Total alkalinity determined through experiments comparing usage of high-density polyethylene (HDPE) and borosilicate glass bottles for collection and storage of water samples collected on the GEOTRACES GP17-OCE cruise (R/V Roger Revelle RR2214)

Website: https://www.bco-dmo.org/dataset/957644
Data Type: Cruise Results, experimental
Version: 1
Version Date: 2025-04-02

Project
» US GEOTRACES GP17-OCE and GP17-ANT: Inorganic Carbon Cycling in the South Pacific and Southern Oceans by Direct Measurement (GP17-OCE and GP17-ANT Inorganic Carbon)

Contributors	Affiliation	Role
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Abstract
Total alkalinity plays an important role in buffering seawater and determining how much anthropogenic carbon dioxide the oceans can absorb and mitigate the rise in atmospheric concentrations. Total alkalinity varies with location, depth, and time making it an important variable needed to quantify and monitor ocean acidification, and potentially for ocean alkalinity enhancement interventions. Currently, best practices are to use expensive high quality borosilicate glass bottles for collecting and storing these samples. However, unlike other carbon system variables, total alkalinity is not affected by gas exchange meaning plastic bottles may be suitable for total alkalinity sample storage. Plastic bottles are lighter, cheaper, and less prone to breakage making them easier to handle and ship. Here, we test the suitability of high-density polyethylene (HDPE) for collection and long-term storage of total alkalinity samples. Duplicate samples were collected in standard borosilicate glass bottles and HDPE bottles on GEOTRACES GP17-OCE. The samples were analyzed in the laboratory over a year later and the storage methods were compared. It was determined that HDPE is not suitable for long-term storage of total alkalinity samples as there were large changes in total alkalinity over time and precision of duplicate samples was very poor. We hypothesize that HDPE plastic is slightly porous leading to leaching of alkalinity either into or out of the bottle over time impacting the value of the sample. Use of HDPE bottles for total alkalinity samples is not recommended for long term sample storage.

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Coverage

Spatial Extent: **N**:-19.99984 **E**:-75.09732 **S**:-67.00024 **W**:-152.00026
Temporal Extent: 2022-12-04 - 2023-01-24

Methods & Sampling

Water samples were collected on R/V Roger Revelle cruise RR2214, the GEOTRACES GP17-OCE expedition, using the ODF CTD rosette.

125-milliliter (mL) high-density polyethylene (HDPE) oblong wide-mouth bottles certified to meet EPA performance-based standards for metals, cyanide, and fluoride (Fisher Scientific product number 05-721-147) and 250 mL borosilicate glass bottles with ground glass stoppers (Corning Inc., 1500-250) were used to collect samples from the CTD rosette. Samples were filled and poisoned with 0.04% saturated HgCl2 following best practices procedures (Dickson et al. 2007). A precise ~1% headspace was created using a pipette. Samples were stored in boxes at room temperature until analysis ~17-19 months after collection. More details can be found in Woosley et al. (submitted).

Instrumentation:
Samples were analyzed in the lab for total alkalinity using a custom-designed open cell titration with non-linear least squares fitting designed and built by the laboratory of Andrew G. Dickson (University of California, San Diego) and described in detail in Dickson et al. (2003).

Data Processing Description

Data were quality controlled and flagged for any known analytical issues that occurred for a given sample. Sample profiles and comparisons to other biogeochemical parameters, and internal consistency calculations using dissolved inorganic carbon and pHt (total scale) were used to flag outliers or questionable data.

BCO-DMO Processing Description

- Imported original file "HDPE & Glass TA Sumit to BCODMO.xlsx" into the BCO-DMO system.
- Marked "-999" and "-999.00" as missing data values (missing data are empty/blank in the final csv file).
- Renamed fields to comply with BCO-DMO naming conventions.
- Created date-time UTC column in ISO 8601 format.
- Saved final file as "957644_v1_ta_hdpe_glass_bottle_comparison.csv".

Problem Description

No known issues occurred aside from changes in sample total alkalinity during storage, which is what the experiment was meant to determine.

WOCE quality flags were used (2 = good, 3 = questionable, 4 = bad, 5 = missing, 6 = average of two duplicates, 9 = not sampled).

Cruise values were flagged based on known analytical issues, inspection of profiles, and internal consistency checks.

For HD,PE which had storage problems, a large number are flagged as 3 or 4 because they are significantly off, but all values were used in data analysis as storage capacity is what was being tested.

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Data Files

File	
957644_v1_ta_hdpe_glass_bottle_comparison.csv	(Comma Separated Values (.csv), 80.83 KB) MD5:5d7e8e6d346edde9d0085ad8a30b3b44
Primary data file for dataset ID 957644, version 1	

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Related Publications

Dickson, A. G., Afghan, J. D., & Anderson, G. C. (2003). Reference materials for oceanic CO2 analysis: a method for the certification of total alkalinity. Marine Chemistry, 80(2), 185–197. https://doi.org/10.1016/S0304-4203(02)00133-0
Methods

Dickson, A.G.; Sabine, C.L. and Christian, J.R. (eds) (2007) Guide to best practices for ocean CO2 measurement. Sidney, British Columbia, North Pacific Marine Science Organization, 191pp. (PICES Special Publication 3; IOCCP Report 8). DOI: https://doi.org/10.25607/OBP-1342
Methods

Woosley, R.J., J.A. Bruno, D. Neithardt, Z.A. Wang, N. Fujiki, and A. Murata. (submitted, 2025) Comparison of open cell and single-step total alkalinity titration methods and implications for organic alkalinity. Limnol. Ocenogr. Meth.
Results

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Related Datasets

IsRelatedTo

Woosley, R., Bruno, J. A., Neithardt, D. (2025) **Open cell and single-step method for total alkalinity titrations from samples collected on R/V Mirai cruises MR23-06C and MR23-07 in the North Pacific and Western Arctic from September to November 2023.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 2) Version Date 2025-07-29 doi:10.26008/1912/bco-dmo.957527.2 [view at BCO-DMO]

Woosley, R., Neithardt, D., Bruno, J. A. (2025) **Total alkalinity from an experiment testing the suitability of high-density polyethylene (HDPE) for collection and long-term storage of total alkalinity samples using laboratory-manipulated oligotrophic Atlantic surface water.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2025-04-03 doi:10.26008/1912/bco-dmo.957694.1 [view at BCO-DMO]

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Parameters

Parameter	Description	Units
GEOTRACES_sample	GEOTRACES sample number	unitless
Event_number	GEOTRACES event number	unitless
Date	Sample collection date	unitless
Time	Sample collection time in UTC	unitless
ISO_DateTime_UTC	Sample collection date and time (UTC) in ISO8601 format	unitless
Sample_ID	Sample identifier composed of formula ("Station"*1000)+("Cast"*100)+("Niskin")	unitless
Station	Station number	unitless
Cast	Cast identifier	unitless
Niskin	Niskin bottle identifier	unitless
Lat	Latitude	decimal degrees
Long	Longitude	decimal degrees
Pressure	Pressure	decibars (db)
Practical_Salinity	Practical salinity in Practical Salinity Units\	PSU
Total_Alkalinity_glass_bottle	Total Alkalinity (glass bottle)	micromoles per kilogram seawater (umol/kg_sw)
Total_Alkalinity_Flag_glass_bottle	WOCE QC flagging scheme	unitless
Total_Alkalinity_HDPE_bottle	Total Alkalinity (HDPE bottle)	micromoles per kilogram seawater (umol/kg_sw)
Total_Alkalinity_Flag_HDPE_bottle	WOCE QC flagging scheme	unitless

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Instruments

Dataset-specific Instrument Name	high-density polyethylene (HDPE) oblong wide-mouth bottles
Generic Instrument Name	High density polyethylene water bottle
Dataset-specific Description	125 mL HDPE oblong wide-mouth bottles certified to meet EPA performance-based standards for metals, cyanide, and fluoride (Fisher Scientific product number 05-721-147) and 250 mL borosilicate glass bottles with ground glass stopper (Corning Inc., 1500-250) were used to collect samples from the CTD rosette.
Generic Instrument Description	A high density polyethylene (HDPE) water bottle. Often used for surface sampling from small boats. HDPE has a somewhat higher chemical resistance than low density polyethylene (LDPE). HDPE is also somewhat harder and more opaque and it can withstand higher temperatures (120 degrees Celsius for short periods, 110 degrees Celsius continuously).

Dataset-specific Instrument Name	Corning Inc., 1500-250
Generic Instrument Name	Pyrex borosilicate water bottle
Dataset-specific Description	125-milliliter (mL) high-density polyethylene (HDPE) oblong wide-mouth bottles certified to meet EPA performance-based standards for metals, cyanide, and fluoride (Fisher Scientific product number 05-721-147) and 250 mL borosilicate glass bottles with ground glass stoppers (Corning Inc., 1500-250) were used to collect samples from the CTD rosette.
Generic Instrument Description	A Pyrex water sampling bottle manufactured by Corning, Inc.

Dataset-specific Instrument Name	custom-designed open cell titration
Generic Instrument Name	Titrator
Dataset-specific Description	Samples were analyzed in the lab for total alkalinity using a custom-designed open cell titration with non-linear least squares fitting designed and built by the laboratory of Andrew G. Dickson (University of California, San Diego) and described in detail in Dickson et al. (2003).
Generic Instrument Description	Titrators are instruments that incrementally add quantified aliquots of a reagent to a sample until the end-point of a chemical reaction is reached.

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Deployments

RR2214

Website	https://www.bco-dmo.org/deployment/905754
Platform	R/V Roger Revelle
Report	https://www.bodc.ac.uk/resources/inventories/cruise_inventory/reports/rogerrevelle_rr2214.pdf
Start Date	2022-12-01
End Date	2023-01-25
Description	The U.S. GEOTRACES GP17-OCE expedition departed Papeete, Tahiti (French Polynesia) on December 1st, 2022 and arrived in Punta Arenas, Chile on January 25th, 2023. The cruise took place in the South Pacific and Southern Oceans aboard the R/V Roger Revelle with a team of 34 scientists led by Ben Twining (Chief Scientist), Jessica Fitzsimmons, and Greg Cutter (Co-Chief Scientists). GP17 was planned as a two-leg expedition, with its first leg (GP17-OCE) as a southward extension of the 2018 GP15 Alaska-Tahiti expedition and a second leg (GP17-ANT; December 2023-January 2024) into coastal and shelf waters of Antarctica's Amundsen Sea. The GP17-OCE section encompassed three major transects: (1) a southbound pseudo-meridional section (~152-135 degrees West) from 20 degrees South to 67 degrees South; (2) an eastbound zonal transect from 135 degrees West to 100 degrees West; (3) and a northbound section returning to Chile (100-75 degrees West). Additional cruise information is available from the following sources: R2R: https://www.rvdata.us/search/cruise/RR2214 CCHDO: https://cchdo.ucsd.edu/cruise/33RR20221201 More information can also be found at: https://usgeotraces.ldeo.columbia.edu/content/gp17-oce

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Project Information

US GEOTRACES GP17-OCE and GP17-ANT: Inorganic Carbon Cycling in the South Pacific and Southern Oceans by Direct Measurement (GP17-OCE and GP17-ANT Inorganic Carbon)

Coverage: South Pacific and Amundsen Sea

NSF Award Abstract

The oceans help to slow climate change by absorbing about a quarter of the carbon dioxide (CO2) produced by burning of fossil fuels and other human activities. The Pacific and Southern Oceans are known to take up and store significant amounts of anthropogenic CO2, but many questions regarding the amount, variability, and biogeochemical and ecological impacts remain unanswered. This research will focus on answering some of those questions in two areas of the Pacific by analyzing samples for total CO2, total alkalinity, and pH on two GEOTRACES cruises, GP17-OCE and GP17-ANT. The project will support several undergraduate student researchers and create educational modules on ocean acidification for general public and K-12 students.

On the GP17-OCE expedition in the south Pacific, sub-decadal scale variability in the uptake of CO2 and resulting decrease in pH (termed ocean acidification) will be examined by comparing data collected on this expedition with data from prior occupations of the line in 1991, 2005 and 2014. An extended multilinear regression technique will be used to separate natural variability from human induced changes. The second expedition, GP17-ANT, covers the Amundsen Sea, an area with few prior carbon measurements. This sea is perennially ice-covered with several seasonal polynyas (areas of open water surrounded by sea ice) and exhibits complex water circulation making the contribution to the global carbon cycle uncertain. The data collected from this expedition will examine several hypotheses regarding how carbon is taken up, mixed, and recirculated in the region, how glacial ice melt, sea ice, and biological productivity influence the carbon cycle, and provide baseline measurements against future data to determine changes in the carbon cycle of the region over time. Both expeditions will leverage the myriad of other parameters being measured, particularly trace metals such as iron and zinc, to examine how cycling of carbon and trace metals are interlinked through pH.

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.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2148468

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