Results of x-ray diffraction (XRD) analyses collected for various Oceanic Flux Program (OFP) samples and end members for the for OFP/fish carbonate study

Website: https://www.bco-dmo.org/dataset/960297
Data Type: Cruise Results, Other Field Results
Version: 1
Version Date: 2025-05-08

Project
» OCE-PRF: Towards Quantifying Calcium Carbonate Sediment Dissolution During Marine Diagenesis (Marine CaCO3 and ocean chemistry)

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Abstract
These data include results of x-ray diffraction (XRD) analyses, such as mineral abundances and magnesium (Mg) content in calcite, that were collected for various Oceanic Flux Program (OFP) samples and end members such as fish carbonates, bryozoan, and coccolithophore for OFP/fish carbonate study. The sources of samples are included in the dataset, and for samples that were obtained from cruises, the cruise number is included. The raw data are included as supplemental files.

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Coverage

Spatial Extent: **N**:31.9167 **E**:145.4464 **S**:-14.6786 **W**:-76.3272

Methods & Sampling

Measurements were conducted using a PANalytical X'Pert PRO X-ray powder diffractometer using a copper (Cu) anode and an X'Celerator Scientific 1D position-sensitive detector in Bragg-Brentano geometry and were processed using the fundamental-parameters Rietveld refinement software TOPAS V7 (Coelho, 2018).

Data Processing Description

Data were processed using Rietveld refinement using TOPAS V7. The raw data are included as supplemental files.

BCO-DMO Processing Description

- Imported original file "XRD results.xlsx" into the BCO-DMO system.
- Flagged "NA" as a missing data identifier (missing data are blank/empty in the final CSV file).
- Made south latitude values negative.
- Made west longitude values negative.
- Renamed fields to comply with BCO-DMO naming conventions.
- Saved the final file as "960297_v1_xrd_results.csv".
- Opened original data file "Raw XRD data.xlsx" and created separate files for each run; then, saved the 3 supplemental files in CSV format.

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Data Files

File	
960297_v1_xrd_results.csv	(Comma Separated Values (.csv), 6.74 KB) MD5:c32222f4ff94cfd2ea31bcc5ebc9ce33
Primary data file for dataset ID 960297, version 1	

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Supplemental Files

File	
raw_xrd_run_04-25-23.csv	(Comma Separated Values (.csv), 991.71 KB) MD5:c13f6db76c852884d8c15f10c366ca9d
Supplemental file for dataset ID 960297, version 1. Raw Xay diffraction data; from run on 04-25-23.	
raw_xrd_run_06-03-04-23.csv	(Comma Separated Values (.csv), 892.18 KB) MD5:59b675f2b7897214a3c7c9b64fdbc446
Supplemental file for dataset ID 960297, version 1. Raw Xay diffraction data; from runs on 06-03-23 and 06-04-23.	
raw_xrd_run_08-23-23.csv	(Comma Separated Values (.csv), 234.55 KB) MD5:622c2936ab60e2593f969b08cc74390a
Supplemental file for dataset ID 960297, version 1. Raw Xay diffraction data; from run on 08-23-23.	

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Related Publications

Coelho, A. A. (2018). TOPAS and TOPAS-Academic: an optimization program integrating computer algebra and crystallographic objects written in C++. Journal of Applied Crystallography, 51(1), 210–218. https://doi.org/10.1107/s1600576718000183 https://doi.org/10.1107/S1600576718000183
Software

Hashim, M., Conte, M., Salter, M., A., Pedrosa-Pamies, R. Weber, J. C., Hayden M., Wilson R., Perry, C., Crowley, S.F., Dennis, P.F., Bish, D., and Subhas, A.V. 2025. Fish Carbonates in the Open Ocean and Their Role in the Carbon Cycle. In revision at Global Biogeochemical Cycles.
Results

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Parameters

Parameter	Description	Units
Sample_ID	The ID of the analyzed sample	unitless
Sample_type	The category the sample belongs to	unitless
Sample_source	Source of the sample	unitless
Trap_depth	Trap depth	meters (m)
Latitude	Latitude of sample collection	decimal degrees
Longitude	Longitude of sample collection	decimal degrees
Phase	Phase: A or B. Most samples contained more than one calcite phase, each with a separate peak in the XRD data. The intensity and peak position for each phase were used to determine the phase abundance and calcite Mg content. Phases are given a purely descriptive term: "A" or "B".	unitless
Mg_content	The Mg content in calcite	mol percent
calcite_phase	The weight percent of calcite	weight percent
calcite_phase_error	The error of the weight percent of calcite	weight percent

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Instruments

Dataset-specific Instrument Name	PANalytical X'Pert PRO X-ray powder diffractometer
Generic Instrument Name	X-ray diffractometer
Generic Instrument Description	Instruments that identify crystalline solids by measuring the characteristic spaces between layers of atoms or molecules in a crystal.

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Deployments

OFP_Time-Series

Website	https://www.bco-dmo.org/deployment/704779
Platform	OFP_mooring
Start Date	1978-04-06
Description	The Oceanic Flux Program (OFP) time-series began in 1978 at the Hydrostation S hydrographic time-series site (32 05N, 64 15W), located approximately 45 km southeast of Bermuda. The time-series was originally called the SCIFF (Seasonal Changes in Isotopes and Flux of Foraminifera) program. Location: 1978-1984: 31deg 10min N, 64deg 30min W, 3300m (SCIFF site) 1984-2010: 31deg 50min N, 64deg 10min W, 4500m 2011-present: 31deg 55 N, 64deg 05 W, 4550m

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Project Information

OCE-PRF: Towards Quantifying Calcium Carbonate Sediment Dissolution During Marine Diagenesis (Marine CaCO3 and ocean chemistry)

NSF Award Abstract:
OCE-PRF Towards Quantifying Calcium Carbonate Sediment Dissolution During Marine Diagenesis The goal of the project is to investigate dissolution of calcium carbonate (CaCO3) in sediments below the seafloor and determine its importance to the chemistry of seawater. This project uses sediment samples and chemical data collected from different parts of the ocean during the past five decades by scientific ocean drilling programs. Sediment dissolution of carbonate can lessen the impact of ocean acidification, the process that causes the pH of the ocean to decrease due to the uptake of carbon dioxide (CO2) from the atmosphere. Ocean acidification threatens the survival of marine organisms, such as oysters, clams, and coral reefs, which could alter marine food chains and food supply to humans. By improving understanding of carbonate dissolution in the ocean, results from this project will enable better predictions of the effects of ocean acidification on marine organisms. This will advance the progress of science and contribute to the knowledge that can inform public policy. In addition, understanding carbonate sediment dissolution serves other important purposes. For example, dissolution can create small spaces between sediments that may get filled with groundwater once sediments convert to rocks over millions of years. Thus, understanding the occurrence and spatial distribution of spaces within rocks may help determine the volume and movement of groundwater in subsurface aquifers. This project provides support for a postdoctoral research fellow and research training opportunities for students through the Summer Student Fellowship and Woods Hole-wide Partnership Education Programs at the Woods Hole Oceanographic Institution.

Carbonate mineral dissolution is an integral part of the alkalinity and carbon cycles in the ocean and is expected to play an increasingly significant role in mediating changes in ocean chemistry as atmospheric CO2 continues to rise. The goal of this project is to provide thermodynamic constraints necessary for quantifying carbonate sediment dissolution in marine diagenetic environments. Specifically, the CaCO3 saturation state of pore fluids will be calculated in 365 globally distributed sites from previous scientific ocean drilling expeditions using a specially developed Pitzer ion activity model which is particularly useful for calculating activity coefficients in

high ionic strength solutions such as those that characterize most diagenetic environments. These calculations will be substantiated with geochemical and textural analyses of sediment samples from four representative sites to identify the specific diagenetic processes (e.g., dissolution, precipitation, and recrystallization) and document the conditions responsible for their occurrence and prevalence. The immediate advantage of calculating the saturation state of pore fluids is that such data can be used to estimate carbonate sediment dissolution below the seafloor and quantify its contribution to the alkalinity and carbon cycles, which will lead to more accurate predictions of the consequences of ocean acidification. Another benefit of the global saturation state dataset is that it will improve our understanding of authigenic carbonate precipitation and its link to the carbon cycle over Earth history, which has been proposed as a significant sink for carbon. Furthermore, by complementing the thermodynamic calculations with textural and geochemical analyses, this project will parse out various diagenetic processes and identify the sedimentological and geochemical conditions responsible for their occurrence. Such knowledge is crucial for evaluating the impact of diagenesis on the carbonate-hosted paleoenvironmental proxies. Collectively, this project will pave the way towards a mechanistic understanding of carbonate diagenesis. This will provide important constraints on the oceanic alkalinity cycle, carbon burial rates, and geochemical proxies, which ultimately help us better understand the future of our ocean system in the context of climate change.

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-2205984

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