NOAA Technical Report, OAR-AOML-57

https://doi.org/10.25923/kgzg-0w86

GO-SHIP A13.5 2024:

NOAA Quality Control and Data Analysis

Report for the Inorganic Carbon Parameters

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Miami, Florida

October 2025

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Suggested Citation

Schockman, K.M. 2025; GO-SHIP A13.5 2024: NOAA quality control and data analysis report for the inorganic carbon parameters. NOAA Technical Report, OAR-AOML-57 (doi: 10.25923/kgzg-0w86), 40 pp.

Acknowledgements

The GO-SHIP cruises are sponsored by NOAA's Global Ocean Monitoring and Observing Program (GOMO) and the National Science Foundation (NSF). KS acknowledges funding from NOAA's GOMO (Fund Reference Number 100018302, https://ror.org/037bamf06). Data were collected and made publicly available by the U.S. GO-SHIP (https://usgoship.ucsd.edu/) and the programs that contribute to it. Thank you to the many individuals on shore and on the *R/V Marcus G. Langseth* who contributed to the successful completion of the cruise. Thanks also to the science party analysts, including Charles Featherstone, Evan Josza, Patrick Mears, Dr. Yifan Li, Dr. Bo Yang, Clara Haughey-Gramazio, and Eva Jundt for their work measuring the inorganic carbon parameters. This research was carried out in part under the auspices of the Cooperative Institute for Marine and Atmospheric Studies (CIMAS), a Cooperative Institute of the University of Miami and the National Oceanic and Atmospheric Administration, cooperative agreement #NA20OAR4320472.

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Report for the Inorganic Carbon Parameters

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October 2025

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NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION
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Acronyms

GO-SHIP	Global Ocean Ship-Based Hydrographic Investigations Program
AOML	Atlantic Oceanographic and Meteorological Laboratory
CIMAS	Cooperative Institute for Marine and Atmospheric Studies
GOMO	Global Ocean Monitoring and Observing Program
NSF	National Science Foundation
QC	Quality control
CRM	Certified reference material
CO_2	Carbon dioxide
DIC	Total dissolved inorganic carbon
TA	Total alkalinity
fCO_2	Fugacity of carbon dioxide
WOCE	World Ocean Circulation Experiment
CTD	Conductivity/temperature/depth
CCHDO	Clivar and Carbon Hydrographic Data Office
PI	Principal investigator
RSMAES	Rosenstiel School of Marine, Atmospheric, and Earth Science
PMEL	Pacific Marine Environmental Laboratory
CICOES	Cooperative Institute for Climate, Ocean, and Ecosystem Studies
mCP	meta-cresol purple
K_1, K_2	Carbonic acid dissociation constants
K_{HSO4}	Bisulfate dissociation constant
K_{HF}	Hydrogen fluoride dissociation constant
B_T/S	Total boron to salinity ratio
S_P	Salinity, practical scale
O_2	Oxygen
Stdev	Standard deviation

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Abstract

The Global Ocean Ship-Based Hydrographic Investigations Program (GO-SHIP) A13.5 2024 cruise took place onboard the *R/V Marcus G. Langseth* from February 1 to March 23, 2024, traveling between Mindelo, Cabo Verde and Cape Town, South Africa. This technical report documents and details the quality control (QC) procedures and data analyses of the inorganic carbon parameter measurements (total alkalinity, TA (μmol kg^{-1}); total dissolved inorganic carbon, DIC (μmol kg^{-1}); pH on the total scale at 25 °C, $pH_T(25)$; and fugacity of CO_2 at 20 °C, $fCO_2(20)$ (μatm)) from 112 conductivity/temperature/depth (CTD) stations. After preliminary QC analyses at sea, secondary QC analyses and internal consistency assessments were conducted in this report as a means to standardize the QC protocols and ensure a fully consistent dataset for all four inorganic carbon parameters. Analyses highlight that the inorganic carbon measurements for the A13.5 2024 cruise follow best-practice measurement protocols.

1. Introduction

The U.S. Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP) A13.5 2024 cruise, led by Chief Scientist Dr. Zachary Erickson and Co-Chief Scientist Dr. Jesse Anderson, took place onboard the *R/V Marcus G. Langseth* from February 1 to March 23, 2024, traveling between Mindelo, Cabo Verde and Cape Town, South Africa (Fig. 1). Conductivity/temperature/depth (CTD) casts were conducted at 112 stations, and included measurements of physical properties (salinity (via conductivity), temperature, depth (via pressure)), inorganic carbon parameters (total alkalinity, TA; total dissolved inorganic carbon, DIC; pH on the total scale at 25 °C, $pH_T(25)$; fugacity of carbon dioxide (CO_2) at 20 °C, $fCO_2(20)$), nutrient concentrations (nitrate, nitrite, phosphate, silicate), dissolved oxygen concentration, trace gases (chlorofluorocarbons, CFCs; sulfur hexafluoride, SF_6; nitrous oxide, N_2O), and other ancillary measurements including biological sampling, organic concentrations (dissolved organic carbon), and isotopes (carbon, nitrogen, oxygen). The full cruise report and complete dataset are available for download on the Clivar and Carbon Hydrographic Data Office (CCHDO) website (EXPOCODE: 33H320240201; https://cchdo.ucsd.edu/cruise/33H320240201). This report documents and details the quality control (QC) procedures and data analyses of the inorganic carbon parameter measurements (TA (µmol kg^{-1}), DIC (µmol kg^{-1}), $pH_T(25)$, and $fCO_2(20)$ (µatm)).

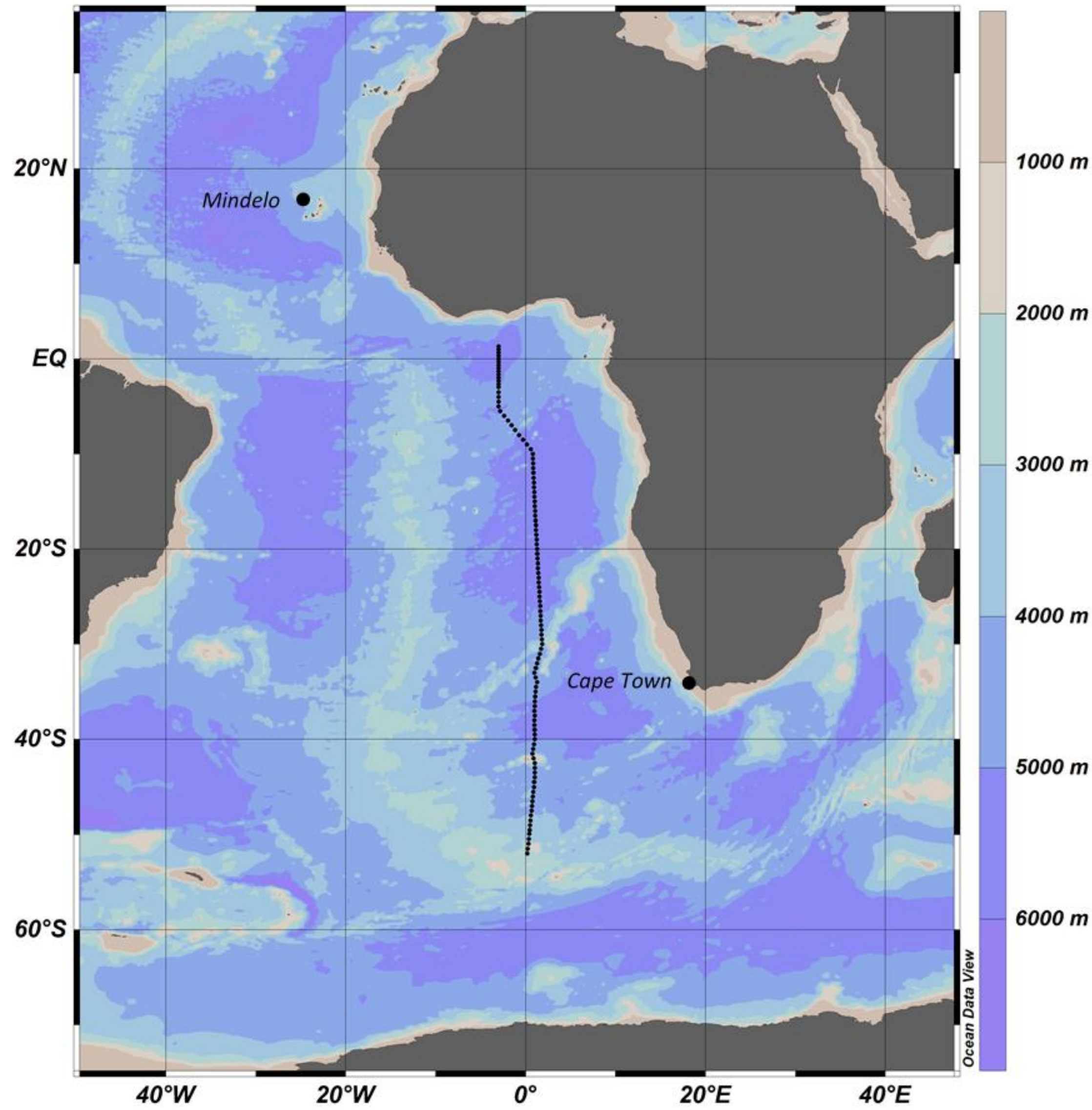

Fig. 1. GO-SHIP A13.5 2024 cruise track.

2. Methods

2.1 Data Collation and Primary QC

Details of the measurement protocols for all parameters can be found in the full cruise report. The principal investigators (PI) and analysts for the four inorganic carbon parameters are given in Table 1, with a full list of PIs and analysts for all cruise measurements in the full cruise report. Every sample on the cruise was assigned a sample ID: sample ID = 10000*station + 100*cast + bottle number. While onboard, initial quality flags were assigned to each inorganic carbon measurement following the World Ocean Circulation Experiment (WOCE) protocols as defined in Table 2 (WHP, 1998).

Table 1

PIs and analysts, along with their affiliated institutions, for each of the inorganic carbon parameter measurements. Note: RSMAES – Rosenstiel School of Marine, Atmospheric, and Earth Science; PMEL – Pacific Marine Environmental Laboratory; AOML – Atlantic Oceanographic and Meteorological Laboratory; CICOES – Cooperative Institute for Climate, Ocean, and Ecosystem Studies; and CIMAS – Cooperative Institute for Marine and Atmospheric Studies.

Parameter	PI(s)	Institution	Analyst	Institution
TA	Dr. Chris Langdon	U. Miami (RSMAES)	Dr. Bo Yang	U. Miami (RSMAES)
DIC	Dr. Richard Feely Dr. Rik Wanninkhof	NOAA PMEL NOAA AOML	Charles Featherstone Evan Josza	NOAA AOML U. Washington (CICOES)
$pH_T(25)$	Dr. Chris Langdon	U. Miami (RSMAES)	Clara Haughey-Gramazio Eva Jundt	U. Miami (RSMAES) U. Miami (RSMAES)
$fCO_2(20)$	Dr. Rik Wanninkhof	NOAA AOML	Patrick Mears Dr. Yifan Li	U. Miami (CIMAS) U. Delaware

Table 2
WOCE data quality flags used in the GO-SHIP A13.5 2024 dataset for inorganic carbon water samples (WHP, 1998).

Flag Value	Definition
2	Acceptable measurement
3	Questionable measurement
4	Bad measurement
5	Not reported
6	Mean of replicate measurements
9	Sample not drawn for this measurement from this bottle

During and after the cruise, some adjustments were made to the inorganic carbon measurements unique to each parameter. For pH_T, measurements were performed near 25 °C, with the exact temperature recorded, and then adjusted to a temperature of 25 °C for reporting purposes (denoted as $pH_T(25)$). Additionally, pH_T measurements were corrected onboard for small perturbations caused by the indicator dye (meta-cresol purple, mCP) on the sample (for more details, see the full cruise report). For $f\mathrm{CO_2}$, measurements were performed near 20 °C, with the exact temperature recorded, and then adjusted to a temperature of 20 °C for reporting purposes (denoted as $f\mathrm{CO_2}(20)$). Additionally, $f\mathrm{CO_2}$ samples were calibrated using standard gases measured before and after each set of up to 12 samples (for more details, see the full cruise report). Subsequent QC checks were performed by the parameter leads after all corrections and adjustments were made to flag any noticeable outliers.

The precision of measurements for each of the inorganic carbon parameters was assessed through routine duplicate measurements on a subset of samples throughout the cruise (Tables 3–6; see Additional Tables section below). For full, 24-bottle Niskin casts, TA and $pH_T(25)$ generally selected two sets of duplicates randomly throughout the cast. Each duplicate pair was run back-to-back during analysis. TA and $pH_T(25)$ used one sample bottle for both measurements, so the duplicate pairs were generally the same for both parameters. For DIC, typically three sets of duplicates were randomly selected from near the bottom, mid-depth, and surface Niskin bottles. Each duplicate pair was spread out throughout the titration cell run, with duplicate measurements specifically not run back-to-back. For $f\text{CO}_2(20)$, generally one set of duplicates was randomly selected throughout the cast. The duplicate pair was run back-to-back during analysis. To read more details about duplicate measurements, please see the full cruise report.

2.2 Secondary QC

After the primary QC discussed above, the inorganic carbon data were collated to perform secondary QC checks. Measurements of TA, DIC, $\text{pH}_\text{T}(25)$, and $f\text{CO}_2(20)$ with WOCE quality flags of 2, 3, 4, and 6 (Table 2) were kept for this analysis. Internal consistency of these measurements was assessed by comparing measured and calculated values for each of the inorganic carbon parameters. Generally, the closer measured and calculated values are to one another, the more internally consistent the dataset is said to be. Calculations of the inorganic carbon parameters were made using CO2SYS (Pierrot et al., 2006; Van Heuven et al., 2011) version 3.1.1 for MATLAB (Sharp et al., 2020). All calculations were performed on the total pH_T scale using the following parameters: carbonic acid dissociation constants (K_1 and K_2) of Lueker et al. (2000), bisulfate dissociation constant (K_{HSO4}) of Dickson (1990), hydrogen fluoride dissociation constant (K_{HF}) of Perez and Fraga (1987), and total boron to salinity ratio (B_T/S) of Lee et al. (2010). Calculations generally utilized the salinities (practical scale; S_P) from discrete bottles measured onboard unless the measured salinity value was not flagged as 2 or 6, in which case the salinity value from the CTD sensor was used.

Calculated values of a parameter X obtained using inputs of Y and Z are denoted throughout the document as 'X(Y,Z)'. The difference between measured X and X(Y,Z) is a residual of X and is denoted as 'ΔX' (i.e., $\Delta X = X - X(Y,Z)$). As all four inorganic carbon parameters were measured, and only two parameters are required for a single calculation, each inorganic carbon parameter was generally calculated using three sets of combination pairs (i.e., TA can be calculated using (DIC, $pH_T(25)$), (DIC, $fCO_2(20)$), and ($pH_T(25)$, $fCO_2(20)$)). If any of the inorganic carbon parameter measurements were missing for that sample, only the available combination pairs were used. Calculations using the ($pH_T(25)$, $fCO_2(20)$) input pair were used for analyses in some situations, especially where one of the other inorganic carbon parameters was missing, but are generally not shown throughout the document as they are not recommended according to best practices (Patsavas et al., 2015). The residuals for each of the inorganic carbon parameters were analyzed to check for outlier sample values via a quantitative process described below.

For all 112 stations, depth profiles were created for measurements of discrete oxygen (O_2), CTD sensor O_2, discrete S_P, CTD sensor S_P, TA, DIC, $pH_T(25)$, and $fCO_2(20)$. These depth profiles were used in this work for visual indication of potential outliers and/or Niskin bottles fired/closed at incorrect depths.

2.3 Certified Reference Material (CRM) Checks Throughout the Cruise

CRMs provided by Dr. Andrew Dickson's laboratory at Scripps Institution of Oceanography were used to assess the accuracy of both TA and DIC measurements throughout the cruise. For TA measurements, CRMs were used to standardize the HCl acid concentration used in the TA titrations and to check that the system was functioning properly. For each DIC system, CRMs were run at the beginning of a subset of sample measurements corresponding to a specific titration cell, which typically was used for one station's worth of samples. The difference between the measured CRM DIC value and certified CRM DIC value was used to adjust the system for that specific subset of measurements. For more details, see the full cruise report.

3. Results

3.1 Primary and Secondary QC Checks

The duplicate measurements of TA, DIC, $pH_T(25)$, and $fCO_2(20)$ are provided in Tables 3–6, including both individual duplicate values and the absolute difference between the two measurements. The average ± standard deviation (stdev; 1σ) of the absolute differences between duplicates for each parameter is as follows — TA: 1.2 ± 1.0 µmol kg^{-1} (n = 123 duplicate measurement pairs); DIC: 1.3 ± 1.0 µmol kg^{-1} (n = 319 duplicate measurement pairs); $pH_T(25)$: 0.0025 ± 0.0034 (n = 194 duplicate measurement pairs); and $fCO_2(20)$: 1.7 ± 2.6 µatm (0.2% ± 0.2%) (n = 147 duplicate measurement pairs) (Table 7).

Table 7
Inorganic carbon parameter statistics from the primary and secondary QC checks. Data include the average absolute difference between duplicate measurements ± 1σ stdev for each parameter. Also shown are the mean calculated residuals (measured – calculated) ± 3σ stdev threshold values for each parameter subsetted by input pair used in the calculations.

Parameter	Measurements: Avg. duplicate difference ± 1σ stdev	Calculations: Mean residual ± 3σ stdev
TA ($\mu mol\ kg^{-1}$)	1.2 ± 1.0 (n = 123)	DIC, pH_T(25): –1 ± 13 DIC, fCO_2(20): –6 ± 12
DIC ($\mu mol\ kg^{-1}$)	1.3 ± 1.0 (n = 319)	TA, pH_T(25): 1 ± 12 TA, fCO_2(20): 5 ± 15
pH_T(25)	0.0025 ± 0.0034 (n = 194)	TA, fCO_2(20) and DIC, fCO_2(20): –0.01 ± 0.02 TA, DIC: 0.00 ± 0.03
fCO_2(20) (µatm)	1.7 ± 2.6 (n = 147)	TA, pH_T(25) and DIC, pH_T(25): –3% ± 4% TA, DIC: –3% ± 7%

Residuals of TA, DIC, pH_T(25), and fCO_2(20) were calculated with the full dataset using all available sets of input pairs. The mean residuals ± 3σ stdev for residuals calculated using various sets of input pairs are provided in Table 7. These mean residuals ± 3σ stdev values were used as a quantitative threshold for quality control purposes. Any residual greater than 3σ from the mean residual value was flagged for further analysis. A list of samples was collated based on these residual flagging guidelines and sent to each of the responsible PIs for additional inspection. Also included in the list were sample points originally flagged as 3 or 4 onboard, but had calculated residuals within the thresholds and no visual indications of an outlier. In these cases, the recommendation was for the PI to check the original data to determine if any of these flags should be changed to a 2.

In general, residuals calculated using one temperature independent parameter (i.e., TA or DIC) and one temperature dependent parameter ($pH_T(25)$ or $fCO_2(20)$) were preferred for flagging purposes. Due to the availability of multiple residuals for each inorganic carbon parameter, it was often clear which, if any, of the four parameters was an incorrect value. As an example, for sample ID #130101, ΔDIC was –22.6 $\mu mol\ kg^{-1}$ using the (TA, $pH_T(25)$) pair and –1.6 $\mu mol\ kg^{-1}$ using the (TA,$fCO_2(20)$) pair. Similarly, ΔTA was 23.3 $\mu mol\ kg^{-1}$ using the (DIC, $pH_T(25)$) pair and 1.8 $\mu mol\ kg^{-1}$ using the (DIC,$fCO_2(20)$) pair. Furthermore, $\Delta pH_T(25)$ residuals calculated using all input pairs were on the order of –0.05, which is larger than the 3σ stdev threshold. It would be reasonable to state that the $pH_T(25)$ value for this sample is likely an outlier, while the TA, DIC, and $fCO_2(20)$ measurements are more internally consistent with one another. In this instance, the recommendation would be to flag this $pH_T(25)$ sample as a 4. In cases where multiple residuals for an individual sample were large and it was unclear which parameter may be incorrect, additional data and visual identification were used for further inspection.

All points visually identified as outliers in the depth profiles of TA, DIC, $pH_T(25)$, and $fCO_2(20)$ were included in the list of sample points sent to PIs for additional inspection. Depth profiles of CTD sensor O_2 and discrete O_2 were used to determine if a Niskin bottle had been misfired at an incorrect depth and/or if a Niskin bottle had leaked. Comparisons of CTD sensor S_P and discrete S_P were also used as a secondary check for Niskin bottle issues. The sampling log sheets and CTD console log sheets were checked for any reported issues at the time of the CTD cast and/or sampling during the cruise. The combination of depth profiles and log sheet checks was used to assign Niskin bottle flags for each sample to be included in the full dataset on CCHDO.

Overall, the recommendations for flag changes were assembled and sent to each of the PIs/parameter leads who checked the data points and had the ultimate say for which (if any) flags should be changed. The number of recommended flag changes and the percentage of these flag changes accepted for each parameter are provided in Table 8. In some cases, the PI/parameter leads concluded that a flagged parameter value in question was incorrect, and an updated value was provided in lieu of changing the flag designation (these values were still counted as "accepted flag changes" in Table 8). Once the data values and flags were updated, the final inorganic carbon data were submitted to CCHDO to be included with the full cruise dataset.

Table 8
The number of flag changes recommended to each inorganic carbon PI and the number of flag changes accepted (both as a number and as a percentage of the total recommended).

Parameter	Recommended flag changes	Accepted flag changes	Percentage of recommended flag changes accepted
TA	32	30	94%
DIC	14	13	93%
$pH_T(25)$	26	26	100%
$fCO_2(20)$	5	5	100%

3.2 CRM Checks Throughout the Cruise

For A13.5 2024 DIC measurements, 115 CRMs were run on two identical systems denoted as AOML3 (n = 59) and AOML4 (n = 56). The average absolute difference between the measured CRM DIC and certified CRM DIC values was 2.7 ± 1.2 μmol kg^{-1} (1σ) for AOML3 and 1.2 ± 0.9 μmol kg^{-1} (1σ) for AOML4. The differences between measured CRM DIC and certified CRM DIC values remained generally constant throughout time for both systems, with measured CRM DIC value being consistently larger than the respective certified CRM DIC values (Fig. 2). For additional details regarding CRM usage for HCl standardization in TA measurements, please reach out to the individual PI (Table 1).

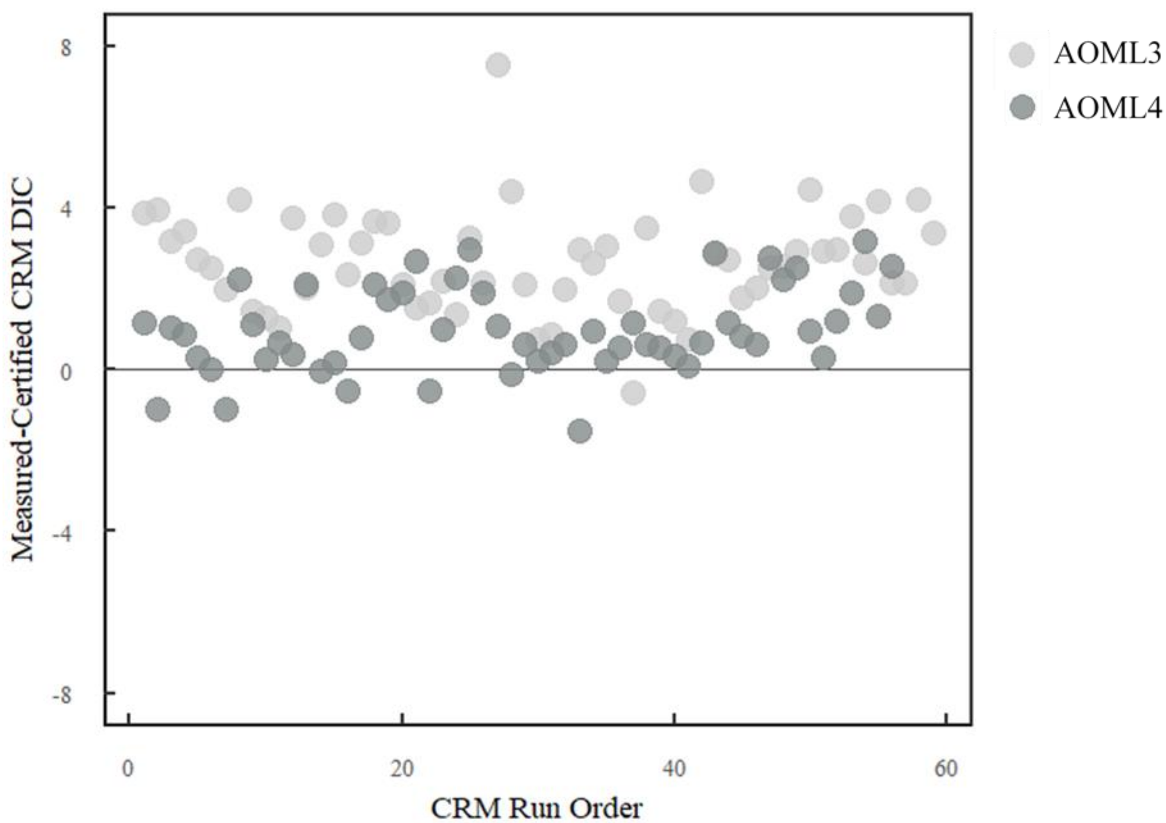

Fig. 2. Differences between measured CRM DIC and certified CRM DIC values shown in terms of the order the CRMs were measured (i.e., throughout the duration of the cruise). As specified above, each difference value between the measured CRM DIC and certified CRM DIC was used to adjust the corresponding subset of measurements for that titration cell, which was replaced approximately every 12 hours. Color denotes the DIC system (AOML3 or AOML4) that corresponds to the CRM measurement.

3.3 CO_2-System Internal Consistency

Internal consistency assessments shown below were made using the final dataset of inorganic carbon parameters on CCHDO after PI flag changes were incorporated (https://cchdo.ucsd.edu/cruise/33H320240201). Residuals were calculated for all samples where at least three or more inorganic carbon parameters were measured using all available sets of input parameters. Only data with good (2) or duplicate (6) data flags were used for these final internal consistency assessments. (Initial internal consistency assessments were used as a means of secondary QC as described above. However, the data ultimately determined to be questionable (3) or bad (4) quality were removed from this final assessment.)

Residuals of TA and DIC (denoted as ΔTA and ΔDIC) are generally evenly distributed about zero for the full range of measured TA and DIC (Figs. 3 and 4). For calculations of both TA and DIC, residuals calculated using $fCO_2(20)$ as one of the input parameters are in general further from zero compared to residuals calculated using $pH_T(25)$ as one of the input parameters. ΔTA and ΔDIC values calculated using the ($pH_T(25)$, $fCO_2(20)$) input pair are not shown as they are larger in magnitude and not recommended according to best practices (Patsavas et al., 2015).

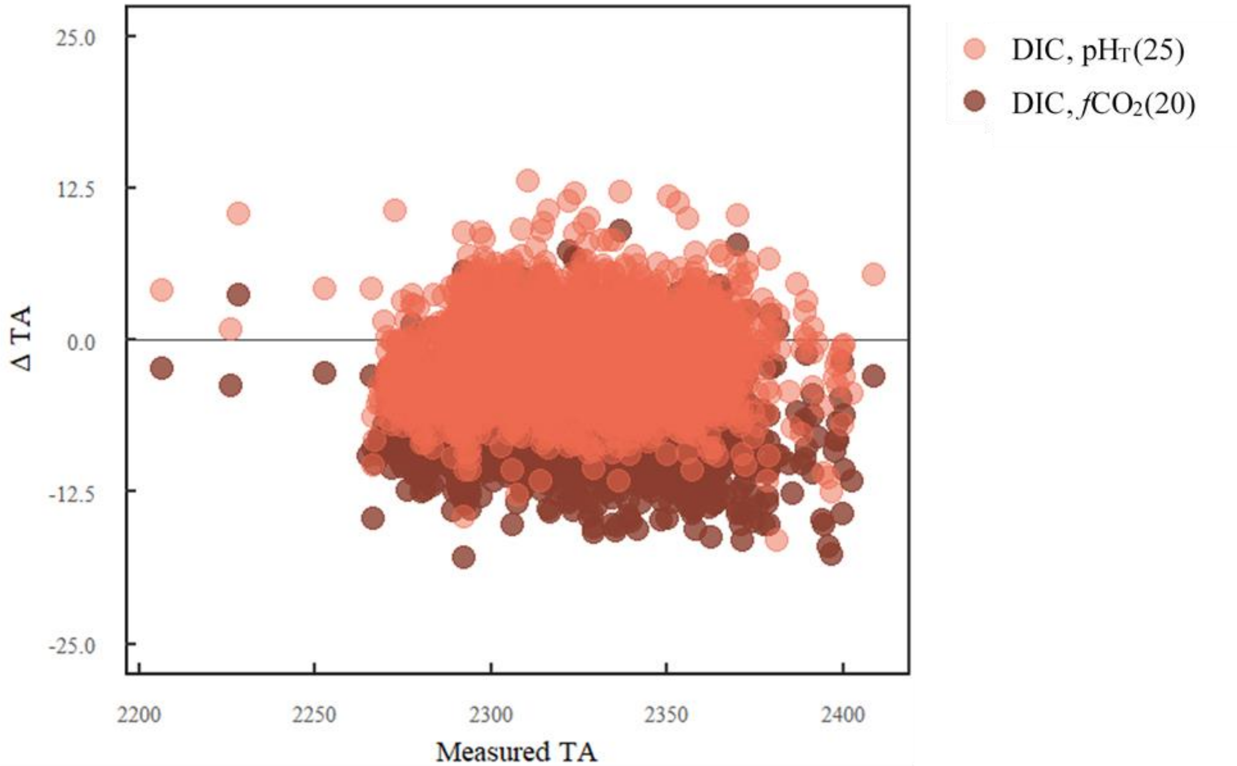

Fig. 3. Residuals of TA (ΔTA = measured TA – calculated TA; µmol kg^{-1}) shown in terms of measured TA. Color denotes the input pair used for TA calculations: (DIC, pH$_T$(25)) or (DIC, $f CO_2$(20)).

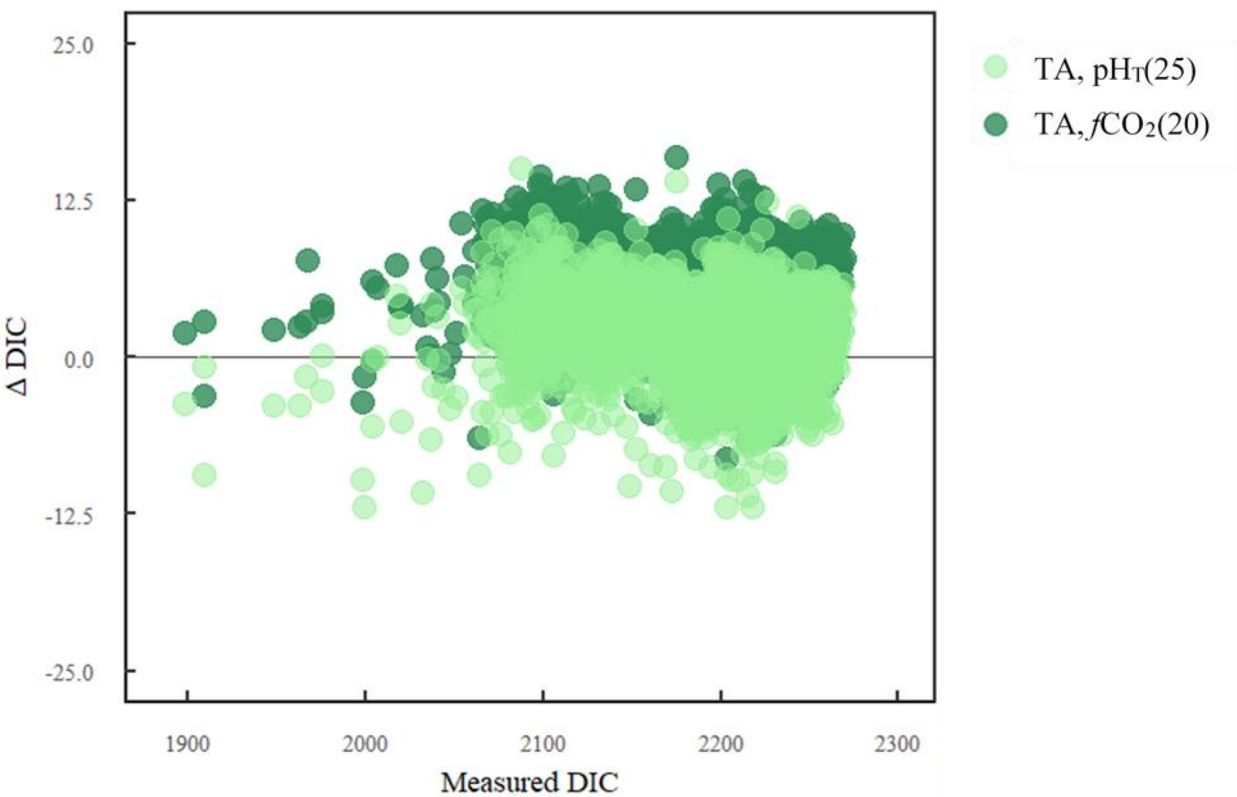

Fig. 4. Residuals of DIC (ΔDIC = measured DIC – calculated DIC; µmol kg^{-1}) shown in terms of measured DIC. Color denotes the input pair used for DIC calculations: (TA, pH$_T$(25)) or (TA, fCO$_2$(20)).

Residuals of pH$_T$(25) (denoted as ΔpH$_T$(25)) generally show an even distribution of residuals for the full range of measured pH$_T$(25) (Fig. 5). ΔpH$_T$(25) values calculated using the (TA, DIC) input pair encompass a larger magnitude than ΔpH$_T$(25) values calculated using (DIC, fCO$_2$(20)) and (TA, fCO$_2$(20)). This finding is expected as it is generally recommended to pair one temperature-independent parameter (i.e., TA or DIC) with one temperature-dependent parameter (i.e., pH$_T$(25) or fCO$_2$(20)) in calculations. ΔpH$_T$(25) values calculated using the (TA, DIC) input pair are generally evenly spread about zero for the full range of measured pH$_T$(25) with no apparent slope. Hence, the previously reported pH-dependent pH offset detected between measured pH and pH(TA, DIC) in many large-scale, oceanographic datasets (McElligott et al., 1998; Williams et al., 2017) is not observed for A13.5 2024 data. $\Delta pH_T(25)$ values calculated using both (DIC, $fCO_2(20)$) and (TA, $fCO_2(20)$) are evenly distributed for the full range of measured $pH_T(25)$ though there is a consistent, slightly negative offset in the residual values. However, this negative offset is smaller in magnitude compared to another recent GO-SHIP cruise A16N 2023 which also contained measurements of all four inorganic carbon parameters (Schockman, 2025a; Schockman, 2025b). This finding suggests that calculated $pH_T(25)$ values using $fCO_2(20)$ as one of the input parameters are consistently overestimated compared to the respective measured $pH_T(25)$ values.

Residuals of $fCO_2(20)$ as a percentage of measured $fCO_2(20)$ (denoted as $\Delta fCO_2(20)$ (%)) generally show an even distribution of residuals for the full range of measured $fCO_2(20)$ (Fig. 6). $\Delta fCO_2(20)$ (%) values calculated using all three sets of input pairs have a consistent, slightly negative offset in the residual values. However, this negative offset is smaller in magnitude compared to another recent GO-SHIP cruise A16N 2023 which also contained measurements of all four inorganic carbon parameters (Schockman, 2025a; Schockman, 2025b). Similar to $\Delta pH_T(25)$ (TA, DIC), $\Delta fCO_2(20)$ (%) values calculated using the (TA, DIC) input pair encompass a larger magnitude than $\Delta fCO_2(20)$ (%) values calculated using (DIC, $pH_T(25)$) and (TA, $pH_T(25)$), which is an expected observation.

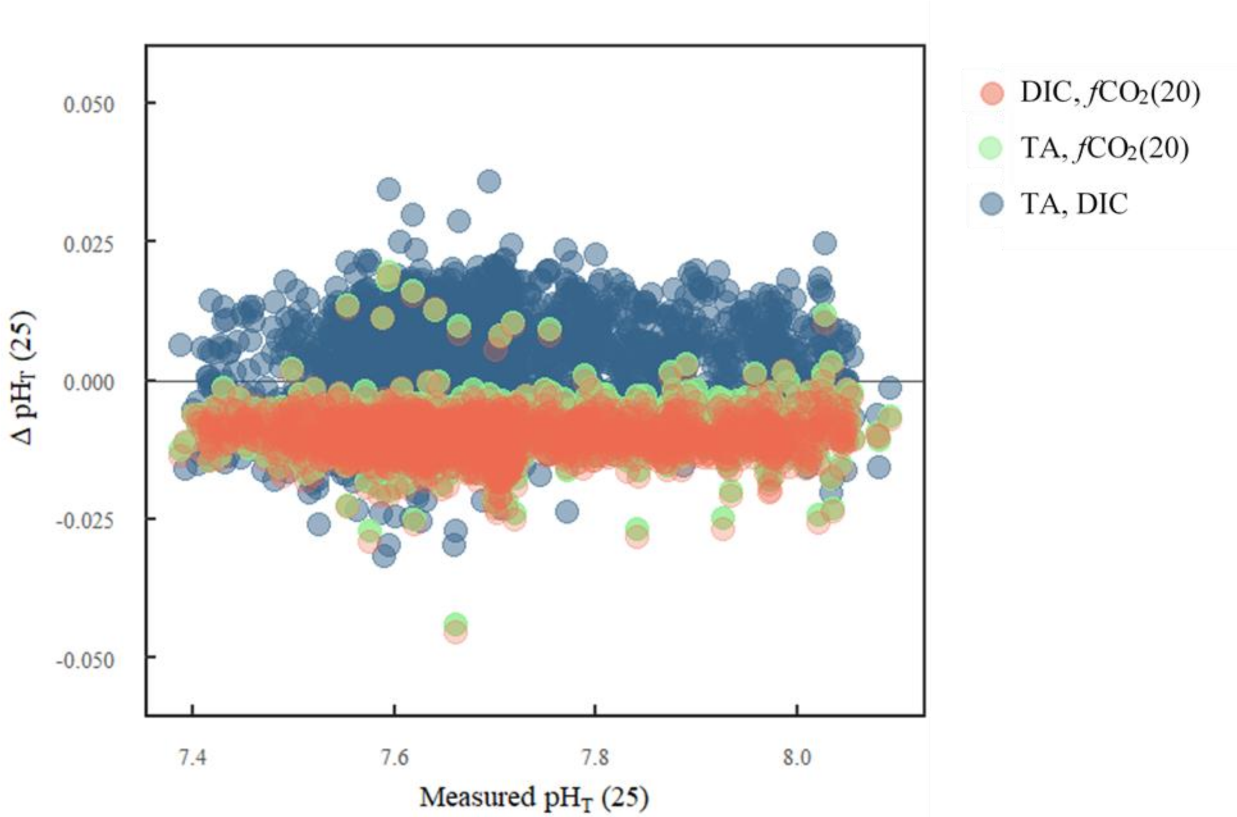

Fig. 5. Residuals of $pH_T(25)$ ($\Delta pH_T(25)$ = measured $pH_T(25)$ – calculated $pH_T(25)$) shown in terms of measured $pH_T(25)$. Color denotes the input pair used for $pH_T(25)$ calculations: (DIC, $fCO_2(20)$), (TA, $fCO_2(20)$), or (TA, DIC). Note that the (DIC, $fCO_2(20)$) and (TA, $fCO_2(20)$) points overlap such that (TA, $fCO_2(20)$) symbols are masked.

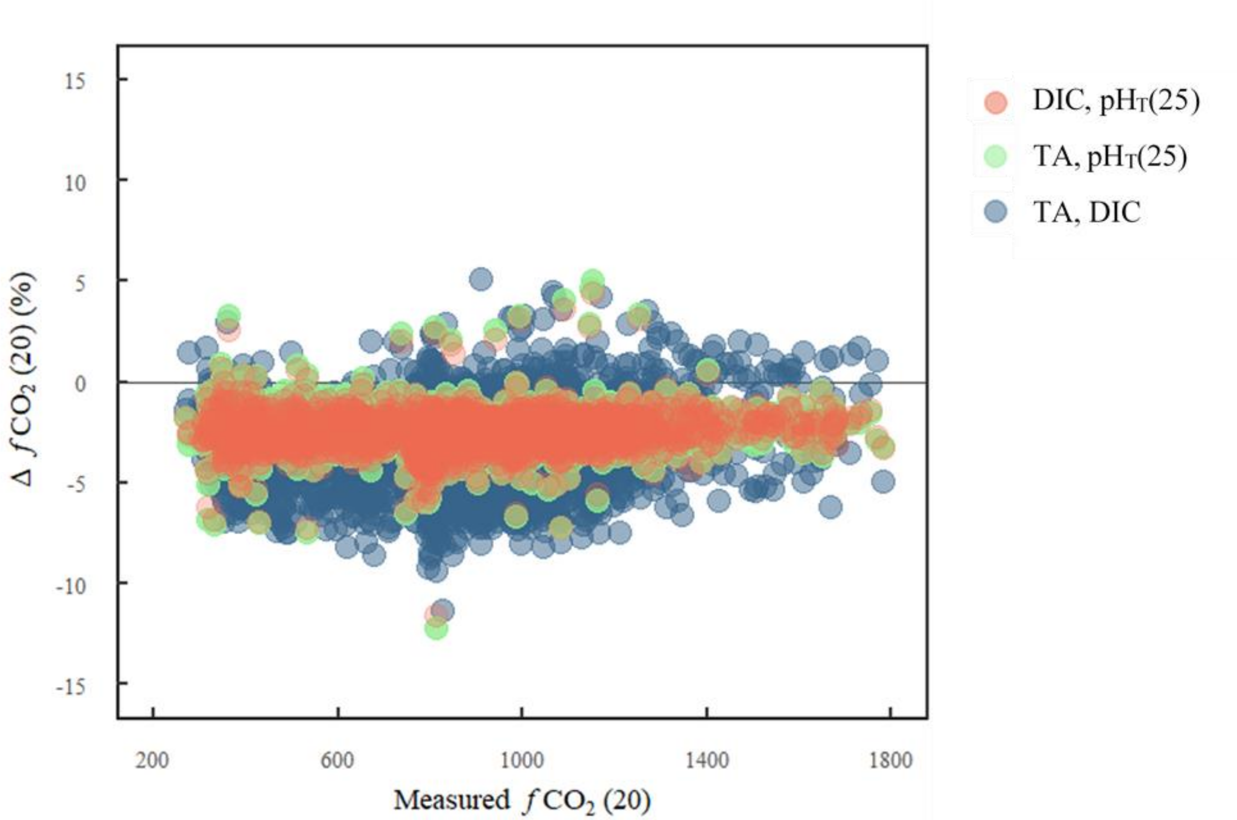

Fig. 6. Residuals of $fCO_2(20)$ as a percentage of measured $fCO_2(20)$ ($\Delta fCO_2(20)$ (%) = (measured $fCO_2(20)$ – calculated $fCO_2(20)$) / measured $fCO_2(20)$ *100) shown in terms of measured $fCO_2(20)$ (µatm). Color denotes the input pair used for $fCO_2(20)$ calculations: (DIC, $pH_T(25)$), (TA, $pH_T(25)$), or (TA, DIC). Note that the (DIC, $pH_T(25)$) and (TA, $pH_T(25)$) points overlap such that (TA, $pH_T(25)$) symbols are masked.

4. Conclusions

This report highlights and describes the quality control measures of the inorganic carbon parameters for the A13.5 2024 dataset. The full cruise report located on CCHDO's website contains additional information regarding measurement details and techniques. In general, the inorganic carbon system measurements appear to be of the highest quality standard expected of

GO-SHIP cruises. This cruise contains measurements of all four inorganic carbon parameters, allowing for a thorough internal consistency analysis with multiple sets of calculations for each parameter. Important observations include the systematic offset observed when using $fCO_2(20)$ as an input parameter for calculations, and the corresponding offset between measured and calculated $fCO_2(20)$ values. These offsets have also been detected to a greater extent in another recent GO-SHIP cruise A16N 2023 which also contained measurements of all four inorganic carbon parameters (Schockman, 2025a; Schockman, 2025b). Several reasons for these differences, including known inconsistencies in the inorganic carbon system calculations, have been described elsewhere (Woosley and Moon, 2023; Carter et al., 2024; Schockman et al., 2024; Schockman, 2025a). The similar pattern of inconsistency between measured and calculated $fCO_2(20)$ values now described in multiple cruises highlights the need for more routine measurements of $fCO_2(20)$ to conduct these types of comparisons. Future work should investigate if there are aspects of a particular cruise that result in this systematic offset between measured and calculated $fCO_2(20)$ values being larger or smaller in magnitude compared to other similar cruises.

5. Additional Tables

Table 3
Individual duplicate measurement values of TA (µmol kg^{-1}; duplicate one and duplicate two), measured back-to-back, as well as the absolute difference between duplicates. Measurements are provided according to their sample ID.

Sample ID	TA: Duplicate One	TA: Duplicate Two	Absolute Difference
20107	2332.2	2335.0	2.8
20114	2307.9	2307.4	0.5
30118	2289.1	2290.8	1.7
40114	2307.7	2308.7	1.0
50101	2347.3	2346.9	0.4
50124	2252.9	2251.9	1.0
60116	2295.8	2297.4	1.6
70123	2359.6	2360.7	1.1
80103	2338.6	2340.4	1.8
90212	2307.4	2307.7	0.3
100107	2334.8	2336.6	1.8
110403	2340.5	2337.2	3.3
120115	2303.7	2299.8	3.9
140108	2332.5	2332.9	0.4
150123	2354.9	2360.1	5.2
160110	2321.0	2319.9	1.1
170102	2343.3	2344.7	1.4
180122	2324.8	2325.5	0.7
190104	2344.3	2345.3	1.0
220118	2311.6	2312.5	0.9
230106	2333.4	2336.2	2.8
240120	2332.5	2331.3	1.2
250116	2291.0	2290.7	0.3
260101	2353.2	2352.0	1.2
270103	2356.2	2355.6	0.6
280107	2336.1	2335.6	0.5
280115	2293.6	2293.4	0.2
290117	2294.7	2293.7	1.0
290119	2304.9	2305.5	0.6
300121	2330.2	2330.9	0.7
310121	2311.7	2310.5	1.2
320105	2348.0	2348.2	0.2
330101	2352.6	2351.1	1.5
340123	2380.3	2377.7	2.6
350111	2320.1	2320.0	0.1

360102	2356.9	2357.3	0.4
370115	2295.2	2295.8	0.6
370123	2384.6	2384.5	0.1
380107	2338.9	2339.1	0.2
390105	2350.4	2350.8	0.4
400105	2353.2	2353.3	0.1
410110	2322.1	2322.6	0.5
420108	2330.4	2329.2	1.2
430106	2346.2	2347.5	1.3
440121	2336.4	2337.8	1.4
450105	2352.7	2349.9	2.8
450119	2311.1	2311.5	0.4
460123	2366.5	2362.9	3.6
470117	2292.1	2292.5	0.4
480106	2344.8	2345.2	0.4
480121	2362.9	2362.1	0.8
490104	2356.5	2356.1	0.4
490124	2380.7	2381.5	0.8
500106	2344.2	2343.9	0.3
510105	2349.5	2348.4	1.1
520103	2357.6	2358.9	1.3
530106	2346.0	2345.8	0.2
540117	2304.3	2304.2	0.1
550106	2350.3	2351.5	1.2
550121	2354.9	2354.9	0.0
560108	2336.7	2337.7	1.0
560119	2317.4	2316.5	0.9
570104	2357.8	2356.6	1.2
570118	2316.7	2315.9	0.8
580111	2318.1	2318.8	0.7
590113	2302.4	2302.5	0.1
600110	2321.5	2321.9	0.4
610124	2377.4	2378.9	1.5
620115	2291.4	2291.8	0.4
630109	2323.8	2322.2	1.6
640113	2291.8	2290.4	1.4
650113	2290.3	2287.4	2.9
660105	2341.1	2339.1	2.0
670103	2347.9	2345.5	2.4
680112	2295.0	2296.0	1.0
690123	2373.6	2370.8	2.8
710110	2329.6	2331.4	1.8
710120	2343.7	2346.6	2.9
720122	2360.5	2360.2	0.3

730118	2327.1	2329.5	2.4
740101	2370.5	2370.4	0.1
750102	2364.3	2367.8	3.5
760210	2337.2	2337.1	0.1
770116	2317.1	2319.1	2.0
780117	2316.8	2319.8	3.0
790103	2363.1	2366.0	2.9
790116	2304.2	2303.7	0.5
800111	2335.2	2334.3	0.9
810107	2342.9	2342.0	0.9
820104	2365.8	2365.4	0.4
820120	2316.1	2315.8	0.3
830104	2364.5	2363.7	0.8
840108	2337.8	2339.1	1.3
850109	2339.4	2341.2	1.8
860124	2317.1	2314.7	2.4
870108	2337.5	2335.6	1.9
880122	2307.8	2309.1	1.3
890120	2299.4	2298.9	0.5
900114	2280.5	2279.9	0.6
910115	2277.7	2278.3	0.6
920104	2345.8	2348.3	2.5
930116	2293.0	2290.5	2.5
940103	2354.2	2354.0	0.2
950110	2307.9	2310.8	2.9
960119	2290.8	2291.5	0.7
970109	2335.1	2338.0	2.9
980104	2352.8	2352.2	0.6
990124	2273.4	2272.9	0.5
1000122	2273.8	2271.6	2.2
1010121	2270.6	2270.4	0.2
1020117	2280.1	2279.5	0.6
1030111	2338.1	2338.7	0.6
1040113	2297.5	2301.6	4.1
1050124	2271.8	2271.2	0.6
1060109	2345.5	2344.9	0.6
1070113	2296.2	2297.3	1.1
1080122	2272.4	2271.4	1.0
1090107	2352.1	2351.0	1.1
1100119	2285.6	2284.4	1.2
1110116	2289.3	2289.0	0.3
1120105	2346.6	2345.8	0.8
1130106	2359.1	2359.0	0.1
1130111	2343.2	2345.0	1.8

Table 4
Individual duplicate measurement values of DIC (μmol kg^{-1}; duplicate one and duplicate two), measured randomly throughout a cell run, as well as the absolute difference between duplicates. Also included is the system on which each set of duplicates was run (AOML3 or AOML4). Measurements are provided according to their sample ID.

Sample ID	DIC: Duplicate One	DIC: Duplicate Two	Absolute Difference	System
20112	2170.52	2171.69	1.17	AOML4
20122	2175.05	2174.50	0.55	AOML4
30101	2215.12	2211.03	4.09	AOML3
30112	2171.77	2172.01	0.24	AOML3
30124	1909.43	1908.59	0.84	AOML3
40101	2213.83	2212.26	1.57	AOML4
40113	2178.90	2179.78	0.88	AOML4
40122	2189.00	2189.17	0.17	AOML4
50102	2207.90	2205.76	2.14	AOML3
50114	2204.80	2202.55	2.25	AOML3
50122	2173.47	2173.11	0.36	AOML3
60101	2212.28	2209.63	2.65	AOML4
60112	2176.23	2173.68	2.55	AOML4
60124	1968.35	1965.70	2.65	AOML4
70101	2211.34	2209.98	1.36	AOML3
70112	2168.31	2170.76	2.45	AOML3
70124	1966.19	1966.95	0.76	AOML3
80101	2212.82	2211.93	0.89	AOML4
80113	2187.96	2187.01	0.95	AOML4
80122	2172.03	2171.24	0.79	AOML4
90201	2212.55	2211.39	1.16	AOML3
90213	2190.52	2192.07	1.55	AOML3
90222	2168.00	2169.04	1.04	AOML3
100102	2210.20	2209.70	0.50	AOML4
100112	2173.67	2173.76	0.09	AOML4
110401	2212.06	2210.89	1.17	AOML3
110412	2174.28	2172.15	2.13	AOML3
110423	2172.36	2171.61	0.75	AOML3
120101	2210.44	2210.12	0.32	AOML4
120114	2210.92	2211.83	0.91	AOML4
120124	2005.63	2007.51	1.88	AOML4
130101	2207.02	2206.04	0.98	AOML3
130113	2177.84	2176.09	1.75	AOML3
130122	2177.51	2180.09	2.58	AOML3
140101	2209.31	2209.31	0.00	AOML4
140112	2172.58	2172.48	0.10	AOML4
140123	2192.53	2194.05	1.52	AOML4
150102	2205.69	2206.97	1.28	AOML3

150113	2191.97	2191.84	0.13	AOML3
150123	2090.07	2089.22	0.85	AOML3
160101	2209.41	2209.66	0.25	AOML4
160124	2016.97	2018.20	1.23	AOML4
170101	2206.67	2206.09	0.58	AOML3
170113	2182.65	2183.16	0.51	AOML3
170122	2199.52	2199.46	0.06	AOML3
180102	2206.41	2209.16	2.75	AOML4
180112	2179.74	2179.57	0.17	AOML4
180123	2074.36	2073.89	0.47	AOML4
190101	2207.64	2206.93	0.71	AOML3
190112	2184.55	2184.44	0.11	AOML3
190124	2035.32	2033.51	1.81	AOML3
200101	2210.78	2212.44	1.66	AOML4
200110	2181.07	2181.15	0.08	AOML4
200122	2157.11	2157.45	0.34	AOML4
210112	2200.58	2202.90	2.32	AOML3
210123	2048.88	2046.64	2.24	AOML3
220102	2208.68	2208.99	0.31	AOML4
220112	2231.15	2232.53	1.38	AOML4
220123	2062.49	2059.39	3.10	AOML4
230101	2206.63	2204.80	1.83	AOML3
230111	2217.73	2217.05	0.68	AOML3
230124	2039.87	2041.58	1.71	AOML3
240101	2216.73	2215.04	1.69	AOML4
240112	2233.63	2237.20	3.57	AOML4
240123	2067.95	2067.48	0.47	AOML4
250101	2211.10	2209.99	1.11	AOML3
250112	2186.04	2186.05	0.01	AOML3
250123	2136.62	2135.50	1.12	AOML3
260101	2212.89	2214.63	1.74	AOML4
260114	2232.94	2233.33	0.39	AOML4
260124	2041.88	2039.01	2.87	AOML4
270122	2173.23	2174.06	0.83	AOML4
280101	2213.57	2213.98	0.41	AOML3
280112	2193.94	2193.67	0.27	AOML3
280123	2134.85	2136.28	1.43	AOML3
290101	2213.82	2215.26	1.44	AOML4
290115	2253.99	2256.17	2.18	AOML4
290124	2068.12	2067.75	0.37	AOML4
300101	2211.27	2209.68	1.59	AOML3
300113	2227.18	2226.38	0.80	AOML3
300122	2102.67	2100.93	1.74	AOML3
310101	2214.70	2215.77	1.07	AOML4
310112	2199.48	2198.54	0.94	AOML4
310123	2090.92	2091.13	0.21	AOML4

320101	2212.99	2210.65	2.34	AOML3
320113	2222.72	2222.02	0.70	AOML3
320123	2080.45	2079.42	1.03	AOML3
330101	2216.05	2219.32	3.27	AOML4
330113	2233.35	2233.61	0.26	AOML4
330123	2084.61	2083.36	1.25	AOML4
340101	2210.36	2211.26	0.90	AOML3
340112	2196.85	2197.24	0.39	AOML3
340123	2094.01	2095.15	1.14	AOML3
350101	2216.01	2215.97	0.04	AOML4
350112	2209.26	2209.62	0.36	AOML4
350122	2209.34	2210.09	0.75	AOML4
360101	2215.81	2213.33	2.48	AOML3
360114	2232.20	2232.96	0.76	AOML3
360123	2088.40	2090.02	1.62	AOML3
370102	2216.05	2217.25	1.20	AOML4
370113	2222.01	2220.50	1.51	AOML4
370122	2147.82	2150.22	2.40	AOML4
380101	2213.56	2214.16	0.60	AOML3
380112	2207.33	2207.28	0.05	AOML3
380123	2075.63	2077.74	2.11	AOML3
390101	2219.87	2219.30	0.57	AOML4
390112	2220.32	2220.30	0.02	AOML4
390122	2105.16	2102.16	3.00	AOML4
400101	2213.27	2213.94	0.67	AOML3
400113	2220.33	2221.50	1.17	AOML3
400123	2092.76	2092.89	0.13	AOML3
410101	2221.82	2218.85	2.97	AOML4
410113	2234.11	2233.15	0.96	AOML4
410122	2130.34	2131.32	0.98	AOML4
420101	2216.76	2214.37	2.39	AOML3
420112	2220.68	2222.41	1.73	AOML3
420122	2115.36	2115.89	0.53	AOML3
430101	2224.09	2221.96	2.13	AOML4
430114	2233.75	2234.86	1.11	AOML4
430124	2096.41	2094.42	1.99	AOML4
440101	2215.89	2213.37	2.52	AOML3
440112	2204.39	2208.11	3.72	AOML3
440123	2089.05	2088.16	0.89	AOML3
450102	2221.88	2218.55	3.33	AOML4
450112	2218.85	2215.77	3.08	AOML4
450122	2103.43	2104.33	0.90	AOML4
460101	2217.41	2215.30	2.11	AOML3
460114	2226.69	2226.12	0.57	AOML3
460123	2086.78	2084.95	1.83	AOML3
470102	2215.81	2216.72	0.91	AOML4

470113	2219.39	2219.75	0.36	AOML4
470122	2098.91	2096.60	2.31	AOML4
480102	2214.31	2216.76	2.45	AOML3
480112	2210.58	2212.31	1.73	AOML3
480122	2089.81	2093.07	3.26	AOML3
490103	2215.35	2217.06	1.71	AOML4
490113	2215.72	2215.37	0.35	AOML4
490122	2117.31	2114.52	2.79	AOML4
500101	2218.15	2218.42	0.27	AOML3
500112	2208.22	2209.22	1.00	AOML3
500124	2087.13	2085.16	1.97	AOML3
510102	2217.44	2218.19	0.75	AOML4
510114	2230.63	2232.97	2.34	AOML4
510122	2083.80	2081.87	1.93	AOML4
520101	2218.65	2219.16	0.51	AOML3
520113	2216.88	2216.69	0.19	AOML3
520122	2098.41	2095.73	2.68	AOML3
530102	2219.79	2221.93	2.14	AOML4
530112	2207.67	2208.97	1.30	AOML4
530124	2091.50	2090.33	1.17	AOML4
540101	2218.27	2218.59	0.32	AOML3
540113	2222.20	2223.31	1.11	AOML3
540122	2092.75	2089.44	3.31	AOML3
550102	2220.57	2220.87	0.30	AOML4
550112	2203.58	2204.87	1.29	AOML4
560101	2221.37	2219.86	1.51	AOML3
560112	2198.78	2199.94	1.16	AOML3
560123	2088.78	2086.90	1.88	AOML3
570102	2215.54	2217.26	1.72	AOML4
570113	2223.63	2223.87	0.24	AOML4
570123	2091.85	2091.60	0.25	AOML4
580113	2224.11	2224.85	0.74	AOML3
580122	2103.63	2102.74	0.89	AOML3
590102	2215.47	2216.96	1.49	AOML4
590112	2221.01	2222.04	1.03	AOML4
590123	2097.24	2097.36	0.12	AOML4
600101	2221.19	2221.06	0.13	AOML3
600114	2212.29	2212.44	0.15	AOML3
600124	2105.32	2102.71	2.61	AOML3
610102	2220.93	2220.37	0.56	AOML4
610114	2204.74	2206.30	1.56	AOML4
610122	2099.25	2099.37	0.12	AOML4
620102	2219.85	2220.87	1.02	AOML3
620113	2226.97	2229.78	2.81	AOML3
620122	2095.87	2093.85	2.02	AOML3
630102	2220.96	2221.03	0.07	AOML4

630113	2209.72	2212.02	2.30	AOML4
630124	2097.80	2095.95	1.85	AOML4
640101	2219.66	2218.60	1.06	AOML3
640112	2225.07	2226.14	1.07	AOML3
640123	2084.72	2085.15	0.43	AOML3
650112	2218.98	2220.55	1.57	AOML4
650122	2088.19	2088.15	0.04	AOML4
660102	2218.54	2220.32	1.78	AOML3
660112	2205.57	2206.37	0.80	AOML3
660122	2085.83	2082.45	3.37	AOML3
670102	2216.27	2217.96	1.69	AOML4
670114	2163.26	2163.27	0.01	AOML4
670124	2085.87	2087.46	1.59	AOML4
680101	2220.19	2219.60	0.59	AOML3
680112	2169.67	2171.65	1.98	AOML3
680124	2099.02	2098.84	0.18	AOML3
690102	2217.15	2216.16	0.99	AOML3
690122	2089.62	2090.87	1.25	AOML3
700102	2219.62	2219.86	0.24	AOML4
700112	2188.12	2189.02	0.90	AOML4
700122	2094.57	2094.13	0.44	AOML4
710101	2254.68	2256.85	2.17	AOML3
710114	2182.85	2182.74	0.11	AOML3
710124	2101.08	2101.73	0.65	AOML3
720101	2259.20	2258.02	1.18	AOML4
720114	2173.82	2175.48	1.66	AOML4
720123	2094.03	2093.70	0.33	AOML4
730102	2236.36	2238.95	2.59	AOML3
730113	2192.04	2191.57	0.47	AOML3
730122	2093.09	2095.17	2.08	AOML3
740102	2236.15	2235.60	0.55	AOML4
740113	2179.79	2181.24	1.45	AOML4
740122	2088.95	2089.37	0.42	AOML4
750101	2259.42	2258.61	0.81	AOML3
750112	2206.42	2208.12	1.70	AOML3
750123	2084.02	2083.59	0.43	AOML3
760202	2256.58	2256.03	0.55	AOML4
760212	2228.23	2228.83	0.60	AOML4
760224	2092.63	2093.49	0.86	AOML4
770101	2260.64	2261.26	0.62	AOML3
770113	2189.91	2194.66	4.75	AOML3
770123	2094.05	2095.57	1.52	AOML3
780102	2257.29	2257.70	0.41	AOML4
780112	2232.38	2230.76	1.62	AOML4
780122	2083.82	2083.84	0.02	AOML4
790101	2256.02	2259.28	3.26	AOML3

790113	2198.96	2200.40	1.44	AOML3
790123	2081.86	2081.90	0.04	AOML3
800101	2259.33	2260.21	0.88	AOML4
800113	2219.40	2219.63	0.23	AOML4
800124	2087.75	2086.77	0.98	AOML4
810101	2260.24	2257.19	3.05	AOML3
810113	2205.87	2205.17	0.70	AOML3
810123	2071.58	2069.98	1.60	AOML3
820101	2260.57	2259.62	0.95	AOML4
820111	2234.13	2233.34	0.79	AOML4
820124	2072.94	2072.36	0.58	AOML4
830101	2261.09	2260.76	0.33	AOML3
830113	2229.31	2231.15	1.84	AOML3
830123	2068.89	2068.98	0.09	AOML3
840102	2256.03	2256.35	0.32	AOML4
840113	2202.80	2205.29	2.49	AOML4
840124	2079.71	2080.59	0.88	AOML4
850102	2258.89	2259.42	0.53	AOML3
850112	2240.92	2241.88	0.96	AOML3
850123	2080.66	2080.67	0.01	AOML3
860102	2256.32	2255.11	1.21	AOML4
860113	2215.95	2216.01	0.06	AOML4
860123	2067.16	2065.23	1.93	AOML4
870102	2256.44	2257.31	0.87	AOML3
870113	2211.88	2213.07	1.19	AOML3
870123	2071.91	2071.34	0.56	AOML3
880101	2261.41	2259.95	1.46	AOML4
880113	2231.89	2231.65	0.24	AOML4
880124	2067.49	2065.75	1.74	AOML4
890102	2256.18	2258.44	2.26	AOML3
890112	2244.92	2245.16	0.24	AOML3
890123	2063.37	2062.28	1.09	AOML3
900101	2259.86	2259.16	0.70	AOML4
900113	2189.66	2189.51	0.15	AOML4
900124	2061.61	2061.04	0.57	AOML4
910101	2259.32	2259.30	0.02	AOML3
910113	2190.32	2191.37	1.05	AOML3
910124	2068.18	2068.94	0.76	AOML3
920102	2253.76	2254.27	0.51	AOML4
920113	2185.25	2186.63	1.38	AOML4
920123	2092.37	2093.56	1.19	AOML4
930101	2237.05	2236.44	0.61	AOML3
930116	2078.36	2076.23	2.13	AOML3
940101	2255.76	2255.35	0.41	AOML4
940113	2175.19	2175.47	0.28	AOML4
940124	2074.24	2075.01	0.77	AOML4

950101	2256.19	2254.04	2.15	AOML3
950113	2172.16	2175.41	3.25	AOML3
950124	2084.95	2082.61	2.34	AOML3
960102	2255.76	2258.24	2.48	AOML4
960112	2211.22	2211.48	0.26	AOML4
960123	2085.30	2082.90	2.40	AOML4
970102	2256.32	2259.82	3.50	AOML3
970112	2200.84	2199.28	1.56	AOML3
970123	2082.55	2082.38	0.17	AOML3
980101	2264.10	2260.30	3.80	AOML4
980113	2182.73	2180.43	2.30	AOML4
980124	2079.92	2080.71	0.79	AOML4
990101	2267.25	2266.39	0.86	AOML3
990113	2210.90	2210.48	0.42	AOML3
1000101	2264.44	2266.53	2.09	AOML4
1000112	2242.58	2241.68	0.90	AOML4
1000124	2100.36	2101.86	1.50	AOML4
1010102	2260.07	2264.21	4.14	AOML3
1010113	2214.24	2214.32	0.08	AOML3
1010123	2107.17	2106.50	0.67	AOML3
1020101	2262.83	2263.94	1.11	AOML4
1020113	2232.47	2233.25	0.78	AOML4
1020124	2104.50	2104.36	0.14	AOML4
1030101	2267.21	2268.39	1.18	AOML3
1030113	2232.92	2232.94	0.02	AOML3
1030124	2110.38	2105.67	4.71	AOML3
1040102	2261.78	2260.82	0.96	AOML4
1040112	2234.61	2235.95	1.34	AOML4
1040123	2107.58	2106.41	1.17	AOML4
1050113	2209.61	2211.47	1.86	AOML3
1050123	2114.57	2115.12	0.55	AOML3
1060102	2260.48	2263.63	3.15	AOML4
1060112	2242.97	2241.82	1.15	AOML4
1060124	2112.24	2113.85	1.61	AOML4
1070102	2266.78	2266.40	0.38	AOML3
1070112	2235.43	2233.94	1.49	AOML3
1080102	2259.29	2261.81	2.52	AOML4
1080111	2249.27	2250.13	0.86	AOML4
1080123	2112.51	2113.88	1.37	AOML4
1090101	2270.30	2267.83	2.47	AOML3
1090113	2232.52	2231.01	1.51	AOML3
1090124	2125.61	2126.98	1.37	AOML3
1100101	2264.13	2264.57	0.44	AOML4
1100113	2245.16	2246.50	1.34	AOML4
1100124	2137.48	2138.08	0.60	AOML4
1110102	2257.28	2257.12	0.16	AOML3

1110115	2144.99	2144.75	0.24	AOML3
1120116	2147.99	2145.15	2.84	AOML4
1130101	2270.12	2268.43	1.69	AOML3
1130113	2265.20	2268.49	3.29	AOML3
1130123	2158.45	2155.70	2.76	AOML3

Table 5
Individual duplicate measurement values of $pH_T(25)$ (duplicate one and duplicate two), measured back-to-back, as well as the absolute difference between duplicates. Measurements are provided according to their sample ID.

Sample ID	$pH_T(25)$: Duplicate One	$pH_T(25)$: Duplicate Two	Absolute Difference
20107	7.7118	7.7131	0.0013
20114	7.6134	7.6086	0.0048
30118	7.5141	7.5106	0.0035
40114	7.6343	7.6341	0.0002
50101	7.6995	7.6987	0.0008
50124	8.0555	8.0566	0.0011
60116	7.5479	7.5463	0.0016
70123	7.8526	7.8505	0.0021
80102	7.7084	7.7065	0.0019
90212	7.6991	7.7001	0.0010
100107	7.7099	7.7093	0.0006
110403	7.7108	7.7079	0.0029
120115	7.5787	7.5782	0.0005
130121	7.7038	7.7050	0.0012
140108	7.7118	7.7136	0.0018
150123	7.9542	7.9730	0.0188
160110	7.7214	7.7192	0.0022
170102	7.7075	7.7059	0.0016
180122	7.6765	7.6769	0.0004
190104	7.7061	7.7087	0.0026
210111	7.6878	7.6916	0.0038
220118	7.6157	7.6212	0.0055
230106	7.7084	7.7072	0.0012
240120	7.6679	7.6653	0.0026
250116	7.4331	7.4355	0.0024
260101	7.7103	7.7091	0.0012
270103	7.7102	7.7036	0.0066
280107	7.7056	7.7066	0.0010
280115	7.4879	7.4906	0.0027
290117	7.4196	7.4144	0.0052
290119	7.5188	7.5170	0.0018
300104	7.7085	7.7089	0.0004
300121	7.6532	7.6522	0.0010
310111	7.6876	7.6862	0.0014
310121	7.5596	7.5588	0.0008
320105	7.7076	7.7086	0.0010
320109	7.7047	7.7048	0.0001

330101	7.7118	7.7038	0.0080
330123	8.0191	8.0285	0.0094
340108	7.7029	7.7075	0.0046
340123	7.9848	7.9858	0.0010
350111	7.6724	7.6718	0.0006
350121	7.5710	7.5708	0.0002
360102	7.7129	7.7135	0.0006
360117	7.4480	7.4500	0.0020
370115	7.4858	7.4818	0.0040
370123	8.0225	8.0204	0.0021
380107	7.7044	7.7034	0.0010
380117	7.4480	7.4427	0.0053
390105	7.7034	7.6998	0.0036
400105	7.7048	7.7076	0.0028
400114	7.5188	7.5213	0.0025
410110	7.6934	7.6916	0.0018
410121	7.6771	7.6785	0.0014
420108	7.7007	7.7019	0.0012
430106	7.7013	7.6993	0.0020
430118	7.4529	7.4486	0.0043
440115	7.4758	7.4779	0.0021
440121	7.8461	7.8406	0.0055
450105	7.7054	7.7045	0.0009
450119	7.6343	7.6360	0.0017
460102	7.7133	7.7109	0.0024
460123	7.9799	7.9778	0.0021
470101	7.7130	7.7081	0.0049
470117	7.6062	7.6083	0.0021
480106	7.7002	7.7042	0.0040
480121	7.9197	7.9205	0.0008
490104	7.7079	7.7095	0.0016
490124	8.0070	8.0464	0.0394
500106	7.7068	7.7071	0.0003
500115	7.5162	7.5193	0.0031
510105	7.7070	7.7066	0.0004
510112	7.6076	7.6042	0.0034
520103	7.7113	7.7155	0.0042
520116	7.5852	7.5860	0.0008
530106	7.7095	7.7058	0.0037
530121	7.9432	7.9473	0.0041
540114	7.5504	7.5509	0.0005
540117	7.7285	7.7305	0.0020
550106	7.7082	7.7086	0.0004
550121	7.9293	7.9304	0.0011

560108	7.7025	7.7009	0.0016
560119	7.7994	7.7960	0.0034
570104	7.7089	7.7065	0.0024
570118	7.7965	7.7969	0.0004
580111	7.6783	7.6826	0.0043
580117	7.6807	7.6775	0.0032
590113	7.5702	7.5696	0.0006
590119	7.9031	7.9043	0.0012
600110	7.6850	7.6849	0.0001
600122	7.9778	7.9714	0.0064
610112	7.6031	7.6015	0.0016
610124	7.9811	7.9815	0.0004
620105	7.7058	7.7083	0.0025
620115	7.5914	7.5960	0.0046
630109	7.6843	7.6816	0.0027
630120	7.9096	7.9101	0.0005
640103	7.7124	7.7123	0.0001
640113	7.5982	7.6035	0.0053
650106	7.6886	7.6882	0.0004
650113	7.6014	7.6016	0.0002
660105	7.6908	7.6963	0.0055
660117	7.8115	7.8026	0.0089
670103	7.7017	7.6989	0.0028
670120	7.9176	7.9199	0.0023
680112	7.6822	7.6784	0.0038
680124	7.9750	7.9726	0.0024
690112	7.6661	7.6673	0.0012
690123	7.9738	7.9688	0.0050
700105	7.6890	7.6862	0.0028
700115	7.7801	7.7791	0.0010
710110	7.6277	7.6314	0.0037
710120	7.9093	7.9102	0.0009
720113	7.6141	7.6159	0.0018
720122	7.9735	7.9719	0.0016
730103	7.6984	7.7002	0.0018
730118	7.8598	7.8621	0.0023
740101	7.6374	7.6373	0.0001
740109	7.6214	7.6245	0.0031
750102	7.6466	7.6440	0.0026
750114	7.6823	7.6865	0.0042
760210	7.6124	7.6102	0.0022
760224	7.9708	7.9689	0.0019
770103	7.6529	7.6539	0.0010
770116	7.8001	7.8009	0.0008

780111	7.5804	7.5804	0.0000
780117	7.8146	7.8172	0.0026
790103	7.6550	7.6578	0.0028
790116	7.7430	7.7438	0.0008
800111	7.6024	7.6060	0.0036
800117	7.7300	7.7297	0.0003
810107	7.6734	7.6729	0.0005
810122	7.9211	7.9228	0.0017
820104	7.6386	7.6389	0.0003
820120	7.8160	7.8182	0.0022
830104	7.6446	7.6457	0.0011
830111	7.6002	7.5970	0.0032
840108	7.6604	7.6604	0.0000
840113	7.5939	7.5987	0.0048
850112	7.5726	7.5693	0.0033
860101	7.6334	7.6296	0.0038
860124	7.9447	7.9398	0.0049
870108	7.6639	7.6658	0.0019
870119	7.8055	7.8022	0.0033
880102	7.6301	7.6322	0.0021
880122	7.8549	7.8522	0.0027
890103	7.6384	7.6349	0.0035
890120	7.7881	7.7930	0.0049
900108	7.6451	7.6469	0.0018
900114	7.6410	7.6405	0.0005
910115	7.6465	7.6492	0.0027
910122	7.7930	7.7943	0.0013
920104	7.6669	7.6711	0.0042
920118	7.7689	7.7699	0.0010
930107	7.6382	7.6403	0.0021
930116	7.8935	7.8978	0.0043
940103	7.6407	7.6429	0.0022
950110	7.5697	7.5747	0.0050
950120	7.7922	7.7880	0.0042
960108	7.6286	7.6255	0.0031
960119	7.7771	7.7723	0.0048
970101	7.6212	7.6217	0.0005
970109	7.5862	7.5862	0.0000
980104	7.7712	7.7742	0.0030
980119	7.6309	7.6347	0.0038
990101	7.5975	7.5997	0.0022
990124	7.8334	7.8329	0.0005
1000110	7.5875	7.5886	0.0011
1000122	7.7296	7.7250	0.0046

1010114	7.6213	7.6205	0.0008
1010121	7.7464	7.7529	0.0065
1020117	7.6416	7.6426	0.0010
1020123	7.7921	7.7925	0.0004
1030111	7.5702	7.5687	0.0015
1030117	7.6437	7.6433	0.0004
1040103	7.6080	7.6074	0.0006
1040113	7.5775	7.5779	0.0004
1050102	7.5992	7.6013	0.0021
1050124	7.7850	7.7851	0.0001
1060109	7.5982	7.5962	0.0020
1060119	7.6603	7.6627	0.0024
1070105	7.6158	7.6136	0.0022
1070113	7.5834	7.5790	0.0044
1080108	7.6147	7.6155	0.0008
1080122	7.7798	7.7775	0.0023
1090107	7.6140	7.6140	0.0000
1090118	7.6239	7.6263	0.0024
1100103	7.5981	7.5983	0.0002
1100119	7.6437	7.6453	0.0016
1110106	7.5711	7.5724	0.0013
1110116	7.7425	7.7440	0.0015
1120105	7.5942	7.5933	0.0009
1130106	7.5950	7.5935	0.0015
1130111	7.5529	7.5534	0.0005

Table 6
Individual duplicate measurement values of $fCO_2(20)$ (µatm; duplicate one and duplicate two), measured back-to-back, as well as the absolute and relative differences between duplicates (relative difference = absolute difference / average duplicate value * 100). Measurements are provided according to their sample ID.

Sample ID	$fCO_2(20)$: Duplicate One	$fCO_2(20)$: Duplicate Two	Absolute Difference	Relative Difference (%)
20118	1284.84	1285.56	0.72	0.06
30106	786.42	784.03	2.39	0.30
40113	827.08	826.61	0.47	0.06
50118	1318.77	1323.73	4.96	0.38
60102	804.41	805.98	1.57	0.19
70104	797.31	796.69	0.62	0.08
80114	994.22	1000.23	6.01	0.60
90221	747.91	745.45	2.46	0.33
100122	779.29	778.85	0.44	0.06
110408	785.35	785.00	0.35	0.04
120113	875.59	874.38	1.21	0.14
130102	804.93	808.03	3.10	0.38
140115	1113.50	1115.89	2.39	0.21
150101	806.11	808.60	2.49	0.31
160108	788.41	790.26	1.85	0.23
170119	1215.21	1220.58	5.37	0.44
180121	847.13	847.60	0.47	0.06
190102	803.16	805.04	1.88	0.23
200104	798.39	799.70	1.31	0.16
210104	797.48	798.98	1.50	0.19
220111	1043.20	1044.91	1.71	0.16
230106	793.37	795.25	1.88	0.24
240113	1501.19	1508.74	7.55	0.50
250105	798.69	801.85	3.16	0.39
260117	1556.86	1569.53	12.67	0.81
270104	816.72	818.36	1.64	0.20
270116	1661.92	1672.88	10.96	0.66
280116	1672.82	1682.91	10.09	0.60
280124	327.25	322.40	4.85	1.49
290117	1659.25	1678.48	19.23	1.15
290124	332.86	330.42	2.44	0.74
300117	1609.13	1611.72	2.59	0.16
310103	803.97	804.96	0.99	0.12
310120	1254.81	1253.43	1.38	0.11
320105	807.56	807.61	0.05	0.01
320116	1668.17	1676.68	8.51	0.51

330104	808.16	809.56	1.40	0.17
330118	1329.42	1339.18	9.76	0.73
340109	803.29	803.60	0.31	0.04
340124	345.74	346.03	0.29	0.08
350106	821.57	822.08	0.51	0.06
350120	1196.34	1196.30	0.04	0.00
360105	822.11	822.34	0.23	0.03
360120	1264.32	1263.27	1.05	0.08
370103	804.64	803.94	0.70	0.09
370116	1606.76	1609.07	2.31	0.14
380108	807.10	806.61	0.49	0.06
380119	1469.87	1469.55	0.32	0.02
390107	814.67	815.05	0.38	0.05
390117	1626.03	1626.86	0.83	0.05
400104	804.73	805.46	0.73	0.09
400119	1510.26	1509.96	0.30	0.02
410102	803.53	804.20	0.67	0.08
410122	466.81	467.92	1.11	0.24
420103	806.50	806.34	0.16	0.02
420118	1510.32	1510.52	0.20	0.01
430107	821.52	820.35	1.17	0.14
430120	1154.98	1154.18	0.80	0.07
440116	1599.72	1605.07	5.35	0.33
440122	450.77	449.10	1.67	0.37
450106	818.45	818.69	0.24	0.03
450120	629.45	626.87	2.58	0.41
460103	802.93	803.38	0.45	0.06
460117	1125.85	1123.99	1.86	0.17
470103	801.04	802.19	1.15	0.14
470121	486.55	485.04	1.51	0.31
480101	795.68	798.40	2.72	0.34
480123	357.84	358.00	0.16	0.04
490102	803.08	803.03	0.05	0.01
490116	1224.82	1226.14	1.32	0.11
500103	801.62	802.44	0.82	0.10
500116	1363.84	1364.21	0.37	0.03
510101	797.33	798.50	1.17	0.15
510113	1142.81	1148.41	5.60	0.49
520103	800.39	800.94	0.55	0.07
520115	1213.41	1216.47	3.06	0.25
530102	798.80	799.52	0.72	0.09
530117	839.55	838.59	0.96	0.11
540115	1061.37	1060.48	0.89	0.08
540118	657.12	656.15	0.97	0.15

550107	806.57	806.66	0.09	0.01
550123	382.38	382.59	0.21	0.05
560106	804.91	804.92	0.01	0.00
560117	830.47	831.24	0.77	0.09
570109	816.50	816.84	0.34	0.04
570121	417.64	416.74	0.90	0.22
580110	822.51	823.28	0.77	0.09
580118	683.97	682.25	1.72	0.25
590105	808.12	808.92	0.80	0.10
590112	1075.93	1076.86	0.93	0.09
600103	797.05	796.70	0.35	0.04
600120	459.62	460.06	0.44	0.10
610113	1136.54	1139.39	2.85	0.25
610116	828.55	827.00	1.55	0.19
620120	517.29	518.07	0.78	0.15
630109	847.87	848.93	1.06	0.12
640116	716.35	716.07	0.28	0.04
650107	865.84	866.33	0.49	0.06
660116	686.63	687.23	0.60	0.09
670112	873.90	873.67	0.23	0.03
680112	849.68	849.33	0.35	0.04
690113	739.59	739.39	0.20	0.03
700101	929.51	933.08	3.57	0.38
710104	816.78	816.49	0.29	0.04
720102	931.94	933.66	1.72	0.18
730120	515.81	515.46	0.35	0.07
740117	534.26	533.63	0.63	0.12
750114	840.09	839.38	0.71	0.08
760213	989.92	989.99	0.07	0.01
770109	966.31	967.35	1.04	0.11
780112	1133.95	1133.13	0.82	0.07
790104	882.46	884.19	1.73	0.20
790117	658.96	658.27	0.69	0.10
800121	498.24	497.79	0.45	0.09
810111	1102.74	1102.61	0.13	0.01
820121	562.11	561.29	0.82	0.15
830108	887.38	887.37	0.01	0.00
840101	987.29	989.49	2.20	0.22
850103	983.68	984.62	0.94	0.10
860111	1098.35	1097.95	0.40	0.04
870122	504.26	503.86	0.40	0.08
880116	905.10	904.64	0.46	0.05
890107	876.66	876.90	0.24	0.03
900101	988.38	989.32	0.94	0.10

910114	948.30	947.82	0.48	0.05
920109	1092.21	1093.54	1.33	0.12
930101	995.92	997.10	1.18	0.12
940116	714.69	713.94	0.75	0.10
950121	580.43	579.80	0.63	0.11
960112	1085.20	1084.55	0.65	0.06
970105	934.76	935.30	0.54	0.06
980123	503.49	502.55	0.94	0.19
990115	944.15	943.87	0.28	0.03
1000105	1007.47	1004.30	3.17	0.32
1010114	997.69	996.02	1.67	0.17
1020118	931.43	931.35	0.08	0.01
1030103	1073.85	1073.50	0.35	0.03
1040106	995.27	994.46	0.81	0.08
1050116	953.08	953.91	0.83	0.09
1060113	1142.97	1147.79	4.82	0.42
1070119	861.77	861.02	0.75	0.09
1080110	1162.20	1162.04	0.16	0.01
1090105	1054.94	1053.07	1.87	0.18
1100122	717.75	717.81	0.06	0.01
1110103	1036.53	1036.06	0.47	0.05
1120115	743.79	741.29	2.50	0.34
1130102	1112.05	1113.52	1.47	0.13

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