Carbon near edge X-ray absorption fine structure (NEXAFS) spectra of standard compounds

Website: https://www.bco-dmo.org/dataset/815362
Data Type: experimental
Version: 1
Version Date: 2020-06-15

Project
» Geochemical controls on organic carbon quantity and quality in the deep subsurface (Org C Sed II)
» Elucidating the extent and composition of mineral-hosted carbon in the deep biosphere (Org C Sed I)

Programs
» Center for Dark Energy Biosphere Investigations (C-DEBI)
» Center for Dark Energy Biosphere Investigations (C-DEBI)

Contributors	Affiliation	Role
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Abstract
Carbon near edge X-ray absorption fine structure (NEXAFS) spectra of standard compounds. These data contain incident energy and absorption values at that energy for a standard compounds.

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Coverage

Temporal Extent: 2016-01

Dataset Description

Carbon near edge X-ray absorption fine structure (NEXAFS) spectra of standard compounds. These data contain incident energy and absorption values at that energy for a standard compounds.

These data were published in Estes et al. (2019).

Methods & Sampling

See Estes el al. (2019) for complete methods.

1–10 µL of standard compounds was pipetted onto silicon wafers and air-dried. The beamline was operated

with a 500 l mm–1 spherical grating monochromator and entrance and exit slits set to 40 µm, which yielded an absolute energy resolution of less than 0.3 eV. The samples were attached to an aluminium sample stick in a single load and analysed under ultrahigh vacuum conditions (pressure ~10−9 mbar). The measurements were made in the total electron yield (TEY) mode on a spot size of less than 1 mm2 using a grazing incidence angle of 45°, where previous trials determined that the incidence angle did not yield a difference in results. The TEY mode was selected instead of fluorescence as we observed dampening of the fluorescence signal, probably due to matrix-induced absorption.

Spectra were collected around the C 1s edge, from 260 to 340 eV, with a dwell time of 0.2 s. To avoid beam damage and variation of the background due to charging, scans were taken at different positions on the sample. The spectra analysed were the average of 2–3 scans taken at different positions on the sample. The dark current was measured prior to the collection of each spectrum and subtracted from the raw data. Spectra were then normalized to no load current measured by a mesh upstream of the chamber with freshly evaporated gold.

Instruments:

Bulk carbon NEXAFS spectroscopy was conducted on beamlines 8-2 and 10-1 at the Stanford Synchrotron Radiation Lightsource.

The absolute energy calibration of the carbon spectra was achieved by shifting the energy such that the first dip in the incoming intensity due to carbon contamination on the beamline optics (carbon dip) occurred at 284.7 eV.

Data Processing Description

Spectral processing was completed by subtracting a line fit to the pre-edge region (281–283 eV), followed by an area normalization between 282 and 310 eV with the high-energy intensity kept constant (atomic normalization). The entire pre-edge region appeared linear; fitting and background subtraction was conducted over a smaller energy range due to the presence of oxygen harmonic peaks. All the data normalization was conducted in Igor Pro (WaveMetrics).

BCO-DMO Data Manager Processing Notes:
* exported data in xlsx file "Estes_NEXAFSstds_data.xlsx" to csv file
* added a conventional header with dataset name, PI name, version date
* modified parameter names to conform with BCO-DMO naming conventions
* blank values in this dataset are displayed as "nd" for "no data." nd is the default missing data identifier in the BCO-DMO system.

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Data Files

File
nexafs_stds.csv (Comma Separated Values (.csv), 125.90 KB) MD5:925201313dd82766cf6f2c82fbc00e12 Primary data file for dataset ID 815362

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Related Publications

Estes, E. R., Pockalny, R., D'Hondt, S., Inagaki, F., Morono, Y., Murray, R. W., … Hansel, C. M. (2019). Persistent organic matter in oxic subseafloor sediment. Nature Geoscience, 12(2), 126–131. doi:10.1038/s41561-018-0291-5

Results

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Parameters

Parameter	Description	Units
eV	incident energy	electron volts (eV)
BSA	absorption values for protein (bovine serum albumin (BSA)). arbitrary units (normalized)	unitless
phenylalanin	absorption values of phenylalanin. arbitrary units (normalized)	unitless
leucine	absorption values of leucine. arbitrary units (normalized)	unitless
agarose	absorption values of agarose. arbitrary units (normalized)	unitless
alginate	absorption values of alginate. arbitrary units (normalized)	unitless
lipo	absorption values of lipo. arbitrary units (normalized)	unitless
phospholipid	absorption values of phospholipid. arbitrary units (normalized)	unitless
HMWDOM	absorption values of high molecular weight dissolved organic matter (HMWDOM). arbitrary units (normalized)	unitless
humic_acid	absorption values of humic acid. arbitrary units (normalized)	unitless

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Instruments

Dataset-specific Instrument Name	
Generic Instrument Name	Spectrometer
Dataset-specific Description	Bulk carbon synchrotron-based near edge x-ray fine structure (NEXAFS) spectroscopy was conducted on beamlines 8-2 and 10-1 at the Stanford Synchrotron Radiation Lightsource.
Generic Instrument Description	A spectrometer is an optical instrument used to measure properties of light over a specific portion of the electromagnetic spectrum.

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Project Information

Geochemical controls on organic carbon quantity and quality in the deep subsurface (Org C Sed II)

Website: https://www.darkenergybiosphere.org/award/3d-spatial-mapping-of-the-energetic-return-of-1000-metabolisms-within-the-compositional-variation-of-oceanic-crusts-near-mid-ocean-ridges/

Coverage: North Atlantic gyre, South Pacific gyre

Abstract from the C-DEBI project page:

Sediment underlying ocean gyres receives minimal input of fresh organic matter yet sustains a small but active heterotrophic microbial community. The concentration and composition of the organic carbon (OC) available to this deep biosphere however is unknown. We analyzed the content and composition of OC in pelagic sediment in order to identify mechanism(s) that dictate the balance between OC preservation and utilization by microorganisms. Sediment cores from the North Atlantic gyre (KN223), South Pacific Gyre (Knox02-RR), and Peru Basin (IODP site 1231) allowed for a global comparison and a test of how sediment lithology and redox state affect OC preservation. OC was present in low concentrations in all samples (0.01—0.61%), at depths up to 112 meters below seafloor and estimated sediment ages of up to 50 million years. Synchrotron-based near edge X-ray absorption fine structure (NEXAFS) spectroscopy was conducted on over 100 samples, one of the first applications of NEXAFS to sedimentary environments. NEXAFS revealed an OC reservoir dominated by amide and carboxylic functionalities in a scaffolding of O-alkyl and aliphatic carbons. Detection of extractable, extracellular proteins supports this composition and suggests that sedimentary OC is protein-derived. This composition was common across all sites and depths, implicating physical rather than chemical mechanisms in OC preservation on long timescales. This study thereby points to physical access rather than energy or metabolic potential as a key constraint on subsurface heterotrophic life.

Elucidating the extent and composition of mineral-hosted carbon in the deep biosphere (Org C Sed I)

Website: https://www.darkenergybiosphere.org/award/elucidating-the-extent-and-composition-of-mineral-hosted-carbon-in-the-deep-biosphere/

Coverage: North Atlantic gyre, South Pacific gyre

Abstract from the C-DEBI project page:

Minerals have recently been identified as a primary host for organic carbon (OC) within marine sediments. This strong physical and chemical carbon-mineral association is believed to reduce, and in some cases completely eliminate, the bioavailablilty of this carbon for microbial life. The paucity of information regarding the nature of this carbon-mineral association and the composition of the hosted carbon, however, precludes our ability to predict the ultimate fate of this OC and its involvement in deep subsurface life. Here, we addressed this knowledge gap by using a suite of bulk and spatially-resolved geochemical and mineralogical techniques to characterize OC-mineral associations within the deep subsurface. We characterized sediment samples collected on the 2014 North Atlantic long coring expedition (KN223) in the western subtropical North Atlantic that included three geochemically distinct long cores to a depth of 24-30 m and spanned OC-limited oxic to anoxic sediments. We find measurable and relevant OC concentrations throughout the sediment cores, that decreases linearly over ~25 meters burial depth, from ~0.15 to 0.075 mol OC/kg solid. OC within the sediments is compositionally complex on both a macro- and micro-scale, spanning a gradient of lability even at depth. Proteins are observed throughout the sediment depth profiles, where they appear to constitute a substantial fraction of the TOC. Correspondingly, a low C:N ratio is observed, consistent with proteinaceous carbon within the sediments. In sum, these findings point to a substantial mineral-hosted OC reservoir within the deep subsurface that may fuel the deep biosphere and select for protein-based heterotrophy.

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Program Information

Center for Dark Energy Biosphere Investigations (C-DEBI)

Website: http://www.darkenergybiosphere.org

Coverage: Global

The mission of the Center for Dark Energy Biosphere Investigations (C-DEBI) is to explore life beneath the

seafloor and make transformative discoveries that advance science, benefit society, and inspire people of all ages and origins.

C-DEBI provides a framework for a large, multi-disciplinary group of scientists to pursue fundamental questions about life deep in the sub-surface environment of Earth. The fundamental science questions of C-DEBI involve exploration and discovery, uncovering the processes that constrain the sub-surface biosphere below the oceans, and implications to the Earth system. What type of life exists in this deep biosphere, how much, and how is it distributed and dispersed? What are the physical-chemical conditions that promote or limit life? What are the important oxidation-reduction processes and are they unique or important to humankind? How does this biosphere influence global energy and material cycles, particularly the carbon cycle? Finally, can we discern how such life evolved in geological settings beneath the ocean floor, and how this might relate to ideas about the origin of life on our planet?

C-DEBI's scientific goals are pursued with a combination of approaches:
(1) coordinate, integrate, support, and extend the research associated with four major programs—Juan de Fuca Ridge flank (JdF), South Pacific Gyre (SPG), North Pond (NP), and Dorado Outcrop (DO)—and other field sites;
(2) make substantial investments of resources to support field, laboratory, analytical, and modeling studies of the deep subseafloor ecosystems;
(3) facilitate and encourage synthesis and thematic understanding of submarine microbiological processes, through funding of scientific and technical activities, coordination and hosting of meetings and workshops, and support of (mostly junior) researchers and graduate students; and
(4) entrain, educate, inspire, and mentor an interdisciplinary community of researchers and educators, with an emphasis on undergraduate and graduate students and early-career scientists.

Note: Katrina Edwards was a former PI of C-DEBI; James Cowen is a former co-PI.

Data Management:
C-DEBI is committed to ensuring all the data generated are publically available and deposited in a data repository for long-term storage as stated in their Data Management Plan (PDF) and in compliance with the NSF Ocean Sciences Sample and Data Policy. The data types and products resulting from C-DEBI-supported research include a wide variety of geophysical, geological, geochemical, and biological information, in addition to education and outreach materials, technical documents, and samples. All data and information generated by C-DEBI-supported research projects are required to be made publically available either following publication of research results or within two (2) years of data generation.

To ensure preservation and dissemination of the diverse data-types generated, C-DEBI researchers are working with BCO-DMO Data Managers make data publicly available online. The partnership with BCO-DMO helps ensure that the C-DEBI data are discoverable and available for reuse. Some C-DEBI data is better served by specialized repositories (NCBI's GenBank for sequence data, for example) and, in those cases, BCO-DMO provides dataset documentation (metadata) that includes links to those external repositories.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-0939564

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