

Bottle sample TA, pH, and DIC collected during an inter-comparison of autonomous in situ instruments for ocean CO₂ measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016

Website: <https://www.bco-dmo.org/dataset/870368>

Data Type: experimental, Other Field Results

Version: 1

Version Date: 2022-03-01

Project

» [A new tool for ocean carbon cycle and ocean acidification studies](#) (Bermuda Biochem Timeseries)

Contributors	Affiliation	Role
DeGrandpre, Michael	University of Montana	Principal Investigator
Martz, Todd R.	University of California-San Diego (UCSD-SIO)	Co-Principal Investigator
Shangguan, Qiwei	University of Montana	Student, Contact
York, Amber D.	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract

This dataset contains total alkalinity (TA), pH, and dissolved inorganic carbon (DIC) from bottle samples collected 3 to 4 times a day. These data were part of an inter-comparison of autonomous in situ instruments for ocean CO₂ measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in August of 2016. These data were published in Shangguan et al. (2022).

Table of Contents

- [Coverage](#)
- [Dataset Description](#)
 - [Methods & Sampling](#)
 - [Data Processing Description](#)
- [Data Files](#)
- [Related Publications](#)
- [Related Datasets](#)
- [Parameters](#)
- [Project Information](#)
- [Funding](#)

Coverage

Temporal Extent: 2016-08-16 - 2016-08-27

Methods & Sampling

Bottle samples are analyzed following descriptions:

The pH samples were analyzed by spectrophotometry immediately after collection using purified mCP. The AT and DIC samples were poisoned and stored following standard protocol (Dickson et al., 2007), and were analyzed within three days using CRMs for quality assurance (Batch 156; see Dickson et al., 2003). AT was determined by open-cell potentiometric titration (Gran, 1952) and a nonlinear least squares approach (Dickson et al., 2007). DIC was determined by acidifying samples and quantifying the extracted CO₂ gas by infrared detection (Goyet and Snover, 1993).

Data Processing Description

Data is output directly from instrumentation.

BCO-DMO Data Manager Processing Notes:

* Data from source file "2016 bottle samples.xlsx" Sheet1 were imported into the BCO-DMO data system. Value "na" in the source file was classified as a missing data identifier.

* Parameters (column names) renamed to comply with BCO-DMO naming conventions. See <https://www.bco-dmo.org/page/bco-dmo-data-processing-conventions>

[[table of contents](#) | [back to top](#)]

Data Files

File
bottle_2016.csv (Comma Separated Values (.csv), 1.98 KB) MD5:f89d037b453be30471028b3891eb6ffe Primary data file for dataset ID 870368

[[table of contents](#) | [back to top](#)]

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](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

Goyet, C., & Snover, A. K. (1993). High-accuracy measurements of total dissolved inorganic carbon in the ocean: comparison of alternate detection methods. *Marine Chemistry*, 44(2–4), 235–242.

[https://doi.org/10.1016/0304-4203\(93\)90205-3](https://doi.org/10.1016/0304-4203(93)90205-3)

Methods

Gran, G. (1952). Determination of the equivalence point in potentiometric titrations. Part II. *The Analyst*, 77(920), 661. doi:10.1039/an9527700661 <https://doi.org/10.1039/AN9527700661>

Methods

Shangguan, Q., Prody, A., Wirth, T. S., Briggs, E. M., Martz, T. R., & DeGrandpre, M. D. (2022). An inter-comparison of autonomous in situ instruments for ocean CO₂ measurements under laboratory-controlled conditions. *Marine Chemistry*, 240, 104085. <https://doi.org/10.1016/j.marchem.2022.104085>

Results

[[table of contents](#) | [back to top](#)]

Related Datasets

IsRelatedTo

Shangguan, Q., DeGrandpre, M., Martz, T. R. (2022) **A pCO₂ time series from a SAMI-CO₂ instrument during an inter-comparison of autonomous in situ instruments for ocean CO₂ measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-01 doi:10.26008/1912/bco-dmo.870390.1 [[view at BCO-DMO](#)]

Relationship Description: Data from different sensors in the same inter-comparison study of autonomous in situ instruments for ocean CO₂ measurements under laboratory-controlled conditions.

Shangguan, Q., DeGrandpre, M., Martz, T. R. (2022) **A pCO₂ time series from a SuperCO₂ benchtop**

instrument during an inter-comparison of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016. Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-01 doi:10.26008/1912/bco-dmo.870401.1 [[view at BCO-DMO](#)]

Relationship Description: Data from different sensors in the same inter-comparison study of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions.

Shangguan, Q., DeGrandpre, M., Martz, T. R. (2022) **Temperature and salinity by a MicroCAT CTD during an inter-comparison of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-01 doi:10.26008/1912/bco-dmo.870412.1 [[view at BCO-DMO](#)]

Relationship Description: Data from different sensors in the same inter-comparison study of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions.

Shangguan, Q., DeGrandpre, M., Martz, T. R. (2022) **Total alkalinity from SAMI-alks during an inter-comparison of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-01 doi:10.26008/1912/bco-dmo.870352.1 [[view at BCO-DMO](#)]

Relationship Description: Data from different sensors in the same inter-comparison study of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions.

Shangguan, Q., DeGrandpre, M., Martz, T. R. (2022) **pH time-series from SAMI-pH and SeapHOx instruments during an inter-comparison of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions at Scripps Institution of Oceanography in 2016.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-03-01 doi:10.26008/1912/bco-dmo.870379.1 [[view at BCO-DMO](#)]

Relationship Description: Data from different sensors in the same inter-comparison study of autonomous in situ instruments for ocean CO2 measurements under laboratory-controlled conditions.

[[table of contents](#) | [back to top](#)]

Parameters

Parameter	Description	Units
time	Timestamp with time zone (UTC) in ISO 8601 format YYYY-MM-DDThh:mmZ	unitless
Bottle_AT	Total alkalinity measured by benchtop instruments	micromoles per kilogram (umol/kg)
Bottle_DIC	DIC measured by benchtop instruments	micromoles per kilogram (umol/kg)
Bottle_pH	pH measured by benchtop instruments	pH scale

[[table of contents](#) | [back to top](#)]

Project Information

A new tool for ocean carbon cycle and ocean acidification studies (Bermuda Biochem Timeseries)

Coverage: Bermuda

NSF abstract:

The ocean inorganic carbon system is of great interest to marine scientists, and indeed all people, because it contains important information about ocean productivity, the sources and sinks of anthropogenic carbon dioxide, and ocean acidification. Total alkalinity is one of the critical inorganic carbon parameters and has been widely measured through ship and laboratory-based methodologies. At this time, there are no commercially-

available in situ sensors for total alkalinity. In this project, researchers at the University of Montana will further develop and test a new autonomous system, known as the SAMI-alk, for measuring total alkalinity. This new system will expand understanding of total alkalinity and the inorganic carbon cycle by making near continuous measurements in locations not frequented by ships. The development of this instrument will have important broader implications for the oceanographic community and ocean acidification research by providing a novel instrument for ocean research. This project will also provide training opportunities to graduate and undergraduate students, and will continue to support public outreach on ocean acidification through a university-affiliated museum.

Studies focused on the marine carbon cycle and ocean acidification pose a number of measurement challenges. While pH is the ocean acidification "smoking gun" and partial pressure of CO₂ is critical for gas exchange calculations, the full inorganic carbon system must be quantified for most inorganic carbon studies. Using autonomous sensors to accurately and precisely quantify all of the inorganic carbon species has been a long-standing objective for marine biogeochemists, but full characterization of the inorganic carbon system has, until recently, been limited to ship and laboratory-based measurements. Total alkalinity is one such parameter as its research has been limited by the lack of instrument capable of making in situ measurements. This research will address this problem and advance inorganic carbon studies through the further development of an autonomous, in situ system to measure seawater total alkalinity, known as the submersible autonomous moored instrument for total alkalinity (SAMI-alk). Preliminary testing of the instrument showed great promise, and through this project, researchers will conduct lab experiments to improve its performance. Two new prototype instruments will be tested in laboratory and field evaluations.

[[table of contents](#) | [back to top](#)]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1459255

[[table of contents](#) | [back to top](#)]