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From spectra to structure: ATR-FTIR analysis of conodont elements

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Conodonts are common Paleozoic and Mesozoic microfossils of presumably early vertebrates, that are widely used in biostratigraphy, paleoclimate reconstructions, and hydrocarbon exploration. Conodont elements consist mainly of fluorapatite and can be divided into an albid crown (white matter), a hyaline crown with enamel-like properties, and an organic-enriched basal body. A detailed description of the compositional characteristics of these hard tissues is crucial, given the increasing intensity of conodont research using secondary ion mass spectrometry (SIMS). In this context, estimating the carbonate and hydroxyl contents in conodonts is of key importance, as oxygen isotope analysis using the SIMS method provides information on the pooled isotopic composition of various oxygen-bearing components (e.g., PO_4, CO_3, H_2O, and OH), which may have different isotope signatures due to diagenetic overprint.

The main goal of this study is to test and refine an *in-situ* method for determining CO_2 and H_2O mass fractions in conodonts using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR). ATR-FTIR analyses were conducted following the recipe initially designed for inorganic minerals of the apatite supergroup [1], while data evaluation was performed using the software SpecXY [2].

Different conodont hard tissues, distinguished based on optical microscopy – both reflected light and fluorescence imaging – correlate well with spectral bands originating from vibrational modes of: $(PO_4)^{3-}$ (740–1130 cm^{-1}), OH^- (~3550 cm^{-1}), $(CO_3)^{2-}$ (1320–1535 cm^{-1}), CO_2 (2300–2400 cm^{-1}), and organic components (2755–3010 cm^{-1}). Clear correlations are observed between the bands in the $(CO_3)^{2-}$ region and organic matter, as well as between the peaks in the $(CO_3)^{2-}$ and $(PO_4)^{3-}$ regions. The observed carbonate content increases in the following order: albid crown < hyaline crown < basal body. Thus, the applied ATR-FTIR method can help to delineate structural zones of conodont elements and has the potential to integrate various *in-situ* analytical techniques to identify optimal sites for isotopic investigations of conodonts, contributing to the challenges of solving paleoclimate conditions.

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[1] Hammerli *et al.* (2021), *Contrib Mineral Petrol* 176, 105. [2] Gies *et al.* (2024), *Comput Geosci* 189, 105626.