Vibrational spectroscopy of biominerals: combining computer models and experiments to understand structural features

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Computer models are nowadays able to provide a fundamental understanding of the atomic arrangement and properties of minerals in a wide range of conditions, including those not accessible by experimental techniques. Within this context, Density Functional Theory has been recently shown to provide satisfactory results in predicting structural and vibrational properties of biominerals such as anhydrous and hydrated calcium carbonates [1-3].

With regard to vibrational properties, infrared and Raman spectroscopies are two of the most widely employed investigation tools for minerals and materials. Though it is possible to obtain extremely accurate experimental spectra, the nature of the samples and the presence of impurities often impede a complete assignment of the peaks [4,5].

This work reports a combined experimental and theoretical study of calcium carbonate vibrational spectra that provides new insights into the structure of its crystallization intermediates [3]. This analysis allows several hypotheses to be tested [6,7] regarding the structure of vaterite against the spectra measured for both biogenic and abiogenic samples.

[1] Carteret *et al* (2013) *J. Chem. Phys.* **138**, 014201 [2] Demichelis *et al* (2013) *J. Phys. Chem. C* **117**, 17814-17823 [3] Demichelis *et al* (2014) *J. Cryst. Growth* doi: 10.1016/j.jcrysgro.2013.10.064 [4] Wehrmeister *et al* (2010) *J. Raman Spectrosc.* **41**,193–201 [5] Coleyshaw *et al* (2003) Spectrochim. Acta A **59** (2003) 2231-2239 [6] Kabalah-Amitai *et al* (2013) *Science* **340**, 454-457 [7] Demichelis *et al*. (2013) *Cryst. Growth Des.* **13**, 2247-2251