

THE CHEMIN DATABASE: A COLLABORATIVE TOOL FOR MINERALOGY AND PLANETARY SCIENCE. D. F. Blake¹, T. F. Bristow¹, B. Lafuente^{2,3}, R. T. Downs⁴, G. Downs², P. Sarrazin^{2,3}, N. Stone⁵.¹Exobiology Branch, MS 239-4, NASA Ames Research Center, Moffett Field, CA USA (david.blake@nasa.gov; 650-604-4816); ²SETI Institute, Mountain View, CA USA; ³eXaminArt LLC, Mountain View, CA USA; ⁴Department of Geosciences, Univ. of Arizona, Tucson, AZ USA; ⁵The Open Data Repository, Main, MA, USA

Introduction: The CheMin X-ray Diffractometer (XRD) onboard the Mars Science Laboratory (MSL) rover Curiosity is the first crystallographic instrument deployed on another planet. The CheMin database [1], published using the Open Data Repository (ODR) [2], is a living repository of CheMin and related MSL data integrated with tools and procedures for visualization and analysis. The goal is to give researchers, students, and educators the ability to reduce, analyze, and interpret CheMin mineralogical data from ~3.7-billion-year-old sediments drilled from lake deposits in Gale crater, Mars.

CheMin: The first X-ray Diffraction instrument to analyze rocks and soil on another planet: The CheMin instrument on the MSL rover Curiosity [3] determines the mineralogy and elemental composition of powdered Martian soil and rock using XRD. As the first crystallographic instrument flown in space, CheMin's mineralogical analyses have revolutionized our understanding of early Mars [4]. CheMin data have proven key in reconstructing ancient habitable surficial environments on Mars, preserved in ~3.7 Ga fluvial-lacustrine strata at Gale crater. The mineralogy and compositions of primary detrital minerals in these sediments provide novel insights into the nature of martian igneous rocks and styles of volcanism. Evidence of syn-depositional, early diagenetic and late-stage diagenetic aqueous alteration influencing these rocks is recorded in the secondary minerals they contain. The mineral abundances and compositions determined from CheMin comprise the only full mineralogical data set for Mars surface materials that is currently available.

Data Archiving: During a mission such as MSL, all data from the *Curiosity* rover are archived in the Planetary Data System (PDS) for use by the broader planetary science community. However, data archived in the PDS are relatively difficult to access except by those knowledgeable of the system. The result is that most of the MSL publications are authored by the science teams themselves. Indeed, even these papers and the data contained in them are generally only available to individuals who belong to a research university or institution that has paid a subscription fee to the publisher. Papers written by the planetary science community at large commonly reanalyze data published in science team papers

or PDS “reduced data records” created by the science teams, not the original raw data. This is the result of:

1. Complexity associated with finding / downloading instrument data from the PDS,
2. Lack of access to the software tools necessary to create “reduced data records” from the original “engineering data records” (the raw data) and,
3. Lack of access to either the software packages necessary to analyze the data, or to the databases of reference standards or terrestrial analogs useful for interpreting the results.

The CheMin Database: As summarized by an *American Mineralogist* “Highlights and Breakthroughs” article [5], “...*The mineral abundances and compositions determined from MSL Curiosity CheMin data are the most complete mineralogical data set for Mars surface materials until a Mars Sample Return mission (MSR) which is still at least a decade away.*”

A primary goal of the CheMin science team has been to ensure that all of CheMin's raw data are readily available to the planetary science and education communities. To that end, data collected by CheMin on Mars including contextual information, XRD patterns, images and geochemical data can be downloaded from the CheMin ODR database [1], analyzed with cloud-based software [6], and reinterpreted by anyone with access to the web, without the need for proprietary analytical software or mineralogical databases.

Infrastructure: The CheMin Database uses the Open Data Repository (ODR) [2], a universal data publication platform supported by NASA through the Astrobiology Habitable Environments Database (AHED) project [7,8]. The ODR platform is an open-source, data storage and data publication system that supports the use of metadata standards, templates for rapid dataset design and construction, diverse display and data interaction capabilities, and the ability to integrate plug-in applications for data analysis.

Database structure. Each data record in the database includes:

1. Sample description;
2. Interactive XRD and XRF patterns with associated metadata and downloadable files;

3. Mineral abundances derived from diffraction data;
4. Access to the library of CIF files used in diffraction pattern analysis;
5. Links to raw data and results from other MSL instruments (such as elemental composition data from APXS) for each of the samples analyzed by CheMin;
6. Library of downloadable open source references publications associated with each analysis;
7. Access to the Experiment Data Records (EDRs) for each sample;
8. A detailed narrative of how the analysis was performed;
9. Access to QAnalyze [6], an automated cloud-based application for quantitative analysis of mineral samples using XRD.

With this database and its integrated software, anyone can reproduce the analyses that were published by the CheMin team, and even explore alternative models.

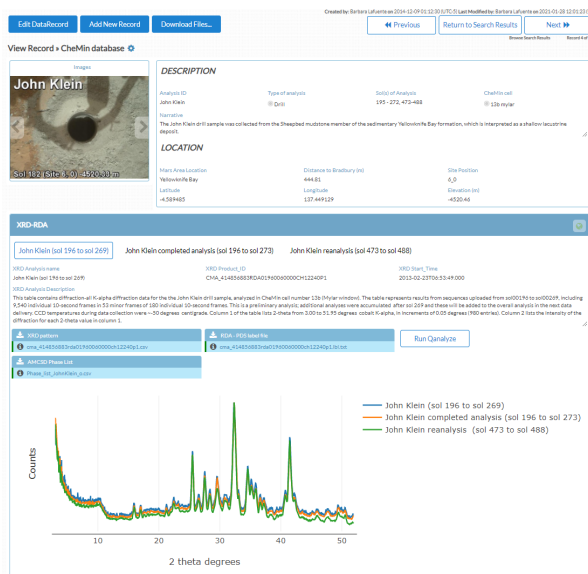


Figure 1. Example of a portion of a CheMin data record view.

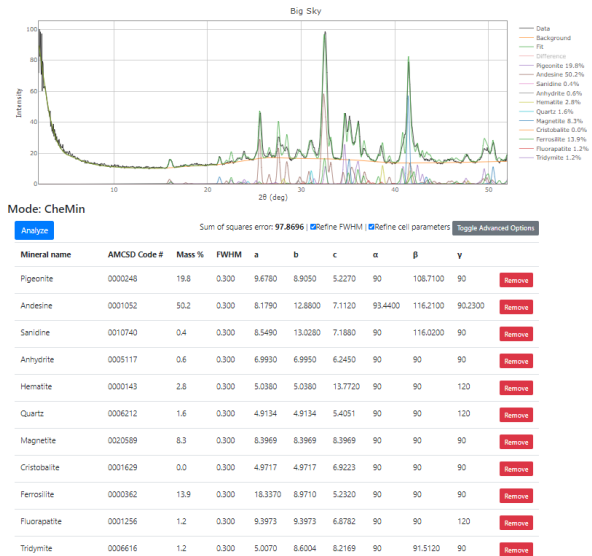


Figure 2. Example of CheMin XRD data processed by the web-based application QAnalyze.

Acknowledgments: We gratefully acknowledge the support for this work by the NASA NNX11AP82A, Mars Science Laboratory Investigations, and University of Arizona Geosciences.

References: [1] <https://odr.io/CheMin> [2] Lafuente B. et al. (2018) *AGU Fall Meeting*, Abstract # IN53E-0653 [3] Blake, D. F. et al. (2012) *Space Sci. Rev.*, 170, 341–399. [4] Rampe, E. B. et al. (2020) *Geochemistry*, 80, 125605. [5] Velbel, M. A. (2018). *Am. Min.*, 103, 837–838 [6] <https://www.qanalyze.com/> [7] Detweiler et al (2019) *Abscicon*, Abstract # 319-213 [8] Bristow et al. (2020) *White Paper PSA Decadal Survey 2023-2032*.