

# Raw pH data acquired during the pH internal consistency experiment.

**Website:** <https://www.bco-dmo.org/dataset/905235>

**Data Type:** experimental

**Version:** 1

**Version Date:** 2023-07-28

## Project

» [Improving Accuracy and Precision of Marine Inorganic Carbon Measurements](#) (Inorganic Carbon Measurements)

Contributors	Affiliation	Role
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## Abstract

These data include the measured pH<sub>T</sub>, total alkalinity, dissolved inorganic carbon, raw pH<sub>T</sub> absorbance, and calculated pH<sub>T</sub> of 25 batches of seawater as a function of temperature, salinity, and pCO<sub>2</sub>. These data were used to evaluate the internal consistency of 120 different possible combinations of CO<sub>2</sub> system constants. The marine inorganic carbon system can be calculated with two measured parameters due to thermodynamic relationships. However, there are many different parameterizations for the required constants and the most accurate or best is not known. These data were used to evaluate the constants and make recommendations for which constants to use, and how to perform CO<sub>2</sub> system calculations.

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## Coverage

**Spatial Extent:** Lat:39.773433 Lon:-70.884417

**Temporal Extent:** 2019-10-10

## Methods & Sampling

Oligotrophic Atlantic surface seawater was collected from 39° 46.406' N and 70° 53.065' W on October 10, 2019.

The surface seawater was modified to five different salinities and 5 different pCO<sub>2</sub> values for a total of 25 batches. Salinity was modified through dilution or evaporation. pCO<sub>2</sub> was modified by bubbling CO<sub>2</sub> gas of different pCO<sub>2</sub> concentrations (balance air).

The water was then bottled and sealed into 250 mL borosilicate glass bottles following SOPs (Dickson et al. 2007). Each batch consisted of 44 bottles.

## Data Processing Description

For each batch the pH<sub>T</sub> was measured at 9 different temperatures.

pH<sub>T</sub> was measured spectrophotometricly using purified meta-cresol indicator dye with an Agilent 8454 spectrophotometer following SOP (Dickson et al. 2007 and Woosley (2021)) and the indicator calibration equations of Liu et al. (2011).

## BCO-DMO Processing Description

- \* Related data DIC, TA, equilibrium pCO<sub>2</sub> can be found in the related summary dataset.
- \* Adjusted column names to fit database requirements.

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## Data Files

File
<b>905235_v1_rawph.csv</b> (Comma Separated Values (.csv), 303.87 KB) MD5:adefcb2cbac5a23c4dfd118660c19f20
Primary datafile for dataset 905235

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## Related Publications

Dickson, A.G.; Sabine, C.L. and Christian, J.R. (eds) (2007) Guide to best practices for ocean CO<sub>2</sub> 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*

Liu, X., Patsavas, M. C., & Byrne, R. H. (2011). Purification and Characterization of meta-Cresol Purple for Spectrophotometric Seawater pH Measurements. Environmental Science & Technology, 45(11), 4862–4868. doi:[10.1021/es200665d](https://doi.org/10.1021/es200665d)

*Methods*

Woosley, R. J. (2020). Evaluation of the temperature dependence of dissociation constants for the marine carbon system using pH and certified reference materials. Marine Chemistry, 103914.

doi:[10.1016/j.marchem.2020.103914](https://doi.org/10.1016/j.marchem.2020.103914)

*Methods*

Woosley, R. J., & Moon, J.-Y. (2023). Re-evaluation of carbonic acid dissociation constants across conditions and the implications for ocean acidification. Marine Chemistry, 250, 104247.

<https://doi.org/10.1016/j.marchem.2023.104247>

*Results*

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## Related Datasets

### IsSourceOf

Woosley, R. (2023) **Measured pH and nutrient data acquired during the pH internal consistency experiment**. Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version

Date 2023-08-01 doi:10.26008/1912/bco-dmo.905357.1 [[view at BCO-DMO](#)]  
*Relationship Description: Contains raw data as basis for the summary table.*

## IsRelatedTo

Woosley, R. (2023) **Total alkalinity and dissolved inorganic carbon data measured during the pH internal consistency experiment.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2023-07-31 doi:10.26008/1912/bco-dmo.905278.1 [[view at BCO-DMO](#)]  
*Relationship Description: Data is part of the same experiment.*

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## Parameters

Parameter	Description	Units
Batch	Seawater batch number	unitless
Bottle	sample bottle number	unitless
Rep	Sample measurement repetition	unitless
Practical_Salinity	Salinity	unitless
Calculated_Temperature	Temperature used to calculate pH	Degrees Celsius (°C)
Measured_Temperature	Measured Temperature	Degrees Celsius (°C)
A434	Absorbance at 434 nm	Absorbance units (AU)
A578	Absorbance at 578 nm	Absorbance units (AU)
A730	Absorbance at 730 nm	Absorbance units (AU)
A488	Absorbance at 488 nm	Absorbance units (AU)
R	Absorbance Ratio	Absorbance units (AU)
raw_pHt	measured pHt without indicator perturbation corection	unitless
flag	quality control flag (2 = good, 3 = questionable, 4 = bad, 5 = missing)	unitless
flag_reason	reason for QC flags 3-5	unitless

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## Instruments

<b>Dataset-specific Instrument Name</b>	Agilent 8454 spectrophotometer
<b>Generic Instrument Name</b>	Spectrophotometer
<b>Generic Instrument Description</b>	An instrument used to measure the relative absorption of electromagnetic radiation of different wavelengths in the near infra-red, visible and ultraviolet wavebands by samples.

## Project Information

### Improving Accuracy and Precision of Marine Inorganic Carbon Measurements (Inorganic Carbon Measurements)

**Coverage:** Lab studies

#### *NSF Award Abstract:*

The oceans absorb about one third of the CO<sub>2</sub> humans release into the atmosphere from the burning of fossil fuels and other activities. While ocean uptake of CO<sub>2</sub> slows its rate of increase in the atmosphere, it comes with costs for the oceans and the organisms that live there. Once in seawater, CO<sub>2</sub> reacts with water to produce bicarbonate and hydrogen ions. The increase in hydrogen ions lowers the pH in a process called ocean acidification. Not all areas of the ocean are affected equally. The solubility of CO<sub>2</sub> is greater in the cold waters of the Arctic making them more prone to ocean acidification. However, due to the low temperatures and low salinities in the Arctic, the uncertainties in pH values are much larger there than for the other oceans. This project evaluates pH at low temperatures and salinities, and develops best practice recommendations to improve the ability to compare measurements among laboratory groups and studies and reduce overall uncertainty in the measurements. The project provides training for an undergraduate student and promotes awareness of ocean acidification through public outreach.

Having highly accurate and precise measurements are important for monitoring changes to pH and CO<sub>2</sub> uptake through time and the effects on marine life. In order to improve pH measurements for polar waters, several different experiments will be conducted. The temperature dependence of pH will be determined from 30°C to near freezing for low salinity waters. The results will be compared to current chemical models to quantify offsets and biases. Recommendations will be made for the best physical chemical model to use for low temperature and salinity seawater. Moreover, pH is measured spectrophotometrically using an indicator dye. Preparation and calibration of the indicator is important to standardize studies across space and time and ensure comparability. Indicator quality is essential for detecting ocean acidification, but its stability is currently unknown. If the dye degrades after production, biases or artifacts in pH measurements may result as the dye ages. Experiments will be undertaken using batches of dyes from weeks to over 10 years old to resolve its degradation characteristics. The experiments will establish how long a batch of dye remains valid once it is prepared without biasing the measurements. This is particularly important for long term studies such as extended research expeditions and autonomous systems where a batch of dye may be used over a year. Together, by both investigating the validity of chemical models for seawater pH at low temperature and salinity and examining the stability of the pH indicator dye, methodological uncertainties can be reduced to permit better monitoring of changes in global ocean 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.

## Funding

Funding Source	Award
<a href="#">NSF Division of Ocean Sciences (NSF OCE)</a>	<a href="#">OCE-1923312</a>