

Dissolved iron speciation results from 2019 Bermuda Atlantic Iron Time-series (BAIT) cruises EN631, AE1909, AE1921, AE1930 in the Western Subtropical North Atlantic Gyre from March to November 2019 (BAIT Project)

Website: <https://www.bco-dmo.org/dataset/869081>

Data Type: Cruise Results

Version: 1

Version Date: 2022-02-14

Project

» [NSFGEO-NERC: Collaborative Research: Using Time-series Field Observations to Constrain an Ocean Iron Model](#) (BAIT)

Program

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

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Abstract

Dissolved iron-binding organic ligand concentrations and conditional stability constants from GO-FLO water column samples collected in 2019 during four Bermuda Atlantic Iron Time-series (BAIT) cruises in the Bermuda Atlantic Time-series Study (BATS) region.

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Coverage

Spatial Extent: N:32.151 E:-63.5796 S:31.1769 W:-64.8147

Temporal Extent: 2019-03-11 - 2019-11-21

Methods & Sampling

Sampling and analytical methodology:

Sample collection and filtering: Water column samples were collected by the BAIT sampling team from 12 trace metal clean modified 6-L Niskin-X samplers (General Oceanics Inc.) deployed on a clean CTD rosette system (Sedwick et al. 2005). The BAIT sampling team filtered the samples through 0.2 μm Supor Acropak filter cartridges (Pall) inside a clean-air laboratory van.

Filtered seawater samples for iron speciation (organic complexation) were collected in 500 mL acid-cleaned Nalgene narrow-mouth fluorinated high-density polyethylene (FPE) bottles that had been filled with Milli-Q for at least two weeks after acid cleaning and rinsed three times with filtered seawater prior to sample collection (Buck et al. 2012). All filtered seawater samples for dissolved iron speciation were frozen at -20 °C shipboard and shipped to the University of South Florida for laboratory-based analyses post cruise.

Dissolved iron speciation (organic complexation) analyses:

Dissolved iron speciation (organic complexation) was analyzed using competitive ligand exchange- adsorptive cathodic stripping voltammetry (CLE-AdCSV) with salicylaldoxime as the added competing ligand (Buck et al. 2015), modified from the original Rue and Bruland (1995) method. A borate-ammonium buffer was added to all vials, for a final pH of 8.2 (NBS scale; Buck et al. 2007, 2012). Dissolved iron additions of 0 to 10 nM were used in the titrations, for a total of 15 points in each titration. CLE-AdCSV analyses were performed on Bioanalytical Systems (BAS) Controlled Growth Mercury Electrodes (static mercury drop setting, size 14) with Epsilon e2 (BAS) electrochemical analyzers. Deposition time of 120 s was applied to the analyses. There are no reference samples available for iron speciation measurements of iron in seawater, though this method has been shown to compare well with other labs and techniques in GEOTRACES intercalibration exercises (Buck et al. 2012, 2016).

Data Processing Description

Science Data Processing Notes:

CLE-AdCSV data was interpreted using a freely available interpretation program, ProMCC (Omanovic et al. 2015; <https://sites.google.com/site/daromasoft/home/promcc>), which employs matrix based optimization of titration data fitting to obtain ligand concentrations and conditional stability constants for each sample. Uncertainties in the fitted parameter are presented as the 95% confidence interval provided by the interpretation program. When replicate titrations were conducted, results are presented as averages of the replicates.

Dissolved iron (DFe) concentrations determined by inductively coupled plasma-mass spectrometry (ICP-MS) by Bettina Sohst in project PI Peter Sedwick's lab at Old Dominion University were used in the ProMCC interpretation program to calculate ligand concentrations and conditional stability constants from the sample titrations. The DFe values used for this dataset are provided in the speciation submission for reference, please see Sedwick's dataset for the complete dissolved iron data and metadata.

The detection limit for the electroactive Fe-SA complex has been found to be 0.01 nM (Buck et al. 2007), calculated as three times the standard deviation of measured peak height from a 0.05 nM Fe addition to UV-oxidized and chelexed seawater with a 900 s deposition time. For a 90 s deposition time, the detection limit for Fe-SA is ~0.1 nM (Buck et al. 2018).

Data flag notes:

The standard Ocean Data View qualifying flags were used within the flag columns of the dataset (reference all flags at https://www.bodc.ac.uk/resources/delivery_formats/odv_format/):

- 1: Good Value: Good quality data value that is not part of any identified malfunction and has been verified as consistent with real phenomena during the quality control process. [Used when data were shown to be reproducible]
- 2: Probably Good Value: Data value that is probably consistent with real phenomena but this is unconfirmed or data value forming part of a malfunction that is considered too small to affect the overall quality of the data object of which it is a part. [Used when the reported value reflects analysis of a single or unverified replicate]
- 3: Probably Bad Value: Data value recognized as unusual during quality control that forms part of a feature that is probably inconsistent with real phenomena. [Not used]
- 4: Bad Value: An obviously erroneous data value. [Not used]
- 5: Changed Value: Data value adjusted during quality control. [Not used]
- 6: Value Below Detection Limit: The level of the measured phenomenon was too small to be quantified by the technique employed to measure it. The accompanying value is the detection limit for the technique or zero if that value is unknown. [Not used]
- 7: Value in Excess: The level of the measured phenomenon was too large to be quantified by the technique

employed to measure it. The accompanying value is the measurement limit for the technique. [Not used]

8: Interpolated Value: This value has been derived by interpolation from other values in the data object. [Not used]

9: Missing Value: The data value is missing. Any accompanying value will be a magic number representing absent data. [Any missing data reflect samples that were not analyzed or were analyzed but results are not (or not yet) reported; "nd" = "no data" used in these cases]

A: Value Phenomenon Uncertain: There is uncertainty in the description of the measured phenomenon associated with the value such as chemical species or biological entity.

BCO-DMO Processing Notes

- Spaces within column headers were replaced with underscores
- Special characters removed from column name (% changed to Percent)

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Data Files

File
dataset_buckcaprara_bait_fespeciation-1.csv (Comma Separated Values (.csv), 18.05 KB) MD5:2e845a19096ade65dff0d100fc995c07
Primary data file for dataset ID 869081

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Related Publications

Buck, K. N., Gerringa, L. J. A., & Rijkenberg, M. J. A. (2016). An Intercomparison of Dissolved Iron Speciation at the Bermuda Atlantic Time-series Study (BATS) Site: Results from GEOTRACES Crossover Station A. *Frontiers in Marine Science*, 3. doi:[10.3389/fmars.2016.00262](https://doi.org/10.3389/fmars.2016.00262)

Methods

Buck, K. N., Lohan, M. C., Berger, C. J. M., & Bruland, K. W. (2007). Dissolved iron speciation in two distinct river plumes and an estuary: Implications for riverine iron supply. *Limnology and Oceanography*, 52(2), 843-855. doi:[10.4319/lo.2007.52.2.0843](https://doi.org/10.4319/lo.2007.52.2.0843)

Methods

Buck, K. N., Moffett, J., Barbeau, K. A., Bundy, R. M., Kondo, Y., & Wu, J. (2012). The organic complexation of iron and copper: an intercomparison of competitive ligand exchange-adsorptive cathodic stripping voltammetry (CLE-ACSV) techniques. *Limnology and Oceanography: Methods*, 10(7), 496-515. doi:[10.4319/lom.2012.10.496](https://doi.org/10.4319/lom.2012.10.496)

Methods

Buck, K. N., Sedwick, P. N., Sohst, B., & Carlson, C. A. (2018). Organic complexation of iron in the eastern tropical South Pacific: Results from US GEOTRACES Eastern Pacific Zonal Transect (GEOTRACES cruise GP16). *Marine Chemistry*, 201, 229-241. <https://doi.org/10.1016/j.marchem.2017.11.007>

Methods

Buck, K. N., Sohst, B., & Sedwick, P. N. (2015). The organic complexation of dissolved iron along the U.S. GEOTRACES (GA03) North Atlantic Section. *Deep Sea Research Part II: Topical Studies in Oceanography*, 116, 152-165. doi:[10.1016/j.dsr2.2014.11.016](https://doi.org/10.1016/j.dsr2.2014.11.016)

Methods

Cutter, G. A., & Bruland, K. W. (2012). Rapid and noncontaminating sampling system for trace elements in global ocean surveys. *Limnology and Oceanography: Methods*, 10(6), 425-436. doi:[10.4319/lom.2012.10.425](https://doi.org/10.4319/lom.2012.10.425)

Methods

GEOTRACES, 2010. Sample and sample-handling protocols for GEOTRACES Cruises, in: *Standards and Intercalibration Committee* (Ed.), 1.0 ed.

Methods

Omanović, D., Garnier, C., & Pižeta, I. (2015). ProMCC: An all-in-one tool for trace metal complexation studies.

Marine Chemistry, 173, 25–39. doi:[10.1016/j.marchem.2014.10.011](https://doi.org/10.1016/j.marchem.2014.10.011)
Methods

Rue, E. L., & Bruland, K. W. (1995). Complexation of iron(III) by natural organic ligands in the Central North Pacific as determined by a new competitive ligand equilibration/adsorptive cathodic stripping voltammetric method. *Marine Chemistry*, 50(1-4), 117–138. doi:[10.1016/0304-4203\(95\)00031-l](https://doi.org/10.1016/0304-4203(95)00031-l)
Methods

Sedwick, P. N., Church, T. M., Bowie, A. R., Marsay, C. M., Ussher, S. J., Achilles, K. M., Lethaby, P. J., Johnson, R. J., Sarin, M. M., & McGillicuddy, D. J. (2005). Iron in the Sargasso Sea (Bermuda Atlantic Time-series Study region) during summer: Eolian imprint, spatiotemporal variability, and ecological implications. *Global Biogeochemical Cycles*, 19(4), n/a-n/a. <https://doi.org/10.1029/2004gb002445>
<https://doi.org/10.1029/2004GB002445>
Methods

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Parameters

Parameter	Description	Units
CRUISE	cruise number	unitless
PROJECT_CRUISE	BAIT project cruise number	unitless
Cast_Number	cast number	unitless
SAMPLE_ID	sample identifier	unitless
DATE	GMT date when rosette cast or towfish sampling was started, in format YYYY-MM-DD.	unitless
LATITUDE	position when sampling cast was started in decimal °N (2 m sample = underway sample collected typically on approach to station).	lat
LONGITUDE	position when sampling cast was started in decimal °E (2 m sample = underway sample collected typically on approach to station).	lon
DEPTH	sample collection depth below sea surface. GeoFish sample assigned 2 m depth.	meters (m)
Fe_D_CONC_BOTTLE	dissolved iron (Fe) concentration value used in the speciation data interpretation. Data received from project PI Peter Sedwick's lab at Old Dominion University, contact Sedwick for additional information.	nM
L1Fe_D_CONC_BOTTLE	concentration of strongest dissolved iron-binding ligand detected. Units: nM (10 ⁻⁹ M). "nd" for "no data" used when no data available for this sample.	nM
L1_FLAG	Standard Ocean Data View qualifying flags were used (1 = Good Value, 2 = Probably Good Value, 3 = Probably Bad Value, 4 = Bad Value, 5 = Changed Value, 6 = Value Below Detection Limit, 7 = Value in Excess, 8 = Interpolated Value, 9 = Missing Value, A = Value Phenomenon Uncertain). See Processing Notes for full flag details.	unitless
L1_95_Percent_CI	95% confidence limit of [L1] determined from data fit by ProMCC.	nM
L1Fe_D_LogK_BOTTLE	log conditional stability constant of L1 complexes with iron (log K cond FeL1, Fe1).	unitless
log_K1_FLAG	Standard Ocean Data View qualifying flags were used (1 = Good Value, 2 = Probably Good Value, 3 = Probably Bad Value, 4 = Bad Value, 5 = Changed Value, 6 = Value Below Detection Limit, 7 = Value in Excess, 8 = Interpolated Value, 9 = Missing Value, A = Value Phenomenon Uncertain). See Processing Notes for full flag details.	unitless
log_K1_95_Percent_CI	95% confidence limit of log K1 determined from data fit by ProMCC. No units, K1 has units of M ⁻¹ . "nd" for "no data" used when no data available for this sample.	unitless

L2Fe_D_CONC_BOTTLE	concentration of second (weaker) dissolved iron-binding ligand. Units: nM (10 ⁻⁹ M).	unitless
L2_FLAG	Standard Ocean Data View qualifying flags were used (1 = Good Value, 2 = Probably Good Value, 3 = Probably Bad Value, 4 = Bad Value, 5 = Changed Value, 6 = Value Below Detection Limit, 7 = Value in Excess, 8 = Interpolated Value, 9 = Missing Value, A = Value Phenomenon Uncertain). See Processing Notes for full flag details.	unitless
L2_95_Percent_CI	95% confidence limit of [L2] determined from data fit by ProMCC. Units: nM (10 ⁻⁹ M). "nd" for "no data" used when no data available for this sample.	unitless
L2Fe_D_LogK_BOTTLE	log conditional stability constant of L2 complexes with iron (log K cond FeL2, Fe1). No units, K2 has units of M ⁻¹ . "nd" for "no data" used when no data available for this sample.	unitless
log_K2_FLAG	Standard Ocean Data View qualifying flags were used (1 = Good Value, 2 = Probably Good Value, 3 = Probably Bad Value, 4 = Bad Value, 5 = Changed Value, 6 = Value Below Detection Limit, 7 = Value in Excess, 8 = Interpolated Value, 9 = Missing Value, A = Value Phenomenon Uncertain). See Processing Notes for full flag details.	unitless
log_K2_95_Percent_CI	95% confidence limit of log K2 determined from data fit by ProMCC. No units, K2 has units of M ⁻¹ . "nd" for "no data" used when no data available for this sample.	unitless

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Instruments

Dataset-specific Instrument Name	Bioanalytical Systems (BASi) Controlled Growth Mercury Electrodes
Generic Instrument Name	BASi Controlled Growth Mercury Electrode
Dataset-specific Description	CLE-AdCSV analyses were performed on Bioanalytical Systems (BASi) Controlled Growth Mercury Electrodes (static mercury drop setting, size 14) with Epsilon e2 (BASi) electrochemical analyzers. Deposition time of 120 s was applied to the analyses.
Generic Instrument Description	Bioanalytical Systems (BASi) Mercury drop electrodes are generated by the BASi Controlled Growth Mercury Electrode (CGME) in three modes: DME (Dropping Mercury Electrode) - mercury is allowed to flow freely from the reservoir down the capillary and so the growth of the mercury drop and its lifetime is controlled by gravity. (The optional 100 um capillary is recommended for this mode.) SMDE (Static Mercury Drop Electrode) - the drop size is determined by the length of time for which the fast-response capillary valve is opened, and the drop is dislodged by a drop knocker. The dispense/knock timing is microprocessor-controlled and is typically coordinated with the potential pulse or square-wave waveform. This mode can also be used to generate the Hanging Mercury Drop Electrode required for stripping experiments. CGME (Controlled Growth Mercury Electrode) - the mercury drop is grown by a series of pulses that open the capillary valve. The number of pulses, their duration, and their frequency can be varied by PC control, providing great flexibility in both the drop size and its rate of growth. This CGME mode can be used for both polarographic and stripping experiments. http://www.basinc.com/products/ec/cgme.php

Dataset-specific Instrument Name	6-L Niskin-X samplers (General Oceanics Inc.)
Generic Instrument Name	Niskin bottle
Dataset-specific Description	Water column samples were collected by the BAIT sampling team from 12 trace metal clean modified 6-L Niskin-X samplers (General Oceanics Inc.) deployed on a clean CTD rosette system (Sedwick et al. 2005). The BAIT sampling team filtered the samples through 0.2 µm Supor Acropak filter cartridges (Pall) inside a clean-air laboratory van.
Generic Instrument Description	A Niskin bottle (a next generation water sampler based on the Nansen bottle) is a cylindrical, non-metallic water collection device with stoppers at both ends. The bottles can be attached individually on a hydrowire or deployed in 12, 24, or 36 bottle Rosette systems mounted on a frame and combined with a CTD. Niskin bottles are used to collect discrete water samples for a range of measurements including pigments, nutrients, plankton, etc.

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Deployments

EN631

Website	https://www.bco-dmo.org/deployment/869159
Platform	R/V Endeavor
Report	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/endeavor_en631.pdf
Start Date	2019-03-10
End Date	2019-03-15
Description	See additional cruise information at the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/EN631

AE1909

Website	https://www.bco-dmo.org/deployment/869175
Platform	R/V Atlantic Explorer
Report	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/atlanticexplorer_ae1909.pdf
Start Date	2019-05-11
End Date	2019-05-17
Description	See additional cruise information at the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/AE1909

AE1921

Website	https://www.bco-dmo.org/deployment/869176
Platform	R/V Atlantic Explorer
Report	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/atlanticexplorer_ae1921.pdf
Start Date	2019-08-16
End Date	2019-08-22
Description	See additional cruise information at the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/AE1921

AE1930

Website	https://www.bco-dmo.org/deployment/869177
Platform	R/V Atlantic Explorer
Report	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/atlanticexplorer_ae1930.pdf
Start Date	2019-11-15
End Date	2019-11-21
Description	See additional cruise information at the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/AE1930

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Project Information

NSFGEO-NERC: Collaborative Research: Using Time-series Field Observations to Constrain an Ocean Iron Model (BAIT)

Coverage: Bermuda Atlantic Time-Series Study region, waters of the western Subtropical North Atlantic Gyre (ca. 30°N-33°N, 62°W-65°W)

NSF and NERC Award Abstract:

Iron is an essential nutrient for the growth of phytoplankton in the oceans. As such, iron plays key roles in regulating marine primary production and the cycling of carbon. It is thus important that models of ocean biology and chemistry consider iron, in order to explore past, present and future variations in marine productivity and the role of the ocean in the global carbon cycle. In this joint project involving researchers in the U.S. and the U.K., supported by both NSF and the Natural Environment Research Council (U.K.), field data from the Bermuda Atlantic Time-series Study (BATS) region will be combined with an established, state-of-the-art ocean biogeochemical model. By leveraging the known seasonal-scale physical, chemical and biological changes in the BATS region, the oceanographic context provided by the BATS core data, and an existing model of the regional physical circulation, the proposed study will yield process-related information that is of general applicability to the open ocean. In particular, the proposed research will focus on understanding the atmospheric input, biological uptake, regeneration and scavenging removal of dissolved iron in the oceanic water column, which have emerged as major uncertainties in the ocean iron cycle. The project will include significant educational and training contributions at the K-12, undergraduate, graduate and postdoctoral levels, as well as public outreach efforts that aim to explain the research and its importance.

The ability of ocean models to simulate iron remains crude, owing to an insufficient understanding of the mechanisms that drive variability in dissolved iron, particularly the involvement of iron-binding ligands, colloids and particles in the surface input, biological uptake, regeneration and scavenging of dissolved iron in the upper ocean. Basin-scale data produced by the GEOTRACES program provide an important resource for testing and improving models and, by extension, our mechanistic understanding of the ocean iron cycle. However such data provide only quasi-synoptic 'snapshots', which limits their utility in isolating and identifying the processes that control dissolved iron in the upper ocean. The proposed research aims to provide mechanistic insight into these governing processes by combining time-series data from the BATS region with numerical modeling experiments.

Specifically, seasonally resolved data on the vertical (upper 2,000 meters) and lateral (tens of kilometers) distributions of particulate, dissolved, colloidal, soluble and ligand-bound iron species will be obtained from the chemical analysis of water column samples collected during five cruises, spanning a full annual cycle, shared with the monthly BATS program cruises. These data, along with ancillary data from the BATS program, will be used to test and inform numerical modeling experiments, and thus derive an improved understanding of the mechanisms that control the distribution and dynamics of dissolved iron in the oceanic water column.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

This is a project jointly funded by the National Science Foundation's Directorate for Geosciences (NSF/GEO) and the National Environment Research Council (NERC) of the United Kingdom (UK).

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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.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1829777

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