

International Conference on Space Optics—ICSO 2014

La Caleta, Tenerife, Canary Islands

7–10 October 2014

Edited by Zoran Sodnik, Bruno Cugny, and Nikos Karafolas



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International Conference on Space Optics — ICSO 2014, edited by Zoran Sodnik, Nikos Karafolas, Bruno Cugny, Proc. of SPIE Vol. 10563, 105634L · © 2014 ESA and CNES
CCC code: 0277-786X/17/\$18 · doi: 10.1117/12.2304234

HIGH RESOLUTION MIDDLE INFRARED SPECTROMETER, A PART OF ATMOSPHERIC CHEMISTRY SUITE (ACS) FOR EXOMARS 2016 TRACE GAS ORBITER

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ABSTRACT

The Atmospheric Chemistry Suite (ACS) package is a part of Russian contribution to ExoMars ESA-Roscosmos mission for studies of the Martian atmosphere and climate. ACS consists of three separate infrared spectrometers, sharing common mechanical, electrical, and thermal interfaces. The mid-infrared (MIR) channel is a cross-dispersion high resolution echelle instrument dedicated to solar occultation measurements and sensitive studies of trace gases. The MIR channel is a spectrometer working in 2.3-4.2 μm spectral range, covering simultaneously up to almost 300 nm per exposure, targeting the resolving power of 50,000. A cross-dispersion concept on echelle and ordinary diffraction grating allows acquisition of the wide wavelength domain at once. That provides a strategic advantage for maximizing the number of gaseous species detected simultaneously and good spectral resolution of measurements during fast occultation sessions. Moving the second grating allows to switch from one group of the diffraction orders to another prior to a series of measurements, or desired positions during one measurement sequence. The concept of the cross-dispersion echelle instrument, which is widely accepted in astronomy, has been already employed in planetary missions with VIRTIS-H instrument presently in flight on Rosetta and Venus Express missions.

Targeting very high spectral resolution the MIR channel operates in solar occultation only. A telescope with relative aperture of 1:3 forms the image of the solar disk on the slit. The FOV is determined by the slit and it consists 0.1 \times 2.9 mrad. The spectral resolution of the spectrometer is fully slit-limited, and the resolving power of $\lambda/\Delta\lambda \geq 50000$ at 3.3 μm is supported. Two secondary cross-dispersion diffraction gratings (plain, 180 and 361 grooves per mm) are mounted back-to-back on a stepper motor to change observed echelle orders. We have chosen two secondary gratings philosophy to switch between them depending on the long or short wavelength range we are on. Changing the position of the secondary grating in angular steps of 1.8 $^\circ$, from 10 to 30 echelle orders are available for simultaneous record depending on the wavelength. 100 steps are evidently used to switch between gratings prior measurements. The full spectral range is covered on diffraction orders from 142 to 248. For each observation detector area is covered by 10 to 30 stripes, each corresponding to single echelle diffraction order. Given the complexity of the diffraction orders pattern, full detector frames will be transmitted to the ground, with lossless compression. However, the onboard averaging will be possible. Single data frame will be accumulated for 0.5 seconds, stacking of a number of shorter exposures.

I. INTRODUCTION

The studies of the Martian atmosphere and climate have been identified as the primary scientific goal of ExoMars Trace Gas Orbiter (TGO) [1], which is the follow up of the Mars Science Orbiter concept [2]. Since 2011 for the new configuration of the project based on ESA-Roscosmos cooperation, Space Research Institute (IKI) has proposed a suite of spectroscopic instruments for the studies of the Mars atmosphere in the infrared spectral range, the Atmospheric Chemistry Suite (ACS). Selected by the Solar System Panel of the Space Council of Russian Academy of Science this instrument was introduced by Roscosmos as one of two Russian contributions to TGO, the second being collimated neutron detector FRENDA (Fine Resolution Epithermal Neutron Detector) [3]. The new set of TGO instruments has been discussed and approved by the European Space Agency and Russian Federal Space Agency, Roscosmos, during 2012; the final ExoMars cooperation agreement is signed in March, 2013. The new TGO payload includes four payloads: NOMAD, ACS, FRENDA, and CaSSIS (high-resolution color stereo camera).

ACS is the set of three spectrometers being built in Space research Institute (IKI) in Moscow, Russia. Its design capitalizes on the previous developments of high technology readiness: two instruments built for unsuccessful Phobos-Grunt project [4-6] and one instrument flown at the ISS in 2009-2012 [7]. Some components/subsystems are contributed by German Institut für Planetenforschung (DLR) and LATMOS

(CNRS) in France. The present paper briefly describes the concept of the MIR instrument and the planned observations.

A detailed analysis of the MIR and overall ACS' science objectives will be presented elsewhere, but here we still summarize main goals. The spectral range of MIR (2.3-4.2 μm) includes several CO₂ absorption bands allowing to do measurements of density and temperature profiles from 10 to at least 140 km and isotopic ratios of ¹³CO₂/CO₂, CO¹⁸O/CO₂. The D/H ratio in Martian atmosphere is measured only from the ground, with H₂O and HDO lines recorded separately. Also, the vertical profile of the HDO/H₂O ratio has never been measured. MIR is aimed to carry simultaneous measurements HDO in orders 3.42-3.74 μm and H₂O between 3.18-3.45 μm , or/and recruiting H₂O data from NIR 1.38 μm band. D/H ratio and its profiles will give new information on water reservoirs, their history and cloud processes. Another important goal is to do sensitive measurements of methane with detection threshold an order better than 1.3 ppbv (TLS on Curiosity rover, [8]). MIR will measure "at once" spectra in the echelle diffraction orders 187-173, corresponding to 3.18-3.45 μm . The short-wavelength side of MIR's spectral range is extended to cover almost the whole carbon monoxide band. CO is a good tracer of air mass transport due to CO₂ condensation/sublimation and its observed abundances yet greatly differs from existing models. Observing strong and weak lines within the band will allow to retrieve concentrations at high and low altitudes. Besides all that, MIR will be able to so sensitive search for a number of minor species, some yet undetected, some possibly related to volcanic or biologic activity: C₂H₂, C₂H₄, C₂H₆, HO₂, H₂O₂, H₂CO, HCl, SO₂, OCS etc. The most of the MIR science tasks are also tackled by the TIRVIM channel and NOMAD [9], at different spectral resolution and using different instrument concepts. This redundancy increases the overall success of the TGO science mission.

II. MIR IN ACS ARCHITECTURE

ACS includes three separate spectrometers, sharing common mechanical, thermal and electrical interfaces. On the TGO spacecraft the instrument occupies the slot at the upper deck. The ACS architecture and its concept design are shown in Fig. 1.

ACS has several optical openings allowing observations in nadir ($-Y$ in the spacecraft coordinate system), and in solar occultation, at 67° from $-Y$ to $-X$ in the XY plane, and possibly on the limb (using nadir apertures). The accuracy of spacecraft attitude control is ± 1 mrad. The main opening of MIR is pointed to the sun.

The common electronic block (BE) serves as a single electrical interface of the ACS to the spacecraft in terms of power, commands and data. The power interface includes the main power switch, power conditioning, and the specific switches for each scientific channel. The final power distribution is done in the channels using regulated voltage lines from the BE. The command and data interfaces to TGO are MIL1553 and SpaceWire respectively. Fully redundant BE electronics is FPGA-based and includes 32 GB of flash-memory. Control electronics units of each channel are redundant as well. The data/command interfaces between the BE and the scientific channels are LVDS, 8 Mbit/s.

General measurement and interface parameters of ACS are summarized in Table 1. ACS consists of four blocks bolted together and sharing a single mechanical interface to the spacecraft. Roughly two thirds of its mass allocation of 33.5 kg is dedicated to larger channels, MIR and TIRVIM. The remaining mass is shared between the smaller NIR channel, the BE, the mechanical structure, and the thermal regulation system.

Following the spacecraft requirements, the ACS suite regulates its thermal characteristics, minimizing thermal flux to the spacecraft. The thermal control is provided by several radiators placed at the upper plane of TIRVIM and MIR channels, and a radiator at the right surface of MIR (as in the figure; $+X$ and $-Z$ axes of the spacecraft respectively), as well as by independent operational and survival thermal control systems. During the cruise/aerobraking phases of flight the BE is off, and the regulation of survival heaters is provided by dedicated subsystems.

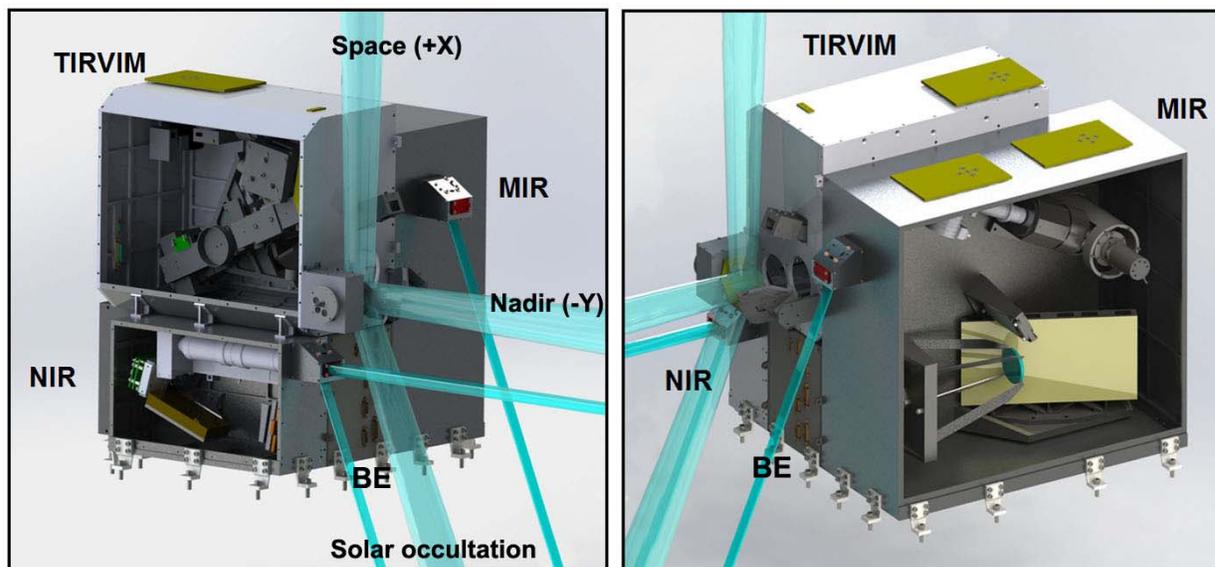


Fig. 1 The concept design of ACS. Suite consists of four blocks: the NIR channel, MIR channel, the TIRVIM channel and the electronic block. The yellow blocs designate the instrument's radiators. The pointing directions of the ACS channels are shown.

Table 1 Measurement and interface parameters of the three scientific channels of ACS and the overall values for the whole instrument. Mass and power allocations are preliminary and in the last column they include maturity margins.

Parameter	NIR	MIR	TIRVIM	ACS
Operation modes	Nadir (dayside and nightside), SO	Solar occultation (SO)	Nadir (dayside and nightside), SO	Nadir, SO, Limb
Field of view (FOV)	2×0.02 °	10×0.5 arc min	3° full solar disk in SO	
Spectral range	0.73-1.6 μm	2.3-4.3 μm 0.2-0.9 μm	2-17 μm 1.7-4 μm Nadir "CH ₄ "	0.25-17 μm full 0.73-17 μm spectral
Instantaneous spectral range	50 × 100 cm ⁻¹ ; 16 nm at 1.37 μm	7 × (0.28-0.32 μm) ex. 3.13-3.46 μm	Full range	
Time to measure one spectrum	1 s Nadir 50 ms SO	0.5-1 s	4 s Nadir 10 s Nadir "CH ₄ " 2 s SO	
Number of spectra per measurement	≤ 10	1 or 2	1 or 2	
Spectral resolution/resolving power	$\lambda/\Delta\lambda \geq 20,000$	$\lambda/\Delta\lambda \geq 50,000$	1.6 cm ⁻¹ Nadir 0.2cm ⁻¹ Nadir "CH ₄ " 0.2 cm ⁻¹ SO ($\lambda/\Delta\lambda \approx 15,000$ at 3.3 μm)	
Mass	3.3 kg	12.2 kg	11.6 kg	33.5 kg
Power	15W	30W	28W	39-85 W survival 22 W
Volume	12×35×25 cm ³	20×50×60 cm ³	20×44×30 cm ³	52×60×47 cm ³
Data rate (prelim. allocation)	0.1 Gb/day	0.7 Gb/day	0.7 Gb/day	1.5 Gb/day

III. MIR CHANNEL

The MIR channel is a cross-dispersion spectrometer working in 2.3-4.2 μm spectral range, and covering simultaneously up to 290 nm per measurement. With a cross-dispersion concept, the echelle orders are dispersed along the x-axis and separated along the y-axis of the focal plane by a secondary dispersion element, making full use of the two dimensions of the detector array. Acquisition of the wide wavelength domain at once provides a strategic advantage for maximizing the number of gaseous species simultaneously mapped. The concept of the cross-dispersion echelle instrument, which is widely accepted in astronomy, has been already employed in planetary missions with VIRTIS-H (Visible and InfraRed Thermal Imaging Spectrometer with High resolution) instrument presently in flight on Rosetta and Venus Express missions [10, 11]. The concept of VIRTIS-H consists in acquiring a broad spectral range of 2-5 μm instantaneously at the 2-D detector using the echelle grating and a prism. With a number of diffraction orders of ~ 10 , the resolving power of VIRTIS-H is $\lambda/\Delta\lambda \approx 2000$.

Targeting much higher resolving power than that of VIRTIS-H, and a broader instantaneous spectral range than that of SOIR-type echelle-AOTF instruments we conceived a new type of an optical scheme: a cross-dispersion echelle-spectrometer with movable secondary dispersion element. This concept allows to achieve high spectral resolution instantaneously in a large number of adjacent diffraction orders (from 10 to 30 in our case), covering only a fraction of the full spectral range. A moving dispersion element allows the instrument to switch from one group of diffraction orders to another prior to a series of measurements, or alternating two desired positions during one measurement sequence. Introducing the moving parts is the main disadvantage of this method. It reduces reliability, and the mechanical switching is slow, comparing to the AOTF tuning. However we consider the advantage of the broad instantaneous coverage against several very narrow spectral intervals is important and justifies spending some time on the mechanism action. Also, the positioner of the secondary disperser could be as reliable as a scanner device; OMEGA (French acronym for Observatory for Minerals, Water, Ices, and Activity) on Mars Express [12] celebrating 10 years in Mars orbit is a good example.

Targeting very high spectral resolution the MIR channel operates in solar occultation only. The optical scheme of MIR can be separated into three main parts, the entry optics, the echelle spectrometer, and the secondary disperser (see Fig. 2). All the refractive elements are designed of ZnSe and CaF_2 , transparent for the visible light, other elements are aluminum alloy mirrors fabricated by diamond turning.

The entry optics consists of a periscope mirror imposed by mechanical constraints. A blocking filter (not shown in Fig. 2) is made of AR-coated Si 5-mm slab. A telescope with relative aperture of 1:4 forms the image of the solar disk on the slit. The FOV is determined by the slit and it consists 0.5×10 arc min (0.1×2.9 mrad).

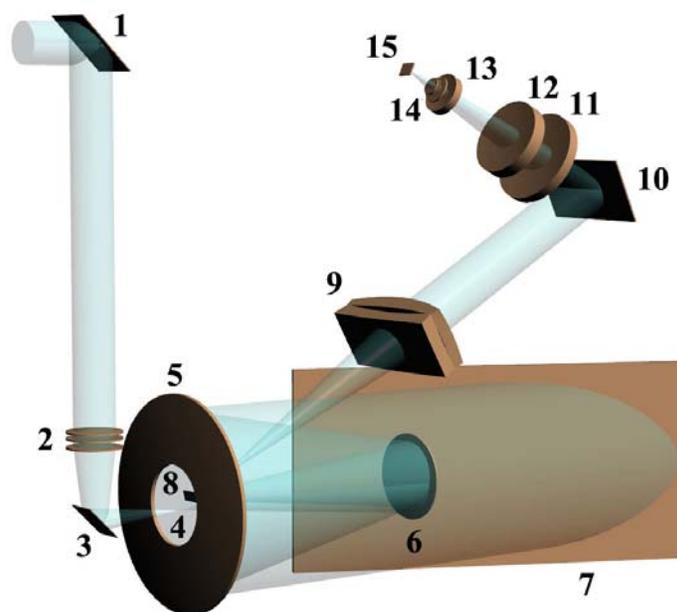


Fig. 2 A simplified optical scheme of the MIR channel. 1, 3, folding mirrors; 2- entry telescope; 4- slit; collimator of the main spectrometer; 5- primary mirror, 6- secondary mirror, 7- echelle diffraction grating, 8 – folding convex, 9- collimator of the secondary grating; 10- steerable secondary gratings; 11-13 detector's focusing lenses; 14- cold filter; 15- detector array.

The echelle-spectrometer employs the autocollimation Littrow scheme. Two conditions needed to achieve the high spectral resolution are the echelle grating large enough, and a high linear dispersion. A diffraction-limited resolving power is

$$R_{DL} = \frac{\lambda}{\Delta\lambda} \approx \frac{2D}{\lambda} \tan \theta, \quad (1)$$

where D is the collimator diameter and θ is the blaze angle. For the worst case of $4.3 \mu\text{m}$ and $\tan \theta = 2$ the requirement of $R \geq 50,000$ implies $D \geq 54 \text{ mm}$, easy to fulfill. The linear dispersion determines a slit-limited resolving power

$$R_{sl} = 2 \tan \theta \frac{f_{col}}{\delta_{sl}}, \quad (2)$$

where f_{col} is the collimator focal length, and δ_{sl} is the slit width. IR arrays with the pitch of less than $15 \mu\text{m}$ are not available, and for a Nyquist slit of $2 \cdot 15 \mu\text{m}$ the requirement of $R \geq 50,000$ results in $f_{col} \geq 750 \text{ mm}$. This value is the principal design driver, which determines the dimensions of the grating and the MIR channel in general.

The large focal length in a reasonable size and volume could be achieved using a two-mirror collimator design. In the precursor compact echelle-spectrometer [5] for the same purpose we have used a segment of Klevtsov-Cassegrain design, a fully spherical combination of a primary mirror and a sub-aperture corrector, a meniscus and a Mangin mirror. In the MIR collimator the both mirrors are aspherical. The aperture of the collimator is chosen as a compromise between the desired etendue of the instrument and the suitable size of the grating given f_{col} of $\sim 750 \text{ mm}$.

We use a large custom-made echelle grating from AMOS (Belguim) with a ruled area of $107 \times 240 \text{ mm}$. The grating is blazed at 63.43° (R2), and has 3 grooves per mm. The grating is ruled on the aluminum substrate using diamond turning. Following Eq. (1) the free spectral range for one diffraction order is $\text{FSR} \approx 16 \text{ cm}^{-1}$ (or 17.7 nm at $3.3 \mu\text{m}$). The full spectral range is covered on 107 diffraction orders, from 142 to 248.

The linear dispersion for the short-wavelength side of the spectral range is 2.0 nm/mm (0.030 nm/pix), and 3.1 nm/mm (0.047 nm/pix) for the long-wavelength edge. The quality of the imaging system is close to the diffraction limit; the spot diagram gives root mean square (RMS) of $6.5 \mu\text{m}$ in the center of the diffraction orders with some worsening to the edges. The spectral resolution of the spectrometer is fully slit-limited, and with a $30\text{-}\mu\text{m}$ slit the resolving power of $\lambda/\Delta\lambda \geq 50000$ at $3.3 \mu\text{m}$ is supported.

Two secondary cross-dispersion diffraction gratings (plain, 180 and 361 grooves per mm) are mounted back-to-back on a stepper motor to change observed echelle orders. The design of the grating positioner capitalizes on MSASI (Mercury Sodium Atmosphere Spectral Imager) scanner development for Bepi Colombo mission [13]. We have chosen two secondary gratings philosophy to switch between them depending on the long or short wavelength range we are on (Table 2). Changing the position of the secondary grating in angular steps of 1.8° , from 10 to 30 echelle orders are available for simultaneous record depending on the wavelength. One hundred steps (180°) are evidently used to switch between gratings prior measurements. The full spectral range is covered on echelle diffraction orders from 142 to 248. For each observation detector area is covered by 10 to 30 stripes, each corresponding to single echelle diffraction order. The height of the stripes ranges from 150 to $200 \mu\text{m}$ depending on the wavelength. It is planned that there is a possibility to change the position of the stepper motor during the occultation measurements, and to register several adjacent groups of diffraction orders.

The detector is a space-grade version of the standard Scorpio MW K508 Sofradir (France) product, with optimized spectral range. Adaptations with respect to this standard detector are: the replacement of standard Scorpio cold filter (band-pass $3.7\text{-}4.8 \mu\text{m}$) by a custom filter; adaptation of the window AR coating; adaptation of the cryo-cooler K508 RICOR (Israel) for operation in space (same as for Venus Express). This detector includes a 640×512 MWIR retina made of a MCT (Mercury Cadmium Telluride, HgCdTe) hybridized onto a silicon ROIC (read-out integrated circuit) by indium bumps. The pixel pitch is $15 \times 15 \mu\text{m}^2$. Given the complexity of the diffraction orders pattern, full detector frames will be transmitted to the ground, with lossless compression. However, similarly to NIR, the onboard averaging will be possible. A single data frame will be accumulated for each 0.5 or 1 second, stacking of a number of shorter exposures.

The thermal regime of MIR is maintained by a passive radiators, and by two separate systems of temperature regulation. During the cruise phase a dedicated temperature control system is powered directly from the TGO survival heater line. During the operations in the Martian orbit, the temperature control is managed by the MIR Control Electronics.

Table 2 Estimated wavelength coverage of MIR in function of angle of the secondary grating.

Secondary grating relative angle, degree	Grating, gr/mm	Minimum wavelength, μm	Maximum wavelength, μm	Wavelength coverage per exposure, nm
7,1	361	2,7669	2,8735	107
5,3	361	2,6325	2,7797	147
3,5	361	2,5000	2,6441	144
1,7	361	2,3614	2,5105	149
-0,1	361	2,3066	2,3708	64
-1,9	“zero” position			
-3,7	180	3,9357	4,2137	278
-5,5	180	3,6469	3,9356	289
-7,3	180	3,3592	3,6467	288
-9,1	180	3,0815	3,3591	278
-10,9	180	2,8059	3,0814	275

IV. ACS OPERATION PLAN

The ExoMars TGO mission phases and their duration are listed in Table 3. The Near Earth Commissioning Phase is dedicated mainly to activation and checkout of each of the ACS' channels and the BE. This involves, amongst other activities, the checkout of the interfaces with the spacecraft, and verification how the overall system performance meets the requirements of Critical operations, e.g. power-up sequences will be at first performed only in ground coverage periods when a real-time control and monitoring of the S/C is possible. All the checkouts performed before the EDM separation will not be fully representative, because the EDM is shading the ACS radiators, and the thermal regime of the instrument would not be nominal. On the top of checkouts, the ACS will perform, depending on schedule, at least one of the following calibration sessions: line of sight mismatch calibration, spectral calibration, stray light calibration and dark sky calibration.

During the Cruise Phase, ACS will be kept off, except for survival heaters, powered directly by TGO. Checkouts, including the Sun pointing are requested at least twice during the cruise. Upon the arrival to the Martian orbit, and after the EDM release, ACS will be finally ready for a checkout and calibration session. It will be important to perform this session after the cruise, so that any issues discovered could be analysed during the following ~230 days of aerobraking phase, in search of solutions, preparation of software patches, etc.

The science operations phase starts after the aerobraking is finished and TGO has reached the nominal operation circular orbit. This orbit is the near-polar 400-km altitude circular orbit, with an inclination of 74°, and an orbital period of approximately two hours. The orbit is optimized for atmospheric observations, allowing diurnal monitoring and to observe solar eclipses at each revolution. With 12 orbits per day, one observation every egress and ingress, up to 24 occultations per day can be observed. The full surface of Mars will be scanned, with the exception of polar areas. Science operations will last at least one Martian Year, before TGO passes into preferentially the relay mode upon the arrival of the 2018 ExoMars landing mission.

The ACS will perform the occultation measurements by all the three channels, and nadir measurements only by NIR and TIRVIM. MIR will operate exclusively in solar occultation. The density of the nadir measurements and the exact number of observed occultations per orbit will be defined in the long term planning (LTP) and specified in the middle term planning (MTP) according to spacecraft resources.

Table 3 ExoMars TGO mission phases and timing.

Launch window	7-27/1/2016
Near Earth Commissioning	L + up to 1 month
Cruise Phase	Approx 250 days
EDM release and Mars orbit insertion	19/10/2016
Aerobraking into 400-km circular orbit	Approx 230 days
On-orbit commissioning	Approx 2 weeks
Science Operations	1 Martian Year
Beginning of Relay Phase	January 2019 (rover arrival)
End of Mission	31/12/2022

Each observation is initiated by a telecommand, which is transmitted by the BE to appropriate ACS channels. For each channel the operation starts with detector pre-cooling procedure, which last at least 5 minutes. Additional time is necessary for internal checks and reserve, so every session starts in advance, 10 min prior to the occultation or to the desired nadir coordinates. Every occultation lasts for 2 minutes that corresponds to altitude range of the tangent point of 0-160 kilometers.

V. CONCLUSIONS

The ACS suite to study the atmosphere of Mars in the spectral range from the near IR (0.73 μm) to $\sim 17 \mu\text{m}$ in various modes of observations is being developed for the launch on ExoMars TGO spacecraft in 2016. The two main features of the instrument are (i) redundant solar occultation measurements in the full spectral range with resolving power from $\lambda/\Delta\lambda \sim 20,000$ in the near IR, $\sim 50,000$ in the 2–4 μm range by MIR and ~ 3000 at the 17- μm edge, and (ii) the sensitive nadir measurements, in the near IR, with $\sim 20,000$ resolving power, and in the 4–17 μm range at a resolution of 1.6 cm^{-1} . The preliminary design review (PDR) is completed in 2013, and the critical design review (CDR) is planned in the second half of the 2014. We present the optical design concepts, and design characteristics of the MIR channel of the instrument, the parameters reported are to be confirmed upon testing of prototypes.

ACKNOWLEDGMENTS

The development and fabrication of ACS is funded by Roscosmos with contributions from LATMOS, France and DLR, Germany. Authors affiliated with MIPT acknowledge the support from grant #11.G34.31.0074 of Ministry for Science and Education of Russian Federation.

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