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 (GA Tech)	Principal Investigator
Rauch, Shannon	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
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Methods & Sampling

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).

Data Processing Description

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

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Data Files

File
Sulfur_NEXFS_Standards.csv (Comma Separated Values (.csv), 16.48 KB) MD5:f4bdfe2146f0bdcae7ffac35b67df266 Primary data file for dataset ID 756682

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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
Results

Ravel, B., & Newville, M. (2005). ATHENA,ARTEMIS,HEPHAESTUS: data analysis for X-ray absorption spectroscopy usingIFEFFIT. Journal of Synchrotron Radiation, 12(4), 537–541. doi:10.1107/s0909049505012719 https://doi.org/10.1107/S0909049505012719
Methods

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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

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Instruments

Dataset-specific Instrument Name	X-ray fluorescence microscope
Generic Instrument Name	Fluorescence Microscope
Dataset-specific Description	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 Description	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.

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Project Information

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

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.

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Funding

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

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