Sulfur Near Edge X-ray Fluorescence Spectroscopy Data for standard materials

Website: https://www.bco-dmo.org/dataset/756682
Data Type: experimental
Version: 1
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Project

» P-NEXFS investigation of the influence of aerosol phosphorus on the Mediterranean Sea (Aerosol P)

| Contributors   | Affiliation                                                                 | Role                      |
|----------------|------------------------------------------------------------------------------|---------------------------|
| Ingall, Ellery | Georgia Institute of Technology (Georgia Tech)                               | Principal Investigator    |
| Rauch, Shannon | Woods Hole Oceanographic Institution (WHOI BCO-DMO)                          | BCO-DMO Data Manager      |

Abstract

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Acquisition Description
Methodology: The sulfur standards were ground using an agate mortar and pestle to the consistency of a fine talcum powder (approximately 10 um). A cellulose acetate filter was then gently dredged through a small quantity (less than 1 mg) of powder placed on a microscope slide. This procedure produced a thin and almost imperceptible coating on the filter in order to limit the thickness and thus self-absorption. S-NEXFS spectra of sulfate standards were collected in bulk mode. Self-absorption must be carefully controlled when measuring fluorescent X-rays from thick specimens; however, the effects of self-absorption are limited to the region of the spectrum above the K-edge. In our repeated measurements, the post-edge features were consistent and reproducible, which allows discrimination of different sulfate standards.

Sampling and analytical procedures: S compounds and minerals were obtained from chemical supply houses or mineral dealers. See papers cited below for details.

Instruments: X-ray fluorescence microscope located at beamline 2-ID-B at the Advanced Photon Source, Argonne National Laboratory. The beamline is optimized to examine samples over a 1–4 keV energy range using a focused X-ray beam with a spot size of approximately 60 nanometers squared. The energy was calibrated using an elemental sulfur standard. The whiteline energy of the elemental sulfur standard was aligned to 2472 eV.

Data processing: S-NEXFS data were normalized to create a relative intensity value of approximately 1 for post-edge area of the spectra. The data were also processed using a three-point smoothing algorithm built into the software package Athena to remove high-frequency noise (Ravel and Newville, 2005).

Processing Description

BCO-DMO Processing: modified parameter names (replaced spaces with underscores, removed special characters).

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Related Publications
Longo, A. F., Vine, D. J., King, L. E., Oakes, M., Weber, R. J., Huey, L. G., … Ingall, E. D. (2016). Composition and oxidation state of sulfur in atmospheric particulate matter. Atmospheric Chemistry and Physics, 16(21), 13389–13398. doi:10.5194/acp-16-13389-2016

Ravel, B., & Newville, M. (2005). ATHENA, ARTEMIS, HEPHAESTUS: data analysis for X-ray absorption spectroscopy using IFEFFIT. Journal of Synchrotron Radiation, 12(4), 537–541. doi:10.1107/S0909049505012719

Parameters
| Parameter               | Description                                                                 | Units                                      |
|------------------------|-----------------------------------------------------------------------------|--------------------------------------------|
| Energy                 | X-ray energy                                                                | electron volts                             |
| Ammonium_Sulfate       | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Barite                 | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Copper_II_Sulfate      | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Gypsum                 | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Iron_Ammonium_Sulfate  | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Iron_III_Sulfate       | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Jarosite               | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Magnesium_Sulfate      | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Potassium_Sulfate      | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
| Sodium_Sulfate         | Name of sulfur standard or mineral analyzed. Units (x-ray fluorescence counts) are normalized to incoming radiation. | x-ray fluorescence counts                  |
## Instruments

| Dataset-specific Instrument Name | Dataset-specific Description                                                                 |
|---------------------------------|---------------------------------------------------------------------------------------------|
| X-ray fluorescence microscope   | X-ray fluorescence microscope located at beamline 2-ID-B at the Advanced Photon Source, Argonne National Laboratory: The beamline is optimized to examine samples over a 1–4 keV energy range using a focused X-ray beam with a spot size of approximately 60 nanometers squared. The energy was calibrated using an elemental sulfur standard. The whiteline energy of the elemental sulfur standard was aligned to 2472 eV. |

| Generic Instrument Name         | Generic Instrument Description                                                               |
|---------------------------------|---------------------------------------------------------------------------------------------|
| Microscope-Fluorescence         | Instruments that generate enlarged images of samples using the phenomena of fluorescence and phosphorescence instead of, or in addition to, reflection and absorption of visible light. Includes conventional and inverted instruments. |
Coverage: Mediterranean

NSF Award Abstract: Primary nutrients, such as nitrogen and phosphorus, are critical for all life on earth, and limited quantities in the marine environment can inhibit primary productivity. Atmospheric aerosols are a significant source of these nutrients to nutrient-poor ocean regions, such as the phosphorus-limited Mediterranean Sea. The availability of phosphorus in aerosols has traditionally been linked to the composition and abundance of different phosphorus phases present. Unfortunately, investigating phosphorus composition in aerosols has been challenging due to methodological limitations until recently. In this study, researchers from Georgia Tech will use a new technique known as synchrotron-based P Near Edge X-ray Fluorescence Spectroscopy, in conjunction with X-ray fluorescence microscopy, to examine the diversity of aerosol phosphorus phases delivered to the Mediterranean Sea. By defining the relationship between air mass source region, aerosol composition, and bioavailability, results from this work will improve current knowledge of the factors regulating productivity in the Mediterranean Sea and help to clarify the potential response of this region to different climate change scenarios. Broader Impacts: In addition to the valuable insights this project will provide on the controls on productivity and nutrient cycling in the Mediterranean Sea, this study will further education of young scientists, broaden participation of under-represented groups in ocean science, and enhance research infrastructure.

Funding

| Funding Source | Award          |
|----------------|---------------|
| NSF Division of Ocean Sciences (NSF OCE) | OCE-1357375   |

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