*A new simulant: JSC Mars-1*

JSC Mars-1 is NASA’s Johnson Space Center simulant developed in 1998 as a laboratory reference for mainly for testing space instrumentations. On the bases of the compositional and physical properties of the landing sites of Vikings and Pathfinder missions on Mars, Allen et al. (1998) identified this material as a Martian simulant and analyzed it. It is a volcanic ash, which underwent aqueous alteration, from Mauna Kea volcan, Hawaii.

We wanted to analyze this further simulant because its spectrum could match with the atmospheric dust spectrum better than the finest part of MGS-1 (see Section 6). It was commercially available in the past, now you need to request NASA.

The dataset of our analysis is contained in the repository in Research Data Unipd (<https://researchdata.cab.unipd.it/id/eprint/1279>; Costa et al., 2024a, b).

The granulometric analysis was conducted by means of Laser Diffraction Particle Size Analyzer (Malvern Panalytical Mastersizer3000) equipped with a large volume liquid dispenser (Hydro LV). Samples were analyzed as reported in Costa et al. (2024b): we added sample until a 4% of light obscuration. Both during the sample addition and the analysis, ultrasound dispersion was activated at the power of 90%, and the stirring speed has been set to 2500 rpm; for other parameters see Tab. 5.7 in Costa et al. (2024b). Firstly, we measured the particle size and size distribution of the original simulants (i.e., the bulk samples). After this first screening, the samples were sieved with an automated vibrating sieve (Retsch) using the following sieve-ranges: <32 µm, 32 – 63 µm, 63 – 250 µm, 250 µm – 1000 µm, > 1000 µm. Each fraction was characterized through the laser diffraction granulometry. For each acquisition, the last five measurements (of 20) have been averaged. The diagram in Fig. 1 highlights the grainsize distribution for the original sample and four different granulometric classes. With the term Original sample, we refer to the simulant powder as it was received in the original package. The 250-1000 µm class was not shown and measured because the presence of several grains with diameter >3.5 µm cause the obstruction of the instrument, avoiding the analysis.

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*Figure 1.* *Granulometric curves of the original JSC Mars-1 and four different granulometric classes (see Supplementary materials).*

Instead of the Inductively Coupled Plasma Mass Spectroscopy Perkin-Elmer NexION 350X (ICP-MS), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) has been employed for the quantitative analysis of inorganics elements of the simulants.

Around 50 mg of sample were weighed using an analytical balance (Practum, Sartorius, 0.01 mg) and transferred into Teflon vessels for acidic microwave-assisted mineralization (Ethos UP, Milestone). A mixture of 6 mL of aqua regia (HCl:HNO₃, 3:1) and 0.1 mL of ultrapure HF was added to each vessel, which was then sealed and subjected to the heating program reported in Tab. 2. After mineralization and cooling to room temperature, 0.5 mL of a saturated H₃BO₃ solution was added to the digests and left to react for 2 h.

|  |  |  |
| --- | --- | --- |
| **Time (min)** | | **Temperature (°C)** |
| **Heating** | 25 | 240 |
| 15 | 240 |
| **Cooling** | 20 | Room Temperature |
| **Program name** | | Granite |

*Table 2.* *Parameters for the microwave used for the preparation of ICP-OES samples.*

The solutions were diluted to a final volume of 50 mL with ultrapure water. Subsequently, aliquots were further diluted (1:10) for the determination of major elements (Al, Ca, Fe, K, Mg, Na, Ti, Si) and (1:2) for the quantification of trace constituents (Ba, Cr, Cu, Mn, Ni, Pb, Sr, Zn).

Elemental analysis was carried out using an ICP-OES instrument (Perkin Elmer Optima 5300DV). Quantification was performed by external calibration using five-point calibration curves (500–10,000 µg/L) for major elements and six-point calibration curves (10–500 µg/L) for minor elements. Calibration data are reported in Tab. 3.

|  |  |  |
| --- | --- | --- |
| **Elements** | **λ** | **Calibration range (µg/L)** |
| Al | 308.215 | 0-10000 |
| Na | 589.592 |
| Mg | 258.213 |
| Ti | 337.279 |
| K | 766.490 |
| Ca | 317.933 |
| Fe | 238.204 |
| Si | 252.851 |
| Cr | 205.560 | 0-500 |
| Ni | 231.604 |
| Mn | 259.372 |
| Sr | 421.552 |
| Cu | 324.752 |
| Zn | 206.200 |
| Ba | 233.527 |
| Pb | 217.000 |

*Tab. 3.* *Elements selected for the chemical analysis and relative parameters used during the acquisition.*

To validate the analytical procedure for the quantification of major and minor elements, a certified basalt standard (Montana II Soil, NIST SRM2711a) was used to optimize the mineralization and analysis conditions. The Tab. 4 shows the concentrations of chemical elements and their relative standard deviations in percent.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Units | mg/gr | | | | | | | | | µg/gr | | | | | | | |
| Chemical element |  | **Al** | **Na** | **Mg** | **Ti** | **K** | **Ca** | **Fe** | **Si** | **Cr** | **Ni** | **Mn** | **Sr** | **Cu** | **Zn** | **Ba** | **Pb** |
| JSC Mars-1 | value | 88.7 | 13.7 | 23.4 | 17.1 | 7.8 | 38.2 | 90.9 | 178.6 | 94.0 | 71.0 | 1772 | 874.0 | 9.0 | 92.0 | 98.0 | 110.0 |
| RSD % | 1.7 | 5.6 | 2.3 | 0.7 | 5.3 | 2.4 | 1.8 | 1.0 | 11.1 | 30.1 | 1.7 | 1.9 | 8.5 | 1.8 | 2.7 | 3.9 |

*Table 4.* *Concentrations of chemical elements and their relative standard deviations in percent (RSD %) for JSC Mars-1.*

The X-ray diffractometer Philips X’Pert PRO (Bragg-Brentano HD optics, cobalt source, detector X’Celerator detector) was used for the mineralogical characterization of the three Martian simulants. We prepared the samples as we have done in Costa et al. (2024b):

* qualitative analysis: manual grinding of dry simulants with agate mortar (<63 µm);
* quantitative analysis – Rietveld method: the samples was weighted and mixed with an appropriate amount of standard zincite ZnO in order to be 10% of the whole sample. A specific amount of ethanol was added to the mixture of JSC Mars-1 + zincite, which was put in the micronizer at the highest speed for 5 minutes. The powder was dried in the air. The result was a uniform and fine powder (<5 µm) ready to be analyzed.

HighScore (Plus) software version 4.9 (PANalytical B.V., 2020, Almelo, The Netherlands; Degen et al., 2014) allowed to identify the mineral species (qualitative phase analysis) while the relative abundance of each phase was calculated using the Rietveld method as implemented in Profex-BGMN v. 5.2.3 (Döbelin et al., 2015; Tab. 5.10 in Costa et al., 2024b). Fig. 2a and Tab. 5a are related to a qualitative analysis excluding the amorphous material, while Fig. 2b and Tab. 5b to a quantitative analysis which however includes the amorphous material. Peaks shown in the diffractograms are linked to specific minerals (Fig. 2a and Fig. 2b).



a

Immagine che contiene testo, schermata, linea, Diagramma

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b

*Figure 2.* *a) XRD pattern related to qualitative analysis of the simulant JSC Mars-1; b) XRD pattern related to quantitative analysis of the simulant JSC Mars-1: minerals detected are shown in different colors. The gray curve at the bottom represents the differences, in terms of intensities, between the measured (black) pattern and the fitted (red) pattern, it shows effectively the goodness of the fit.*

a

|  |
| --- |
| **Components** |
| plagioclase |
| pyroxene |
| olivine |
| magnetite |
| mica |
| quartz |
| gypsum |

b

|  |  |
| --- | --- |
| **Components** | **Amount (m%)** |
| plagioclase | 28.4 |
| pyroxene | 5.7 |
| olivine | 5.4 |
| magnetite | 2.9 |
| mica | 2.8 |
| quartz | 0.7 |
| gypsum | 0.2 |
| amorphous | 54 |

*Table 5.* *a) Table of qualitative analysis of the simulant JSC Mars-1; b) Table of quantitative analysis in mass percentage (in m%) of the simulant JSC Mars-1.*

The hyperspectral imaging cameras used were Headwall Photonics Nano-Hyperspec, that acquired from 400 to 1000 nm and had a sampling of ~2 nm, and Headwall Photonics Micro-Hyperspec camera, that acquired from 900 to 2500 nm and had a sampling of ~10 nm. After setting up parameters in the camera software, original simulants were placed on the motorized stage to acquire their spectra both in VNIR and SWIR range (Tab. 5.11 in Costa et al., 2024b). As white reference for radiance conversion a 99% reflectivity Spectralon (Labsphere, Inc.) was used, we repeated the acquisition twice with each grainsize-class of the simulant, in order to average afterwards. Acquisition output files were imported in ENVI software (Buller, 2023) where Regions of Interest (ROIs) were defined and spectral data extrapolated. The obtained files in ASCII format were opened and processed in Origin software (OriginLab Corporation, 2019). A light smoothing (binomial method) was applied in the VNIR spectra to reduce signal noise and finally VNIR and SWIR acquisitions were merged at 970 nm. For the sieved simulants, merging consisted in a averaging of spectra and downward shift of the SWIR curve. Moreover, following Zhang et al. (2014), the smoothed/ merged data were multiplied by absolute reflectance of the Spectralon white reference (Labsphere, Inc.) in order to mitigate potential artifacts due to its absorption peak at 2100 nm. Thanks to the absorption bands in the graph (Fig. 3) we can identify the main spectral features of the simulant and comprehend the minerals existing within the original simulant and the sieved simulant in the following granulometric classes: 0-32 µm, 32-63 µm, 63-250 µm, 250-1000 µm and >1000 µm.

Immagine che contiene testo, diagramma, linea, Diagramma

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*Figure 3.* *Spectra of the original (i.e., bulk sample) and different grainsize fractions of JSC Mars-1 (see Supplementary materials).*

Supplementary materials

See Research Data Unipd (<https://researchdata.cab.unipd.it/id/eprint/1279>; Costa et al., 2024a, b).

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