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Magnesium location in calcite brachiopod shells by synchrotron analysis: Implications for Mg/Ca thermometry

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Mg/Ca ratios of biogenic calcite of marine invertebrate organisms, such as foraminifera and mollusc shells, have been successfully used to determine seawater temperature, without the influence of salinity such as in the oxygen isotope measurements. Mg/Ca thermometry is based on the principle that there is an increase in Mg²⁺ substituting for Ca²⁺ within the crystal lattice with an increase in temperature. This principle is often not checked and, while a significant fraction of magnesium may be present in the lattice some may be in a different environment such as an associated with organic components (e.g. protein). XANES analyses at the Mg K-edge were carried out to determine the environment of Mg²⁺ within brachiopod species with low and high magnesium shells. Comparison of results with magnesium standards from abiogenic calcium carbonates and organic components, indicate that Mg²⁺ is within the crystal lattice in all brachiopod species studied. However, in high-magnesium shells, Mg²⁺ concentrations cannot be used for Mg/Ca thermometry because the Mg²⁺ concentrations are higher relative to calcium in the shell than in the surrounding water and therefore, would result in an overestimation of calculated seawater temperatures.