

**ELEMENTAL CALIBRATION OF THE PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY (PIXL) OF MARS 2020.** C. M. Heirwegh<sup>1</sup>, W. T. Elam<sup>2</sup>, Y. Liu, K. P. Sinclair<sup>1</sup>, J. A. Hurowitz<sup>3</sup>, A. C. Allwood<sup>1</sup>, <sup>1</sup>Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California USA, <sup>2</sup>Applied Physics Laboratory, University of Washington, Seattle, Washington, USA, <sup>3</sup>Department of Geoscience, Stony Brook University, Stony Brook, New York, USA, [christopher.m.heirwegh@jpl.nasa.gov](mailto:christopher.m.heirwegh@jpl.nasa.gov).

**Introduction:** The Planetary Instrument for X-ray Lithochemistry (PIXL), selected for Mars 2020, is a sub-millimeter scale X-ray fluorescence spectrometer [1,2] capable of generating *in situ* elemental map datasets of Martian rocks or soils. Planetary Scientists will harness PIXL's analytical capabilities to investigate the early geological history of Mars, search for signs of water and bio-signatures and inform on selection of geological samples for caching as part of the mission's sample return objective. In addition to production of fine scale resolution elemental maps, the fidelity of PIXL's *in situ* science capability demands that the spectrometer be capable of delivering highly accurate quantified major (Mg, Al, Si, Ca, Fe) and minor (S, K, Ti, Cr, Mn) elemental compositions of its measured targets.

The PIXL science team has made effort to develop PIXL's quantification capability and has assessed the level of accuracy that can be expected while on Mars. This effort has also elucidated challenges and limitation associated with quantifying geological materials and perhaps, most important of all, indicated areas within PIXL's data treatment procedure in which further efforts are likely to yield an improvement in spectrometer performance.

**Methods:** Elemental calibration involved a series of X-ray measurements performed in Mars-like atmospheric conditions on 6 homogenous standards (Teflon-blank, BHVO2-G, BIR1-G, BCR2-G, NIST 610 and Scapolite) and 7 geological powdered reference materials (LKSD-4, Gyp-B, COQ-1, SRM 694, SARM 6, Mica Mg and JMS-2) at 2 hours integration per target. These samples were chosen as they provided a relatively broad range of elemental abundance for each element.

**Analysis and Results:** Histogram data were processed using the quantification procedure developed to analyze PIXL data [2] which includes use of the PIQUANT fundamental parameters quantification software, developed in-house to analyze PIXL data. The procedure includes first, deriving the polycapillary energy-dependent X-ray transmission profile, second, using the glass standards to develop element-specific correction factors to account for small, consistent deviations in our quantification process and third, using PIQUANT to treat standards as unknowns, quantify their major element components and compare to certificates. It was found that for MgO, Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, CaO and

FeO, these constituents were quantifiable to within 20% or less of the certificate values when their sample's concentrations were 10% or greater. For minor element components, SO<sub>3</sub>, K<sub>2</sub>O, TiO<sub>2</sub>, Cr<sub>2</sub>O<sub>3</sub> and MnO, these constituents were quantified to within 30% or less of the certificate values when their sample's concentrations were 1% or greater.

**Discussion:** Challenges encountered during analysis will be discussed in terms of both plans for improving our approach and more generally, reviewing precautions recommended to analysts when disseminating data products originating from X-ray Spectroscopy systems, including PIXL.

Directions for improvement may include enhancing PIQUANT's signal to background peak filtering process, inclusion of secondary fit models to describe both peak tailing artifacts, that arise due to unavoidable incomplete charge collection in the X-ray detectors, and, other radiative X-ray processes not yet incorporated in the software. Additionally, for several powders in which elements were highly discrepant from the certificates, the science team will measure these using other well-calibrated micro-XRF spectrometers in effort to validate our analysis.

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**References:** [1] Allwood, A. C. et al. (2015) *Proceedings of IEEE Aerospace Conference*. [2] Heirwegh, C. M. et al. (2018) *Powder Diffraction* 33, 162 – 165.