Supplementary Material for

Best Practice Data Standards for Discrete Chemical Oceanographic Observations

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## 1 TEOS-10

In 2010, the Intergovernmental Oceanographic Commission (IOC), the Scientific Committee on Oceanic Research (SCOR), and the International Association for the Physical Sciences of the Oceans (IAPSO) adopted a new standard for calculation of the thermodynamic properties of seawater, namely the International Thermodynamic Equation of Seawater 2010 (TEOS-10, Link: http://www.teos-10.org/) (IOC et al., 2010; McDougall and Barker, 2011). It replaced the 1980 International Equation of State of Seawater (EOS-80) standard (Millero et al., 1980; Millero and Poisson, 1981). TEOS-10 enables a thermodynamically consistent description of seawater properties and is recommended as the primary means by which they are evaluated.

Perhaps the most significant change of the TEOS-10 standard is that it uses Absolute Salinity [*S*A, unit: g kg-1, which is usually estimated from a measured Practical Salinity (*S*P) value together with a regional correction term] instead of Practical Salinity (Practical Salinity Scale 1978, or PSS-78, unitless, based solely on the conductivity ratio) to characterize seawater (IOC et al. 2010; Wright et al., 2011; Le Menn et al., 2018). The thermodynamic properties of seawater, e.g., density and enthalpy, are now expressed as functions of *S*A (although the formulations for the parameters of the carbonate system such as *K*1 and *K*2 are still expressed as functions of the *S*P). The second most significant change of the TEOS-10 standard is the adoption of Conservative Temperature (Θ), which is proportional to the potential enthalpy and more accurately represents the heat content, to replace potential temperature (θ) (Supplementary Figure 1) (IOC et al., 2010; Pawlowicz, 2013).

Note that both Absolute Salinity (*S*A) and Conservative Temperature (Θ) are calculated quantities. The salinity and temperature values that should be reported in cruise data files and archived in national databases continue to be the quantities, Practical Salinity (*S*P), and *in situ* water temperature.

## 2 Recommended dissociation constants and other values for carbon system calculations

As many investigators calculate carbon dioxide (CO2) system parameters, recommended dissociation constants and other relevant quantities are discussed briefly here. Note that it is not recommended to report seawater CO2 parameters that are calculated using CO2SYS or similar programs in a cruise data file. However, if calculated parameters are reported, it is recommended that the dissociation constants used and other choices are clearly indicated in the metadata and that the uncertainties associated with such calculated parameters are reported.

Determination of dissociation constants remain a topic of active research, and the recommended dissociation constants have been revised over time as new data became available and may change in the future. It is important to recognize that there are meaningful uncertainties in all current formulations (Orr et al. 2015). Based on our current understanding, a broad recommendation can be made to use the dissociation constants from Lueker et al. (2000) for carbonic acid at salinities for open ocean situations [*S*P: 19-43, and temperature (T): 2-35°C] and the dissociation constants from Waters et al. (2014) [refitted based on data compiled by Millero (2010)] for brackish-water situations [the range of validity of these constants was stated as *S*P: 1-50, T: 0-50°C]. For samples with *S*P>=19, the choice of Lueker et al. (2000) vs. Waters et al. (2014) could result in a difference of up to 2% for fugacity of carbon dioxide (*f*CO2), 0.01 for pH, and 0.7% for saturation states of aragonite (ΩAr) and calcite (ΩCa), in some situations when calculated from the total alkalinity (TA) and dissolved inorganic carbon content (DIC) pair (Supplementary Figure 2).

The boron-salinity (B/*S*P) ratio of Lee et al. (2010) is recommended over that of Uppström (1974), as it is based on more data and used an improved method of determination. Recent results (Olafsson et al., 2020) also suggest that the internal consistency in surface water (DIC, TA, *f*CO2) seems to be better with the B/*S*P ratio advocated by Lee et al. (2010). When calculated from the TA-DIC pair, surface water *f*CO2, ΩAr, and ΩCa differ by up to 1.5%, and surface pH differs by up to 0.006 in some situations when calculated using the B/*S*P ratios of Uppström (1974) and Lee et al. (2010) (Supplementary Figure 3).

For the dissociation constants of bisulfate (HSO4–), Dickson (1990) is recommended over Khoo et al. (1977). For the dissociation constants of hydrofluoric acid (HF), Perez and Fraga (1987) is recommended over Dickson and Riley (1979). However, the choices of HSO4– and HF parameterizations should have little effect on any calculated results unless one of the input or output parameters is pH on “free” scale.

**Supplementary Table 1.** Additional column header abbreviations, their corresponding World Ocean Circulation Experiment (WOCE) Hydrographic Programme Exchange format terms (in *italic*), recommended units, and brief descriptions, for discrete chemical oceanographic observations (less commonly used). [Credit: The column header abbreviation standards presented here are based on the 30-year-old Exchange format of the WOCE Hydrographic Programme (Joyce and Corry, 1994; Swift and Diggs, 2008) with updates and refinements by the Climate and Ocean-Variability, Predictability, and Change (CLIVAR) and the Carbon Hydrographic Data Office (CCHDO) of the Scripps Institution of Oceanography].

|  |  |  |  |
| --- | --- | --- | --- |
| **Abbreviation** | **WOCE exchange format** | **Full unit** | **Description** |
| PAR  [umol/m2/s] | *PAR* | 10–6 mol m–2 s–1 | Photosynthetically active radiation |
| PAR\_flag | *PAR\_FLAG\_W* | N/A | Quality control flag for PAR |
| POC  [ug/kg] | *POC (UG/KG)* | 10–6 g kg–1 | Particulate organic carbon content |
| POC\_flag | *POC\_FLAG\_W* | N/A | Quality control flag for POC |
| TOC  [umol/kg] | *TOC* | 10–6 mol kg–1 | Total organic carbon content |
| TOC\_flag | *TOC\_FLAG\_W* | N/A | Quality control flag for TOC |
| PIC  [umol/kg] | *N/A* | 10–6 mol kg–1 | Particulate inorganic carbon content |
| PIC\_flag | *N/A* | N/A | Quality control flag for PIC |
| DON  [umol/kg] | *DON(UMOL/KG)* | 10–6 mol kg–1 | Dissolved organic nitrogen content |
| DON\_flag | *DON\_FLAG\_W* | N/A | Quality control flag for DON |
| PON  [ug/kg] | *PON(UG/KG)* | 10–6 g kg–1 | Particulate organic nitrogen content |
| PON\_flag | *PON\_FLAG\_W* | N/A | Quality control flag for PON |
| TON  [umol/kg] | *TON* | 10–6 mol kg–1 | Total organic nitrogen content |
| TON\_flag | *TON\_FLAG\_W* | N/A | Quality control flag for TON |
| TDN  [umol/kg] | *TDN(UMOL/KG)* | 10–6 mol kg–1 | Total dissolved nitrogen content |
| TDN\_flag | *TDN\_FLAG\_W* | N/A | Quality control flag for TDN |
| Delta\_C14\_DOC  [per mille] | *14C-DOC (/MILLE)* | parts per thousand | ∆14C of dissolved organic carbon is a measure of the ratio of the contents of carbon isotopes 14C:12C in the sample to that in the reference standard, reported in parts per thousand (per mille, ‰). Δ14C represents the normalized value of δ14C, with the effect of isotopic fractionation removed. |
| Delta\_C14\_DOC\_error  [per mille] | *C14ERR* | parts per thousand | Error for Delta\_C14\_DOC\* |
| Delta\_C14\_DOC\_flag | *14C-DOC\_FLAG\_W* | N/A | Quality control flag for Delta\_C14\_DOC |
| Delta\_C14\_TOC  [per mille] | *N/A* | parts per thousand | ∆14C of total organic carbon is a measure of the ratio of the contents of carbon isotopes 14C:12C in the sample to that in the reference standard, reported in parts per thousand (per mille, ‰). Δ14C represents the normalized value of δ14C, with the effect of isotopic fractionation removed. |
| Delta\_C14\_TOC\_error  [per mille] | *N/A* | parts per thousand | Error for Delta\_C14\_TOC\* |
| Delta\_C14\_TOC\_flag | *N/A* | N/A | Quality control flag for Delta\_C14\_TOC |
| Delta\_O18  [per mille] | *DELO18 (/MILLE)* | parts per thousand | δ18O of seawater is a measure of the ratio of contents of oxygen isotopes 18O:16O in the sample to that in the reference standard, reported in parts per thousand (per mille, ‰). |
| Delta\_O18\_error  [per mille] | *N/A* | parts per thousand | Error for Delta\_O18\* |
| Delta\_O18\_flag | *DELO18\_FLAG\_W* | N/A | Quality control flag for Delta\_O18 |
| Delta\_N15\_Nitrate  [per mille] | *D15N\_NO3* | parts per thousand | δ15N of nitrate is a measure of the ratio of the contents of nitrogen isotopes 15N:14N in the sample to that in the reference standard, reported in parts per thousand (per mille, ‰). |
| Delta\_N15\_Nitrate\_error  [per mille] | *N/A* | parts per thousand | Error for Delta\_N15\_Nitrate\* |
| Delta\_N15\_Nitrate  \_flag | *D15N\_NO3\_FLAG\_W* | N/A | Quality control flag for Delta\_N15\_Nitrate |
| Tritium  [TU] | *TRITUM (TU)* | TU | Tritium (3H) content is reported as TU (Tritium Units) which refers to a tritium to hydrogen ratio [T]/[H] of 10‑18. |
| Tritium\_error  [TU] | *TRITER (TU)* | TU | Error for Tritium\* |
| Tritium\_flag | *TRITUM\_FLAG\_W* | N/A | Quality control flag for Tritium |
| Delta\_He3  [%] | *DELHE3 (PERCNT)* | percent | δ3He is the percentage enrichment of 3He, above the normal atmospheric values. |
| Delta\_He3\_error  [%] | *N/A* | percent | Error for Delta\_He3\* |
| Delta\_He3\_flag | *DELHE3\_FLAG\_W* | N/A | Quality control flag for Delta\_He3 |
| CH4  [nmol/kg] | *CH4 (NMOL/KG)* | 10–9 mol kg–1 | Methane content |
| CH4\_flag | *CH4\_FLAG\_W* | N/A | Quality control flag for CH4 |
| CH3CL  [pmol/kg] | *CH3CL (PMOL/KG)* | 10–12 mol kg–1 | Chloromethane content |
| CH3CL\_flag | *CH3CL\_FLAG\_W* | N/A | Quality control flag for CH3CL |
| CCL4  [pmol/kg] | *CCL4 (PMOL/KG)* | 10–12 mol kg–1 | Carbon tetrachloride content |
| CCL4\_flag | *CCL4\_FLAG\_W* | N/A | Quality control flag for CCL4 |
| Helium  [nmol/kg] | *HELIUM (NMOL/KG)* | 10–9 mol kg–1 | Helium content |
| Helium\_error  [nmol/kg] | *HELIER* | 10–9 mol kg–1 | Error for Helium\* |
| Helium\_flag | *HELIUM\_FLAG\_W* | N/A | Quality control flag for Helium |
| Neon  [nmol/kg] | *NEON (NMOL/KG)* | 10–9 mol kg–1 | Neon content |
| Neon\_error\_  [nmol/kg] | *NEONER (NMOL/KG)* | 10–9 mol kg–1 | Error for Neon\* |
| Neon\_flag | *NEON\_FLAG\_W* | N/A | Quality control flag for Neon |
| Argon  [umol/kg] | *ARGON (UMOL/KG)* | 10–6 mol kg–1 | Argon content |
| Argon\_flag | *ARGON\_FLAG\_W* | N/A | Quality control flag for Argon |
| DMS  [nmol/kg] | *DMS* | 10–9 mol kg–1 | Dimethylsulfide (C2H6S) content |
| DMS\_flag | *DMS\_FLAG\_W* | N/A | Quality control flag for DMS |
| Methyl\_Chloroform  [pmol/kg] | *MCHFRM (PMOL/KG)* | 10–12 mol kg–1 | Methyl chloroform (1,1,1-trichloroethane) content |
| Methyl\_Chloroform\_flag | *MCHFRM\_FLAG\_W* | N/A | Quality control flag for Methyl\_Chloroform |
| Iodate  [nmol/kg] | *IODATE (NMOL/KG)* | 10–9 mol kg–1 | Iodate (IO3–) content |
| Iodate\_flag | *IODATE\_FLAG\_W* | N/A | Quality control flag for Iodate |
| Iodide  [nmol/kg] | *IODIDE (NMOL/KG)* | 10–9 mol kg–1 | Iodide (I–) content |
| Iodide\_flag | *IODIDE\_FLAG\_W* | N/A | Quality control flag for Iodide |
| Krypton\_85  [dpm/1000 kg] | *KR-85 (DM/MG)* | dpm (1000 kg) –1 | Radioactivity of krypton-85 in the ocean. |
| Krypton\_85\_flag | *KR-85\_FLAG\_W* | N/A | Quality control flag for Krypton\_85 |
| Cesium\_137  [dpm/100 kg] | *CS-137 (DM/.1MG)* | dpm (100 kg) –1 | Radioactivity of cesium-137 in the ocean. |
| Cesium\_137\_flag | *CS-137\_FLAG\_W* | N/A | Quality control flag for Cesium\_137 |
| Radium\_226  [dpm/100 kg] | *RA-226 (DM/.1MG)* | dpm (100 kg) –1 | Radioactivity of radium-226 in the ocean. |
| Radium\_226\_flag | *RA-226\_FLAG\_W* | N/A | Quality control flag for Radium\_226 |
| Radium\_228  [dpm/100 kg] | *RA-228 (DM/.1MG)* | dpm (100 kg) –1 | Radioactivity of radium-228 in the ocean. |
| Radium\_228\_flag | *RA-228\_FLAG\_W* | N/A | Quality control flag for Radium\_228 |
| Radium\_228/Radium\_226 | *RA-8/6 (DM/.1MG)* | dimensionless | The Ra-228/Ra-226 activity ratio |
| Radium\_228/Radium\_226  \_error | *RA-8/6E (DM/.1MG)* | dimensionless | Error for Radium\_228/Radium\_226\* |
| Radium\_228/Radium\_226  \_flag | *RA-8/6\_FLAG\_W* | N/A | Quality control flag for Radium\_228/Radium\_226 |
| Strontium\_90  [dpm/100 kg] | *SR-90 (DM/.1MG)* | dpm (100kg) –1 | Radioactivity of strontium-90 in the ocean. |
| Strontium\_90\_flag | *SR-90\_FLAG\_W* | N/A | Quality control flag for Strontium\_90 |
| Aluminum  [nmol/kg] | *ALUMIN (NMOL/L)* | 10–9 mol kg–1 | Aluminum content |
| Aluminum\_flag | *ALUMIN\_FLAG\_W* | N/A | Quality control flag for Aluminum |
| Barium  [nmol/kg] | *BARIUM (NMOL/KG)* | 10–9 mol kg–1 | Barium content |
| Barium\_flag | *BARIUM\_FLAG\_W* | N/A | Quality control flag for Barium |
| Calcium  [umol/kg] | *CALCIUM* | 10–6 mol kg–1 | Calcium content |
| Calcium\_flag | *CALCIUM\_FLAG\_W* | N/A | Quality control flag for Calcium |
| Copper  [nmol/kg] | *CU* | 10–9 mol kg–1 | Copper content |
| Copper\_flag | *CU\_FLAG\_W* | N/A | Quality control flag for Copper |
| Iron  [nmol/kg] | *FE (NMOL/L)* | 10–9 mol kg–1 | Iron content |
| Iron\_flag | *FE\_FLAG\_W* | N/A | Quality control flag for Iron |
| Manganese  [nmol/kg] | *MN (NMOL/L)* | 10–9 mol kg–1 | Manganese content |
| Manganese\_flag | *MN\_FLAG\_W* | N/A | Quality control flag for Manganese |
| Nickel  [nmol/kg] | *NI* | 10–9 mol kg–1 | Nickel content |
| Nickel\_flag | *NI\_FLAG\_W* | N/A | Quality control flag for Nickel |

**\* The term "error" is used here to retain historical consistency. Measurement error is in general, unknown and unknowable (ISO JGCM, 2008). If this parameter is provided, it requires added metadata to indicate what was meant by this term, and how its value was estimated.**

**Supplementary Table 2.** Column header abbreviations of this study and their corresponding Global Ocean Data Analysis Product (GLODAP) (Olsen et al., 2020) and Climate and Forecast (CF) (Hassell et al., 2017) terms. All rows from Table 1 are preserved in this table for one-to-one correspondence purposes even though some of them do not map to either the GLODAP or the CF terms.

|  |  |  |
| --- | --- | --- |
| **Abbreviation** | **GLODAP** | **Climate and Forecast (CF)** |
| EXPOCODE | N/A | N/A |
| Cruise\_ID | cruise | N/A |
| Section\_ID | N/A | N/A |
| Station\_ID | station | N/A |
| Cast\_number | cast | N/A |
| Rosette\_position | N/A | N/A |
| Niskin\_ID | bottle | N/A |
| Niskin\_flag | N/A | N/A |
| Sample\_ID | N/A | N/A |
| Year\_UTC | year | N/A |
| Month\_UTC | month | N/A |
| Day\_UTC | day | N/A |
| Time\_UTC | hour, minute | time |
| Yearday\_UTC | N/A | N/A |
| Longitude | longitude | longitude |
| Latitude | latitude | latitude |
| Depth\_bottom | bottomdepth | sea\_floor\_depth\_below\_sea\_surface |
| CTDPRES | pressure | sea\_water\_pressure |
| Depth | depth | depth |
| CTDTEMP\_ITS90 | temperature | sea\_water\_temperature |
| CTDTEMP\_flag | N/A | N/A |
| CTDSAL\_PSS78 | salinity | sea\_water\_practical\_salinity |
| CTDSAL\_flag | salinityf | N/A |
| Salinity\_PSS78 | salinity | sea\_water\_practical\_salinity |
| Salinity\_flag | salinityf | N/A |
| CTDOXY | oxygen | moles\_of\_oxygen\_per\_unit\_mass\_in\_sea\_water |
| CTDOXY\_flag | oxygenf | N/A |
| Oxygen | oxygen | moles\_of\_oxygen\_per\_unit\_mass\_in\_sea\_water |
| Oxygen\_flag | oxygenf | N/A |
| DIC | tco2 | mole\_concentration\_of\_dissolved\_inorganic\_carbon\_in\_sea\_water |
| DIC\_flag | tco2f | N/A |
| TA | talk | sea\_water\_alkalinity\_expressed\_as\_mole\_equivalent |
| TA\_flag | talkf | N/A |
| pH\_T\_measured | N/A | sea\_water\_ph\_reported\_on\_total\_scale |
| TEMP\_pH | N/A | N/A |
| pH\_flag | phtsinsitutpf | N/A |
| Carbonate\_measured | N/A | mole\_concentration\_of\_carbonate\_expressed\_as\_carbon\_in\_sea\_water |
| TEMP\_Carbonate | N/A | N/A |
| Carbonate\_flag | N/A | N/A |
| fCO2\_measured | N/A | fugacity\_of\_carbon\_dioxide\_in\_sea\_water |
| TEMP\_fCO2 | N/A | N/A |
| fCO2\_flag | fco2f | N/A |
| Silicate | silicate | moles\_of\_silicate\_per\_unit\_mass\_in\_sea\_water |
| Silicate\_flag | silicatef | N/A |
| Phosphate | phosphate | moles\_of\_phosphate\_per\_unit\_mass\_in\_sea\_water |
| Phosphate\_flag | phosphatef | N/A |
| Nitrate | nitrate | moles\_of\_nitrate\_per\_unit\_mass\_in\_sea\_water |
| Nitrate\_flag | nitratef | N/A |
| Nitrate\_and\_Nitrite | N/A | moles\_of\_nitrate\_and\_nitrite\_per\_unit\_mass\_in\_sea\_water |
| Nitrate\_and\_Nitrite\_  flag | N/A | N/A |
| Nitrite | nitrite | moles\_of\_nitrite\_per\_unit\_mass\_in\_sea\_water |
| Nitrite\_flag | nitritef | N/A |
| Ammonium | N/A | mole\_concentration\_of\_ammonium\_in\_sea\_water |
| Ammonium\_flag | N/A | N/A |
| Chl\_a | chla | mass\_concentration\_of\_chlorophyll\_a\_in\_sea\_water |
| Chl\_a\_flag | chlaf | N/A |
| DOC | doc | mole\_concentration\_of\_dissolved\_organic\_carbon\_in\_sea\_water |
| DOC\_flag | docf | N/A |
| Delta\_C13\_DIC | c13 | N/A |
| Delta\_C13\_DIC\_flag | c13f | N/A |
| Delta\_C14\_DIC | c14 | N/A |
| Delta\_C14\_DIC\_error | c14err | N/A |
| Delta\_C14\_DIC\_flag | c14f | N/A |
| CFC11 | cfc11 | moles\_of\_cfc11\_per\_unit\_mass\_in\_sea\_water |
| CFC11\_flag | cfc11f | N/A |
| CFC12 | cfc12 | mole\_concentration\_of\_cfc12\_in\_sea\_water |
| CFC12\_flag | cfc12f | N/A |
| CFC113 | cfc113 | N/A |
| CFC113\_flag | cfc113f | N/A |
| SF6 | sf6 | mole\_concentration\_of\_sulfur\_hexafluoride\_in\_sea\_water |
| SF6\_flag | sf6f | N/A |
| N2O | N/A | N/A |
| N2O\_flag | N/A | N/A |

**Supplementary Table 3.** WOCE quality control flags for Niskin bottles [adapted from Joyce and Corry (1994)].

|  |  |
| --- | --- |
| **Flag** | **Meaning** |
| 1 | Bottle information unavailable |
| 2 | No problems noted |
| 3 | Leaking |
| 4 | Did not trip correctly |
| 5 | Not reported |
| 6 | Significant discrepancy in measured values between Gerard and Niskin bottles |
| 7 | Unknown problem |
| 8 | Pair did not trip correctly. Either the Niskin bottle tripped at an unplanned depth while the Gerard tripped correctly or vice versa. |
| 9 | Samples not drawn from this bottle |

**Supplementary Table 4.** WOCE quality control flags for variables measured from discrete water samples [adapted from Joyce and Corry (1994)].

|  |  |
| --- | --- |
| **Flag** | **Meaning** |
| 1 | Sample for this measurement was drawn from water bottle but analysis not received. Note that if water is drawn for any measurement from a water bottle, the quality flag for that parameter must be set equal to 1 initially to enable all water samples to be accounted for. |
| 2 | Acceptable measurement |
| 3 | Questionable measurement |
| 4 | Bad measurement |
| 5 | Not reported |
| 6 | Mean of replicate measurements |
| 7 | Manual chromatographic peak measurement |
| 8 | Irregular digital chromatographic peak integration |
| 9 | Sample not drawn for this measurement from this bottle |

**Supplementary Table 5.** WOCE quality control flags for sensor based continuous measurement reported at 1-dbar intervals [adapted from Joyce and Corry (1994)].

|  |  |
| --- | --- |
| **Flag** | **Meaning** |
| 1 | Not calibrated |
| 2 | Acceptable measurement |
| 3 | Questionable measurement |
| 4 | Bad measurement |
| 5 | Not reported |
| 6 | Interpolated over >2 dbar interval |
| 7 | Despiked |
| 8 | Not assigned for CTD data |
| 9 | Not sampled |

**Supplementary Figure 1.** Comparison of potential temperature (θ), conservative temperature (Θ), and potential density anomaly with reference pressure of 0 (σ0) calculated using the EOS-80 and TEOS-10 methods with data from the P02 transect in 2004 (Feely et al., 2013a). (a) the regression of θ from EOS-80 against Θ from TEOS-10. (b) the regression of σ0 from EOS-80 against that from TEOS-10. (c) the differences between θ from EOS-80 and Θ from TEOS-10 against water depth (given as pressure). (d) the differences between σ0 against water depth (given as pressure).



**Supplementary Figure 2.** The differences of fugacity of carbon dioxide (*f*CO2), pH, aragonite saturation state (ΩAr), and calcite saturation state (ΩCa) calculated from DIC, TA, and other parameters that result from using the *K*1 and *K*2 dissociation constants from Lueker et al. (2000) (L) instead of Waters et al. (2014) (W). The left-side panels [(a), (c), (e) and (g)] show these differences against salinity (*S*P) based on surface data collected from three estuaries near the coast of Georgia, USA [temperature: 27-29°C] (Jiang et al. 2008). The right-side panels [(b), (d), (f), (h)] show these differences against temperature based on surface data from a north-to-south transect in the Pacific Ocean (P16S) [*S*P: 33-36] (Feely et al. 2013b). The blue circles and red crosses show the actual differences and the percent differences, respectively.



**Supplementary Figure 3.** The differences of *f*CO2, pH, ΩAr, and ΩCa calculated from DIC, TA, and other parameters that result from using the boron to salinity (B/*S*P) ratios from Uppström (1974) (U) instead of Lee et al. (2010) (L). The left-side panels [(a), (c), (e) and (g)] show these differences against salinity (*S*P) based on surface data collected from three estuaries near the coast of Georgia, USA [temperature: 27-29°C] (Jiang et al. 2008). The right-side panels [(b), (d), (f), (h)] show these differences against temperature based on surface data from a north-to-south transect in the Pacific Ocean (P16S) [*S*P: 33-36] (Feely et al. 2013b). The blue circles and red triangles show the actual differences and the percentage differences, respectively, using the *K*1 and *K*2 dissociation constants from Lueker et al. (2000), and the blue and red dots show the actual differences and the percentage differences, respectively, using the *K*1 and *K*2 dissociation constants from Waters et al. (2014).



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