9.3 Appendix 3: Glossary of Definitions of Terms

Organic carbon – for the purposes of this report, any carbonaceous substance that is not inorganic. Typical definitions include the presence of covalent C-C and/or C-H bonds, average oxidation state < 4, yielding CO_2 upon combustion, and others. All of these definitions comprise (different) subsets of the broader definition that we adopt here. Examples include formic acid, ethanol, glucose, hydrocarbons including methane, lipids, amino acids, purines, pyrimidines, urea, chlorofluorocarbons, Teflon, dimethylsilicone, etc. The term organic carbon does not imply formation by a biological process.

Inorganic carbon – the boundary between "organic" and "inorganic" carbon is ambiguous, and no single definition is broadly accepted. Here we use 'inorganic' to refer primarily to materials comprised of oxygen and carbon. Examples include gaseous CO and CO_2, dissolved CO_3^{2-} and HCO_3^-, and carbonate minerals such as calcite and dolomite. Many definitions of inorganic carbon also include metal and metalloid carbides, cyanides, and elemental carbon, although for clarity we refer here to such materials specifically by name rather than as inorganic carbon.

Elemental carbon – materials that contain only the element carbon, such as graphite, diamond, fullerenes, and graphene.

Macromolecular organic carbon – complex, high molecular weight, organic carbon compounds which are formed by polymerization or cross-linking of smaller subunits. Organic macromolecules include ordered biopolymers such as proteins, DNA, polysaccharides, and lignin; synthetic polymers including polyester, polytetrafluoroethylene (Teflon), and silicone; and irregular geopolymers such as humic acids, asphaltenes, and kerogen.

Organic particulates – macromolecular organic material that can be captured by sieving filters (for example > 1 μm particulates).

Biologically relevant functional groups – atoms other than C or H in an organic molecule that impart functionality to the compound. Examples include: alcohols, carboxylic acids, amines, amides, esters, and phosphate esters. Carbon-carbon double bonds are typically included in this definition.

Amino acid – organic carbon compounds that contain both an amine and carboxylic acid functional group. The linking of amino acids via a peptide bond [(C=O)-(NH)], allows the formation of peptides and proteins in terrestrial biological systems. Terrestrial organisms use only 22 standard amino acids of specific chirality, although many more such compounds exist. Examples include alanine, cysteine, glycine, etc.

Carbohydrate – organic carbon compounds with the generic formula $(CH_2O)_n$, containing multiple hydroxyl and carboxyl functions. Individual monomers (a.k.a. monosaccharides, sugars) can be polymerized via acetal and hemiacetal bonds to form polysaccharides (carbohydrate polymers). Examples include glucose, sucrose, cellulose, and starch.

Lipid – lipids, in comparison to 'hydrocarbons,' are generally inferred to be of biologic origin. They commonly comprise long, hydrophobic hydrocarbon backbones with a polar end group and few functional groups. They can have linear chains (e.g., fatty acids, leaf waxes), branched chains (phytol, methyl-branched fatty acids), cyclic moieties (e.g., alkyl benzenes) or polycyclic moieties (e.g., sterols, lignin).

Hydrocarbon – formally, any molecule containing only the elements H and C. However, usage has expanded to include any hydrophobic molecule originating in rocks or fossil fuels regardless of composition

(e.g., “this rock contains 5 μg/g extractable hydrocarbons”). For this report, we adopt the latter meaning, and use it in conjunction with ‘lipids’ to distinguish between biotic and abiotic sources.

Chirality – a characteristic stemming from the 3-dimensional nature of organic carbon compounds. When a carbon atom is surrounded by four different moieties, it can exist as either of two non-superimposable mirror images (enantiomers). Enantiomers can rotate plane-polarised light in opposite directions and are so designated as "right-" or "left-handed" based on this property.

Homochirality – a collection of structurally similar molecules that are chiral in the same sense i.e. all left-handed (amino acids in terrestrial life) or all right-handed (sugars in terrestrial life). Homochirality is considered a characteristic of terrestrial biological systems.

Chain-length preference in lipids – the synthesis of lipids requires the addition of carbon atoms to a precursor to increase carbon-chain length. In biological systems, these carbons come from two-C donors (such as acetate) or five-C donors (isoprenoids), forming long-chain carbon skeletons with specific chain lengths. Compounds formed from acetate show strong preferences for even or odd numbers of carbon atoms (e.g, C12, C14, C16, C18, etc in fatty acids, or C27, C29, C31, C33, etc in hydrocarbons).

Pyrolysis products – organic compounds generated when a sample is heated, in the absence of oxygen, to the point of thermal decomposition.

Volatile and semi-volatile organic compounds – molecules with substantial vapor pressure either at room temperature (volatile) or at some elevated temperature (semivolatile). Molecules that thermally decompose before entering the gas phase are termed involatile. There is little agreement on precise temperature cutoffs between these categories, hence we adopt the practical definitions above.

Isotopes – atoms of the same element having a different number of neutrons, and hence mass. They are chemically identical and form the same compounds, phases, etc, but the mass difference causes them to react at subtly different rates. Radioactive versus stable isotopes (^{14}C vs ^{13}C, ^{3}H vs ^{2}H) are frequently distinguished, and the relative abundance of certain isotopes (in organic matter, primarily ^{2}H, ^{13}C, ^{15}N, ^{18}O, and ^{34}S) are frequently used to distinguish between materials of terrestrial versus extraterrestrial origin.

Isotopic fractionation – any chemical, physical or biological process that alters the relative abundance of isotopes in a material. An example is the depletion of ^{2}H and ^{18}O in water vapor evaporating from a liquid. Many natural processes have characteristic isotopic fractionations, e.g. fixation of CO_2 in the photosynthesis. The loss of radioactive isotopes (e.g., ^{14}C or ^{3}H) due to decay is not typically regarded as fractionation as it occurs regardless of physical or chemical processes.

CONTAMINATION TERMINOLOGY

Organic contamination – Any substance that significantly interferes with our ability to detect the presence of martian organic compounds or prevents our confidently determining that an organic compound is of martian and not terrestrial origin.

Constant Contamination – background levels, such as in a blank, which are well characterized, constant and can be readily addressed in the evaluation of the compositional analysis. These are often mitigated or controlled by design and selection of materials and processes.

Random or variable contamination – spacecraft are huge systems requiring long periods of building. As a result, there is the potential for contamination to be introduced from entirely unpredicted events (*Black*

swan events). Such variable contamination can be identified, limited or controlled by continuous monitoring of processes, systems and witness plates.

Adventitious carbon – when surfaces are cleaned to a high level, the removal of surface oxidation layers, etc. results in the formation of a charged surface. Adventitious carbon comprises the charged carbon molecules within the atmosphere that are attracted to and bind to cleaned surfaces, therefore the chemistry of this carbon reflects the conditions of the environment in which it forms.

Contamination control – limiting the introduction of contaminants through processes and design.

Contamination knowledge – the use of witness plates, controls and process monitoring to quantitatively and qualitatively characterize and understand the types of contamination such that interpretation of acquired data is possible and the science objectives can be met.

Contaminants of concern – the organic molecules identified by our scientific understanding of the environment, bioburden and process design that provide the best indication of contamination that could interfere with the anticipated sample analyses and defined scientific objectives.

Surface contact transfer – the transfer of contaminants from a sampling surface to the sample. While the efficiency of this transfer is variable (depending on the types and nature of the contaminants and sample matrix), in a worst-case scenario it is assumed to be 100%.

Blank – a measurement designed to establish the amount of analyte due to sources other than the sample. Blanks can have many different contributing components, which may or may not be distinguished, e.g. sample handling and storage blank, processing blank, reagent and solvent blank, instrument blank, etc. Can also be referred to as a ***negative control standard***.

Background – signals detected by the instrument that are due to sources other than the targeted analyte, for example fluorescence or adsorption of sample matrix in optical techniques, contaminants present in the vacuum system of mass spectrometers, etc. The term is often, though not always, used to denote signals that interfere with or degrade measurement capabilities.

Witness plate – provides a background measurement alongside sample measurement to document where, when and what contaminants are introduced during the mission. Witness plates are generally comprised of more that one type of material, each having different adherence properties (such as sapphire and silicone wafers), and can include clean plates, organic check material, or stored materials.

Pristine – in the context of sample collection, pristine can be considered as the level to which background contamination can be removed to within the cost and technical limitations of the time.

Noise floor – the lowest, reasonably achievable limit of contamination.

ANALYTICAL TERMINOLOGY

Analyte - the element, isotope, compound, substance, etc. of interest in an analysis.

Sample matrix – the sample material that surrounds and contains the analytes of interest, e.g. sediment, rock, water, etc. The sample matrix affects the manner in which sample is prepared and introduced into a measurement technique (i.e. liquid vs solid-phase extraction), as well as potentially affecting the analytical measurement itself.

Detection limit – is by convention defined as the quantity of a material yielding a detected signal at some specified level above the blank or noise in the measurement (signal/noise ratio). This may be regarded as the minimum level at which there is sufficient certainty in the measurement to state that the analyte is unambiguously detected; and as the maximum level to state that the analyte is not there. Different signal/noise ratios are adopted for different applications, but typically vary between 3 and 20.

Sensitivity – the amount of analyte required to provide a unit of measurable signal, i.e. picomoles/mV. This term is often confounded with detection limit.

Resolution – the ability to separate or distinguish adjacent signals or compounds. The term has various meanings in different analytical techniques, i.e. in chromatography refers to the ability to separate distinct molecular structures, whereas in spectroscopy refers to the ability to distinguish different wavelengths.

Quantitative analysis – an analysis carried out to measure the amount (or concentration) of analyte in a sample. This is typically achieved by comparing the instrument response from the sample to a calibration curve generated from authentic laboratory standards, although other approaches are possible. Note that the term does not imply that a measurement is free from error or uncertainty.

Qualitative analysis – an analysis carried out to determine the identity, structure, functionality, or other properties of the analyte. Because generating calibrating curves for quantitative analysis typically requires knowing what analytes are targeted, qualitative analysis typically precedes quantitative analysis in the study of unknown materials. Estimates of relative abundance from (typically uncalibrated) qualitative analysis are sometimes called 'semi-quanitative,' although this term is ambiguous.

ANALYTICAL TECHNIQUES

Chromatography – a family of techniques, that relies on different rates of migration of analytes in a fluid phase travelling in a solid or liquid phase, for physically separating analytes in a mixture. The separation relies on differing physical and/or chemical properties of the analyte, such as vapor pressure, solubility, hydrophobicity, ionic strength, size, shape etc. Techniques for organic separations are often distinguished based on the mobile phase used for the separation, i.e. gas chromatography (analytes in a gas phase) vs liquid chromatography (analytes in a liquid phase).

Capillary electrophoresis – a family of analytical separation methods performed in a narrow bore (capillary) where the analytes are separated by migration through an electrolyte solution under the influence of high electric fields.

Magnetic resonance – a family of techniques (generically "**NMR**") that detect the absorption and reemission of electromagnetic energy by atoms in a strong magnetic field, due to spin-flipping of nuclei. The technique is non-destructive, and is widely used for structural elucidation of unknown organic compounds.

Mass spectrometry - a family of analytical techniques based upon the ionization of molecules, followed by manipulation, separation, and detection of those ions in magnetic and/or electrical fields. The technique typically yields the mass/charge ratio of each ion, which is useful in determining identity and structure. A variety of different ionization methods (e.g. electron-impact, chemical ionization, photoionization, electrospray, MALDI, secondary-ion impact, etc) and mass analyzer designs (sector-field, quadrupole, ion trap, time-of-flight, FT-ICR, etc) can be combined. Hyphenated techniques with chromatography (e.g., GC-MS and LC-MS) are very common. Techniques using multiple stages of ion manipulation (i.e., MS-MS or

MS^n) are sometimes used to increase specificity of analysis, or to help elucidate structure. Mass spectrometry is considered a 'destructive' analytical technique.

Optical spectroscopy – a family of analytical techniques that work by observing the interaction of photons (light) with the sample. Techniques can include measuring light reflection or scattering, absorption, fluorescence (absorption and re-emission at a longer wavelength), and Raman scattering (scattering with a minor energy loss arising from stimulation of a vibrational mode). Observations at different wavelengths target different properties of molecules, with x-ray wavelengths targeting atomic (elemental) composition, UV and visible light targeting molecular electronic transitions, and infrared wavelengths targeting molecular rotations and vibrations. Techniques can sometimes provide spatially resolved analysis, as in Raman microscopy. Optical techniques are typically non-destructive.

Mass spectroscopy – a mass/charge versus relative intensity plot used in chemical analysis. Typically, mass spectra are formed using a mass spectrometer when an organic carbon compound is ionized, decomposes according the laws of chemistry. The fragments are separated according to their mass/charge, counted and viewed as a relative abundance plot. Mass spectra, obtained under identical conditions can be a rapid, reliable and sensitive means of identifying unambiguously identifying organic carbon compounds.

Total carbon/total organic carbon analysis – related techniques for the analysis of bulk materials that aim to determine total levels of (organic) carbon via combustion of analytes to CO_2, with quantitation of the evolved CO_2. Because the analysis is operationally defined (i.e., anything that yields CO_2 at a given temperature), techniques that differ in temperature, time, PO_2, etc can include or exclude different materials. For example, graphite would be detected in a total carbon analysis at 1000°C but not at 500°C.

Laser desorption **-** the process by which incident laser radiation results in the separation of a molecule from a surface or matrix, allowing sampling of molecules with fewer matrix effects. This process may result in ionization of the molecules.

Secondary ionization mass spectrometry (SIMS) – a family of techniques in which samples are sputtered and ionized by the impact of a beam of primary ions, typically followed by mass spectrometric analysis. They are particularly useful in providing spatially-resolved mass spectrometric analysis (but see also laser desorption). High-energy primary ion beams (typically Cs^+ or O^-) typically achieve more aggressive sample sputtering (can be used to ablate surface layers) and yield monoatomic ions suitable for elemental and/or isotopic analysis, whereas low-energy ion beams typically sample only surface layers and yield molecular ions suitable for identification and structural analysis. The former technique is commonly known simply as SIMS (or NanoSIMS, depending on the spatial resolution of the primary ion beam), whereas the latter is often known as TOF-SIMS (although the combination of TOF mass spectrometry with low-energy primary ion beam is not required, it is commonly employed). Note that the acronym SIMS is also commonly used for "selection ion mass spectrometry" which is a different technique.

Isotope-ratio mass spectrometry (IRMS) – a subcategory of mass spectrometry in which the specific intent is to provide highly precise measurements of isotopic abundance, usually at the expense of losing structural information because analytes must be converted to a common molecular form (i.e., H_2, CO_2, N_2, SO_2, etc). For organic molecules, such techniques generally employ electron-impact ionization with sector-field spectrometers and multiple parallel detectors. The technique is commonly distinguished from SIMS, even though both provide similar types of information.

Isotope-ratio optical spectroscopy (IROS) – a subcategory of optical spectroscopy in which the specific intent is to provide highly precise mesurements of isotope abundance. Specific techniques typically employ either very-long pathlength absorption cells (integrated cavity-output spectroscopy, ICOS) or cavity-ringdown spectroscopy (CRDS), and both require that analytes be converted to a common molecular form

(i.e., H_2O, CO_2, N_2, etc). Although the optical detection is nondestructive, conversion to common analyte form is destructive.

X-ray Photoelectron Spectroscopy (XPS) – a technique where a surface is irradiated with soft x-rays, leading to ionization of the surface atoms. The subsequent release of emitted photoelectrons allows a spectrum to be obtained of the distribution and kinetic energy of the surface atoms to be determine, the intensity of specific peaks allows a quantitative analysis of each analyzed atom.

PROCESSING TECHNIQUES

Combustion – heating a material in the presence of molecular oxygen, or a source of oxygen, to generate carbon dioxide.

Destructive sampling – sampling or measurement processes, which result in the destruction of the sample.

Solvent Extraction – use of a liquid phase to selectively dissolve (solubilize) and separate particular compound classes from a complex matrix. Solvents of different polarities can be used to differentially extract different compound classes.

Pyrolysis – heating a material in the absence of oxygen to induce thermal decomposition. Typically, this approach relies on a defined temperature regime. Pyrolysis at temperatures up to ~ 600°C is used to convert a solid macromolecular material to smaller, volatile products that were amenable to separation by gas chromatography and identification by mass spectrometric analysis. The composition of these pyrolysis products is used to infer the nature of the macromolecular precursor. Pyrolysis at temperatures exceeding 1000°C typically converts the precursor to its elements (e.g. C, H_2) or small molecules such as CO.

Thin section – a thin slice of sample prepared either for the evaluation of internal composition or to allow access to a technique requiring a thinner cross section of material.

9.3.1 Glossary of Acronyms

	Adventitious Carbon
AC	
ALHT	Apollo Lunar Hand Tools
ALSRC	Apollo Lunar Sample Return Container
ATLO	Assembly, Test, and Launch Operations
ATP	Adenosine triphosphate, the energy storage molecule of a cell
CAPTEM	Curation and Analysis Planning Team for Extraterrestrial Materials, a committee that is part of the NASA advisory structure
DART/MS	Direct Analysis in Real Time - Mass Spectrometry
DNA	Deoxyribonucleic Acid
DRIFT	Diffuse Reflectance Infrared Fourier Transform spectroscopy
EDL	Entry, Descent, and Landing
EDX or EDAX	Energy-Dispersive spectroscopy
FTIR	Fourier Transform Infrared spectroscopy
GCMS	Gas Chromatography - Mass Spectrometry
GSFC	NASA Goddard Space-Flight Center
IR	Infrared
ISO	International Organization for Standardization
ITAR	International Traffic in Arms Regulations
IUPAC	International Union of Pure and Applied Chemistry
JPL	NASA Jet Propulsion Laboratory
LCMS	Liquid Chromatography - Mass Spectrometry
LM	Lunar Module
LOD	Limit Of Detection
LRL	Lunar Receiving Laboratory
Mars 2020	Mars 2020 Mission
M-Mars 2020 SDT	Mars 2020 Science Definition Team
MEP	Mars Exploration Program
MEPAG	Mars Exploration Program Analysis Group
MoE	Meeting of Experts, a process used by the U.S. National Research Council
MOMA	Mars Organic Molecule Analyzer (an instrument on ExoMars 2018)
MSL	Mars Science Laboratory
MSR	Mars Sample Return
MSR SSG (II or 2)	Mars Sample Return Science Steering Group II
NASA	National Aeronautics and Space Administration
NRC	National Research Council
NRC SSB	National Research Council Space Study Board
NVR	Non-Volatile Residue
OCM	Organic Check Material
OCP	Organic Contamination study Panel
OCSSG	Organic Contamination Science Steering Group
OSIRIS-REx	Origins Spectral Interpretation Resource Identification Security -- Regolith Explorer
PAH	Polycyclic Aromatic Hydrocarbons
PCR	Polymerase Chain Reaction
PLSS	Primary Life Support System
PP	Planetary Protection

QCM	Quartz Crystal Microbalance
RAD	Radiation Assessment Detector (instrument on MSL)
RGA	Residual Gas Analyzer
SA/SPAH	Sample Acquisition / Sample Processing And Handling (instrument on MSL)
SAM	Sample Analysis at Mars (an instrument on MSL)
SEM	Scanning Electron Microscopy
SIMS	Secondary Ion Mass Spectrometry
SMD	Science Mission Directorate
S/N	Signal-to-Noise ratio
SRC	Sample Return Capsule
SRF	Sample Receiving Facility
TAGSAM	Touch-And-Go Sample Acquisition Mechanism (instrument on OSIRIS-REx)
TEGA	Thermal and Evolved Gas Analyzer (instrument on Phoenix)
TOC	Total Organic Carbon
TOF-SIMS	Time-of-Flight Secondary Ion Mass Spectrometry
UV	Ultraviolet
WSTF	White Sands Test Facility
WP	Witness Plate
XPS	X-ray Photoelectron Spectroscopy