Ocean Acidification International Coordination Centre
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Guide to Best Practices in Ocean Acidification Research and Data Reporting

Addendum, 2015-11-13

This addendum provides critical information and links to complementary resources for users of the *Guide to Best Practices in Ocean Acidification Research and Data Reporting* (Eds: Riebesell U., Fabry V. J., Hansson L. & Gattuso J.-P., 2010. 260 p. Luxembourg: Publications Office of the European Union). It was initiated following discussions within the SOLAS IMBER Ocean Acidification Working Group and the Advisory Board of the IAEA Ocean Acidification International Coordination Centre.

Contributors: Jean-Pierre Gattuso, Andrew Dickson, Sam Dupont, Jens Nejstgaard and Ulf Riebesell.

The following references, listed according to Chapter, provide important additional information on the various aspects discussed in the Best Practices guide. Users are strongly recommended to consult these articles as a complement to the Guide.

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Annex 1

Guidelines for reporting ocean acidification data in scientific journals

These guidelines were prepared by J.-P. Gattuso (gattuso@obs-vlfr.fr), H. Garcia (hernan.garcia@noaa.gov), C. J. M. Hoppe (Clara.Hoppe@awi.de), J. Orr (James.Orr@lsce.ipsl.fr), H.-O. Pörtner (Hans.Poertner@awi.de) and Y Yang (yangyan@xmu.edu.cn)

This document was prepared in the framework of the data management activity of the Ocean Acidification International Coordination Centre of the International Atomic Energy Agency (OAICC; www.iaea.org/ocean-acidification). Please contact the first author (gattuso@obs-vlfr.fr) in case of any error or omission. It is primarily based on Dickson et al. (2007), Dickson (2010), Nisumaa et al. (2010), Pesant et al. (2010), Pörtner et al. (2010) and Orr et al. (2015).

To ensure reproducibility, it is critical to report at least two variables of the carbonate system of seawater as well as salinity, temperature, and the hydrostatic pressure (if the measurements were not performed at atmospheric pressure). In addition, authors should report concentrations of total dissolved inorganic phosphorus as well as total dissolved inorganic silicon (in $\mu mol\ kg^{-1}$) whenever possible. Furthermore,

- Authors should carefully report how the parameters were measured and, if applicable, which protocol they followed.
- The use of Certified Reference Materials, source, and batch numbers must be mentioned.
- At least two of the following carbonate system parameters should be measured and reported (note the preferred acronyms and units):
    - Dissolved inorganic carbon (C_T; $\mu mol\ kg^{-1}$)
    - Total alkalinity (A_T; $\mu mol\ kg^{-1}$)
    - pH (it is critical to mention its scale; see below)
    - Partial pressure of carbon dioxide (pCO_2; µatm)
    - Fugacity of carbon dioxide (fCO_2; µatm)
    - Carbonate ion concentration (CO_3^{2-}; $\mu mol\ kg^{-1}$)
- The pH scale (NBS, free, total, or seawater) must be mentioned prominently in the manuscript.
- If more than one pH scale is used in a given manuscript, the pH should always be given with the associated scale as a subscript:
    - on the National Bureau of Standards scale (pH_{NBS})
    - on the seawater scale (pH_{SWS})

    - on the free scale (pH_F)
    - on the total scale (pH_T)

- The temperature at the time of sampling and at the time of measurement should both be mentioned, if they differ.
- Salinity is needed (note that it is unitless).
- The formulations used to calculate the following variables should be mentioned:
    - Concentrations of total boron
    - CO_2 solubility (K_0)
    - Dissociation constants of carbonic acid (K_1 and K_2), boric acid (K_b), water (K_w), phosphoric acid (K_{p1}, K_{p2}, K_{p3}), silicic acid (Ksi), hydrogen fluoride (K_f), and bisulfate (Ks)
    - Solubility products of calcite (Kspc) and aragonite (Kspa)
- The software package used to calculate the carbonate chemistry, along with its version number, and any associated options must all be mentioned.
- Average reproducibility of the performed measurements (with number of measurements) should be mentioned.
- Finally, it is strongly recommended that the chemistry and biological data are either archived in an on-line database (preferred) or provided along with the paper as supplementary information.

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