Low-Fe(III) Greenalite Was a Primary Mineral from Neoarchean Oceans

Jena E Johnson*[a], Janet R Muhling[b,c], Julie Cosmidis[a,1], Birger Rasmussen[c], Alexis S Templeton[a]

[a]Dept. of Geosciences, University of Colorado - Boulder, 2200 Colorado Ave, Boulder CO 80309
[b]School of Earth Sciences, The University of Western Australia, 35 Stirling Highway, Crawley WA 6009, Australia
[c]Dept. of Applied Geology, Curtin University, Kent Street, Bentley, Perth WA 6102, Australia
[1]*Currently* Dept. of Geosciences, Pennsylvania State University, University Park, PA 16802

*Corresponding Author: jenaje@umich.edu; *Currently* Dept. of Earth and Environmental Sciences, University of Michigan, Ann Arbor, MI 48109

Accompanying Raw Data

Research Overview: We used multi-scale imaging and spectroscopic techniques to characterize the best-preserved examples of nanoscale iron silicate mineral inclusions from 2.5 billion-year-old BIFs and ferruginous cherts. Combined, our results indicate that these primary minerals were low-Fe(III) greenalite.

The raw data included here are synchrotron-based X-ray transmission and absorption spectroscopy data as well as X-ray diffraction patterns. Please see accompanying publication for details on data acquisition. Note the enclosed data is unprocessed, except for calibration, and analyses or comparative results will be found in the accompanying publication.

This research was funded by the Agouron Institute (Postdoctoral Fellowship to J.E.J.) and the Rock-Powered Life NASA Astrobiology Institute (Cooperative Agreement NNA15BB02A).

Methods: Portions of this data was collected at the Canadian Light Source (CLS), which is supported by the Canada Foundation for Innovation, Natural Sciences and Engineering Research Council of Canada, the University of Saskatchewan, the Government of Saskatchewan, Western Economic Diversification Canada, the National Research Council Canada, and the Canadian Institutes of Health Research. Portions of this research were carried out at the Stanford Synchrotron Radiation Lightsource (SSRL), SLAC National Accelerator Laboratory, which is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract DE-AC02-76SF00515. The SSRL Structural Molecular Biology Program is supported by the DOE Office of Biological and Environmental Research, and by the National Institutes of Health, National Institute of General Medical Sciences (including P41GM103393). The contents are solely the responsibility of the authors and do not necessarily represent the official views of NIGMS or NIH. Bulk rock and standard powders were examined using XRD on a Siemens D500 X-ray diffractometer at the United States Geological Survey in Boulder.

File Inventory:

CLS STXM raw data [zip drive]

Folders with multiple energy map images (5Emap) that can be aligned and compiled into a Fe redox map following Bourdelle et al. (2013)[1], as well as stacks of images of a single area over a sequence of energies. These stacks can be analyzed to extract average Fe L-edge XANES spectra following Bourdelle et al[1] and Cosmidis and Benzerara (2014)[2].

- ABDP9 219m
  - 5Emap
    - Files=A160827065.hdr, A160827065_a000 to …_a004
  - Stack
    - Files=A160827066.hdr, A160827066_a000 to …_0184
- ABDP9 288m
  - 5Emap
    - Files=A160827060.hdr, A160827060_a000 to …_a004
  - Stack
    - Files=A160827058.hdr, A160827058_a000 to …_0184
- ABDP9 288m2
  - 5Emap
    - Files=A160828049.hdr, A160828049_a000 to …_a004
  - Stack
    - Files=A160828051.hdr, A160828051_a000 to …_0184
- Chlorite1
  - Stack
    - Files=A160827102.hdr, A160827102_a000 to …_0184
- Chlorite2
  - Stack
    - Files=A160829009.hdr, A160829009_a000 to …_0184
- GKF 327m
  - 5Emap
    - Files=A160828001.hdr, A160828001_a000 to …_a004
  - Stack
    - Files=A160828002.hdr, A160828002_a000 to …_0184
- Silv 313m
  - 5Emap
    - Files=A160827111.hdr, A160827111_a000 to …_a004
  - Stack
    - Files=A160827112.hdr, A160827112_a000 to …_0184

[1] Bourdelle F, Benzerara K, Beyssac O, Cosmidis J, Neuville DR, Brown GE, Paineau E (2013) Quantification of the ferric/ferrous iron ratio in silicates by scanning transmission X-ray microscopy at the Fe $L_{2,3}$ edge. *Contrib Mineral Petrol*, v. 166, p. 423-434.

[2] Cosmidis J, Benzerara K (2014) Soft x-ray scanning transmission spectromicroscopy. In *Biomineralization Sourcebook: Characterization of Biominerals and Biomimetic Materials* (ed. Gower L) p. 115-133.

SSRL XAS raw data
This dataset includes fluorescence maps of our sample thin sections ABDP9 222m, ABDP9 380m, DDH44 388m, GKF 356m and GKF 357m at 11 keV or 8 keV (.hdf5 files), plotmarker files (.mpm files) that indicate the position of X-ray absorption point spectra, and all point spectra (.xdi or .dat files) collected for each sample on Beam Line 2-3 at SSRL. Also included are bulk spectra collected for iron silicate standards (greenalite, donated from S. Guggenheim and run at both beamlines), minnesotaite, and cronstedtite donated from the Caltech mineralogical collection.

XRD raw data
Most of our XRD patterns derived from the JADE XRD database but they did not have a greenalite standard and so we acquired an XRD pattern on the greenalite standard that was generously given to us by S. Guggenheim. We also share here the bulk XRD spectra of microdrilled chert from the ABDP9 380m and GKF 357m thick sections.

Use and Access:

These files may be examined using a variety of software; however, the authors used the following open-access software to perform plotting and data analyses:

- aXis2000 software for STXM data analyses. aXis2000 is written in Interactive Data Language (IDL). It is available free for non-commercial use from http://unicorn.mcmaster.ca/aXis2000.html/ courtesy of AP Hitchcock (2014).
- SIXPACK and SMAK software for analysis of X-ray fluorescence maps and X-ray absorption spectroscopy data from SSRL. SIXPACK and SMAK were developed by Samuel Webb at SSRL and may be downloaded from https://www.sams-xrays.com free of charge.
- XRD patterns were initially compared to standards using the proprietary JADE software; however, the plots shown in our accompanying manuscript were produced using R which can be downloaded for free from https://www.r-project.org/.

All the above free software have instruction manuals alongside instructions for downloading.

Citation to Related Article:

Johnson, J. E., Muhling, J. R., Cosmidis, J., Rasmussen, B. & Templeton, A. S. (2018). Low-Fe(III) Greenalite Was a Primary Mineral from Neoarchean Oceans. *Geophysical Research Letters*, 45. https://doi.org/10.1002/2017GL076311