

Metadata file

This repository contains data pertaining to the oxidation of mackinawite (FeS) as observed by Mössbauer spectroscopy. The analyzed and plotted data was published here:

Cheng D, Neumann A, Yuan SH, Liao WJ, and Qian A. Oxidative Degradation of Organic Contaminants by FeS in the Presence of O₂. *Environmental Science & Technology* 2020, 54, 7, 4091-4101. [doi: 10.1021/acs.est.9b07012](https://doi.org/10.1021/acs.est.9b07012)

The data contained are:

- Raw Mössbauer data (*.txt)
- Folded Mössbauer spectra (*.fld)
- Fits of the Mössbauer data as published in Fig 3 in above publication (*.vbf)
- Recoil project containing all spectra and corresponding fits (FeS_oxidation.rpj)

To open and view the folded data, fits and project, you will require the software Recoil.

To locate the data files corresponding to the subfigures in Fig 3 use the guide below:

- Fig 3a = 170113 DC wet FeS_1 4.2K v12.*
- Fig 3b = 170224 DC FeS oxidation 0.5h 4.2K.*
- Fig 3c = 170223 DC FeS oxidation 1h 4.2K.*
- Fig 3d = 170208 DC FeS oxidation 4h 4.2K.*
- calibration file (160406 calibration file v12.txt) enables you to fold the raw data if you are using a software other than Recoil

If you have any queries regarding the data, please contact Anke Neumann:

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