CRYSTAL CHEMISTRY OF PRIMARY AND SECONDARY MINERALS IN THE JEZERO CRATER FLOOR.

E. L. Moreland[1], K. S. Siebach[1], G. Costin[1], Y. Jiang[1], M. Tice[2], T. V. Kizovski[3], Y. Liu[4], and A. J. Brown[5], [1]Rice University, Houston, TX 77005 (morelandellie@rice.edu), [2]Texas A&M U. (College Station, TX 77843), [3]Brock U. (Ontario, Canada), [4]JPL-Caltech (Pasadena, CA 91125), [5]Plancius Research (Severna Park, MD).

Introduction: The Mars2020 Perseverance Rover is exploring Jezero crater on Mars to investigate a potential past habitable environment [1]. The rocks in Jezero crater hold key clues to understanding the past habitability of Mars because this crater was once home to a lake environment [1]. To decipher the conditions of this past environment, it is crucial to identify the primary and secondary minerals of the rocks remaining in Jezero crater.

Thus far, the crater floor has been identified as an igneous olivine cumulate from analysis of the primary minerals [2]. Furthermore, presence of secondary minerals preserves information about the water-rock interactions that occurred in the crater [2,3]. Identifying primary and secondary minerals is an important first step for compiling the history of Jezero crater.

Identifying the detailed stoichiometry of mineral assemblages can provide valuable insight into the specific geochemistry of the conditions that formed the rocks. While valuable, it is more challenging to extract the exact crystal chemistry of minerals. However, by utilizing geochemical data from the PIXL instrument [4] onboard the Perseverance rover and a developed mineral identification algorithm [5], we identify and provide the exact stoichiometry of primary and secondary mineralogy of rock targets. This is a meaningful endeavor for constraining the history of Jezero crater and the geochemical interactions that occurred to create the facies.

PIXL Instrument: The Planetary Instrument for X-ray Lithochemistry (PIXL) is onboard the Perseverance rover. The PIXL instrument is an X-ray fluorescence (XRF) spectrometer that retrieves a grid or map of in situ high resolution XRF spectra of rock targets at ~120 µm spot size [4]. These spectra are then quantified into oxide weight percentages to provide high resolution geochemical data that is texturally correlated to the rock target [4,6].

MIST Algorithm: The Mineral Identification for Stoichiometry (MIST) algorithm is a mineral identification algorithm based on the premise that, by definition, every mineral has a unique stoichiometry [5]. The algorithm takes geochemical data and finds if it matches the known stoichiometry of a mineral in the algorithm. This method works when the grain size of the mineral is as large or larger than the measurement spot size (for PIXL, ≳ 120 µm) so that the algorithm analyzes the chemistry of a pure mineral.

Mineral Identification: The rock targets analyzed by PIXL in the Jezero crater floor provide ideal data for the MIST algorithm because these rock targets have coarse grains [2,3]. Here, we focus on two targets in the Séítah formation, which is comprised of olivine cumulate rocks exposed on the crater floor [2,3].

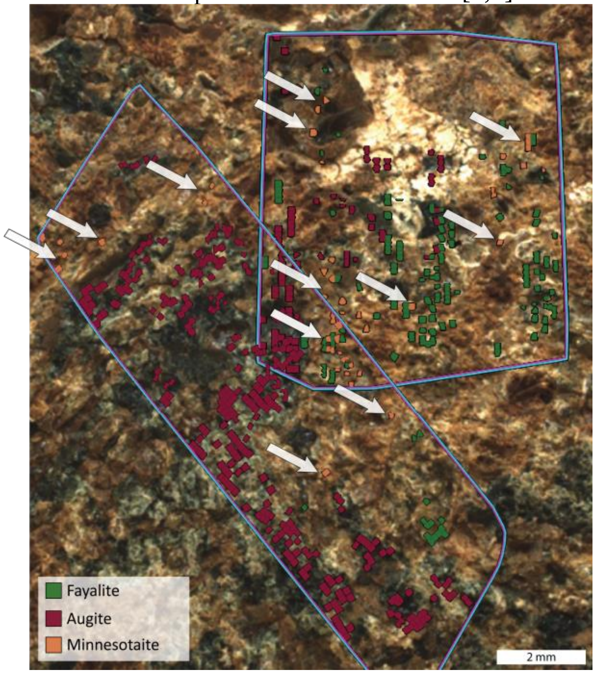

Figure 1*: MIST stoichiometric mineral identifications mapped on top of the footprints of the Quartier PIXL scans (blue outlines). Minnesotaite identifications pointed out with white arrows.*

Primary Mineralogy. PIXL analysis was performed on two rock targets in the Séítah unit. Two PIXL scans were performed on an abraded rock target named Dourbes with a total of 5,685 measurement spots. In line with previously published results, our MIST algorithm identifies olivine with stoichiometry $(Mg_{1.05-1.09}Fe_{0.89})_{\Sigma=1.94-1.98}(SiO_4)$ (Fo_{54}) and augite with $Wo_{36.40-37.03}En_{42.30-43.03}Fs_{20.57-20.66}$. There were also two PIXL scans on the abraded Quartier rock target comprising of 6,603 measurement spots. In Quartier, our MIST algorithm found olivine with stoichiometry $(Fe_{1.04}Mg_{0.85-0.88})_{\Sigma=1.89-1.92}(SiO_4)$ (Fo_{44-45}) and augite with $Wo_{35.55-38.28}En_{38.05-38.24}Fs_{23.48-26.40}$ (Fig. 1). While these two targets are in the same geologic unit, they are separated by ~125 m and this seems to have contributed to the Quartier target becoming more iron rich than its Dourbes counterpart.

Secondary Mineral of Interest. While multiple secondary minerals were identified in these rock targets, we focus on the identification of the mineral minnesotaite for two reasons: 1) There were multiple spots of minnesotaite identified in both Dourbes and Quartier, and 2) minnesotaite was recently identified in Gale crater by the X-ray diffraction instrument onboard the Curiosity rover [7]. Minnesotaite (Mns), the iron-rich structural equivalent of talc, was first identified in the banded iron formation in Minnesota and could provide constraints on the temperature and pH conditions [8].

Minnesotaite Analysis: We investigate our identification of minnesotaite by testing the algorithm and propagating error from the PIXL instrument.

Terrestrial comparison. To ensure our MIST algorithm correctly identifies minnesotaite, we checked a suite of minnesotaite compositions analyzed on Earth. Unfortunately, minnesotaite is an understudied mineral, however we found a suite of 31 well-characterized samples [9-14]. Our MIST algorithm positively identifies all 31 samples as minnesotaite and successfully differentiates talc from minnesotaite (Fig. 2).

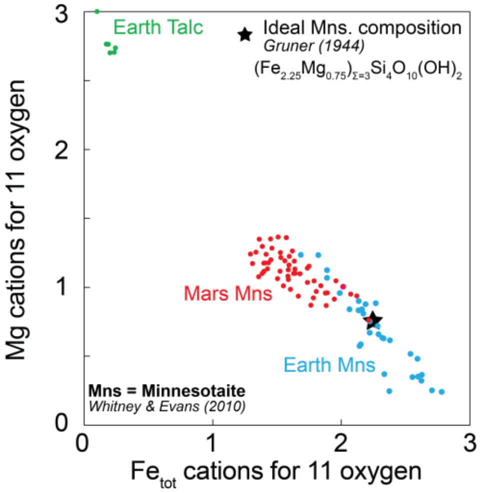

***Figure 2**: Mg vs. Fe graph showing identified Mars minnesotaite points with minnesotaite and talc compositions from Earth.*

Monte Carlo error propagation. Error is introduced into this analysis from the PIXL instrument. Every XRF spectrum that is quantified has an associated error for every reported oxide. To propagate this error, we produce Monte Carlo simulations to randomly vary each oxide within the reported error bounds to produce plausible compositions based on each reported spot composition [15]. With this method, we produce 5000 simulations for each reported PIXL composition that MIST identified as minnesotaite (Fig. 3). We then run these 5000 compositions back through the MIST algorithm to determine how many are still identified as minnesotaite. This allows us to prescribe a confidence estimate based on the percentage of the simulations still stoichiometrically matching minnesotaite, with ≥80% being high confidence.

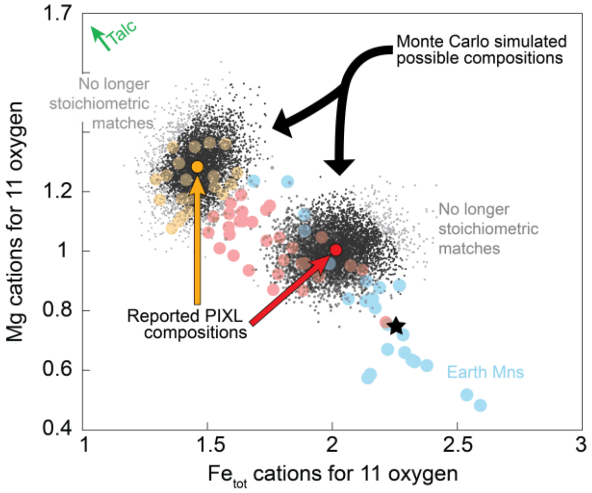

***Figure 3**: Mg vs. Fe graph showing example of Monte Carlo simulated compositions and analysis.*

Conclusions and Future Work: MIST successfully identifies and provides stoichiometry of primary mineralogy. MIST can also provide initial identification of secondary minerals, which are key for constraining the geochemistry of past environments. Further work will utilize PIXL data that have been corrected for diffraction and roughness to eliminate additional sources of error. Similar analyses applied to other secondary minerals identified in the crater floor rocks will provide key mineral assemblages to constrain the history of Jezero crater.

References: [1] Farley, K. A. et al. (2020) *Space Sci Rev*, *216*, 142. [2] Liu, Y. et al. (2022) *Science*, *377*, 1513-1519. [3] Tice, M. M. et al. (2022) *Sci. Adv.*, *8*, 47. [4] Allwood, A. C. et al. (2020) *Space Sci Rev*, *216*, 134. [5] Siebach, K. L. et al. (2022) *AGU Fall Meeting*, V42A-04. [6] Heirweigh, C. M. et al. (2022) *Spectrochem. Acta B*, *196*, 106520. [7] Thorpe, M. T. et al. (2022) *JGR: Planets*, *127*, e2021JE007099. [8] Chevrier, V. et al. (2007) *Nature*, *448*, 60-63. [9] Gruner, J. W. (1944) *Am. Min.*, *29*, 9-10. [10] Guggenheim, S. & Eggleton, R. A. (1986) *Can. Min.*, *24*, 479-497. [11] Klein, C. (1974) *Can. Min.*, *12*, 475-498. [12] Gole, M. J. (1980) *Am. Min.*, *65*, 8-25. [13] Rasmussen, M. G. et al. (1998) *Can. Min.*, *36*, 147-162. [14] Ahn, J. H. & Buseck, P. R. (1989) *Am. Min.*, *74*, 384-393. [15] Treiman, A. H. (2020) *Plan. Sci. Journ.* *1*, 65.