

**Table 1.** Parameters that are included in the data product. CTD is short for conductivity, temperature, and depth, and refers to a package of electronic instruments that measure these properties.

| Abbreviation                | Variable name                                                                                                                                                                                                                                      | Unit                    | Measured/<br>calculated |
|-----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|-------------------------|
| Accession                   | The data package identification number used by NOAA's National Centers for Environmental Information. This ID can be used to retrieve the original cruise data files.                                                                              | -                       | -                       |
| EXPOCODE                    | Expedition code of a research cruise                                                                                                                                                                                                               | -                       | -                       |
| Cruise_flag                 | Flags indicating the overall quality of a cruise data file (refer to Table 2 for more details)                                                                                                                                                     | -                       | -                       |
| Cruise_ID                   | The identification of a research cruise                                                                                                                                                                                                            | -                       | -                       |
| Observation_type            | Whether a sample is collected from Niskin bottles or an onboard flow-through system                                                                                                                                                                | -                       | -                       |
| Profile_number              | A series of sequential number profile identifying a profile                                                                                                                                                                                        | -                       | -                       |
| Station_ID                  | Identification of a sampling station                                                                                                                                                                                                               | -                       | -                       |
| Cast_number                 | Cast number at a sampling station                                                                                                                                                                                                                  | -                       | -                       |
| Niskin_ID                   | Niskin identification number                                                                                                                                                                                                                       | -                       | -                       |
| Sample_ID                   | Sample_ID is a combination of Station_ID, Cast_number, and Niskin_ID. Sometimes it can also be a series of non-repeating numbers to identify each row from a cruise data file.                                                                     | -                       | -                       |
| Depth_bottom                | Depth at bottom of a sampling station                                                                                                                                                                                                              | m                       | measured                |
| Max_sample_depth            | The maximum sampling depth                                                                                                                                                                                                                         | m                       | measured                |
| CTDPRES                     | Water pressure recorded from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, its pressure is equal to the depth of the water inlet. When such info is not available, it is assumed to be 5 dbar.      | dbar                    | measured                |
| Depth                       | The depth at which a sample is collected                                                                                                                                                                                                           | m                       | measured                |
| CTDTEMP_ITS90               | Temperature on the International Temperature Scale of 1990 (ITS-90) from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, temperature has also been merged into the CTDTEMP_ITS90 variable.            | °C                      | measured                |
| CTDSAL_PSS78                | Salinity on the Practical Salinity Scale 1978 (PSS-78) from sensors on a CTD rosette. For surface samples collected from an onboard flow-through system, salinity from the thermosalinograph (TSG) has been merged into the CTDSAL_PSS78 variable. | -                       | measured                |
| Salinity_PSS78              | Discrete salinity on the PSS-78 scale                                                                                                                                                                                                              | -                       | measured                |
| recommended_Salinity_PSS78  | Discrete salinity with some missing values filled in using CTDSAL                                                                                                                                                                                  | -                       | measured                |
| CTDOXY                      | Dissolved oxygen from sensors on a CTD rosette                                                                                                                                                                                                     | $\mu\text{mol kg}^{-1}$ | measured                |
| Oxygen                      | Discrete dissolved oxygen from Winkler titration                                                                                                                                                                                                   | $\mu\text{mol kg}^{-1}$ | measured                |
| recommended_Oxygen          | Discrete dissolved oxygen from Winkler titration with some missing values filled in using CTDOXY                                                                                                                                                   | $\mu\text{mol kg}^{-1}$ | measured                |
| AOU                         | Apparent oxygen utilization                                                                                                                                                                                                                        | $\mu\text{mol kg}^{-1}$ | calculated              |
| DIC                         | Dissolved inorganic carbon                                                                                                                                                                                                                         | $\mu\text{mol kg}^{-1}$ | measured                |
| TALK                        | Total alkalinity                                                                                                                                                                                                                                   | $\mu\text{mol kg}^{-1}$ | measured                |
| pH_TS_measured              | pH on total hydrogen scale (TS) at measurement temperature and ambient pressure                                                                                                                                                                    | -                       | measured                |
| TEMP_pH                     | Temperature of pH measurement                                                                                                                                                                                                                      | °C                      | measured                |
| pH_TS_insitu_measured       | pH on total hydrogen scale (TS) adjusted to in-situ conditions                                                                                                                                                                                     | -                       | measured                |
| pH_TS_insitu_calculated     | pH on total hydrogen scale (TS) at in-situ conditions calculated from DIC, TA and others using CO2SYS                                                                                                                                              | -                       | calculated              |
| Carbonate_measured          | Carbonate ion at measurement temperature and ambient pressure                                                                                                                                                                                      | $\mu\text{mol kg}^{-1}$ | measured                |
| TEMP_Carbonate              | Temperature of carbonate ion measurement                                                                                                                                                                                                           | °C                      | measured                |
| Carbonate_insitu_measured   | Carbonate ion at in-situ conditions adjusted to in-situ conditions                                                                                                                                                                                 | $\mu\text{mol kg}^{-1}$ | measured                |
| Carbonate_insitu_calculated | Carbonate ion at in-situ conditions calculated from DIC, TA and others using CO2SYS                                                                                                                                                                | $\mu\text{mol kg}^{-1}$ | calculated              |
| fCO <sub>2</sub> _measured  | Fugacity of carbon dioxide at measurement temperature and ambient pressure                                                                                                                                                                         | $\mu\text{atm}$         | measured                |

|                                     |                                                                                                  |                       |            |
|-------------------------------------|--------------------------------------------------------------------------------------------------|-----------------------|------------|
| TEMP_fCO <sub>2</sub>               | Temperature of fCO <sub>2</sub> measurement                                                      | °C                    | measured   |
| fCO <sub>2</sub> _insitu_measured   | Discrete fugacity of carbon dioxide adjusted to in-situ conditions                               | µatm                  | measured   |
| fCO <sub>2</sub> _insitu_calculated | Fugacity of carbon dioxide at in-situ conditions calculated from DIC, TA and others using CO2SYS | µatm                  | calculated |
| Aragonite                           | Aragonite saturation state at in-situ conditions calculated from DIC, TA and others using CO2SYS | -                     | calculated |
| Calcite                             | Calcite saturation state at in-situ conditions calculated from DIC, TA and others using CO2SYS   | -                     | calculated |
| Revelle_Factor                      | Revelle Factor calculated from DIC, TA and others using CO2SYS                                   | -                     | calculated |
| Silicate                            | Silicate                                                                                         | µmol kg <sup>-1</sup> | measured   |
| Phosphate                           | Phosphate                                                                                        | µmol kg <sup>-1</sup> | measured   |
| Nitrate                             | Nitrate                                                                                          | µmol kg <sup>-1</sup> | measured   |
| Nitrite                             | Nitrite                                                                                          | µmol kg <sup>-1</sup> | measured   |
| Nitrate_and_Nitrite                 | Nitrate and Nitrite combined                                                                     | µmol kg <sup>-1</sup> | measured   |
| recommended_Nitrate_and_Nitrite     | Nitrate_and_Nitrite, along with Nitrate when Nitrate_and_Nitrite data are not available          | µmol kg <sup>-1</sup> | measured   |
| Ammonium                            | Ammonium                                                                                         | µmol kg <sup>-1</sup> | measured   |

**Table 2.** Cruise flags used for this product.

| Flag value | Meaning                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| A          | These are dedicated OA cruises that are executed following Best Practices for global ocean work as outlined in Hood et al. (2011) and other documents as can be found on GO-SHIP site. Colloquially these are referred to as GO-SHIP quality. Traceable standards and certified reference materials are used and deep stations (≈> 2500 m) are executed to be able to use near constant deep-water concentrations as anchor points. A third inorganic carbon system parameter, such as pH or carbonate ion concentration are often measured, allowing consistency checks.                                                                   |
| B          | These are dedicated OA cruises that have onboard inorganic carbon measurements performed according to Best Practices (Dickson et al. 2007), and many other parameters to highest accuracy through use of standards and certified reference materials. However, the cruises do not necessarily have all other parameters analyzed to highest standards, such as freezing nutrients for shoreside analyses; not taking oxygen and nutrients samples on most Niskins; not normalizing CTD/O <sub>2</sub> trace to Winkler oxygens, insufficient metadata etc. There often are insufficient deep stations to compare data with open ocean data. |
| C          | These are opportunistic cruises where OA parameters are measured in the water column. They include standard hydrographic, carbon, and OA parameters; T, S, O <sub>2</sub> , nutrients, TALK, DIC, pH. Many parameters, including carbon and OA parameters are measured shoreside; CTD oxygen are not adjusted to Winkler oxygen. Generally, no dedicated OA personnel are onboard.                                                                                                                                                                                                                                                          |
| D          | Underway samples only. These cruises have no CTD casts and only have samples taken from the seawater supply line with often a limited amount of other hydrographic parameters. T and S are obtained from thermosalinographs with limited or no salinity check samples.                                                                                                                                                                                                                                                                                                                                                                      |

**Table 3.** World Ocean Circulation Experiment (WOCE) World Hydrographic Program (WHP) (Joyce and Corry, 1994; Swift and Diggs, 2008) QC flags used for this product.

| Flag value | Meaning               |
|------------|-----------------------|
| 2          | Acceptable            |
| 3          | Questionable          |
| 6          | Average of duplicates |
| 9          | Missing value         |

## Methods

When discrete salinity and CTDSAL were merged, data were preferentially chosen from the discrete measurements, provided the QC flag is equal to 2 or 6. The same principles were applied to the oxygen data combination. After merging, all missing values are replaced with “-999”. The merged variables are called “recommended\_Salinity\_PSS78” and “recommended\_Oxygen”, respectively (Table 2).

Apparent oxygen utilization (AOU) was calculated based on absolute salinity, conservative temperature, latitude, longitude, pressure, and recommended\_Oxygen variable using the function “gsw\_O2sol” as described in the International Thermodynamic Equation of Seawater 2010 (TEOS-10) (IOC et al., 2010). Oxygen solubility is the “combined equation: from Garcia and Gordon (1992).

$f\text{CO}_2$ \_insitu\_calculated, Carbonate\_insitu\_calculated, pH\_TS\_insitu\_calculated, aragonite saturation state, calcite saturation state, and Revelle Factor were calculated from *in-situ* temperature, salinity, DIC, TA, silicate, and phosphate using the MATLAB version (Sharp et al., 2020) of the CO2SYS program (Lewis and Wallace, 1998), with the dissociation constants for carbonic acid of Lueker et al., (2000), bisulfate ( $\text{HSO}_4^-$ ) of Dickson (1990), hydrofluoric acid (HF) of Perez and Fraga (1987), and with the total borate equations of Lee et al., (2010).

## References

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