM-specific keywords in Appx A and sample label files in Appx B; added missing values to Appx C	H. Franz/UMBC/ GSFC
2/13/13	2.2; Appx B; Appx C	Eliminated L1C product from table 2-5 and Appx B; changed COMPXXX to ATMCOMP and EGACOMP in the list of valid L2 file descriptors.	H. Franz/UMBC/ GSFC
4/22/13	2.1, 2.3; 3.1; Appx B; Appx C	Minor wording changes; eliminated Appx B and references to it within the text; renamed Appx C to Appx B and modified references to Appx C accordingly.	H. Franz/UMBC/ GSFC
8/13/2013	Tables 2.3, 2.8	Added variants of noble gas and nitrogen enrichment experiment.	H. Franz/UMBC/ GSFC

CONTENTS

ACRONYMS AND ABBREVIATIONS

ASCII	American Standard Code for Information Interchange
CODMAC	Committee on Data Management and Computation
EDR	Experiment Data Record
GC	Gas chromatograph
GDS	Ground Data System
IOT	Instrument Operations Team
JPL	Jet Propulsion Laboratory
MIPL	Multi-mission image Processing Laboratory
MPCS	Mission Data Processing and Control System
MSL	Mars Science Laboratory
NASA	National Aeronautics and Space Administration
OCM	Organic check material
ODS	MSL's Operations Data Store
OPGS	Operations Products Generation Sub-system
PDS	Planetary Data System
QMS	Quadrupole mass spectrometer
RDR	Reduced Data Record
RTO	Real Time Operations (MSL terminology)
SAM	Sample Analysis at Mars
SIS	Software Interface Specification
TBD	To Be Determined
TCD	Thermal Conductivity Detector
TLS	Tunable laser spectrometer

1. INTRODUCTION

1.1 Purpose and Scope

The purpose of this Software Interface Specification (SIS) is to provide suppliers and consumers of the Mars Science Laboratory's (MSL) Sample Analysis at Mars (SAM) instrument with a detailed description of SAM's Reduced Data Records (RDR).

The users for whom this SIS is intended are the scientists who will analyze the data, including those associated with the MSL Project, SAM instrument engineers, and other users in the general planetary science community.

1.2 Contents

This SIS contains a very high level description of how SAM works/operates. It will also describe, at high level, how the SAM data product is acquired by the instrument, and how it is processed, formatted, labeled, and uniquely identified on the ground.

The document discusses standards used in generating the product and software tools that may be used to access the information. The data product structure and organization are described in sufficient detail to enable a user to read the product. Finally, an example of the product's PDS label is provided.

1.3 Applicable Documents and Constraints

This Data Product SIS is responsive to the following MSL documents:

1. Mars Exploration Program Data Management Plan, R. E. Arvidson and S. Slavney, Rev. 4, June 15, 2011.
2. Mars Science Laboratory Project Archive Generation, Validation and Transfer Plan, Joy Crisp, JPL D-35281, November 13, 2006.
3. Planetary Data System Standards Reference, February 27, 2009, Version 3.8, JPL D-7669 Part 2.
4. Planetary Archive Preparation Guide, April 1, 2010, Version 1.4, JPL D-31224, http://pds.nasa.gov/tools/archiving.shtml.
5. SAM Functional Description Document, September 24, 2010, Revision A, JPL D-34225, MSL 375-1235.
6. SAM Science Team and PDS Geosciences Node ICD, Version 3.0, April 5, 2011.
7. SAM RDR Archive Volume Software Interface Specification, May 9, 2012, Version 1.0, JPL D-75417, MSL SIS-SCI030-MSL.

This SIS is meant to be consistent with the contract negotiated between the MSL Project and the Instrument Principal Investigator (PI) in which reduced data records (RDR) and documentation (SIS) are explicitly defined as deliverable products.

1.4 Relationships with Other Interfaces

Changes to this SAM SIS document will affect the following products, software, and/or documents.

Table 1-1. Product and Software Interfaces to this SIS

Name	Type P-product S-software D-document	Owner
Other SAM Programs/Products/Documents	P/S/D	SAM Science Team

2. DATA PRODUCT CHARACTERISTICS AND ENVIRONMENT

2.1 Instrument Overview

This section is included for convenience of PDS data users, but a comprehensive description of the Sample Analysis at Mars (SAM) Suite Investigation in the MSL Analytical Laboratory may be found in Mahaffy et al. (2012). SAM is designed to address the present and past habitability of Mars by exploring molecular and elemental chemistry relevant to life. SAM has the capability to analyze volatiles thermally released from rocks and soils as well as gases from the Martian atmosphere. A primary focus of the suite is the detection and identification of organic compounds. However, SAM will also study the chemical and isotopic state of elements besides carbon that are relevant to life or Mars' geological and environmental history. SAM's science goals are summarized in Table 2-1.

Table 2-1. SAM Science Goals

Science and Measurement Goal	Habitability Question
(1) Survey carbon compound sources and evaluate their possible mechanisms of formation and destruction. (2) Search for organic compounds of biotic and prebiotic importance, including methane.	What does the inventory or lack of carbon compounds near the surface of Mars tell us about its potential habitability?
(3) Reveal the chemical and isotopic state of elements (i.e., N, H, O, S, and others) that are important for life as we know it. (4) Determine atmospheric composition, including trace species that are evidence of interactions between the atmosphere and soil.	What are the chemical and isotopic states of the lighter elements in the solids and in the atmosphere of Mars and what do they tell us about its potential habitability?
(5) Better constrain models of atmospheric and climatic evolution through measurements of noble gas and light element isotopes.	Were past habitability conditions different from today's?

SAM is a suite of three instruments: a Quadrupole Mass Spectrometer (QMS), a Gas Chromatograph (GC), and a Tunable Laser Spectrometer (TLS). The QMS and the GC can operate together in a GCMS mode for separation (GC) and definitive identification (QMS) of organic compounds. The TLS obtains precise isotope ratios for C and O in carbon dioxide, H and O in water, and also measures trace levels of methane and its carbon isotope ratio.

The three SAM instruments are supported by a sample manipulation system (SMS) and a Chemical Separation and Processing Laboratory (CSPL) that includes high-conductance and micro-valves, gas manifolds with heaters and temperature monitors, chemical and mechanical pumps, carrier gas reservoirs and regulators, pressure monitors, pyrolysis ovens, and chemical

scrubbers and getters. The Martian atmosphere is sampled by CSPL valve and pump manipulations that introduce an appropriate amount of gas through an inlet tube to the SAM instruments. Solid phase samples are analyzed by transporting finely sieved materials to one of 74 SMS sample cups that can then be inserted into a SAM oven and thermally processed to release volatiles. The SAM mechanical configuration and a top-level schematic of its sample flow configuration are illustrated in Figures 2-1 and 2-2. SAM instrument components are summarized in Table 2-2.

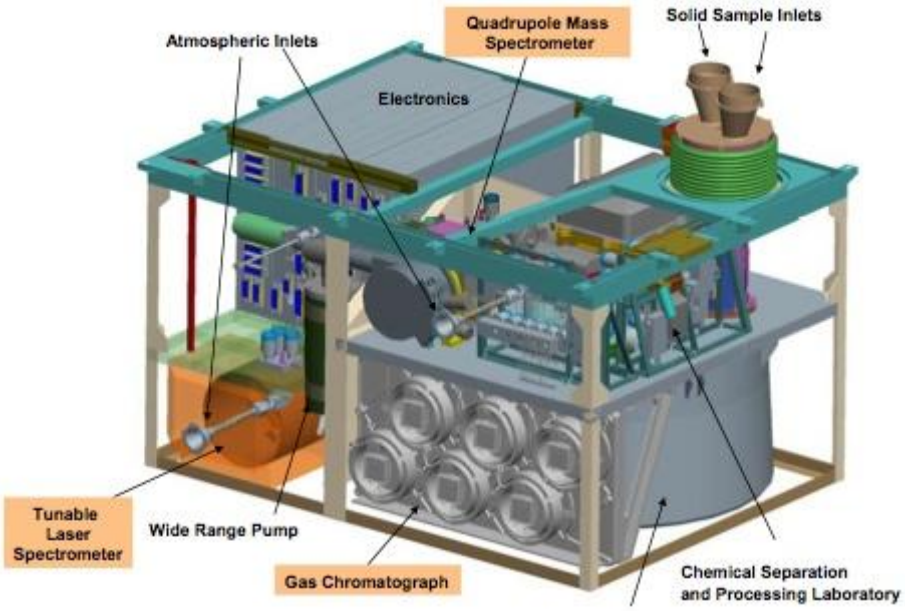

Figure 2-1. The illustration of the mechanical configuration of SAM shows the three instruments and several elements of the Chemical Separation and Processing Laboratory.

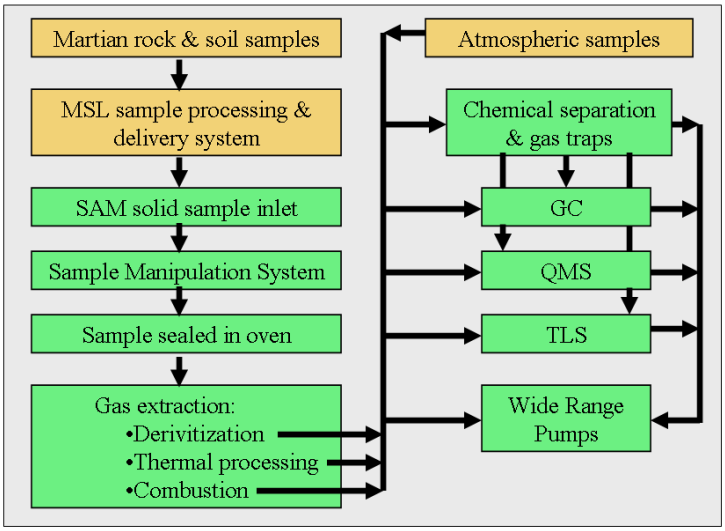

Figure 2-2. The path of solid and gas samples delivered by MSL subsystems to the SAM instruments is shown. Arrows designate the direction of gas and solid transport.

Table 2-2. SAM Instrument Characteristics

Quadrupole Mass Spectrometer			**Tunable Laser Spectrometer**	
Summary: QMS analyzes the atmosphere, gases thermally evolved from solid phase samples to sub ppb sensitivity. QMS is the primary detector for the GC and can operate in static or dynamic mode.			*Summary:* Two-channel Herriott cell design spectrometer that provides high sensitivity, unambiguous detection of targeted species (CH_4, H_2O, and CO_2) and selected isotope ratios. One channel is at a wavelength of 3.27 μm for CH_4, and the second is at 2.78 μm for CO_2 and H_2O.	
Mass Range	2-535 Dalton (Da)		*Sensitivity*	Methane: 2 ppb direct Water: 2 ppm direct CSPL enrichment improves by ~100x.
Detector dynamic range	> 10^{10} with pulse counting and Faraday Cup		*Isotopes*	$^{13}C/^{12}C$ in methane and CO_2 $^{18}O/^{17}O/^{16}O$ in CO_2 and water D/H in methane and water
Crosstalk	< 10^6 adjacent unit mass channels (below 150 Da)		*Isotope precision*	Typically < 10 ‰

Gas Chromatograph	
Summary: GC separates complex mixtures of organic compounds into molecular components for QMS and GC stand-alone analysis. Helium carrier gas is utilized.	
Injection	Injection from traps into the SAM manifold or from 3 GC injection traps incorporated into the GC subsystem.
6 GC Columns	GC1: w/o trap; w/o TCD; MXT20 (C5-C15 organics) GC2: w/o trap; TCD; MXT5 (> C15 organics) GC3: trap; TCD; Carbobond (permanent gases) GC4: trap; TCD; ChirasilDex (chiral compound separation) GC5: trap; TCD; MXT CLP (C5-C15 organics) GC6: trap; TCD; MXTQ (C1-C4 organics, N/S compounds)
Detection Limit	10^{-11} mole

SAM is designed to deliver nine data set types that are acquired via the experiment sequences described in Table 2-3. These experiment sequences may utilize different elements of the SAM suite. In addition to these science sequences, the SAM vacuum elements will be cleaned as necessary during the course of the mission by in situ bakeout.

Pyrolysis is the primary method for detection of organic molecules and examination of mineral content. This approach samples the gas thermally evolved from a small aliquot of sample delivered from the MSL sample acquisition/sample preparation and handling unit (SA/SPaH) to one of 59 quartz cups of the SAM sample manipulation system. Each quartz cup can accommodate up to 0.5 cm^3 of sample and the incremental volume of sample delivered from the SA/SPaH is approximately 0.05 cm^3. This allows delivery of a specified volume of sample to a cup and possible reuse of cups in an extended mission by deposition of fresh sample on the devolatilized residue in a cup. For direct analysis by the QMS or TLS, the sample in the quartz cup is heated from ambient to ~1000 °C with a programmable temperature ramp, nominally 35 °C/min. As gases are released, they are swept through the gas manifold by a helium carrier gas for detection by the spectrometers. Typically, water of hydration is released from samples early in the temperature ramp. Moderately volatile organics are released in the 300 °C to 600 °C range

Table 2-3. SAM Experiment Sequences

Solid Sample Analysis Sequences	
S-PYR Pyrolysis with GCMS (seq. #1)	*Measurement:* Chemical and isotopic analysis of gases evolved from samples as a function of temperature (EGA) and GCMS analysis of organics thermally released from samples. *Experiment Sequence:* Quartz cell cleaned in pyrolysis oven; Sample delivered to cooled cup; Sample heated from ambient to ~1000 °C in helium gas stream while evolved gases are monitored by QMS and TLS; GCMS analysis initiated using gases trapped during gas processing in previous step with detection by QMS and GC thermal conductivity detectors. *Notes:* 59 quartz cups allow this sequence to be repeated many times over the course of the landed mission. Cups can typically be reused several times.
S-DER Derivatization (seq. #2)	*Measurement:* Analysis of chemically derivatized polar compounds such as amino acids and carboxylic acids that would not otherwise be detected by GCMS. *Experiment Sequence:* Foil on metal cup in SMS punctured; Sample delivered to one-cup solvent extraction/derivatization cell; Sample cup moved to oven for thermal processing; Venting of solvent; Thermal injection of derivatized compounds into SAM GC traps; GCMS. *Notes:* 9 derivatization cups in SMS.
S-CMB Combustion (seq. #8)	*Measurement:* Analysis of carbon isotopes in carbon dioxide produced by combustion in oxygen. *Experiment Sequence:* Quartz cell cleaned in pyrolysis oven; Sample delivered to cooled cup; Sample combusted using oxygen gas; Carbon dioxide produced analyzed by TLS for $^{13}C/^{12}C$ isotopic composition.
Atmospheric Analysis Sequences	
A-DIR Direct Atmospheric Measurement (seq. #4)	*Measurement:* QMS and TLS analysis of atmospheric chemical and isotopic composition and seasonal and diurnal variations in trace species abundance. *Experiment Sequence:* Atmospheric gas directed into SAM gas manifold; Analysis by QMS and TLS scans. *Notes:* Duration and number of day time operation may be limited by thermal and energy considerations.
A-ENR Atmospheric Enrichment (seq. #5)	*Measurement:* QMS, TLS, and GCMS analysis of atmospheric trace species. *Experiment Sequence:* Atmospheric gas directed over SAM gas traps for enrichment of trace species; Gases released from traps and analyzed by GCMS for trace species. *Notes:* Direct TLS and QMS measurement also possible during this sequence.
A-MET Methane Enrichment (seq. #6)	*Measurement:* TLS methane analysis with SAM CSPL methane enrichment. *Experiment Sequence:* Atmospheric gas directed over SAM gas scrubbers and cold traps; Methane released into TLS for isotopic and abundance determination. *Notes:* Enrichment sequence may be repeated as necessary for improved methane detection sensitivity.
A-NGE Noble Gas Enrichment (seq. #7)	*Measurement:* Noble gas and nitrogen analysis with SAM CSPL noble gas enrichment. *Experiment Sequence:* Atmospheric gas directed over SAM gas scrubbers; Noble gases and nitrogen analyzed in SAM QMS operated in static mode. *Notes:* Enrichment sequence may be repeated as necessary for improved noble gas and nitrogen detection sensitivity and precision in isotope measurements.
A-DNG Dynamic Noble Gas Enrichment (seq. #7a)	*Measurement:* Noble gas and nitrogen analysis with SAM CSPL noble gas enrichment. *Experiment Sequence:* Atmospheric gas directed over SAM gas scrubbers; Noble gases and nitrogen analyzed in SAM QMS operated in dynamic mode. *Notes:* Variant of A-NG. Enrichment sequence may be repeated as necessary for improved noble gas and nitrogen detection sensitivity and precision in isotope measurements.
A-SNG Semi-static Noble Gas Enrichment (seq. #7b)	*Measurement:* Noble gas and nitrogen analysis with SAM CSPL noble gas enrichment. *Experiment Sequence:* Atmospheric gas directed over SAM gas scrubbers; Noble gases and nitrogen analyzed in SAM QMS operated in semi-static mode, in which high-conductance valve is partially closed. *Notes:* Variant of A-NG. Enrichment sequence may be repeated as necessary for improved noble gas and nitrogen detection sensitivity and precision in isotope measurements.

Calibration Sequences	
CAL-GAS In situ Gas Calibration (seq. #9)	*Measurement:* Calibration gas sampled by QMS, TLS, and GCMS to check instrument performance and changes with time. *Experiment Sequence:* Gas from SAM calibration gas cell released into manifold; QMS and TLS scans; Fluorocarbons trapped on SAM trap; GCMS analysis of fluorocarbons. *Notes:* Calibration sequence repeated on approximately a monthly basis.
CAL-SOL Solid Sample in situ Calibration (seq. #3)	*Measurement:* Identical to S-PYR sequence but using internal calibration standard consisting of carbonate and/or fluorinated carbon compounds. *Experiment Sequence:* Metal cup containing sample opened by SMS foil puncture operation; Sample heated from ambient to ~850 °C in helium gas stream while evolved gases are monitored by QMS and TLS; GCMS analysis initiated to detect fluorocarbons thermally released from cup and trapped during gas processing in previous step; GCMS analysis. *Notes:* 6 solid sample calibration cups will be used during the landed mission to check instrument performance.

due to thermal desorption and the breakdown of macromolecular organic matter. At higher temperatures, gases evolve due to the further pyrolysis of refractory organics and the breakdown of minerals. For example, carbonates and sulfates thermally dissociate to release CO_2 and SO_2, respectively, at temperatures above 500 °C. The temperature at which minerals degrade is often diagnostic of the mineral type.

In addition to direct analysis of the evolved gases, SAM has the option to direct the gas flow over a high-surface-area adsorbent to trap organic molecules, thus separating organic from inorganic volatiles for subsequent analysis by GCMS. Passing the trapped and released organic volatiles through one of six GC columns effectively separates different molecules, allowing for individual detection by the QMS. As a consequence of pyrolysis, the complex refractory organic molecules embedded in a mineral matrix or thermally unstable species may break down during thermal processing to produce lower molecular weight or more stable pyrolysis products. Thus, information on the parent organic molecules must be inferred from the patterns of stable products evolved with temperature. For example, pyrolysis of microbial material typically evolved amines, but the more fragile amino acids are destroyed (Glavin et al., 2006). The detection limit of the SAM GCMS is ~10^{-14} to 10^{-13} mole, depending on the compound and instrument background. The mass range of the QMS is 2-535 Da to sample a wide range of organic compounds.

The second tool used by SAM to understand the state of carbon in Martian rocks and fines is combustion. Reduced carbon in samples delivered to the SAM sample cups may be oxidized by stepped combustion using isotopically pure $^{16}O_2$, with the $^{13}C/^{12}C$ ratio of the CO_2 product determined by QMS and TLS analysis. The $^{13}C/^{12}C$ ratio in organic matter is used as a biomarker on Earth because organisms prefer the lighter ^{12}C isotope and typically incorporate 2-4% more ^{12}C into their cells than is present in the CO_2 carbon source. The utility of these measurements will depend on the ability of SAM to reveal the isotopic composition of the most important reservoirs of inorganic carbon for comparison with organic carbon. Two such reservoirs are the atmosphere itself and carbonates that may be found in rocks or sedimentary materials sampled by MSL. The combined evolved gas and atmospheric sampling should enable this comparison.

In addition to the dry pyrolysis experiments, nine SAM sample cups are dedicated to simple single-step solvent extraction and/or chemical derivatization processes. Resource constraints on

MSL preclude a more ambitious fluid extraction analysis approach. Depending on the chemistries encountered in Martian rocks and soils, this technique may enable analysis of several classes of molecules that could be of biotic or prebiotic relevance, including amino acids, amines, carboxylic acids, and nucelobases. Without derivatization, these compounds would not elute from the GC columns under SAM protocols.

Seven of the SAM wet-chemistry cups use dimethylformamide (DMF) to extract organics from the powdered sample delivered to the cup, while the derivatization agent is a silylation reaction using N,N-Methyl-tert-butyl(dimethylsilyl)trifluoroacetamide (MTBSTFA). The selected volumes of derivatization agent and solvent were mixed together during SAM integration and then hard-sealed into a metal cup. The top cup consists of an electron-beam welded foil that can be punctured on the surface of Mars using the vertical motion of the sample cup into a foil puncture station. The cup is then placed under the SAM sample inlet tube so that these fluids can be mixed with the Martian powdered sample. The cup is next delivered to the pyrolysis oven, where the desired reaction temperature (~80 °C) is set. The hard seal into the pyrolysis chamber ensures that vapor does not escape during the derivatization reaction. After several tens of minutes, much of the solvent is evaporated to the atmosphere through a microvalve and a heated vent, and the chemical products of the derivatization reaction are flash-heated into the injection trap of the gas chromatograph.

The SAM team has exposed the selected solvents and derivatization agents to more radiation than is expected over the course of the mission to ensure that the radiation-induced chemistry is negligible over the course of the nominal MSL mission. The volume of the SAM wet cells enables a substantial excess of derivatization agent to be supplied, to mitigate the impact of side reactions that could compromise the detection of amino acids and carboxylic acids. An internal standard (a fluorinated amino acid compound in a separately punctured dry chamber) will allow evaluation of whether undesired side reactions have fully or partially prevented reaction with organics of interest. See Buch et al. (2006) for further details on the SAM “one-pot” derivatization protocol.

The remaining two SAM wet-chemistry cups are dedicated to thermochemolysis experiments with 25% tetramethyl-ammonium hydroxide (TMAH) in methanol. Thermochemolysis involves concurrent mild thermal bond cleavage and selective base-catalyzed cleavage (hydrolysis) of ester, amide, and ether bonds in high-molecular-weight, complex organics. The free lower molecular-weight carboxylic acid, alcohol, and amine hydrolysis products are subsequently methylated to form highly volatile products amenable to GCMS analysis. During tests of the SAM protocol with Mars analog materials, TMAH thermochemolysis was successful in yielding molecules from samples with challenging mineral matrices or chemistries, including those with oxides, hydroxides, salts, and water. Carboxylates, organic acids, and PAHs are readily detectable with thermochemolysis, although halogenated, alkylated, and other complex free molecules often produce multiple products with this technique. See Eigenbrode et al. (2011) for more details about the SAM thermochemolysis experiment.

An Organic Check Material (OCM) has been developed for SAM as a sample standard for verification of organic cleanliness and characterization of potential sample alteration by the sample acquisition and portioning process of the MSL rover. OCM samples will be acquired

using the same procedures for drilling, portioning, and delivery that are used to study Martian samples during surface operations. Because the SAM suite is highly sensitive to organic molecules, the mission can better verify the cleanliness of sample acquisition hardware if a known material can be processed through SAM and compared with results obtained from Martian samples. The OCM is comprised of amorphous SiO_2 glass doped with fluorinated hydrocarbons (3-fluorophenanthrene and 1-fluoronaphthalene) to ensure that the lack of other detectable molecules is indeed due to their absence, rather than failure of the sample delivery process.

The MSL rover carries five OCM samples, each one a cylindrical brick individually encapsulated in a hermetically sealed can. The five cans are accommodated on the front of the rover and the OCM sample will be acquired by puncturing the top of a can and drilling a brick in place, just as a natural Martian rock is to be sampled. Since the OCM is an expendable resource, the decision to sample an OCM brick will be made by consensus of the MSL project's science operations working group. Possible scenarios for use could include analyzing the OCM immediately after observing any organics in a Martian sample. Perhaps an OCM sample may be acquired if no organics are observed to test whether reduced carbon phases are being destroyed by the drilling, portioning, and delivery process. An OCM sample could be characterized very early in the mission to determine if the EDL processes have contaminated the sampling hardware. See Conrad et al. (2011) for more information about the SAM OCM.

SAM will bring a mixture of several calibration gases to Mars to be used at regular intervals during the mission. The calibration gas cell includes N_2, CO_2, Ar, and a Xe mix heavily spiked with ^{129}Xe to clearly distinguish it from terrestrial or Martian xenon. This cell includes the same fluorocarbon compounds that are incorporated into the OCM bricks, to evaluate the performance of the GCMS before launch and over the duration of the mission.

The SAM Tunable Laser Spectrometer (TLS) offers a direct, non-invasive technique to produce sub ppb sensitivities for gas detection and isotope ratio measurements for samples of small mass and volume, without the mass interferences seen by the QMS. The TLS is a high resolution (0.0005 cm^{-1}) IR spectrometer that includes two semiconductor laser sources: a NIR tunable laser at 2.78 μm from Nanoplus, Germany, that operates at room temperature with a single stage thermoelectric cooler (TEC) and accesses lines of CO_2, water, and their isotopic forms; and a JPL-built interband cascade IC laser at 3.27 μm that operates at 245 K with a two-stage TEC for methane and its isotopic forms $^{13}CH_4$ and $^{12}CH_3D$. Detectors are high-sensitivity HgCdZnTe photovoltaics with immersion linses provided by Vigo Systems S.A. of Poland. The TLS optical head has 3 chambers, the smallest containing the science detectors and their field lenses at the far end. At the near end is a foreoptics chamber that houses the lasers and their collimators, detectors, reference gas cells, beamsplitters that sit outside the main chamber, a multipass gas cell ~5 cm internal diameter and ~20 cm long. The cell volume is ~405 cm^3. This "Herriott" cell contains two internal spherical mirrors with drilled holes for laser entrance and exit, and is fitted with 3 high vacuum valves that connect to SAM. The cell is fitted with two heaters for fringe washing, its own pressure gauge, and temperature sensors. The TLS Herriott cell is designed to provide 81 passes for methane measurements and 43 passes for carbon dioxide and water measurements.

Spectral regions for the TLS were carefully selected for high sensitivity in detection but insensitivity to temperature in line pairs chosen for isotope ratio measurements. TLS employs second harmonic (2f) detection techniques that enhance its sensitivity since the 2f signal is zero-based and the phase sensitive detection regime is moved to higher frequencies (~ 10 kHz) where 1/f noise is lower.

Each channel of the TLS is run by its own microcontroller (8051 CPU) that returns housekeeping data to the SAM CDH computer (including temperatures and cell pressure, fore-optics pressure) and six spectra: 3 from the measurement Herriott cell (direct absorption, 2f low-gain, 2f high-gain) and 3 from the reference channel that contains calibration gases within tiny optical reference cells housed in the fore-optics and sampled by the same laser simultaneously using a beam-splitter. TLS was calibrated during thermal-vacuum testing using NIST-traceable standard calibration gases over a wide range of operating temperatures and pressures. In addition, TLS carries a reference gas cell for each channel with an isotopic standard (checked with IRMS) for in-flight reference to improve isotope ratio precision and accuracy.

Table 2-4 gives the expected measurement capabilities of the SAM TLS with a 15-min integration time, based on actual results from thermal-vacuum testing of the flight instrument. For additional details about the TLS, see Webster and Mahaffy (2011).

Table 2-4. Expected TLS Measurement Capabilities

TLS Channel	Wavelength	Scan Name	Expected Capability in 15-min integration time
1 – IC laser	3.3 μm	Methane	CH_4 to 0.3 ppbv (pptv in SAM) $\delta^{13}C$ to 2‰
2 – Near-IR	2.785 μm	Carbon dioxide	CO_2 to 0.2 ppmv H_2O to 0.2 ppmv $\delta^{13}C$ to 2‰ $\delta^{18}O$ to 3‰ $\delta^{17}O$ to 5‰
		Water	H_2O to 0.1 ppmv δD to 2‰ $\delta^{18}O$ to 3‰ $\delta^{17}O$ to 5‰

2.2 Data Product Overview

Each RDR will have unique PDS detached label files providing all the meta and ancillary data for that RDR. The SAM data files for NASA processing levels 0 through 1B, consisting of variable-width comma-separated-value (CSV) tables and fixed-width CSV tables, will have file extensions of ".CSV" and ".TAB," respectively. The SAM level 2 product will consist of a report file in PDF format that describes the findings of the SAM science team. All associated label files will have file extensions of ".LBL". The data or report file(s) together with the

associated label file(s) are collectively referred to as an RDR. Each RDR product will contain data for a single SAM experiment sequence.

Table 2-5 summarizes SAM standard Reduced Data Record (RDR) data products.

Table 2-5. SAM Standard RDR Data Products

Product Name	NASA Level	Description	PDS Data Set ID
SAM L0	0	Unpacking of telemetry into data numbers as raw ADC values or counts and verification of data integrity	MSL-M-SAM-2-RDR-L0-V1.0
SAM L1A	1A	Conversion of raw ADC values or counts to science units	MSL-M-SAM-3-RDR-L1A-V1.0
SAM L1B	1B	Application of corrections to data, e.g., detector dead time, TCD temperature, noise removal, corrections for saturation and instrument response function. Instrument-specific data may include the following types of information: QMS: time, m/z, signal; oven temperature for EGA runs; GC column temperature for GCMS runs GC: TCD signal vs. retention time; pressure; temperature; column used TLS: direct and harmonic spectra	MSL-M-SAM-4-RDR-L1B-V1.0
SAM L2	2	Results of data interpretation completed by the SAM science team. Instrument-specific data may include the following types of information: QMS: gas composition; isotope ratios; gas composition vs. sample temperature for EGA runs GC/GCMS: species; relative abundance; identification of pyrolysis products and derivatized compounds TLS: abundance and isotope ratios	MSL-M-SAM-5-RDR-L2-V1.0

2.3 Data Processing

2.3.1 Data Processing Level

All SAM RDR products are considered reduced data products as defined by both NASA and "Committee on Data Management and Computation (CODMAC). See Table 2-6 for more details.

2.3.2 Data Product Generation

SAM RDR data products will be generated by the SAM team led by principal investigator Mahaffy at NASA GSFC, co-investigator Cabane at the University of Paris, and co-investigator Webster at JPL. SAM instrument calibration is described in detail in Mahaffy et al. (2012).

Table 2-6. Processing Levels for Science Data Sets

NASA	CODMAC	Description
Packet data	Raw - Level 1	Telemetry data stream as received at the ground station, with science and engineering data embedded.
Level-0	Edited - Level 2	Instrument science data (e.g., raw voltages, counts) at full resolution, time ordered, with duplicates and transmission errors removed.
Level 1A	Calibrated - Level 3	Level 0 data that have been located in space and may have been transformed (e.g., calibrated, rearranged) in a reversible manner and packaged with needed ancillary and auxiliary data (e.g., radiances with the calibration equations applied).
Level 1B	Resampled - Level 4	Irreversibly transformed (e.g., resampled, remapped, calibrated) values of the instrument measurements (e.g., radiances, magnetic field strength).
Level 1C	Derived - Level 5	Level 1A or 1B data that have been resampled and mapped onto uniform space-time grids. The data are calibrated (i.e., radiometrically corrected) and may have additional corrections applied (e.g., terrain correction).
Level 2	Derived - Level 5	Geophysical parameters, generally derived from Level 1 data, and located in space and time commensurate with instrument location, pointing, and sampling.
Level 3	Derived - Level 5	Geophysical parameters mapped onto uniform space-time grids.

2.3.3 Data Flow

Raw data will be delivered to the SAM team as Experiment Data Record (EDR) products generated by the Multi-mission Image Processing Laboratory (MIPL) at JPL under the Operations Products Generation Subsystem (OPGS), using the telemetry processing software MSLEdrGen. Products are created by MIPL during operations from: a) MPCS data products, b) SPICE kernels, and c) a meta-data database. They are created on the MSL Operations Data Store (ODS) and then deposited into MIPL's File Exchange Interface (FEI) for electronic distribution to remote sites/users via a secure subscription protocol. The EDR product is considered NASA packet-level data. SAM EDR data products will be stored at the PDS for safekeeping, but will not be formally archived in PDS. The SAM team will convert raw data to a more manageable format before delivery to the PDS for archiving as the lowest-level RDR product, which is considered to be NASA level 0 data. Higher-level RDR products will represent the results of further data manipulation and interpretation.

2.3.4 Labeling and Identification

A file-naming scheme has been devised for SAM RDR data products, based on the convention used for other MSL products. The file-naming scheme adheres to the Level II 36.3 filename convention to be compliant with PDS standards. It also contains a minimal level of meta-data that retains uniqueness and is searchable.

All MSL data products can be uniquely identified by incorporating key information into the product filename, including the instrument identifier and a version number. Additional fields within the file names have been modified for SAM RDR products to be more suited to the type of data produced by SAM, which differs from that of other MSL instruments.

Each SAM RDR has a detached PDS label associated with the SAM data file. The file-naming scheme for the data products is formed by:

Table 2-7. File naming template

1-2	3-7	8	9-12	13-15	16-17	18	19-22	23	24-26	27	28-34	35	36	37	38-40
instr (2 char)	SAM exp ID (5 alphanumeric)	venue/source (1 char)	sol (4 alphanumeric)	prod (3 char)	level (2 alphanumeric)	_	exp seq (4 char)	_	type (3 char)	_	descr (7 alphanumeric)	_	ver (1 alphanumeric)	.	ext (3 char)

Table 2-8. Detailed description of product name components

<table>
<tr><th>Name</th><th>Description</th></tr>
<tr><td>instr</td><td>(2 characters) MSL science instrument identifier
Valid value: SAM – “SM”</td></tr>
<tr><td>SAM exp ID</td><td>(5 alphanumeric) SAM experiment ID.</td></tr>
<tr><td>venue/
source</td><td>(1 character) Venue and source (Flight Model vs Testbed) identifier
Valid values are:
<table>
<tr><th>Venue/source</th><th>Value</th></tr>
<tr><td>Flight model, pre-launch calibration</td><td>“C”</td></tr>
<tr><td>Flight model, ATLO</td><td>“A”</td></tr>
<tr><td>Flight model, OPS</td><td>“F”</td></tr>
<tr><td>Testbed</td><td>“T”</td></tr>
</table></td></tr>
<tr><td>sol</td><td>(4 alphanumeric) Sol, solar days since first full day on Mars, when data transferred from SAM to rover. Landing day is Sol 0. For pre-launch tests, this field is filled with ASCII lowercase x.

The valid values, in their progression, are as follows (non-Hex):
Range 0000 thru 9999 - “0000”, “0001”, … “9999”
Range 10000 thru 10999 - “A000”, “A001”, … “A999”
Range 11000 thru 11999 - “B000”, “B001”, … “B999”
•
•
Range 35000 thru 35999 - “Z000”, “Z001”, … “Z999”</td></tr>
<tr><td>prod</td><td>(3 characters) Product identifier.

Valid value: SAM RDR - “RDR”</td></tr>
<tr><td>level</td><td>(2 alphanumeric) NASA data processing level.
Valid values:
level 0 – “0_”
level 1A – “1A”
level 1B – “1B”
level 1C – “1C”
level 2 – “2_”</td></tr>
<tr><td>_</td><td>ASCII underscore.</td></tr>
</table>

<table>
<tr><td>exp seq</td><td>(4 characters) SAM experiment sequence.
Valid values:

<table>
<tr><th>SAM Experiment Sequence</th><th>Description</th><th>4-character value</th></tr>
<tr><td>#1</td><td>S-PYR, Solid sample pyrolysis with GCMS</td><td>SPYR</td></tr>
<tr><td>#2</td><td>S-DER, Solid sample derivatization</td><td>SDER</td></tr>
<tr><td>#3</td><td>CAL-SOL, Solid sample calibration</td><td>CSOL</td></tr>
<tr><td>#4</td><td>A-DIR, Direct atmospheric measurement</td><td>ADIR</td></tr>
<tr><td>#5</td><td>A-ENR, Atmospheric enrichment</td><td>AENR</td></tr>
<tr><td>#6</td><td>A-MET, Atmospheric methane enrichment</td><td>AMET</td></tr>
<tr><td>#7</td><td>A-NGE, Atmospheric noble gas enrichment
A-DNG, Dynamic noble gas enrichment
A-SNG, Semi-static noble gas enrichment</td><td>ANGE
ADNG
ASNG</td></tr>
<tr><td>#8</td><td>S-CMB, Solid sample combustion</td><td>SCMB</td></tr>
<tr><td>#9</td><td>CAL-GAS, Gas calibration</td><td>CGAS</td></tr>
</table></td></tr>
<tr><td>_</td><td>ASCII underscore.</td></tr>
<tr><td>type</td><td>(3 char)
Valid values:
<table>
<tr><td>“MSG”</td><td>Message log</td></tr>
<tr><td>“HK_”</td><td>Housekeeping data, levels 0 and 1A only</td></tr>
<tr><td>“QMS”</td><td>QMS data</td></tr>
<tr><td>“GC_”</td><td>GC data</td></tr>
<tr><td>“TLS”</td><td>TLS data</td></tr>
</table></td></tr>
<tr><td>_</td><td>ASCII underscore.</td></tr>
<tr><td>descr</td><td>(7 alphanumeric) Type-dependent; description of file contents. If unused, filled with ASCII X.

Valid values are listed in Appendix B.</td></tr>
</table>

_	ASCII underscore.
ver	(1 alphanumeric) Version identifier, independent of the Special Processing field. The valid values, in their progression, are as follows (non-Hex): Range 1 through 10 - "**1**", "**2**", **…** "**9**", "**0**" Range 11 through 36 - "**A**", "**B**", **…** "**Z**" Range 37 and higher - "**_**" (underscore) The Version number increments by one whenever an otherwise-identical filename would be produced. In general, the highest-numbered Version represents the "best" version of that product.
ext	(3 characters) Product type extension. Valid values for nominal operational data products: Non-imaging instrument data – **"CSV", "TAB", "TXT"** Detached PDS labels for SAM – **"LBL"** Image files – **"TIF"**

Example #1: SM30008F0157RDR1A_SPYR_QMS_MASSXXX_1.TAB

instr	=	"**SM**"	=	SAM
SAM Exp ID	=	"**30008**"	=	SAM Experiment ID 30008
venue / source	=	"**F**"	=	Flight model, ops
sol	=	"**0157**"	=	Sol 157
prod	=	"**RDR**"	=	RDR
level	=	"**1B**"	=	NASA data processing level 1B
exp seq	=	"**SPYR**"	=	Solid sample pyrolysis with GCMS
type	=	"**QMS**"	=	QMS data
descr	=	"**MASSXXX**"	=	Mass spectral data
ver	=	"**1**"	=	Version 1
ext	=	"**TAB**"	=	ASCII data file

Example #2: SM21157F0089RDR0__ADIR_HK_XXXXXXX_1.LBL

MSL instr	=	"**SM**"	=	SAM
SAM exp ID	=	"**21157**"	=	SAM Experiment ID 21157
venue / source	=	"**F**"	=	Flight model, ops
sol	=	"**0089**"	=	Sol 89
prod	=	"**RDR**"	=	RDR
level	=	"**0_**"	=	NASA data processing level 0
exp seq	=	"**ADIR**"	=	Direct atmospheric measurement
type	=	"**HK_**"	=	Housekeeping data
descr	=	"**XXXXXXX**"	=	Unused

ver	=	"**1**"	=	Version 1
ext	=	"**LBL**"	=	PDS label

2.4 Standards Used in Generating Data Products

2.4.5 PDS Standards

SAM data products comply with the PDS standards for file formats and labels, as specified in the PDS Data System Standards Reference, February 27, 2009, Version 3.8, JPL D-7669, Part 2.

2.4.6 Time Standards

The following time standards and conventions are used throughout this document, as well as the MSL project for planning activities and identification of events.

Table 2-9. Time standards

Time Format	*Definition*
SCET	Spacecraft event time. This is the time when an event occurred on-board the spacecraft, in UTC. It is usually derived from SCLK.
SCLK	Spacecraft Clock. This is an on-board 64-bit counter, in units of nano-seconds and increments once every 100 milliseconds. Time zero corresponds to noon on 1-Jan-2000.
ERT	Earth Received Time. This is the time when the first bit of the packet containing the current data was received at the Deep Space (DSN) station. Recorded in UTC format.
Local Solar Time	Local Solar Time (LST). This is the local solar time defined by the local solar days (sols) from the landing date using a 24 "hour" clock within the current local solar day (HR:MN:SC). Since the Mars day is 24h 37m 22s long, each unit of LST is slightly longer than the corresponding Earth unit. LST is computed using positions of the Sun and the landing site from SPICE kernels. If a landing date is unknown to the program (e.g. for calibration data acquired on Earth) then no sol number will be provided on output LST examples: SOL 12 12:00:01 SOL 132 01:22:32.498 SOL 29
RCT	Record Creation Time. This is the time when the first telemetry packet, containing a given data set, was created on the ground. Recorded in UTC format.
True Local Solar Time	This is related to LST, which is also known as the mean solar time. It is the time of day based on the position of the Sun, rather than the measure of time based on midnight to midnight "day". TLST is used in all MIPL/OPGS generated products.

SOL	Solar Day Number, also known as PLANET DAY NUMBER in PDS label. This is the number of complete solar days on Mars since landing. The landing day therefore is SOL zero.

2.4.7 Coordinate Systems

The following coordinate systems are used within the project to refer to the position of the rover and its instruments.

Table 2-10. Coordinate systems

Coordinate System	***Origin***	***Orientation***
Local Level	Same as payload frame, and it moves with the rover	+X North +Z down along gravity vector +Y East
Payload Frame	At the shoulder of the Robotic Arm. Attached and moves with the rover	+X along rover –X (point out into the work space) +Z down along rover (vertical axis) +Y along rover -Y
Site Frame	Same as payload frame when first defined and never moves relative to Mars. Possible to define multiple site frames in case the rover moves/slips.	Same as local level

2.4.8 Data Storage Conventions

SAM low-level RDR products containing housekeeping data will be stored as PDS SPREADSHEET objects, which comprise collections of logically uniform rows containing ASCII values stored in variable-width fields separated by field delimiters. Each row within a SPREADSHEET has the same number of fields, in the same field order, and each field contains the same logical content. Files containing SPREADSHEET objects have the extension CSV.

SAM products containing QMS science data will be stored as ASCII TABLE objects. They will have fixed-length records, although the size of the records in each file may differ depending on the context of the data. Files containing ASCII TABLE objects have the extension TAB.

Label keywords will provide the necessary information to determine the organization of each RDR.

2.5 Data Validation

SAM RDRs, as with all other MSL RDRs, are subject to PDS peer review and verification.

Validation of the SAM RDRs, during production, will be performed according to specifications in the MSL Archive Plan. The SAM Team will validate the science content of the data products. The PDS Geosciences node will validate the archive volumes for compliance with PDS standards and conformance with the design specified in this SIS.

3. DETAILED DATA PRODUCT SPECIFICATIONS

Each of the data products described in Table 2-5 will be saved as a different RDR, as defined in the following sections. Each RDR product will consist of a collection of files that contain data for the different channels or the different SAM instrument components. The SAM RDR file naming convention will uniquely identify each data product component. See Section 2.3.4 for a detailed description of the SAM RDR file naming convention. The structure of the SAM RDR consists of detached ASCII PDS labels and associated data files, as shown in Figure 3-1.

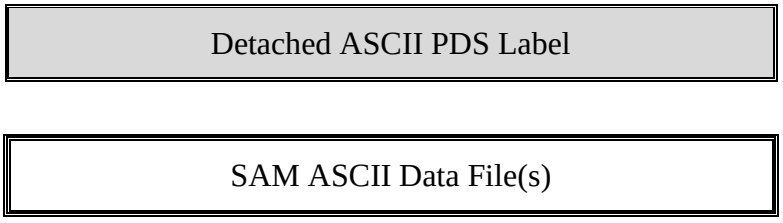

Figure 3-1. The SAM RDR consists of at least two files.

3.1 Label and Header Descriptions

3.1.1 PDS Label

The PDS label, with file extension ".LBL," contains keywords for product identification and table object definitions. The label also contains descriptive information needed to interpret or process the data objects in the file. Detached labels are paired with science data of the same file name, but with different file extensions depending on the data format.

PDS labels are written in Object Description Language (ODL). PDS label statements have the form of "keyword = value". Each label statement is terminated with a carriage return character (ASCII 13) and a line feed character (ASCII 10) sequence to allow the label to be read by many operating systems. Pointer statements with the following format are used to indicate the location of data objects in the file:

^Object = location

Where the carat character (^, also called a pointer) is followed by the name of the specific data object. The location is the starting record number for the data object within the file.

Each PDS label will include all keywords defined for SAM. If a keyword does not have a value, a value of "N/A" will be given. Per PDS rules, "N/A" is used when a keyword exists, but it does not apply to a particular data product, and "UNKNOWN" is used when the value of an applicable keyword cannot be determined at the time the PDS label is generated.

3.1.2 PDS TABLE Object

The TABLE object is a uniform collection of rows containing ASCII or binary values stored in columns. Each field is defined as a fixed-width COLUMN object; the value of the COLUMNS keyword is the total number of COLUMN objects defined in the label. All TABLE objects must have fixed-width records.

3.1.3 PDS SPREADSHEET Object

PDS SPREADSHEET objects are collections of logically uniform rows containing ASCII values stored in variable-width fields separated by field delimiters. Each row within a SPREADSHEET has the same number of fields, in the same field order, and each field contains the same logical content. By definition, the SPREADSHEET object is used only to describe ASCII data objects. The delimiter used for SAM data files is the comma, thus SAM low-level RDR products containing housekeeping data are stored with the file extension ".CSV."

3.1.4 PDS TEXT Object

PDS TEXT objects describe files that contain plain text. Use of the carriage-return/line-feed sequence (<CR><LF>) is required for cross-platform support. The SAM archives may contain text files describing the contents of other files in the archive volume or providing information about experiments that would be helpful in data interpretation by PDS users.

3.1.5 PDS DOCUMENT Object

PDS DOCUMENT objects provide information in support of archived data products. They may consist of one or more files in a single format, such as images to assist PDS users in understanding interpreted SAM science data in the level 2 product.

4. APPLICABLE SOFTWARE

4.1 Utility Programs

There are no SAM-specific utility programs provided with these data products. All products are ASCII text, whether in TABLE, SPREADSHEET, or TEXT objects, and are therefore viewable in any text editor. TABLE and SPREADSHEET products are also suitable for use in spreadsheet and data base management programs.

4.2 Applicable PDS Software Tools

No special PDS software tools are needed to view SAM RDR data products.

4.3 Software Distribution and Update Procedures

There are neither software-distribution nor update procedures associated with these data products.

5. REFERENCES

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APPENDIX A: PDS KEYWORD DEFINITIONS

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
PDS_VERSION_ID	Specifies the version number of the PDS standards document that is valid when a data product label is created. Values for the PDS_version_id are formed by appending the integer for the latest version number to the letters 'PDS'.	String		PDS3	
/* FILE DATA ELEMENTS */	Comment				
RECORD_TYPE	A Specifies the record format of a file. Note: In the PDS, when RECORD_TYPE is used in a detached label file, it always describes its corresponding detached data file and not the label file itself. The use of RECORD_TYPE along with other file-related data elements is fully described in the PDS Standards Reference.	String		FIXED_LENGTH, STREAM	TAB files are FIXED_LENGTH, CSV and TEXT files are STREAM.
RECORD_BYTES	B Specifies the number of bytes in a physical file record, including record terminators and separators. Note: In the PDS, the use of record_bytes, along with other file-related data elements is fully described in the Standards Reference.	Integer		2048	For STREAM record type, RECORD_BYTES is the maximum length of a record

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
FILE_RECORDS	Specifies the number of physical file records, including both label records and data records. Note: In the PDS the use of FILE_RECORDS along with other file-related data elements is fully described in the Standards Reference.	Integer		1038	
/* IDENTIFICATION DATA ELEMENTS */	Comment				
DATA_SET_ID	A unique alphanumeric identifier for a data set or a data product. The DATA_SET_ID value for a given data set or product is constructed according to flight project naming conventions. In most cases the DATA_SET_ID is an abbreviation of the DATA_SET_NAME. Note: In the PDS, the values for both DATA_SET_ID and DATA_SET_NAME are constructed according to standards outlined in the Standards Reference.	String(40)		See example labels for actual values used in each product type	Constant for each data set.
INSTRUMENT_HOST_ID	Specifies a unique identifier for the host where an instrument is located. This host can be either a spacecraft or an earth base (e.g., and observatory or laboratory on the earth). Thus, INSTRUMENT_HOST_ID can contain values which are either SPACECRAFT_ID values or EARTH_BASE_ID values.	String		"MSL"	Scid
INSTRUMENT_HOST_NAME	The full name of the host on which this instrument is based	String		"MARS SCIENCE LABORATORY"	Scid
INSTRUMENT_NAME	Name of the instrument, free format, enclosed in double quotes.	String		"SAMPLE ANALYSIS AT MARS"	EMD: ProductName
PRODUCT_CREATION_TIME	Defines the UTC system format time when a product was created.	String		YYYY-MM-DDThh:mm:ss.fff	Calculated

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
PRODUCT_ID	Represents a permanent, unique identifier assigned to a data product by its producer. See also: source_product_id. Note: In the PDS, the value assigned to product_id must be unique within its data set. The product_id describes the lowest-level data object that has a PDS label.	String(40)		File name, less the extension.	Filename minus the extension
REQUEST_ID	Specifies the Request ID value associated with the Data Product generation command. Unsigned integer.				EMD: RequestId
SEQUENCE_ID	Specifies an identification of the spacecraft sequence associated with the given product. This element replaces the older seq_id, which should no longer be used.			P0171	EMD: SequenceId
SEQUENCE_VERSION_ID	Specifies the version identifier for a particular observation sequence used during planning or data processing.			2	EMD: SequenceVersion
SPACECRAFT_CLOCK_CNT_PARTITION	Specifies the clock partition active for SPACECRAFT_CLOCK_START_COUNT and SPACECRAFT_CLOCK_STOP_COUNT elements.	Integer		1	Static value
SPACECRAFT_CLOCK_START_COUNT	Starting SCLK, smallest, value of all the records contained in the product.	String(30)		Format is "ddddddddddd.ddd", measured in units of seconds stored internally as a floating point number.	- EMD: DvtCourse/DvtFine or - Sclk or - Pulled from instrument data

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
SPACECRAFT_CLOCK_STOP_COUNT	Ending SCLK, largest value of all the records contained in the product.	String(30)		Format is "ddddddddd.ddd", measured in units of seconds stored internally as a floating point number.	- EMD: DvtCourse/DvtFine or - Sclk or - Pulled from instrument data
START_TIME	SPACECRAFT_CLOCK_START_COUNT converted and represented in UTC	String		Formation rule: YYYY-MM-DDThh:mm:ss.fff. No quotation marks.	OnBoardCreationTime – the coarse SCLK in 1-second presentation
STOP_TIME	SPACECRAFT_CLOCK_STOP_COUNT converted and represented in UTC	String		Formation rule: YYYY-MM-DDThh:mm:ss.fff. No quotation marks.	OnBoardCreationTime – the coarse SCLK in 1-second presentation
LOCAL_MEAN_SOLAR_TIME_SOL	TBD	String		Sol-<nnnnn>M<hh>:<mm>:<ss>[.fff] NOTE: Value will be uncalibrated if SPICE kernels are unavailable.	Calculated: - SCLK kernel - Landing site kernel - P kernel
PLANET_DAY_NUMBER	Specifies the number of sidereal days (rotation of 360 degrees) elapsed since a reference day (e.g., the day on which a landing vehicle set down). Days are measured in rotations of the planet in question from the reference day. For MSL, the reference day is “0”, as Landing day is Sol 0. If before Landing day, then value will be less than “1” and can be negative.	Integer			Calculation - SCLK kernel
MISSION_NAME	Specifies a major planetary mission or project. A given planetary mission may be associated with one or more spacecraft.	String		“MARS SCIENCE LABORATORY”	Static Value

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
MISSION_PHASE_NAME	Specifies the commonly-used identifier of a mission phase.	String		"DEVELOPMENT", "LAUNCH", "CRUISE AND APPROACH", "ENTERY, DESCENT, AND LANDING", "PRIMARY SURFACE MISSION", "EXTENDED SURFACE MISSION"	User specified parameter.
OBSERVATION_ID	Specifies a unique identifier for a scientific observation within a data set. It is set via the data product context ID - which doesn't necessarily map to a specific object - it's just used to group various instrument data sets together via a common keyword.	String			TBD
PRODUCER_INSTITUTION_NAME	Specifies the identity of a university, research center, NASA center or other institution associated with the production of a data set. This would generally be an institution associated with the element PRODUCER_FULL_NAME.	String		"MULTIMISSION INSTRUMENT PROCESSING LABORATORY, JET PROPULSION LAB"	Static Value.
PRODUCT_CREATION_TIME	Defines the UTC system format time when a product was created.	String		YYYY-MM-DDThh:mm:ss.fff. No quotation marks.	Calculated
PRODUCT_ID	Represents a permanent, unique identifier assigned to a data product by its producer. See also: source_product_id. Note: In the PDS, the value assigned to product_id must be unique within its data set. The product_id describes the lowest-level data object that has a PDS label.	String(40)		File name, less the extension.	Filename minus the extension

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
PRODUCT_VERSION_ID	Specifies the version of an individual product within a data set. PRODUCT_VERSION_ID is intended for use within AMMOS to identify separate iterations of a given product, which will also have a unique FILE_NAME.	String		"V<*vernum*> D-38107"	User specified parameter
RELEASE_ID	Specifies the unique identifier associated with the release to the public of all or part of a data set. The release number is associated with the data set, not the mission. When a data set is released incrementally, such as every three months during a mission, the RELEASE_ID is updated each time part of the data set is released. The first release of a data set in the mission should have a value of "0001". For example, on MSL the first release of the SSI EDR data set on MSL will have RELEASE_ID = "0001". The next SSI EDR release will have RELEASE_ID = "0002".	String		"0001", "0002", etc., including quotation marks and leading zeroes.	User parameter input.
MSL:REQUEST_ID	Specifies the Request ID value associated with the Data Product generation command. Unsigned integer.				EMD: RequestId
TARGET_NAME	Identifies a target. The target may be a planet, satellite, ring, region, feature, asteroid or comet. See TARGET_TYPE. This is based on mission phase.	String(30)		"MARS", "CALIBRATION"	Calculated by algorithm to determine if looking at the calibration target, if not, then MARS.
TARGET_TYPE	Specifies the type of a named target.	String		CALIBRATION, DUST, N/A, SUN, PLANET	Static value
/* SAM DATA ELEMENTS */	Comment				

Keyword Name	Definition	Type	Units	Valid Values	Location & Source
MSL:SAM_EXPERIMENT_ID	A number that uniquely identifies the SAM experiment that produced the data. The SamExperimentId DPO is the first DPO encapsulated in all the SAM data products (*.csv and *.tab files).	Integer (U16)	n/a	00000 to 99999	DPO: SamExperimentId Field name: id
MSL:SAM_EXPERIMENT_DESCRIPTION	Specifies the type of SAM experiment that produced the data.	String	n/a	maximum length: 64	SAM script
MSL:SAM_GC_COLUMN_NUMBER	Specifies the SAM GC column number used in the experiment.	Integer (U16)	n/a	1 to 6	Message log
MSL:SAM_GC_COLUMN_DESCRIPTION	Specifies the operational configuration of the GC column used in the experiment.	String	n/a	maximum length: 64	SAM script

APPENDIX B: SAM DATA DESCRIPTORS FOR RDR PRODUCT FILE NAMES

Table B-1. Valid descriptors for level 0 and 1A data file names

Data type	Descriptor	File Contents
MSG	MESSAGE	Message log file
HK	CDHHSPD	CDH high-speed housekeeping
	CDHLSPD	CDH low-speed housekeeping
	FSWHKXX	Flight software housekeeping
	GCHKXXX	GC housekeeping
	GPSHKXX	Gas processing system housekeeping
	MISCHKX	Miscellaneous housekeeping
	MOTHKXX	Motor controller housekeeping
	QMSHKXX	QMS housekeeping
	TLSHKXX	TLS housekeeping
	TMHKXXX	General housekeeping
QMS	RAWQMSX	Raw QMS data
	BANDXXX	Band spectral data
	MISCDAC	DAC data
	MASSXXX	Mass spectral data
GC	SIGNALX	TCD signal
	PARAMSX	Parameters for data analysis
	RAWXXXX	Raw data
	TCDOFFX	TCD offset data
TLS	H2O_nnn	H2O data for scan number nnn
	CO2_nnn	CO2 data for scan number nnn
	CH4_nnn	CH4 data for scan number nnn

Table B-2. Valid descriptors for level 1B data file names

Data type	Descriptor	File Contents
QMS	MASSDTC	Dead-time-corrected mass spectral data
	MASSBKG	Background values for mass spectra
	MASSBGS	Background-subtracted mass spectral data
	BANDDTC	Dead-time-corrected band spectral data
	BANDBKG	Background values for band spectra
	BANDBGS	Background-subtracted band spectral data
	PARAMSX	Parameters for data analysis
GC	SIGNALX	TCD signal
	NOISEXX	Noise data
TLS	H2O_nnn	H2O data for scan number nnn
	CO2_nnn	CO2 data for scan number nnn
	CH4_nnn	CH4 data for scan number nnn

Table B-3. Valid descriptors for level 2 data file names

Data type	Descriptor	File Contents
QMS	ATMCOMP	Atmospheric gas composition
	ISOTOPE	Isotope ratios
	EGAXXXX	Evolved gas analysis peaks with sample temperature
	EGACOMP	Abundance estimates for compounds identified by evolved gas analysis
	NOTESXX	Any notes relevant to the QMS data
	IMGnnnn	Any image files relevant to the QMS data, where nnnn = 0001 to 9999
GC	SPECIES	Identified species and relative abundances
	NOTESXX	Any notes relevant to the GC data
	IMGnnnn	Any image files relevant to the GC data, where nnnn = 0001 to 9999
TLS	ABUNDNC	Abundances
	ISOTOPE	Isotope ratios
	NOTESXX	Any notes relevant to the TLS data
	IMGnnnn	Any image files relevant to the TLS data, where nnnn = 0001 to 9999