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Infrared Spectrometer for ExoMars

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INFRARED SPECTROMETER FOR EXOMARS (ISEM), A MAST-MOUNTED INSTRUMENT FOR THE ROVER

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Manuscripts

1 INFRARED SPECTROMETER FOR EXOMARS (ISEM), A MAST- 2 MOUNTED INSTRUMENT FOR THE ROVER

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30 31 32 **Abstract**

33 ISEM (Infrared Spectrometer for ExoMars) is a pencil-beam infrared
34 spectrometer that will measure reflected solar radiation in the near infrared range
35 for context assessment of the surface mineralogy in the vicinity of the ExoMars
36 rover. The instrument will be accommodated on the mast of the rover, and will be

operated together with the PanCam High-Resolution Camera (HRC). ISEM will study the mineralogical and petrographic composition of the martian surface in the vicinity of the rover, and in combination with the other remote sensing instruments, aid the selection of potential targets for close-up investigations and drilling sites. Of particular scientific interest are water-bearing minerals, such as phyllosilicates, sulfates, carbonates, and minerals indicative of astrobiological potential, such as borates, nitrates, and ammonium-bearing minerals. The instrument has a $\sim 1^\circ$ field of view and covers the spectral range between 1.15–3.30 μm with a spectral resolution varying from 3.3 nm at 1.15 μm to 28 nm at 3.30 μm . ISEM’s optical head is mounted on the mast, and its electronics box is located inside the rover’s body. The spectrometer employs an acousto-optic tunable filter (AOTF), and a Peltier-cooled InAs detector. The mass of ISEM is 1.74 kg, including the electronics and harness. The science objectives of the experiment, the instrument design, and operational scenarios are described.

1 Introduction

The ExoMars rover is a mobile laboratory equipped with a drill to sample the surface of Mars to a maximum depth of 2 m, and a suite of instruments to analyze the samples. The drilling device is the only means to access near subsurface materials and introduce them to the internal analytical laboratory. As the number of samples obtained with the drill will be limited, the selection of high value sites for drilling will be crucial. The rover’s mast is therefore equipped with a set of remote sensing instruments to assist the selection process by characterizing the geological and compositional properties of the surrounding terrains. It includes several cameras – a pair of navigation cameras (NavCam), and a panoramic camera (PanCam). PanCam consists of stereo multispectral wide-angle camera pair (the WACs) and a high-resolution color camera (HRC) (Coates et al, this issue) and will provide the context images used to plan travelling and sampling. To complement and enhance the capabilities of the remote sensing suit, an infrared spectrometer able to unambiguously distinguish many rocks and minerals from their spectral reflectance, will allow remote characterization and selection of potential astrobiological targets. This mast-mounted IR spectrometer was proposed during an early discussion of the new ESA-Roscosmos ExoMars configuration as a useful addition to the rover science and to help operations by characterizing from afar the mineralogical interest of targets that the rover could

73 visit.

74

75 ISEM is a derivative of the Lunar Infrared Spectrometer (LIS) (Korablev et al,
76 2015) being developed at the Space Research Institute (IKI) in Moscow for the
77 Luna-25 and Luna-27 Russian landers planned for flight in 2019 and 2021,
78 respectively (Zelenyi et al, 2014). Both the ISEM and LIS instruments have been
79 conceived with similar spectral capabilities. The ISEM design is improved with
80 respect to that of LIS, and modifications were also necessary to comply with the
81 more stringent environmental conditions on the ExoMars rover. A fully
82 operational model of ISEM is not ready at the moment of the paper submission,
83 and the assessment of its measurement performance has been made with the
84 available LIS prototype.

85

86 ISEM is one of two Roscosmos-provided instruments for the ExoMars Rover. It is
87 being predominantly developed at IKI, but includes contributions from the
88 National Research Institute for Physicotechnical and Radio Engineering
89 Measurements (VNIIFTRI) in Russia, Moscow State University, also in Russia,
90 and the Main Astrophysical Observatory, National Academy of Sciences in
91 Ukraine. A calibration target to be used jointly by PanCam and ISEM is being
92 contributed by Aberystwyth University, United Kingdom. Key components, such
93 as the AOTF and the detector, are purchased from NII Micropribor (Russia) and
94 Teledyne (USA). The science team includes researchers from Russia (IKI and
95 Vernadsky Institute), France, Italy, Sweden, Germany, UK, and Canada. The
96 team shares science team members with the PanCam and MicrOmega rover
97 instrument teams. A full list of the ISEM Science and Technical teams is given at
98 the end of the paper.

99

100 After a brief summary of the major objectives of the ExoMars mission, we
101 describe the scientific goals of the ISEM instrument. The technical design is then
102 detailed. Measured performances of LIS prototype and and expected
103 performances of ISEM are presented subsequently. We conclude the paper by
104 addressing the operational scenarios and related environmental constraints.

105

106 2 Science Objectives

107 2.1 Contribution to overall rover mission science

108 The scientific objectives of the ExoMars Program are defined as (Vago et al, this

109 issue):

- 110 1. To search for signs of past and present life on Mars;
- 111 2. To investigate the water/geochemical environment as a function of depth
- 112 in the shallow subsurface;
- 113 3. To study martian atmospheric trace gases and their sources;
- 114 4. To characterize the surface environment

115
116 The first two objectives are the most relevant to the ExoMars rover. The ISEM
117 experiment will contribute to achieving each of these objectives in the following
118 ways:

- 119 1. Many of the minerals and rocks detectable by ISEM are good indicators of
120 past habitable conditions, and of biological processes (e.g, carbonates,
121 oxalates, borates, nitrates, NH₄-bearing minerals (Applin et al, 2015; Berg
122 et al, 2016; Cloutis et al, 2016)) and may even contain biomolecules in
123 detectable concentrations. These include a class of biogenic minerals
124 which are further known to provide a substrate for, and catalyze pre-biotic
125 reactions. Organic compounds, including Polycyclic Aromatic
126 Hydrocarbons (PAHs) and those containing aliphatic C-H molecules, can
127 also be distinguished by ISEM (e.g, Clark et al, 2009; Izawa et al, 2014).
- 128 2. The ISEM instrument is capable of recognizing minerals and rocks, which
129 are indicative of the presence of water as well as geochemical
130 environmental indicators. ISEM can also be used to analyze the drill
131 cuttings excavated by the ExoMars drill system. The operating drill
132 obscures ISEM’s view, and observing the cuttings is only possible after
133 the rover moves off and revisits the drilling site.
- 134 3. If present, ISEM could detect organic-bearing materials, possibly evolving
135 trace gases, such as hydrocarbons.
- 136 4. ISEM can carry out atmosphere observations, providing information on
137 dust and clouds, and contributing to characterization of the atmospheric
138 humidity. ISEM is capable of identifying and monitoring surface frost, and
139 may assess the diversity and stability of various minerals on the martian
140 surface, e.g, by monitoring changes in the spectral properties of drill
141 cuttings over time.

142
143 In terms of where the rover will land, ESA has issued the following scientific
144 criteria for landing site selection (Vago et al, 2015):

145

146 For the ExoMars Rover to achieve results regarding the possible existence of
147 biosignatures, the mission has to land in a **scientifically appropriate setting**:

- 148 1. The site must be **ancient** (older than 3.6 Ga) — from Mars' early, more
149 life-friendly period: the Noachian to the Noachian/Hesperian boundary;
- 150 2. The site must show abundant morphological and mineral evidence for
151 long-term, or frequently reoccurring, **aqueous activity**;
- 152 3. The site must include numerous **sedimentary outcrops**;
- 153 4. The outcrops must be **distributed** over the landing ellipse to ensure the
154 rover can get to some of them (typical rover traverse range is a few km);
- 155 5. The site must have **little dust** coverage.

156

157 ISEM addresses these criteria in the following ways:

- 158 1. The suite of samples that we have used to characterize ISEM in laboratory
159 tests includes materials similar to those found in Noachian terrains (e.g,
160 phyllosilicates, carbonates, etc.)
- 161 2. ISEM will be able to identify minerals that are indicative of aqueous
162 activity, such as phyllosilicates and hydrated sulfates.
- 163 3. Rocks and minerals presumed to have formed in sedimentary
164 environments are the main focus of our investigation and ISEM is
165 particularly well suited to detect and characterize them.
- 166 4. ISEM as a remote instrument is well adapted to characterize the
167 stratification at the outcrop scale.
- 168 5. Our investigation will assess the obscuring effects of dust, first of all on
169 the target areas, but also observing dust accumulation on the calibration
170 target, excavated drill cuttings (e.g, Rice et al, 2011).

171

172 2.2. Synergies with other instruments

173 The main goal of ISEM is to establish the mineral composition of Mars' surface
174 materials remotely. ISEM, together with PanCam (Fig. 1) offer high potential for
175 the remote identification and characterization of any scientifically high-value
176 targets in the vicinity of the rover, including proximal and distant rocks, outcrops,
177 and other geological formations. ISEM will help to establish the geological
178 context of each site along the rover traverse, discriminating between various
179 classes of minerals and rocks. ISEM will also be important in order to select
180 promising sites for subsurface sampling.

181
182 Infrared reflectance spectroscopy allows the study of the composition in the
183 uppermost few millimeters of a rock’s surface. It allows discriminating between
184 various classes of silicates, (hydr-)oxides, hydrated/hydroxilated salts and
185 carbonates. As shown in Fig. 2, the 1.3° Field of View (FOV) of ISEM lies within
186 the 5° FOV of the color PanCam high-resolution camera (HRC), and they both
187 are within a much wider FOV (38.6°) of the Wide Angle Cameras (WACs) with
188 multispectral capabilities (Coates et al, this issue). The multispectral data are
189 produced using a filter wheel with 11 filter positions for each of the two WACs.
190 Out of the 22 filters, six are devoted to red, green, and blue broadband color,
191 duplicated in the both cameras, 12 are optimized for mineralogy in the 400-1000
192 nm range, and four “solar” filters are dedicated to atmospheric studies. By
193 extending the wavelength range beyond PanCam, ISEM will enable many more
194 spectral features diagnostic of specific mineralogy to be detected. Together
195 PanCam and ISEM provide spectrally resolved information from 0.4 to 3.3 μm.

196
197 The identification and mapping of the distribution of aqueous alteration products
198 in the upper surface layer, combined with subsurface data from the neutron
199 detector ADRON and the ground-penetrating radar WISDOM, will help to
200 understand the subsurface structure and the exobiology potential at each
201 prospective drilling site.

202
203 The collected drill samples will be analyzed in the rover’s Analytical Laboratory
204 Drawer (ALD) by several instruments. The first is an infrared hyperspectral
205 microscope MicrOmega (Bibring et al, this issue). The principle of MicrOmega is
206 very similar to that of ISEM. The reflectance spectroscopy is performed in the
207 near-IR, but the analysis is done at the microscopic scale and the sample is
208 illuminated by monochromatic light source. In contrast to MicrOmega, ISEM has
209 a much wider field of view and range of detection. The distance to a target is not
210 really limited, and practically may reach hundreds of meters. Thus, ISEM is better
211 suited for accommodation on the rover mast, where it can be employed for target
212 identification of far away objects, but also for investigating outcrop, rock, and soil
213 mineralogy at close range.

214
215 There is no specific instrument dedicated to environmental characterization on the
216 rover. Although hampered by the limited number of observation cycles, ISEM,

217 jointly with PanCam, will deliver information regarding atmospheric aerosol
218 opacity and the atmospheric gaseous composition. The data on water vapor
219 content and aerosol will be retrieved as a by-product of reflectance spectra, from
220 in-flight calibration, from the direct Sun imaging by PanCam, and from sky
221 observations by PanCam and ISEM.

222

223

224 Figure 1. Schematic view of the ExoMars Rover mast instruments: PanCam,
225 navigation cameras, and ISEM.

226

227

Figure 2. Schematic representation of possible ISEM and PanCam joint observation scenario showing a sequence of ISEM measurements acquired together with WAC and HRC PanCam frames.

2.3 The method

Near-IR spectroscopic observations of the Mars surface have not been performed from any surface platform to date. Spectroscopy was employed on the Mars Exploration Rovers (MER) in the thermal IR range (the radiation emitted by the surface, 5-29 μm) with the Mini-TES instrument (Christensen et al, 2003, 2004a,b). These remote observations proved very useful for selecting targets for *in situ* analyses by the Alpha Proton X-Ray Spectrometer (APXS) and Mossbauer instruments on Spirit and Opportunity (e.g, Squyres et al, 2004). They also allowed the identification of carbonates in Gusev Crater (Morris et al, 2010), and undertook a number of atmospheric investigations (Smith et al, 2006).

Conversely, the near-IR spectral range (i.e. the infrared solar reflected radiation) is being widely used in orbital observations, as it allows for significantly better characterization of aqueous minerals than does the thermal infrared. To illustrate this point, the TES instrument on Mars Global Surveyor (MGS) in the wavelength range from 6 to 50 μm has mapped the distribution of both mafic and anhydrous high-silica minerals (Bandfield et al, 2000; Christensen et al, 2001), but could not unambiguously detect clay/clay-like minerals and salts, including carbonates. In the near-IR, the OMEGA hyperspectral instrument on Mars Express (MEx) measured the martian surface reflectance from 0.5 to 5.2 μm , and was able to recognize a number of different phyllosilicates and sulfates (Bibring et al, 2006). Building on OMEGA's success, the higher spatial resolution of the CRISM instrument on Mars Reconnaissance Orbiter (MRO), which measures reflectance from 0.362 to 3.92 μm , permitted the first detections of carbonates and serpentine (Ehlmann et al, 2008, 2010). One shortcoming of the orbital observations is the limited surface resolution (300-500 m per pixel for OMEGA/MEx and ~20 m for CRISM/MRO), hindering the detection of small-scale exposures. In addition, such instruments suffer from limited detection sensitivity owing to the combination of the subtle nature of aqueous mineral spectroscopic features and to the short dwell time of orbiting spacecraft. The wide variety of minerals on Mars detected by the higher spatial resolution CRISM instrument compared to the lower resolution

OMEGA instrument demonstrates the greater mineralogical diversity that can be identified as spatial resolution improves. Therefore the close-up near-IR capability of ISEM on the ExoMars rover offers a very high diagnostic potential.

The small size and low mass of the ISEM instrument allows it to be accommodated more easily on a rover platform. A similar AOTF-based near IR spectrometer has been selected to enhance the capabilities of the successor to the ChemCam instrument on the Curiosity Rover (Fouchet et al, 2015). The new SuperCam instrument planned for the NASA 2020 rover utilizes a combination of the Laser-Induced Breakdown Spectrometer (LIBS), Raman, and near-IR reflectance spectroscopy, offering complementary elemental and mineralogical analysis techniques.

Spectral range: An optimal spectral range for a near-IR mineralogical characterization is 0.9-4.0 μm to encompass a broad absorption centered in the 0.95-1.1 μm region characteristic for pyroxene or olivine, and 3.4-3.9 μm for carbonate overtones. The spectral range of the prototype LIS spectrometer is a compromise of science requirements and technical limitations. Its longwave bound of 3.3 μm allows for detection of hydration features in the 3 μm region that can be used to discriminate different types of phyllosilicates and other water/hydroxyl-bearing materials (e.g, Clark et al, 1990). The broad absorption in the 3 μm region has contributions from the long wavelength wing of a hydroxyl (OH) fundamental stretch usually centered near 2.7-2.8 μm , H₂O fundamental stretches, and the first overtone of the H₂O bending fundamental (Clark et al, 1990). On Mars, hydration is strong enough that it can be detected at shorter wavelengths. Clays and other hydrated minerals can be detected and discriminated from overtones and combinations absorption features, at $\sim 1.4 \mu\text{m}$, $\sim 1.9 \mu\text{m}$, and 2.2-2.3 μm . Detection of carbonates by ISEM will be possible using correlated 2.3- and 2.5- μm region bands, similar to CRISM/MRO (Ehlmann et al, 2008). Beyond 3.3-3.4 μm the signal is complicated by the thermal radiation of the surface (and from the instrument itself, detectors with longer-wavelength bound are much less sensitive because of thermal background). On the short wavelength bound, the sensitivity of detectors optimized for 3- μm range falls abruptly below 1 μm , hampering mafic silicate identification and characterization. However mafic silicates can be recognized and discriminated by the shape of the long wavelength wing of the 1- μm ferrous iron absorption band and the

300 wavelength position of the 2- μm ferrous iron absorption (see the following
301 section for the details).

302
303 Taking into account the advantages of the heritage design, we choose using the
304 same 1.15-3.3 μm range for ISEM on ExoMars as for the lunar instrument.

305
306 Spectral resolution. The spectral features of Mars surface materials will generally
307 include a mixture of several minerals, and are usually broad (>20 nm full width at
308 half maximum), so that there is no stringent requirement on the spectral resolution
309 for orbital instruments (see Table 1). With increasing spatial resolution, individual
310 minerals may become more apparent, with deeper characteristic absorption
311 features. Pure minerals can likely be observed only at the scale of individual
312 grains, e.g, with the microscope-spectrometer MicrOmega. Given that the ISEM
313 FOV will typically encompass an area of few cm^2 , a mixture of minerals will
314 likely be present, therefore a spectral resolution requirement of 25 cm^{-1} was
315 chosen that corresponds to 3.3 nm at 1.15 μm , 16 nm at 2.5 μm , and 28 nm at 3.3
316 μm .

317
318 In mineralogical studies, the best approach is the acquisition of the full available
319 spectral range. Nyquist sampling (two measured points per spectral resolution) of
320 the full 1.15-3.30 μm ($3030\text{-}8696\text{ cm}^{-1}$) range with a spectral resolution of 25 cm^{-1}
321 results in 453 (512 with margin) spectral points. With a one-second exposure for
322 each spectral point, a complete spectrum is therefore measured in 8.5 minutes.
323 Customable or random wavelength access by the AOTF (see below) allows
324 oversampling, selecting different portions of the spectrum, and focusing on the
325 most interesting or diagnostic spectral intervals.

326
327 The color and IR reflectance of the Mars surface are what one would expect of
328 iron-bearing mineral species that are either primary or formed by hydrous or
329 anhydrous chemical weathering. The infrared reflectance varies from 5% to 35%,
330 with typical values being 15-20% for low albedo regions and 25-30% for high-
331 albedo regions (Erard 2001). A characteristic feature of Mars spectra is a deep
332 absorption feature starting beyond the 2.7- μm CO_2 saturated atmospheric band.
333 Its depth reflects the degree of hydration of the martian surface. An increase in
334 measured reflectance toward longer wavelengths signifies an increasing
335 contribution from emitted thermal radiation. Observations from the ExoMars

rover mast will be carried out using a broad range of phase angles, preferably at high Sun. There is no Sun avoidance requirement for ISEM.

Table 1. Near-IR spectrometers used and planned to study Mars surface

Instrument	Spectral range, μm	Spectral resolution, nm	Surface resolution	Ref.
ISM/Phobos 2	0.8 -3.1	50	20x30 km	Bibring et al, 1990
OMEGA/MEx	0.35-1 1-2.5 2.5-5.1	7 14 20	0.3-5 km	Bibring et al, 2004
CRISM/MRO	0.362-3.92	6.6/pix	18 m	Murchie et al, 2007
ISEM/ExoMars	1.1-3.3	3.3 at 1.15 μm 16 at 2.5 μm 28 at 3.3 μm	3-10 cm	This study
MicrOmega/ExoMars	0.5-3.65	2 at 1.0 μm 25 at 3.6 μm	20 μm	Bibring et al, this issue
SuperCam/2020 Rover	1.3-2.6	5 at 1.3 μm , 20 at 2.6 μm	1.3-7 mm	Fouchet et al, 2015

2.4 Potentially detectable mineral groups

The greatest share of what we know about martian mineralogy has been gleaned from orbital near- and thermal-infrared spectroscopy measurements. The infrared instruments have been successful in identifying igneous minerals, while the near-IR instruments were more important for detecting ancient hydrated minerals, such as phyllosilicates, as well as carbonates and sulfates, which could be used to develop a timeline of changing environmental conditions on Mars and evidence of previous more clement epochs on Mars. The capabilities of ISEM can be gauged against these detections to assess its expected science return, as well as expectations for detecting other mineral species of high scientific value, all in the context of the proposed ExoMars landing sites.

1. Phyllosilicates: The identification of hydrated phyllosilicates on the martian surface is one of the discoveries driving *in situ* exploration of Mars.

Phyllosilicates are commonly detected in ancient, Noachian-aged martian terrains (Poulet et al, 2005). Various types of phyllosilicates have been observed, including Fe/Mg and Al-rich smectites, micas, vermiculites, kaolinite, chlorite, and serpentine (Ehlmann et al, 2009; Murchie et al, 2009; Carter et al, 2013). The presence of these minerals likely indicates that conditions in the past were favorable for the presence of liquid water at or near the surface. They are considered good reaction templates for organic molecules and excellent for biosignature preservation (Bishop et al, 2013, and references therein). Phyllosilicates have been detected from orbit within the ellipse of two out of the three candidate landing sites for the ExoMars rover, Oxia Planum and Mawrth Vallis (Vago et al, this issue). They have not been detected in Aram Dorsum yet; even if they are there, it may be difficult to see them from orbit. ISEM will have the capabilities to detect sharp features between 1.35 and 2.6 μm in phyllosilicate reflectance spectra, which are related to combinations and overtones of OH-M stretching and bending bound to various cations (M) as well as the H-O-H stretch and bend from water bound in interlayer regions or adsorbed on mineral surfaces (Clark et al, 1990) (Figures 3a, b, and c).

2. Carbonates have been discovered on Mars at a number of locations from orbit (Ehlmann et al, 2008, Wray et al, 2016), by surface rovers (Morris et al, 2010), and in martian meteorites (e.g, McKay et al, 1996). The precise species are not always known, but various Mg-Fe-Ca carbonates provide the best match for observed spectral features. Carbonates are important minerals for identification as they often indicate the presence of habitable (circum-neutral) environments. They are also widely implicated in explaining the loss of a substantial fraction of the presumed early Mars dense carbon dioxide atmosphere. Carbonate detection and characterization is possible in a number of wavelength regions. The 2.2-2.6 μm region is one of the best because it is not affected by thermal emission, and absorption bands in this region vary in their positions for different carbonate species (Figure 3d). ISEM may also be able to identify Fe-bearing from Fe-free carbonates on the basis of the presence or absence of a ferrous iron absorption band near 1.2 μm .

3. Sulfates: A number of sulfate minerals have been observed on Mars, both from orbit and in situ, including poorly ($\leq 2 \text{ H}_2\text{O}$) hydrated species (gypsum, kieserite, bassanite), and polyhydrated varieties (Squyres et al, 2004; Gendrin et al, 2005;

Wang et al, 2006; Flahaut et al, 2014; Nachon et al, 2014) as well as hydroxylated species (copiapite, jarosite, alunite and the dehydrated form of amaranthite $\text{FeSO}_4(\text{OH})$). These sulfates are all water/hydroxyl-bearing and several are also indicative of circum-neutral, perhaps habitable environments. Sulfates also have the potential to preserve microfossils (e.g, Allwood et al, 2013) and concentrate organic compounds (Noe Dobrea et al, 2016). Specific sulfates can be powerful indicators of environmental conditions on Mars, past and present (e.g, Leftwich et al, 2013). Sulfate discrimination is possible using a number of wavelength intervals in the ISEM range. For example, gypsum is characterized by a uniquely-shaped absorption band in the 1.4- μm region, jarosite and alunite by absorption bands in the 1.8- μm region, and other sulfates by S-O associated absorption bands in the 2.0-2.5 μm region (Cloutis et al, 2006) (Figures 3e and f).

4. Silica: Silica, in a variety of forms, is present in a number of terrains on Mars (Bandfield et al, 2004; Smith and Bandfield, 2012; Smith et al, 2013, Carter et al, 2013). Differences in reflectance spectra can be used to distinguish different forms of silica, some of which are associated with habitability (Rice et al, 2013). The region most useful for distinguishing different forms of silica is located near 2.2 μm and is due to Si-OH overtones. The nature and abundance of these bonds varies among different types of silica (Rice et al, 2013). This diagnostic feature can be clearly seen in the reflectance spectra of two different grain sizes of quartz (Figure 3g).

5. Igneous minerals. Petrologic investigations of martian rocks have been accomplished by mineralogical, geochemical, and textural analyses by remote sensing observations, in situ investigations, and laboratory analyses of martian meteorites. Igneous rocks are found in numerous settings; NIR spectroscopy from orbiting spacecraft has been an effective mineralogic tool to identify and to map at a global scale various rock-forming minerals such as olivines, pyroxenes and iron-bearing plagioclases (Poulet et al. 2009; Ody et al. 2013; Carter and Poulet 2013). (Figure 3h and i).

6. Ferrous oxides/hydroxides. These minerals are the widespread weathering products of primary iron-bearing materials (Ody et al, 2012). In the ISEM spectral range, they manifest themselves mainly in the shape of the continuum. Hydroxides exhibit shallow absorption features, including near 1.41 and 1.93 μm ,

and several species have been reported from NIR orbital investigations. Some iron-bearing species, such as goethite, exhibit Fe-OH absorption bands longward of the same band in Fe-free minerals (Beck et al, 2011) (Figure 3j).

Several other potential candidates that are amenable to detection and analysis by ISEM, and are of high scientific value, are described below.

Organic ompounds –PAHs. Infrared spectroscopy is potentially sensitive to the presence of organic compounds, which have already been identified *in situ*, though in trace quantities, within Mars samples (Freissinet et al, 2015). PAHs are generally a stable form of organic molecules, and if organic compounds are or were present on the surface of Mars, they have likely transformed to PAHs (Anders et al, 1996). PAHs are also the dominant form of organic material in Archaean terrestrial rocks (Marshall et al, 2007; and references therein). Their reflectance spectra exhibit absorption features that are largely associated with a number of functional groups that may be present, particularly aliphatic C-H molecules (Izawa et al, 2014). They can exhibit absorption bands near 1.69 μm due to CH overtones, 1.50 μm due to N-H stretching overtones, and numerous other overtone and combination bands beyond 2.1 μm . A shoulder of the fundamental 3.2-3.35 μm aromatic band could be also detectable in the spectra, though complicated by a deep 3- μm absorption, characteristic for Mars reflectance in general, see below.

Perchlorates and chlorides. Perchlorates are strongly suspected to be present on Mars on the basis of analytical results from the Phoenix lander in the polar region (Hecht et al, 2009; Cull et al, 2010) and from the MSL Curiosity rover in the near-equatorial region (Farley et al, 2016). Perchlorates have been linked both to the destruction of organic compounds, and to liquid water. They can absorb atmospheric water and allow for the existence of stable liquid water brines (Martin-Torres et al, 2015). Their spectral properties have been the focus of multiple studies (Bishop et al, 2014; Hanley et al, 2015) since the presence of perchlorates could have strong implications for the (non) preservation of biosignatures. Reflectance spectra are characterized by possible Cl-O-H₂O-associated absorption bands near 1.35, 1.75, and 2.15 μm . The 3-micron signature of water is present in IR spectra of perchlorate samples in the form of hydrate, ice or liquid brine (Zorzano et al, 2009). Spectral features in a more suitable NIR

range have possibly been detected from orbit (Ojha et al, 2015), the efforts to confirm this are under way. While anhydrous chloride salts are mostly featureless in the wavelength range of ISEM, chlorinated species have been detected in abundance at Mars (Osterloo et al, 2010), and their hydrated forms would be detectable in the NIR (Hanley et al, 2011).

Oxalates. Oxalates are carbon-bearing minerals that new evidence suggests may be present on Mars in addition to, or instead of, carbonates (Applin et al, 2015). Terrestrial oxalates are typically formed in biological processes (Applin et al, 2016, and references therein). Their presence on Mars would suggest past habitability and possibly biological processes. Oxalates have some similarities with carbonates in terms of multiple C-O associated absorption bands, but their wavelength positions and shapes differ from carbonates and can be used to discriminate different oxalate species. Major oxalate absorption bands are present in the 2.2-2.5 and 3.2-3.3 μm regions.

Water ice. The presence of water ice at the landing site during daytime observations is unlikely, but cannot be excluded (Carrozzo et al, 2009). Seasonal frost, if present at the landing site, will be readily identifiable by ISEM, allowing study of its season deposition cycle and dependence on local conditions. Unambiguous signatures of water ice are present in the ISEM wavelength range with diagnostic absorption bands at 1.25, 1.5, 2.0 and 3.0 μm .

Nitrates. Nitrates may have been detected *in situ* on Mars (Navarro-Gonzalez et al, 2013). They are important minerals because they may indicate the operation of biological processes and/or can serve as a bioavailable source of nitrogen. Their spectral reflectance properties have recently been studied (Cloutis et al, 2016). The NO_3 molecule gives rise to multiple absorption bands that can be detected down to as low as 1.8 μm .

Phosphates. Phosphates are important as a potential indicator of biological processes. They are a likely possibility to explain phosphorus, which has been detected on Mars (Blake et al, 2013), but its form is not yet determined. Their spectral properties are only partially known (Lane et al, 2011). They share some similarities with some other mineral groups, including ferrous iron-associated absorption bands in the 1- μm region and weak P-O absorption bands in the 2-2.5

500 μm region. Robust phosphate detection by ISEM may not be feasible.

501
502 Borates. Borates are another important mineral group that can be associated with
503 habitability and biological processes (Stephenson et al, 2013). Boron cannot be
504 detected with an APXS instrument (Cloutis et al, 2016), but it has been detected
505 and quantified in clays from martian meteorite MIL090030 (Stephenson et al,
506 2013). Borate deposits on Earth are often associated with enclosed evaporitic
507 deposits and might be present in association with martian chlorides and sulfate
508 salts. Borates exhibit B-O associated absorption bands in the 1.55, and 2.15-2.25
509 μm regions, enabling their detection using multiple wavelength intervals and
510 absorption features measurable by ISEM. Absorption band positions and shapes
511 vary between different borates.

512
513 Ammonium-bearing minerals. The presence of the ammonium (NH_4) molecule in
514 various minerals leads to strong absorption bands in the 1.6, 2.0-2.2 and 3.1 μm
515 regions. Band shapes and positions can be used to discriminate different
516 ammonium-bearing minerals (Berg et al, 2016). Ammonium-bearing minerals are
517 of astrobiological importance for a number of reasons. Ammonium is often of
518 biological origin, has high thermal stability, and can withstand some level of
519 metamorphism (Boyd, 2001). Ammonium-bearing minerals on Mars have
520 possibly been detected from spectroscopic observations made from orbit (Sefton-
521 Nash et al, 2012), and a nitrogen cycle on Mars has been suggested to operate
522 (Manning et al, 2008). Low concentrations of ammonium in soil have been
523 reported for the Phoenix landing site (Quinn et al, 2011).

524
525 One of the limitations of spectrally characterizing Mars-relevant minerals with
526 ISEM under ambient terrestrial conditions is that these mineral spectra display a
527 nearly ubiquitous broad and frequently deep absorption feature in the 3- μm region.
528 This is normally attributable to water that may be present in various forms,
529 including adsorbed, fluid inclusions, impurities or accessory phases, or due to
530 incipient alteration. This feature is normally seen even in nominally anhydrous
531 minerals, such as olivine and pyroxene (see Figure 3h and i; more examples of
532 Mars background material spectra are presented in Figure 3 j, k, and l). When
533 such minerals are exposed to Mars-like surface conditions, the 3- μm feature
534 commonly shows a reduction in both depth and width, but rarely disappears
535 completely (Cloutis et al, 2007; Cloutis et al, 2008). It may be possible to use

characteristics of the 3- μ m absorption feature to constrain or determine water content (Milliken and Mustard, 2005), but in multicomponent targets, such determinations will be more difficult. Small amounts of water in the near subsurface and on the surface of Mars also seems to be ubiquitous, displaying seasonal variations (Milliken et al, 2007). Collectively these results suggest that the 3- μ m region may not be best suited for mineralogical determinations using ISEM. However, as discussed above, other wavelength regions accessible to ISEM have significant diagnostic potential for a wide range of minerals, as demonstrated effusively from terrestrial and Mars orbital studies.

Figure 3. Example spectra of minerals and rocks in the ISEM spectral range, which may be expected at the ExoMars landing sites (from CRISM spectral library, http://pds-geosciences.wustl.edu/missions/mro/spectral_library.htm; sample labels from this library). The upper half of the figure (a-f) shows the spectra of minerals the most significant for habitability, while the spectra shown

in the lower half (g-i) are more relevant to background minerals and dust. The spectral resolution of CRISM is close to that of ISEM in the center of the range; ISEM resolution is better at shorter wavelengths, and coarser at 3 μm (see Table 1).

2.5 Atmospheric studies (aerosol, gaseous content)

There is no dedicated instrument, such as e.g. meteorological station on the ExoMars rover to characterize the environmental conditions. Therefore any information available by other means is of particular value. Spectrally resolved data in the visible-NIR and in the thermal IR ranges have been used to assess the atmospheric state from Mars Pathfinder and Mars Exploration Rovers. In the spectral range of ISEM there are absorption bands of atmospheric CO_2 (at 1.43, 1.6, 2.0, and 2.7 μm) and H_2O (at 1.38 and 2.56 μm), and it is well suited, in particular its short-wave sub-range to characterize the main mode of the martian dust (Fedorova et al, 2014). The condensation clouds in the equatorial region consist predominantly of water ice (Vincendon et al, 2011), with multiple absorption bands within the ISEM spectral range (see section 2.4). Carbon dioxide clouds if present at high altitudes may be detected by distinct features of solid CO_2 near 1.2, 1.4, 1.5, 2.0, 2.7, and 3.0 μm .

The gaseous absorptions will be measured by ISEM as a by-product of every surface measurement. Depth of the CO_2 absorptions can be used to determine the surface pressure, and the H_2O absorptions quantify the total column water contents in the atmosphere above the site. To disentangle the possible overlapping atmospheric and mineral features in the reflected surface spectra, preferentially the observations of the *in situ* calibration target will be interpreted. The estimate of accuracy to retrieve the atmospheric pressure by ISEM is given by OMEGA study of the 2- μm CO_2 absorption from the orbit: 7-10 Pa ($\sim 1\%$) 1-sigma. (Forget et al, 2007). With the optical path being half of the OMEGA case, our retrieval accuracy will be comparable.

More precise measurements of surface pressure, minor gases, and better characterization of the atmospheric dust and cloud situation by ISEM will be possible using dedicated atmospheric observations. They will be coordinated with those by PanCam. The PanCam atmospheric study (Coates et al, this issue) will include direct solar observations just prior to sunset (to take advantage of the

590 maximal atmospheric path lengths) and cross sky brightness measurements. Such
591 observations, e.g. performed with Mars Pathfinder camera (Titov et al, 1999;
592 Markiewicz et al, 1999) or MERs (Lemmon et al, 2004; Smith et al, 2006) can be
593 significantly strengthened by extending the spectral range to the near-IR.

594
595 Direct solar observations by ISEM are not so far in the baseline. Their
596 implementation would allow for high-accuracy pressure and water retrievals,
597 better optical characterization of dust, direct and localized detection of H₂O ice
598 and, if present, the CO₂ ice clouds. Observing the Sun at different zenith angles
599 helps putting constraints on the vertical distribution of water vapor. However
600 ISEM is optimized for weak reflected light, and measuring the direct Sun signal
601 may not be feasible. We successfully tested this possibility with the lunar
602 prototype, but the ISEM aperture is larger, and a solar-blind filter within the
603 foreoptics might become necessary. Such a filter would cause a several percent
604 signal loss for the baseline ISEM observations. A final assessment of the direct
605 Sun mode will be done during the characterization of the flight model.

606
607 The cross-sky brightness measurements by ISEM are the best suited for
608 characterizing the aerosol component of the Mars atmosphere. Because of quasi-
609 permanent aerosol loading, the brightness of the martian sky at low zenith angles
610 is not significantly lower than that from light scattered from the surface.
611 Measurements at a range of phase angles will allow to extract the size distribution,
612 optical properties, and even to assess the shape of aerosols suspended in the
613 atmosphere. Water vapor absorption at 2.56 μm is much stronger than that at 0.94
614 μm to be observed by WAC in solar filters, and the ISEM data might put
615 additional constraints on the vertical distribution of water in the boundary layer of
616 atmosphere.

617
618 The variety of atmospheric measurements by ISEM calibrated using an *in situ*
619 calibration target will allow the refinement of atmospheric scattering models and
620 therefore refinement of the calibration of orbital spectral measurements of the
621 martian surface.

622
623 **3 Instrument Description**

624 **3.1 Instrument concept**

625 The measurement principle of ISEM is based on the use of an AOTF. The core

element of an AOTF is a birefringent crystal (typically of paratellurite, TeO_2 , due to the combination of acoustic and optical properties) with a welded piezotransducer. The radio frequency (RF) applied to the transducer generates an acoustic field in the crystal, implementing acousto-optic interactions in Bragg's regime. The spectral selectivity of the acousto-optic diffraction allows the filtering of light. The diffraction occurs for a single wavelength, and there are no diffraction orders. The applied RF controls the tuning of the AOTF. AOTFs are technologically mature and widely used for spectral analysis. The robust design, small dimensions and mass, coupled to the absence of moving parts in an AOTF-based spectrometer, makes them popular for space applications. So far AOTF-based spectrometers have been used in space science: (i) to study the atmospheric composition of Mars and Venus (Korablev et al, 2006, 2012); (ii) on the Moon within the Chang'e-3 VNIS spectrometer ($0.45\text{-}2.4\text{ }\mu\text{m}$) mounted on the Yutu rover (He et al, 2014); (iii) for isolation of echelle-spectrometer diffraction orders in high-resolution instruments (Nevejans et al, 2006; Korablev et al, 2011, 2014; Neefs et al, 2015); and (iv) to illuminate the sample of an IR microscope with monochromatic light (Pilorget and Bibring 2013).

Wider application of the AOTFs in remote sensing is hampered by the inherent requirement to sequentially scan the spectrum. On an orbital mission with a short dwell time, this scanning interferes with the spacecraft or line of sight motion, complicating the analysis. Even for a pencil-beam device, different parts of the acquired spectrum would correspond to different observed areas. Conversely, observations from a static point, such as a planetary lander, or a rover, which remains immobile during the measurement, are well suited for AOTF-based instruments.

As described in the Introduction, ISEM is a close equivalent of LIS being developed for two Russian lunar landers. The LIS development is more advanced with respect to that of ISEM — by about two years. LIS benefited from the experience gained from the pencil-beam spectrometer design of the Mars Express and Venus Express instruments, and from the early developments of MicrOmega. SPICAM-IR AOTF spectrometer with the spectral range $0.9\text{-}1.7\text{ }\mu\text{m}$ (Korablev et al, 2006) has been operating in Mars orbit since 2004. A similar SPICAV-IR instrument employing a double-range AOTF operated in Venus orbit from 2006 to 2014 (Korablev et al, 2012). A double-range AOTF for the spectral range of

0.7-4.1 μm serving as a prototype to the LIS and ISEM’s AOTFs was developed for the Phobos Grunt mission (Leroi et al, 2009).

In order to reduce the influence of the extreme temperature conditions at the rover’s mast on the electronics, the instrument is implemented as two separate boxes, a mast-mounted Optical Box (OB) and the Electronics Box (EB) (Fig. 4). The thermally stabilized EB is mounted within the rover’s body.

Figure 4. The ISEM instrument, the photographs of the optical and electronics box structural and thermal models.

Table 1. ISEM main characteristics and resources

Parameter	Value
Spectral range	1.15-3.3 μm
Spectral resolution	better than 25 cm^{-1} 3.3 nm at 1.15 μm , 16 nm at 2.5 μm , 28 nm at 3.3 μm
FOV	1.3°
Temperature range, operational	-45°C...+30°C (Optical box, OB) -40°C...+50°C (Electronics box, EB)
Temperature range, non-operational	-60°...+60°C (OB and EB) -130°...+60°C for OB pending final confirmation
AOTF	
Material	TeO ₂
Spectral range	1.15-3.39 μm

Parameter	Value
Effectiveness	>50 % (in polarized light)
Aperture	Ø 5 mm, 5°×5°;
Mean RF power	5 W
RF frequency range	23-82 MHz
Detector	InAs photodiode, Ø1 mm, 1-3.45 µm Teledyne Judson Technologies J12TE3-66D-R01M, 3-stage Peltier cooler
ADC	16-bit
Number of points per spectral range	variable, by default 1024 for one observation
Data volume	variable, by default 20 Kbit for one observation
Data/command interface	RS-422
Powers supply voltage	28 V
Power consumption, W	
Peak	14
Average	11.5
Standby	9
Dimensions	160×80×96 mm OB 116×84×55 mm EB
Mass, overall	1.740 kg
OB	0.690 kg
EB	0.560 kg
Calibration target (ISEM part)	0.014 kg
Harness	0.476 kg including 20% margin (TAS-I data)

3.1 The Optical Box

Though most of the electronics are in the EB, some electronics such as the detector's preamplifier, and the RF conditioning electronics remain in the OB. Neither the weak photodiode current, nor the power RF can be transmitted via the 5-m harness. The block-diagram of ISEM is presented in Fig. 5.

The OB contains all the optical elements, the AOTF with associated electronics (ultrasound frequency synthesizer and amplifier boards), the photo detector and the photo detector board (Fig. 6).

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Figure 5. The block diagram of the ISEM control electronics.

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Figure 6. The 3D model open view of the ISEM Optical Box. The main elements are visible: 1- baffle, 2- entry optics; 3, 7- AOTF collimating optics; 4, 6- polarizers; 5- AOTF crystal; 8- detector; 9- detector's preamplifier; 10- AOTF RF

proximity electronics.

The spectrometer is built following a standard layout for an AOTF spectrometer, with the AOTF in the path of a quasi-parallel beam. The optical scheme is based on a Galileo system with remote pupil built using CaF_2 and ZnSe lenses and it is presented in Fig. 7. The image is transferred through the optical system, and the field-of-view (FOV) of 1.3° is formed on the detector sensitive area. The achromatic lens entry telescope (1) has the aperture of 25 mm. The AOTF crystal (5) is placed in a quasi-parallel beam between collimating lenses (3, 7), and a pair of polarizers (4, 6); the output collimating lens (8) serves also as a focusing optic for the detector (8).

Figure 7. ISEM optical scheme. The numbering is the same as in Fig. 6. 2- foreoptics; 3, 7- AOTF collimating optics; 4, 6- polarizers; 5- AOTF crystal; 8- sensitive area of the detector.

A wide-angle AOTF from NII Micropribor in Zelenograd, Russia is manufactured on the base of a tellurium dioxide crystal. The ultrasound frequency range of 23-82 MHz provides a spectral range from $1.15\ \mu\text{m}$ to $3.3\ \mu\text{m}$ with two piezotransducers. The transducers operate in the sub-bands of 23-42 MHz and 42-82 MHz. The crystal cut-off angle is 12.5° in the (110) crystallographic plane. The anisotropic Bragg diffraction regime is used. The incident optical radiation has ordinary polarization and the diffracted optical beam has the extraordinary polarization. The angle between the passed and diffracted optical beams is 6° at the output of the AO crystal. A pair of polarizers with crossed polarizing planes is used to filter out the non-desired zero diffraction order.

724
725 The AOTF and its electronics are assembled in a single functional unit, which
726 includes the acousto-optic cell, the polarizers, a proximity RF matching board, an
727 RF synthesizer, the driver of the AO crystal (the RF power amplifier), and a
728 dedicated internal microcontroller, which communicates with the Main Controller
729 (MC) in the EB and controls all the functions of the acousto-optic module
730 (AOM). Commands define magnitude and frequency of the RF signal applied, as
731 well as the RF driver ON/OFF states. Within the RF range of 23-82 MHz, the
732 minimum step of frequency sweeping is 10 kHz (5900 frequency points). The RF
733 amplitude is may be set at one of 16 even levels. The AOM transmits back to the
734 MC a few housekeeping parameters, such as measured RF voltage, AO crystal
735 temperature, etc. The MC and the AOM are connected via an RS-485 interface
736 running at a speed of 115.2 Kbit/s.

737
738 During the measurement, the RF level is being alternated between ON and OFF
739 states, with the cadence being defined by integration time. The measured signal is
740 then processed as the AC allowing to remove offsets caused by the detector's dark
741 current and stray light, and improving the dynamic range of the instrument.

742
743 The detector is a single-pixel InAs thermo-electrically cooled photodiode. A
744 detector module J12TE3-66D-R01M from Teledyne Judson Technologies is used.
745 The built-in three-stage thermo-electric Peltier cooler maintains a detector
746 temperature about 90°C below that of the hot side. For the ISEM OB operating in
747 the range from -10° to +30°C, it results in the detector's temperature ranging
748 between -100° and -60°C, the corresponding detector's shunt resistance is
749 therefore 60-400 kOhms. The temperature of the sensitive area is monitored by a
750 built-in thermistor.

751
752 The detector's photocurrent is amplified with a two-stage circuit. The first stage is
753 a trans-impedance amplifier, AC-coupled (1 s time constant) to the second stage.
754 The second stage has a gain of 83 and a time constant of 80 µs and is based on an
755 ADA4610 (Analog Devices) operational amplifier characterized by low current
756 and voltage noise (50 fA Hz^{-1/2}, 7.5 nV Hz^{-1/2}). Its output signal is transmitted via
757 the harness to the Electronic Box.

758
759 **3.2 The Electronics Box**

760 The EB is mounted inside the rover at the rear balcony, and it is thermally
761 stabilized. It includes the ADC, the main and auxiliary controllers, power
762 conditioning (power supply unit, PSU), and the interface and bridge boards,
763 which support RS-422 communication between the ISEM and the Rover data and
764 command system.

765
766 The two ISEM blocks are connected via a 5-m harness running from the inside of
767 the Rover to the mast. It is fabricated by Thales Alenia Space-Italy (TAS-I). The
768 cable includes the analog signals from the detector and the thermal sensor, the
769 power supply lines and a digital RS-485 connection to control the AOFT RF
770 synthesizer and the power amplifier.

771
772 The Main Controller (MC) located in the EB commands the operation of all
773 modules of the instrument. It uses a MSP430FR5739 Texas Instruments circuit
774 running at 19.68 MHz. The controller is equipped with 1 Kbyte of RAM and 16
775 Kbyte of ferroelectric memory (FRAM) used for program and data storage.
776 Compared to commonly used FLASH memory, the FRAM has better radiation
777 immunity. A 10-bit internal ADC of the Main controller is used to digitize the
778 signal from the detector's thermistor.

779
780 The main ADC serves to digitize the signal from the detector, amplified in the OB.
781 A 16-bit ADC (ADS8320, Texas Instruments) is used. The full-scale range of the
782 ADC is 2.9 V and the peak-to-peak noise is 3 LSB (22 μ V RMS). The Main
783 Controller receives the ADC output data via a serial interface operating at 2
784 Mbit/s. The preamplifier and the ADC contribute little to the total noise in the
785 signal path, thus the Johnson noise of the detector controls the limit of signal
786 detection.

787
788 The Auxiliary controller, based on C8051F121 Silicon Laboratories circuit
789 operating at 12.25 MHz, incorporates a 12-bit ADC, and serves to monitor power
790 supply voltages and to dispatch the operation of different memory devices. In all,
791 ISEM employs two built-in FLASH memories within the microcontroller, and
792 two external chips of ferroelectric (FRAM) and magneto-resistive (MRAM)
793 memory.

794

795 The two microcontrollers hold four identical copies of their firmware in program
796 memories. At the start of operation, the controllers check the copies, repair
797 damaged ones and run a validation program. In order to increase its reliability,
798 ISEM contains two redundant main controller units. After turning on, first the
799 MC1 is powered. Its sequence, if performed correctly, commands the PSU to keep
800 power at MC1. If not commanded in 5 seconds, the PSU automatically powers on
801 the MC2, and so on.

802
803 The rover Onboard Computer (OBC) controls ISEM operations via RS-422
804 interface. There are two (nominal and redundant) RS-422 links. Communication
805 via only one of the links is available at a given time. The baud rate is 112.179
806 $\pm 1\%$ Kbit/s.

807
808 **3.3 The Calibration Target**

809 In order to determine the incident solar illumination spectrum for deriving I/F data,
810 and to verify the in-flight performance and stability of the instrument, ISEM will
811 observe the radiometric calibration target prior to each measurement. The target is
812 used for the in-flight radiometric calibration of both PanCam and ISEM, and will
813 be located on the front deck of the rover as shown in Fig. 8. At this location it will
814 be interrogated by ISEM from a distance of 1.1 m at an emittance angle of 24° .
815 The calibration target occupies an area of $67 \times 76 \text{ mm}^2$ and has a mass of 40 g.

816
817 The target includes 8 stained glass diffuse reflectance calibration patches with
818 different spectral reflectance properties. Two of these calibration patches will be
819 used by ISEM - the “white” which has a reflectance near 100% in the $0.4\text{-}3.0 \mu\text{m}$
820 spectral range, and the multiband patch, which has distinct spectral features. The
821 white patch is manufactured from Pyroceram provided by the Vavilov State
822 Optical Institute in St. Petersburg and the multiband patch is manufactured from
823 WCT-2065 — a rare earth doped glass manufactured by Schott and supplied by
824 Avian Technologies in the USA. The calibration patches will be calibrated for
825 absolute total hemispherical reflectance and Bidirectional Reflectance
826 Distribution Function (BRDF) and all measurement will be traceable to
827 photometric standards.

828
829 Dust deposition on the radiometric calibration target during the ExoMars mission
830 will be accounted for in the data processing by developing a model of the

831 calibration target and dust system, building on the results of previous missions,
832 measurements of settling rates on the rover panels, solar arrays, etc. (Kinch et al.
833 2007, 2015), and from PanCam calibration results.
834

835
836 Figure 8. PanCam and ISEM calibration target and its location on the rover.
837 Larger circles ($\varnothing 30$ mm) are for both ISEM and PanCam. The smaller circles
838 ($\varnothing 18$ mm) and the shadow posts will be used by PanCam only.
839

841 4 Measurement Scenario

842 4.1 The Experiment Cycle

843 The Experiment Cycle (EC) consists of one spectrum measurement by ISEM. It is
844 explained in Figure 9.
845

846 In order to eliminate the dark signal of the detector and any possible stray light
847 signal, the instrument measures photocurrents when the AOTF RF is OFF (the
848 dark signal) and when it is ON (the full signal). A subtraction of the two values
849 gives the true signal corresponding to the spectrally filtered radiation on the
850 detector.

851
852 During both the ON and OFF states, the main ADC continuously samples signals
853 at a 20 kHz rate. The MC stacks all the measured values and makes the ON–OFF
854 subtraction. This elementary measurement can be repeated up to 256 times
855 (“accumulation factor” parameter), effectively increasing the integration time. All
856 resulting values are stacked as well. Each elementary measurement includes a
857 dead time of ~0.6 ms needed to turn the AOTF ON or OFF. These overheads are
858 mostly the result of remote commanding of the acousto-optic module in the OB,
859 but also include two 0.12-ms transients in the AOTF. An additional dead time of
860 0.45 ms is needed to change the RF. The integration time, variable between 1 and
861 256 ms and defining the ON/OFF timing, and the number of repeated ON/OFF
862 cycles for a given RF value (the accumulation factor) are set by a command.

863
864 As discussed above, the measurement time is a critical factor. To achieve
865 flexibility in spectral sampling, up to 8 “windows” can be defined for one
866 measurement of a spectrum. Every window can be placed anywhere in the AOM
867 frequency range and it has its own number of spectrum points, frequency steps,
868 and accumulation factors.

869
870 During an elementary measurement the 16-bit ADC readings add up to a 24-bit
871 value, and further accumulation, up to 256 times, results in a 32-bit value for each
872 spectrum point. Only 16 bits out of it are used, three options being (i) to transfer
873 merely the 16 LSBs, or (ii) 16 bits starting from a certain bit in order to remove
874 noise, or (iii) to normalize within one spectrum so that the maximum fits exactly
875 within 16 bits. In the latter case the risk is that an errant spike distorts the entire
876 spectrum.

877
878 The exchange of commands between ISEM and the OBC proceeds as follows.
879 The OBC transmits a command (TC) and Rover Elapsed Time (RET). The TC
880 defines ISEM operation parameters and triggers the spectrum measurement. The
881 RET command synchronizes ISEM’s internal time. In the course of operation, the

ISEM sends scientific and housekeeping packets to the OBC and these data are stored into the OBC memory.

Figure 9. A diagram showing timing and breakdown of one spectrum measurement.

4.2 Operations on the surface

ISEM operations over the course of the Reference Surface Mission (RSM) are intimately connected those of the mast and PanCam. All operations are to be guided by the mast's pointing. Three basic operating regimes have been identified:

1) Operations to support sampling.

ISEM will work in parallel with PanCam, as shown in Fig. 2. First the WAC observes an area panoramically, and then the HRC is pointed to the most interesting spots. The spot must be illuminated by direct sunlight. At least one

ISEM spectrum is planned be acquired together with every HRC image, and ISEM measurements may be also conducted separately. The ISEM data will be used to characterize the mineral composition. Sometimes ISEM will be used together with the WAC “geology” filters; however, full analysis with the PanCam WAC geological filters is slower and produces much more data so this capability cannot be used regularly.

2) Operations to assess the geology value of targets

A number of geologically interesting scenes may be distant from the planned rover track or inaccessible for rover sampling, such as crater rims, outcrops, etc. Remote characterization is the only possibility in this case. ISEM will be operated in the same manner as in the first case. There is no theoretical limit on the sounding range provided the illumination conditions (including the phase angle) are acceptable. For instance, illuminated hill slopes may be observed from dozens of km. A practical limit is determined by the ISEM’s FOV, a ~1-meter spot is observed from 44-meter distance. This mode could be used for rover-orbiters coordinated measurements and validations. For a favorable scene ISEM may provide cross-validation over the area covering multiple CRISM pixels.

3) Dedicated environmental operations

ISEM data may be used to characterize atmospheric humidity and aerosol loading. Some information will be obtained as a by-product of geological measurements intermitted with observations of the calibration target. The information about the gaseous atmospheric absorption will be assured by dense spectral sampling of the appropriate spectral intervals. Aerosols are best characterized by cross sky observations. PanCam WAC plans direct Sun observations and cross sky viewing atmospheric campaigns. As discussed in Section 2.5, the ISEM capability to observe the direct Sun is not confirmed. At the same time, following preliminary laboratory characterization we do not expect any operational constraints placed by ISEM on PanCam solar imaging.

In the case of cross sky imaging the ISEM line of sight will be oriented above the horizon, and a special ISEM data acquisition sequence will be implemented. The HRC measurements are not needed, and ISEM will observe in parallel with WAC. The elevation and phase angle for these measurements needs to be carefully planned, targeting as much as possible range of phase angles for WAC and

937 detectable scattered signal in the IR for ISEM.

938

939 **4.2 Resources required**

940 ISEM's data volume is relatively small. One spectrum is only two kilobytes in
941 size (see Table 1 and Section 3). The factor most affecting the rover operations is
942 the measurement time. Fixed surface platforms are better suited for lengthy
943 operations, generally allowing significant accumulation of measurements.
944 However, sequential acquisition of spectra effectively increases the recording
945 time, and, as a result, required measurement times become an important factor for
946 the rover operation cycle.

947

948 The allocated duration of measurements is from 2.5 min (minimum case) to 8.0
949 minutes (optimal case) for a single target. During the whole sequence, ISEM will
950 consume ~12W, requiring an energy of 0.5-4.4 Watts per hour. As described in
951 section 3.3 the length of the spectrum, or the number of points in the spectrum,
952 can be selected. For a "geology" target we will always measure across the full
953 spectral range of ISEM, which may be divided into 1-8 intervals with different
954 sampling. The total number of points in one spectrum will vary between 256 and
955 1024. Within the spectral range, some portions of the spectrum will be measured
956 more accurately, where e.g. a narrow mineral absorption feature or important
957 atmospheric absorption are expected, while other portions of smooth continuous
958 character can be undersampled.

959

960 **4.3 Measurement performance, examples, comparison with state of the art**

961 As the full working prototype of ISEM has not been built yet, the performance of
962 the instrument was verified using the closest prototype, the qualification model
963 (QM) of LIS for the Luna 25 lander. The ISEM hardware involves some
964 improvements with respect to LIS, including better optical throughput (and more
965 sensitive detector featuring the three-stage Peltier cooler. The spectral properties
966 of the AOTF remain the same.

967

968 Spectral range and spectral resolution. The bounds of the spectral range were
969 verified using He-Ne 1.152 μm and 3.39 μm laser lines. The theoretical shape of
970 an AOTF spectral instrument function is close to sinc^2x . Side lobes of this
971 function modify the measured spectrum, but this could be readily accounted for
972 once the bandpass is properly characterized. More dangerous are distant side

lobes, which manifest themselves as a sort of stray light and may reduce the apparent depth of spectral features. More discussion on this aspect of AOTF characterization may be found in Korablev et al. (2013). The measured band pass transmission function of the ISEM prototype is shown in Fig. 10a. The evolution of the resolving power $\lambda/\Delta\lambda$ through the spectral range measured at multiple wavelengths using light sources with sharp emission features (different He-Ne laser, single-mode laser diodes, low-pressure gas-filled lamps) is shown in Fig. 10b.

Figure 10. (a) Normalized transmission function of the instrument measured at 1.523 μm laser line. The FWHM is 19 cm^{-1} (2.7 nm). (b) The resolving power measures through the full spectral range.

A simulation measurement of a mineral spectrum of a Mars analogue by LIS prototype is presented in Fig. 11. Crystalline gypsum was manually ground and sieved to obtain ~1-mm grains, and the resulting sample was illuminated with a 150-W halogen lamp from a distance of 18 cm. The full time to measure this spectrum was 30 min, and the effective exposure to measure one spectral point was 1 s in the long-wave AOTF sub-range, and 0.6 s in the short-wave sub-range. The spectrum shown is normalized by a spectrum of a Lambertian screen (metal surface covered by special reflective coating). The differences between the library and measured spectra might be attributed to different origin of the samples; the difference between the FTS and ISEM spectra are likely due to different observation geometry.

Figure 11. A reflectance spectrum of crystalline gypsum measured by the closest equivalent of ISEM: LIS qualification prototype, and a laboratory Fourier-spectrometer (Bruker), compared to a CRISM library spectrum (LASF41A).

Signal-to-noise ratio estimation. The signal-to-noise ratio (S/N) of ISEM and its LIS prototype is limited by the detector background noise (see section 3.1), so we

1007 may estimate the S/N for ISEM based on LIS prototype testing. With 3 ms
1008 integration time repeated 6 times per point LIS provides the S/N~10 in the center
1009 of the spectral range and 3-5 on the edges. This estimation using the reflected
1010 sunlight and laboratory light sources involves many uncertainties, including
1011 transparency of the terrestrial atmosphere, scaling to the Sun intensity at Mars
1012 distance, and extrapolation. In turn there remains a margin on the duration of the
1013 measurement. The real time to measure one spectral point is not 18 ms, but
1014 $(3 \cdot 2 + 0.6) \cdot 6 + 0.45 = 40.05$ ms, because the light measurement is alternated with
1015 dark measurement, and there are some extra delays in the system (see section 4.1.)
1016 With 3 ms integration time the full spectrum is measured in 41 s, while the
1017 measurements at the surface of Mars may last 2.5-8 min (see section 4.2) that
1018 translates in sensitivity gain of 2-3.

1020 The improvements in ISEM with respect to LIS are i) the deeply cooled detector
1021 with a peak sensitivity attaining a factor of 10 better, and ii) the larger throughput
1022 of the entry optics and the AOTF: The LIS f-number is F:6; the improved ISEM
1023 throughput is ~F:1.7, but vignetting in the AOTF results in effective throughput of
1024 ~F:2. The resulting gain factor is therefore ~90. The detector's peak sensitivity is
1025 at 3.3 μ m in both cases but the curve for the LIS detector is somewhat more flat.
1026 The AOTF characteristics may vary as well. Using more conservative factor of 30
1027 the resulting S/N of ISEM can be estimated as ~300 in the center of the range, and
1028 100-150 at the edges.

1030 Estimation of detection capabilities. Starting from the S/N estimation above we
1031 may estimate minimum detectable abundance for minerals discussed in section
1032 2.4 (see Fig. 1). Precaution factors in the measurement time (2-3), and in
1033 sensitivity (~3) allow sufficient margin to account for, e.g, unfavorable phase
1034 angle, or other factors. We used spectra of different minerals of interest (Fig. 1 a-
1035 f) , on the background spectra of “bright” and “dark” regions of Mars (Erard
1036 1997) to simulate the reflectance of an admixture to the bulk spectrum of the
1037 martian surface. The preliminary sensitivity estimates to detect the fraction of the
1038 selected mineral are presented in Table 3. Given relatively high ISEM S/N ratio
1039 deduced above, these estimates based on the relative depth of individual spectral
1040 features are very conservative. A better sensitivity analysis is planned in the
1041 future, involving analysis of martian mineral analogues, and multicomponent
1042 analysis.

1043
1044 Table. 3. Preliminary estimation of the ISEM sensitivity to detect different
1045 minerals and mineral groups from CRISM spectral library (Fig. 1) on the
1046 background of bright and dark region Mars spectra (Erard, 1997). Mineral
1047 features used to estimate the sensitivity are listed in the last column.

Mineral or mineral group	Bright region	Dark region	Comment
Kaolinite (Fig. 1a)	<5%	5-10%	1.4, 2.2, 2.4 μm
Montmorillonite (Fig. 1b)	5-10%	10-15%	1.4, 1.9, 2.2-2.3 μm
Serpentine (Fig. 1c)	5-10%	5-10%	1.4, 2, 2.35 μm
Carbonates (Fig. 1d)	5-10%	~10%	2.3, 2.5, 3.4 μm
Gypsum (Fig. 1e)	~5%	5-10%	1.4-1.6, 1.8, 2.2 μm
Kieserite (Fig. 1e)	<5%	~10%	Broad structure 1.4-2.4 μm
Jarosite (Fig. 1f)	<5%	5-10%	1.48, 1.75, 2.25 etc. μm

1048
1049 The issue of detection capabilities can be divided into two broad categories: (1)
1050 characterization of a target in the presence of windblown dust; and (2) detection
1051 of a phase or phases of interest in a multicomponent assemblages. There are a
1052 number of studies that have examined detection limits for various components
1053 that are relevant to this issue, and these are supplemented by ongoing studies by
1054 our team that are designed to specifically address this issue. The results of these
1055 studies are summarized in Table 4 below. Some selected examples are shown in
1056 Figures 12-14.

1057
1058 Detection limits depend on a wide variety of factors, beside end member
1059 abundances. These include factors such as relative grain size, the availability of
1060 diagnostic absorption bands, the relative intensity of diagnostic absorption bands,
1061 and physical properties such as whether phases of interest are physically mixed,
1062 or whether an obscuring phase, such as dust cover is present.

1063
1064 We have found that, at least for the variety of mixtures examined, detection limits
1065 are on the order of 10-25 wt.%. For some phases, such as certain organic
1066 compounds, detection limits are much lower (e.g, 1 wt.% adenine is detectable in
1067 the presence of 99 wt.% nontronite (an iron-bearing clay) or hematite (an iron
1068 oxide) (Figures 13 and 14)). Further extensive tests of mineral mixtures and

1069 detection limits are ongoing and planned.

1070

1071 Table 4. Summary of some studies concerning detection limits and discrimination
1072 of different phases relevant to the capabilities of ISEM

Mixture type	Detection limit	Characteristic spectral features	Source
Orthopyroxene + clinopyroxene	~15% of either phase	2 μ m region	Cloutis and Gaffey (1991)
Olivine + orthopyroxene	~20% olivine, 5% pyroxene	2 μ m region	Cloutis et al. (1986)
Orthopyroxene + clinopyroxene	~15% of either phase	2 μ m region	Cloutis and Gaffey (1991)
Pyroxene + palagonitic dust (spectral equivalent of Mars dust) or hematite	~10% pyroxene	2 μ m region	Cloutis and Bell (2004)
Carbonate + basalt	~20% carbonate	2.3-2.6 μ m region	Palomba et al. (2009) and this study
Carbonate + palagonitic dust (Fig. 12)	~15% carbonate	2.3-2.6 μ m region	Palomba et al. (2009) and this study
Palagonitic dust on carbonate (Fig. 12)	<~500 μ m thick palagonite coating required	2.3, 2.5 μ m regions	This study
Palagonitic dust on basalt	<~250 μ m thick palagonite coating required		This study
Kaolinite + illite	~20% of either phase	2.2-2.5 μ m region	This study
Gypsum + basalt	~5% gypsum	1.4, 1.9 μ m regions	This study
Gypsum + palagonitic dust	~5% gypsum	1.4, 1.9 μ m regions	This study
Pyroxene + volcanic glass	~15% pyroxene	2 μ m region	This study
Palagonitic dust + carbonate	~20% carbonate	2.3, 2.5 μ m regions	This study
Nontronite + adenine (Fig. 13)	~1% adenine	1.65, 2.2 μ m regions	This study
Hematite + adenine	~1% adenine	1.65, 2.2 μ m	This study

(Fig. 14)		regions	
-----------	--	---------	--

Figure 12. Reflectance spectra of palagonitic dust sprinkled on a powdered carbonate (magnesite). The most diagnostic absorption band, near 2.33 μm is indicated by an arrow. Note that the band is clearly present with a 260 μm palagonitic dust coating. It is still present, but barely discernible for a 525 μm thick dust coating.

Figure 13. Reflectance spectra of intimate mixtures of nontronite (an Fe-rich clay) and adenine (a component of DNA). The brown arrows indicate spectral regions where adenine absorption bands are still detectable when only 1 wt.% of adenine is present in the mixtures.

Figure 14. Reflectance spectra of intimate mixtures of hematite (an Fe-oxide) and adenine (a component of DNA). The brown arrows indicate spectral regions where adenine absorption bands are still detectable when only 1.3 wt.% of adenine is present in the mixtures.

4.4. Environmental requirements and characterization

The placement of the ISEM optical head on the Rover mast with no possibility of thermal control imposes stringent requirements on survival temperature. The AOTF is a critical device involving bonding of highly anisotropic materials, such as TeO_2 and LiNbO_3 . Anisotropic thermal expansion makes the AOTF devices vulnerable to large temperature excursion, in particular at low temperatures. AOTF technology has demonstrated survival and even operation down to -130°C and below (Leroi et al, 2009; Mantsevich et al, 2015). Several non-operational thermal cycles attaining -130°C lower bound were also performed on two dedicated ISEM acousto-optic components; more testing to fully validate the technology is to be completed.

1109 An important aspect of the AOTF spectrometer characterization is the thermal
1110 calibration, because the optical heads are intended for operations across a
1111 relatively wide temperature range. Some results of thermal characterization of the
1112 acousto-optic module are described in Mantsevich et al. (2015). The operation of
1113 the AO filters was tested in the range of -50° to $+40^{\circ}\text{C}$. The temperature affects
1114 the elastic properties of TeO_2 , changing the ultrasound velocity and birefringence.
1115 The variation of the TeO_2 refraction coefficient as a function of temperature is
1116 negligible. In turn, the change of the slow acoustic wave velocity causes a
1117 noticeable shift of the dispersion curve, comparable with the AO filter pass band
1118 in the operating temperature range. The characterization of the flight instrument
1119 will therefore include calibration of the dispersion curve within the operational
1120 temperature range.

1121
1122 **5. Conclusions**

1123 Sampling from beneath the martian surface to reach and to analyze material
1124 unaltered or minimally affected by cosmic radiation is a significant feature and
1125 perhaps the strongest advantage of the ExoMars rover. The selection of the
1126 sampling sites and, in more general terms, the remote reconnaissance and studies
1127 of the landing site area, are a major part of the Rover’s mission. ISEM offers a
1128 method of mineralogical characterization using IR reflectance spectroscopy, a
1129 technique well proven in orbital studies, and expected to be even more valuable
1130 and precise at the local scale.

1131
1132 In the coming year we aim to deliver field-compatible hardware and to participate
1133 in tests at terrestrial analogue sites and in other joint validations of instrument
1134 performance with the ExoMars team.

1135
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