The MarChemSpec software package can be used to calculate chemical speciation in natural waters containing the ions present in seawater. MarChemSpec is not restricted to standard seawater composition, as is CO2SYS and similar software. Thus carbonate equilibria, for example, can be calculated for natural waters with any major ion composition, and the same is true for the complexation of the trace metals that are the focus of GEOTRACES. The results include estimated uncertainties. These are lowest for calculations of the effect of a change in composition (relative to seawater for example).

The chemical components included in MarChemSpec are:

- Seawater electrolyte (H^+, Na^+, Mg^{2+}, Ca^{2+}, K^+, Sr^{2+}, Cl^-, SO_4^{2-}/HSO_4^-, Br^-, F^-/HF, $B(OH)_3$/$B(OH)_4^-$, CO_2/HCO_3^-/CO_3^{2-}
- Trace metal cations Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Pb^{2+}, Al^{3+}, Fe^{3+}

Background: MarChemSpec was developed in SCOR Working Group 145, and since January 2023 the continued maintenance and development of MarChemSpec is the responsibility of the Chemical Speciation Group of the IAPSO/SCOR/IAPWS Joint Committee on the Properties of Seawater.

For more information about the MarChemSpec project visit our website http:\\marchemspec.org. The software can be downloaded from our website or from our Zenodo archive https://zenodo.org/records/8373046.

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