

# Spectral magnitude data for 0.0008 ppm bands from aerosol water soluble organic matter 1H NMR spectra from R/V Knorr GEOTRACES cruises KN199-04 and KN204-01 in the Subtropical northern Atlantic Ocean in 2010 and 2011

**Website:** <https://www.bco-dmo.org/dataset/652808>

**Data Type:** Cruise Results

**Version:** 29 Dec 2015

**Version Date:** 2015-12-29

## Project

» [U.S. GEOTRACES North Atlantic Transect \(GA03\)](#) (U.S. GEOTRACES NAT)

» [Role of Organic Matter in Determining the Solubility of Atmospherically-Delivered Iron](#) (GEOTRACES Aerosol OM)

## Program

» [U.S. GEOTRACES](#) (U.S. GEOTRACES)

Contributors	Affiliation	Role
<a href="#">Wozniak, Andrew S.</a>	Old Dominion University (ODU)	Principal Investigator
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## Dataset Description

The sampling details and identities of each of the samples is provided in addition to the NMR data. This includes: starting and ending locations (latitudes and longitudes) and times (Greenwich mean time) as well as the sampling rates ( $\text{m}^3 \text{min}^{-1}$ ) and calculated sample volumes ( $\text{m}^3$ ) for each of the aerosol samples. The run times (measured in hours) and sample volumes account for periods when the sampler was stopped due to potential contamination from the ship's stack. The NMR data are reported as spectral intensity units, which are non-quantitative, and chemical shift - at parts per million difference from a reference signal, the hydrogens in tetramethylsilane. Spectral images are also provided as JPEG files. These images show the NMR spectra from which the numerical data are derived.

## Methods & Sampling

The analytical and data processing methodology have been described in Wozniak et al. (2013, 2015). The full citations for these references are below. A summary of the methods is quoted here:

Aerosol WSOM was minimally diluted with D<sub>2</sub>O and analyzed on a Bruker Biospin Avance III 400 MHz NMR with a broadband inverse solution state probe at ODU's College of Sciences Major Instrumentation Cluster facility using a water suppression technique described previously (e.g., Wozniak et al., 2013). WSOM samples were

diluted to a final composition of 9:1 sample:D2O and 500  $\mu$ L of this solution was added to 5 mm glass NMR tubes and analyzed without further manipulation. Spectra were acquired using a 2 s recycle delay, a 119 ms acquisition time, a time domain of 16 k, and co-adding 8000 scans. The summed free induction decay signal was exponentially multiplied and zero-filled once. The spectra were processed with a line broadening of 3 Hz.

\* During data processing for publications from this work (Wozniak et al., 2013, 2015), spectral chemical shifts corresponding to potential solvent interferences from hydrogens in residual water (region excluded: 4.6 ppm to 4.8 ppm), methanol (region excluded: 3.28 ppm to 3.46 ppm), and tetramethylsilane (region excluded: <0.095 ppm) were set to 0. The data archived here do not have these sections set to 0.

\*\* The data for samples 7587, 8044, and 8045 have been flagged as bad and are not included here. Multiple attempts were made to rerun these samples, but adequate spectra were not obtained.

### References:

Wozniak, A. S., R. L. Sleighter, H. Abdulla, A. S. Priest, P. L. Morton, R. U. Shelley, W. M. Landing, and P. G. Hatcher. 2013. Relationships among aerosol water soluble organic matter, iron and aluminum in European, North African, and Marine air masses from the 2010 US GEOTRACES cruise. *Marine Chemistry*, 154, 24-33. doi:[10.1016/j.marchem.2013.04.011](https://doi.org/10.1016/j.marchem.2013.04.011)

Wozniak, A. S., R. U. Shelley, S. M. McElhenie, A. S. Willoughby, W. M. Landing, P. G. Hatcher. 2015. Insights into potential Fe-binding aerosol water soluble organic ligands from the 2011 US GEOTRACES cruise. *Marine Chemistry*, 173, 162-172, doi:[10.1016/j.marchem.2014.11.002](https://doi.org/10.1016/j.marchem.2014.11.002)

## Data Processing Description

### BCO-DMO Processing:

- Modified parameter names to conform with BCO-DMO naming conventions;
- added cruise id, event numbers, and station numbers from BCO-DMO GEOTRACES NAT master event file;
- replaced missing data with 'nd';
- converted date-time fields to ISO format;
- changed longitude values to negative.

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## Data Files

File
<b>GT10-11_NMR.csv</b> (Comma Separated Values (.csv), 121.92 MB) MD5:99984908bd14ef499aee19e850f9d6e8
Primary data file for dataset ID 652808

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## Parameters

Parameter	Description	Units
cruise_id	Cruise identifier	unitless
sample_GEOTRC	GEOTRACES sample number	unitless
event_GEOTRC	GEOTRACES event number; added from the BCO-DMO GEOTRACES NAT master events file.	unitless
station	Station number; added from the BCO-DMO GEOTRACES NAT master events file.	unitless
filter_size	Filter size. Whatman QMA filters are typically sold as 8"x10" sheets in the U.S.	inches
filter_type	Filter type	unitless
lat_start	Latitude at the start of the sampling event.	decimal degrees
lon_start	Longitude at the start of the sampling event.	decimal degrees
ISO_DateTime_UTC_Start	Date and time, formatted to ISO8601 standard, at the start of the sampling event. Format: YYYY-mm-ddTHH:MM:SS.xx	unitless
lat_end	Latitude at the end of the sampling event.	decimal degrees
lon_end	Longitude at the end of the sampling event.	decimal degrees
ISO_DateTime_UTC_End	Date and time, formatted to ISO8601 standard, at the end of the sampling event. Format: YYYY-mm-ddTHH:MM:SS.xx	unitless
run_time	Run time in hours	hours
flow_rate	Sampling rate	cubic meters per minute (m <sup>3</sup> min <sup>-1</sup> )
total	Total sample size	cubic meters (m <sup>3</sup> )
NMR_spectral_image	Link to spectral image (JPEG file) showing the NMR spectra from which the data are derived.	unitless
chemical_shift	Chemical shift measured as parts per million difference from a reference signal, the hydrogens in tetramethylsilane.	parts per million (ppm)
spectral_intensity	Spectral intensity	spectral intensity units (non-quantitative)

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## Instruments

<b>Dataset-specific Instrument Name</b>	
<b>Generic Instrument Name</b>	Aerosol Sampler
<b>Generic Instrument Description</b>	A device that collects a sample of aerosol (dry particles or liquid droplets) from the atmosphere.

<b>Dataset-specific Instrument Name</b>	Bruker Biospin Avance III 400 MHz NMR
<b>Generic Instrument Name</b>	Nuclear Magnetic Resonance Spectrometers
<b>Dataset-specific Description</b>	Aerosol WSOM was minimally diluted with D2O and analyzed on a Bruker Biospin Avance III 400 MHz NMR with a broadband inverse solution state probe at ODU's College of Sciences Major Instrumentation Cluster facility.
<b>Generic Instrument Description</b>	Instruments that identify and quantify magnetically active chemical entities by subjecting a sample to orthogonal magnetic and electrical fields.

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## Deployments

### KN199-04

<b>Website</b>	<a href="https://www.bco-dmo.org/deployment/58066">https://www.bco-dmo.org/deployment/58066</a>
<b>Platform</b>	R/V Knorr
<b>Report</b>	<a href="http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/Cruise_Report_for_Knorr_199_Final_v3.pdf">http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/Cruise_Report_for_Knorr_199_Final_v3.pdf</a>
<b>Start Date</b>	2010-10-15
<b>End Date</b>	2010-11-04
<b>Description</b>	<p>This cruise constitutes the first survey section as part of the U.S. participation in an international program named GEOTRACES. Funding: NSF OCE award 0926423 Science Objectives: To obtain state of the art trace metal and isotope measurements on a suite of samples taken on a mid-latitude zonal transect of the North Atlantic. In particular, sampling targeted the oxygen minimum zone extending off the west African coast near Mauritania, the TAG hydrothermal field, and the western boundary current system along Line W. For additional information, please refer to the GEOTRACES program Web site (<a href="https://www.geotraces.org/">https://www.geotraces.org/</a>) for overall program objectives and a summary of properties measured. Science Activities include seawater sampling via GoFLO and Niskin carousels, in situ pumping (and filtration), CTDO2 and transmissometer sensors, underway pumped sampling of surface waters, and collection of aerosols and rain. Hydrography, CTD and nutrient measurements were supported by the Ocean Data Facility (J. Swift) at Scripps Institution of Oceanography and funded through NSF Facilities. They provided an additional CTD rosette system along with nephelometer and LADCP. A trace metal clean Go-Flo Rosette and winch were provided by the group at Old Dominion University (G. Cutter) along with a towed underway pumping system. Additional cruise information is available from the Rolling Deck to Repository (R2R): <a href="https://www.rvdata.us/search/cruise/KN199-04">https://www.rvdata.us/search/cruise/KN199-04</a> Other Relevant Links: List of cruise participants: [ PDF ] Cruise track: JPEG image (from Woods Hole Oceanographic Institution, vessel operator) ADCP data are available from the Currents ADCP group at the University of Hawaii: KN199-04 ADCP</p>

### KN204-01

<b>Website</b>	<a href="https://www.bco-dmo.org/deployment/58786">https://www.bco-dmo.org/deployment/58786</a>
<b>Platform</b>	R/V Knorr
<b>Report</b>	<a href="http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/STS_Prelim_GT11_Doc.pdf">http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/STS_Prelim_GT11_Doc.pdf</a>
<b>Start Date</b>	2011-11-06
<b>End Date</b>	2011-12-11
<b>Description</b>	<p>The US GEOTRACES North Atlantic cruise aboard the R/V Knorr completed the section between Lisbon and Woods Hole that began in October 2010 but was rescheduled for November-December 2011. The R/V Knorr made a brief stop in Bermuda to exchange samples and personnel before continuing across the basin. Scientists disembarked in Praia, Cape Verde, on 11 December. The cruise was identified as KN204-01A (first part before Bermuda) and KN204-01B (after the Bermuda stop). However, the official deployment name for this cruise is KN204-01 and includes both part A and B. Science activities included: ODF 30 liter rosette CTD casts, ODU Trace metal rosette CTD casts, McLane particulate pump casts, underway sampling with towed fish and sampling from the shipboard "uncontaminated" flow-through system. Full depth stations are shown in the accompanying figure (see below). Additional stations to sample for selected trace metals to a depth of 1000 m are not shown. Standard stations are shown in red (as are the ports) and "super" stations, with extra casts to provide large-volume samples for selected parameters, are shown in green. Station spacing is concentrated along the western margin to evaluate the transport of trace elements and isotopes by western boundary currents. Stations across the gyre will allow scientists to examine trace element supply by Saharan dust, while also contrasting trace element and isotope distributions in the oligotrophic gyre with conditions near biologically productive ocean margins, both in the west, to be sampled now, and within the eastern boundary upwelling system off Mauritania, sampled last year. Funding: The cruise was funded by NSF OCE awards 0926204, 0926433 and 0926659. Additional cruise information is available from the Rolling Deck to Repository (R2R): <a href="https://www.rvdata.us/search/cruise/KN204-01">https://www.rvdata.us/search/cruise/KN204-01</a> Other Relevant Links: ADCP data are available from the Currents ADCP group at the University of Hawaii at the links below: KN204-01A (part 1 of 2011 cruise; Woods Hole, MA to Bermuda) KN204-01B (part 2 of 2011 cruise; Bermuda to Cape Verde)</p>

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## Project Information

### U.S. GEOTRACES North Atlantic Transect (GA03) (U.S. GEOTRACES NAT)

**Website:** <https://www.geotraces.org/>

**Coverage:** Subtropical western and eastern North Atlantic Ocean (GA03)

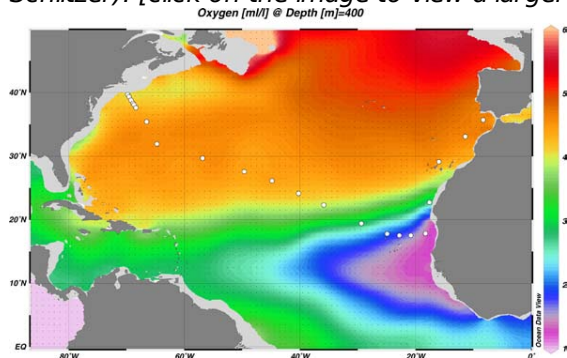
*Much of this text appeared in an article published in OCB News, October 2008, by the OCB Project Office.*

The first U.S. GEOTRACES Atlantic Section will be specifically centered around a sampling cruise to be carried out in the North Atlantic in 2010. Ed Boyle (MIT) and Bill Jenkins (WHOI) organized a three-day planning workshop that was held September 22-24, 2008 at the Woods Hole Oceanographic Institution. The main goal of the workshop, sponsored by the National Science Foundation and the U.S. GEOTRACES Scientific Steering Committee, was to design the implementation plan for the first U.S. GEOTRACES Atlantic Section. The primary cruise design motivation was to improve knowledge of the sources, sinks and internal cycling of Trace Elements and their Isotopes (TEIs) by studying their distributions along a section in the North Atlantic (Figure 1). The North Atlantic has the full suite of processes that affect TEIs, including strong meridional advection, boundary scavenging and source effects, aeolian deposition, and the salty Mediterranean Outflow. The North Atlantic is particularly important as it lies at the "origin" of the global Meridional Overturning Circulation.

It is well understood that many trace metals play important roles in biogeochemical processes and the carbon cycle, yet very little is known about their large-scale distributions and the regional scale processes that affect them. Recent advances in sampling and analytical techniques, along with advances in our understanding of their

roles in enzymatic and catalytic processes in the open ocean provide a natural opportunity to make substantial advances in our understanding of these important elements. Moreover, we are motivated by the prospect of global change and the need to understand the present and future workings of the ocean's biogeochemistry. The GEOTRACES strategy is to measure a broad suite of TEIs to constrain the critical biogeochemical processes that influence their distributions. In addition to these "exotic" substances, more traditional properties, including macronutrients (at micromolar and nanomolar levels), CTD, bio-optical parameters, and carbon system characteristics will be measured. The cruise starts at Line W, a repeat hydrographic section southeast of Cape Cod, extends to Bermuda and subsequently through the North Atlantic oligotrophic subtropical gyre, then transects into the African coast in the northern limb of the coastal upwelling region. From there, the cruise goes northward into the Mediterranean outflow. The station locations shown on the map are for the "fulldepth TEI" stations, and constitute approximately half of the stations to be ultimately occupied.

Figure 1. The proposed 2010 Atlantic GEOTRACES cruise track plotted on dissolved oxygen at 400 m depth. Data from the World Ocean Atlas (Levitus et al., 2005) were plotted using Ocean Data View (courtesy Reiner Schlitzer). [click on the image to view a larger version]

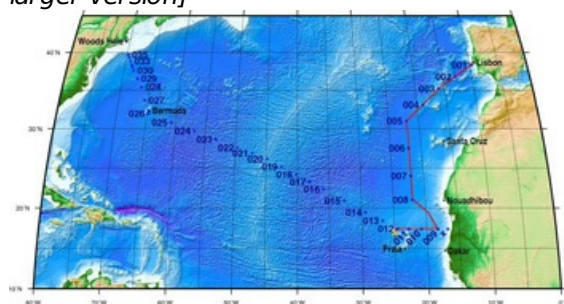


Hydrography, CTD and nutrient measurements will be supported by the Ocean Data Facility (J. Swift) at Scripps Institution of Oceanography and funded through NSF Facilities. They will be providing an additional CTD rosette system along with nephelometer and LADCP. A trace metal clean Go-Flo Rosette and winch system will be provided by the group at Old Dominion University (G. Cutter) along with a towed underway pumping system.

The North Atlantic Transect cruise began in 2010 with KN199 leg 4 (station sampling) and leg 5 (underway sampling only) (Figure 2).

[KN199-04 Cruise Report \(PDF\)](#)

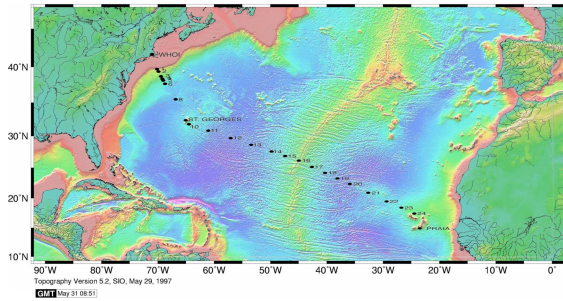
Figure 2. The red line shows the cruise track for the first leg of the US Geotraces North Atlantic Transect on the R/V Knorr in October 2010. The rest of the stations (beginning with 13) will be completed in October-December 2011 on the R/V Knorr (courtesy of Bill Jenkins, Chief Scientist, GNAT first leg). [click on the image to view a larger version]



The section completion effort resumed again in November 2011 with KN204-01A,B (Figure 3).

[KN204-01A,B Cruise Report \(PDF\)](#)

Figure 3. Station locations occupied on the US Geotraces North Atlantic Transect on the R/V Knorr in November 2011. [click on the image to view a larger version]



Data from the North Atlantic Transect cruises are available under the Datasets heading below, and consensus values for the SAFe and North Atlantic GEOTRACES Reference Seawater Samples are available from the GEOTRACES Program Office: [Standards and Reference Materials](#)

**ADCP data** are available from the Currents ADCP group at the University of Hawaii at the links below:

- [KN199-04](#) (leg 1 of 2010 cruise; Lisbon to Cape Verde)
- [KN199-05](#) (leg 2 of 2010 cruise; Cape Verde to Charleston, NC)
- [KN204-01A](#) (part 1 of 2011 cruise; Woods Hole, MA to Bermuda)
- [KN204-01B](#) (part 2 of 2011 cruise; Bermuda to Cape Verde)

### **Role of Organic Matter in Determining the Solubility of Atmospherically-Delivered Iron (GEOTRACES Aerosol OM)**

**Website:** <http://wozniakresearch.com/geotraces/>

**Coverage:** 2010 and 2011 US GEOTRACES North Atlantic Transect cruises

#### *Description from NSF award abstract:*

The atmospheric delivery of soluble Fe to the ocean is an important process contributing to oceanic primary production and the drawdown of atmospheric CO<sub>2</sub>. Combustion influenced air masses carry highly soluble Fe, but the reasons for this increased solubility remain unclear despite the importance to global carbon cycling. Acidic organic matter (OM) components (e.g., -COOH groups) can complex with trace metals, yet no study to date has investigated the comprehensive molecular characteristics of aerosol OM for their role as a determinant of Fe solubility.

In this project, researchers at Old Dominion University will study the relationship between the molecular characteristics of marine aerosol water soluble OM (WSOM) and Fe solubility. Marine particulate aerosols collected during GEOTRACES cruises will be examined to identify WSOM characteristics that may play a role in delivering soluble and bioavailable Fe to the N. Atlantic Ocean. Aerosol WSOM will be characterized using advanced molecular and chemometric techniques to test whether:

- (1) continental combustion-influenced aerosol samples show molecular characteristics unique from those of continental dust influenced samples, having characteristics consistent with higher contributions from OM with acidic functional group;
- (2) aerosol WSOM examined along a gradient of Fe solubility show concurrent changes in the relative magnitude of highly oxygenated compounds and contributions from acidic functional groups; and
- (3) 2D HMBC NMR reveal unique components in composite continental combustion influenced samples relative to marine and dust-influenced samples, and these unique components include OM with carboxyl functional groups that can bind Fe.

This project will be the first of its kind to extensively examine WSOM molecular characteristics and Fe solubility on concurrently collected aerosol samples. The results will be useful for understanding Fe distributions and biogeochemical cycling in the ocean. A potentially transformative aspect of this proposal will be the identification of aerosol WSOM molecular components unique to combustion influenced air masses that have the potential to facilitate aerosol Fe solubility.

The findings of this project are expected to be highly relevant to oceanic and global biogeochemical cycling of OM and many trace metals that form organic complexes. Combustion-influenced OM associations may help explain patterns in the global oceanic distribution of other trace metals and provide key insights into oceanic processes (e.g., primary production, biological pump).

## Program Information

### U.S. GEOTRACES (U.S. GEOTRACES)

**Website:** <http://www.geotraces.org/>

**Coverage:** Global

**GEOTRACES** is a [SCOR](#) sponsored program; and funding for program infrastructure development is provided by the [U.S. National Science Foundation](#).

GEOTRACES gained momentum following a special symposium, S02: Biogeochemical cycling of trace elements and isotopes in the ocean and applications to constrain contemporary marine processes (GEOSECS II), at a 2003 Goldschmidt meeting convened in Japan. The GEOSECS II acronym referred to the Geochemical Ocean Section Studies To determine full water column distributions of selected trace elements and isotopes, including their concentration, chemical speciation, and physical form, along a sufficient number of sections in each ocean basin to establish the principal relationships between these distributions and with more traditional hydrographic parameters;

- \* To evaluate the sources, sinks, and internal cycling of these species and thereby characterize more completely the physical, chemical and biological processes regulating their distributions, and the sensitivity of these processes to global change; and

- \* To understand the processes that control the concentrations of geochemical species used for proxies of the past environment, both in the water column and in the substrates that reflect the water column.

GEOTRACES will be global in scope, consisting of ocean sections complemented by regional process studies. Sections and process studies will combine fieldwork, laboratory experiments and modelling. Beyond realizing the scientific objectives identified above, a natural outcome of this work will be to build a community of marine scientists who understand the processes regulating trace element cycles sufficiently well to exploit this knowledge reliably in future interdisciplinary studies.

Expand "Projects" below for information about and data resulting from individual US GEOTRACES research projects.

## Funding

Funding Source	Award
<a href="#">NSF Division of Ocean Sciences (NSF OCE)</a>	<a href="#">OCE-1234166</a>