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Supplementary information:

From synthetic to biogenic Mg-containing calcite: a comparative study using FTIR microspectroscopy

Xia Long,[a] Michael J. Nasse,[b,c] Yurong Ma,[a*] Limin Qi[a*]

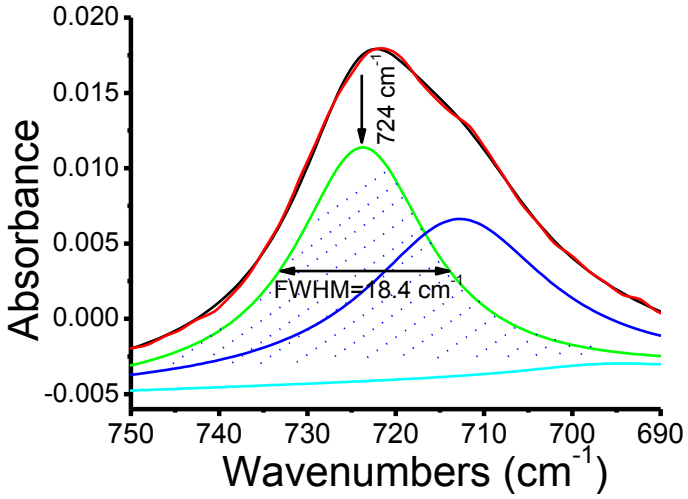

Fig. S1. The peak position and FWHM of ν_4-3 of synthetic Mg-calcite-1 is shown as an example for multi-peak fitting. The red curve is the measured spectrum, the black curve corresponds to the result/sum of all singlet bands from the multi-peak fitting, and the other colours are singlet Lorentzian bands. The peak position, FWHM, and peak area of the Lorentzian fitting curves were calculated with OMNIC from Thermo Scientific. The FWHM of ν_4-3 is 18.4 cm^{-1}. The peak position at 724 cm^{-1} was marked with a black arrow.

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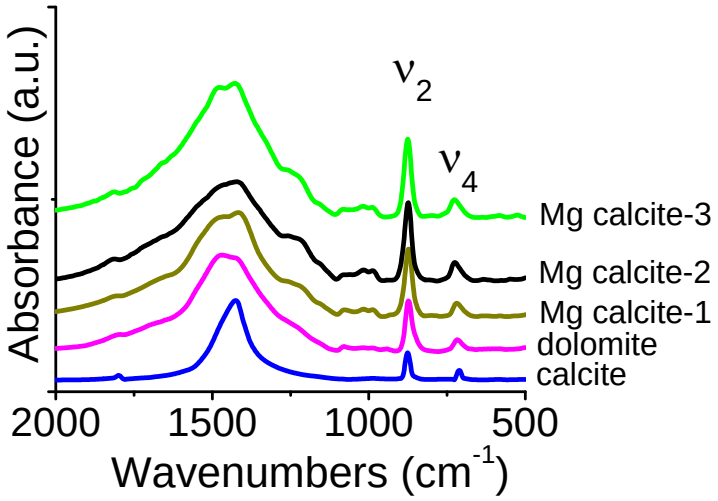

Fig. S2 KBr pellet FTIR spectra of geogenic calcite with 0 mol-% Mg, synthetic Mg calcite-1, -2, and -3 with 20, 30, and 39 mol-% Mg, and dolomite with 50 mol-% Mg, respectively.

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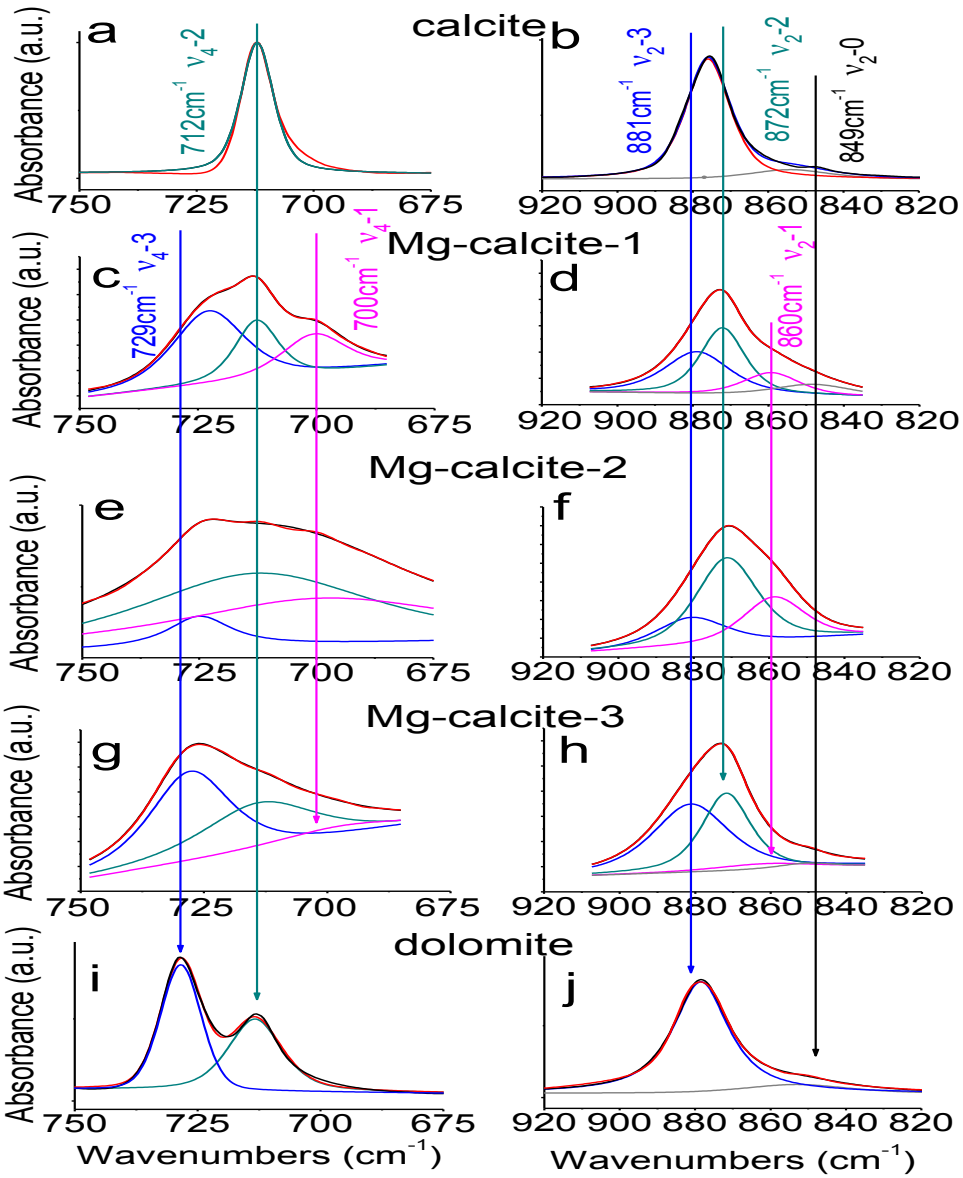

Fig. S3 Lorentzian multi-peak fitting of the ν_4 (a, c, e, g, i) and ν_2 (b, d, f, h, j) spectral bands of the KBr pellet FTIR spectra from Fig. S2: geogenic calcite with 0 mol-% Mg (a, b), synthetic Mg calcite-1 with 20 mol-% Mg (c, d), Mg calcite-2 with 30 mol-% Mg (e, f), Mg calcite-3 with 39 mol-% Mg (g, h), and dolomite with 50 mol-% Mg (i, j). The red curve is the measured spectrum, the black curve corresponds to the result/sum of all single peaks from the multi-peak fit, and the other colours are single Lorentzian peaks.

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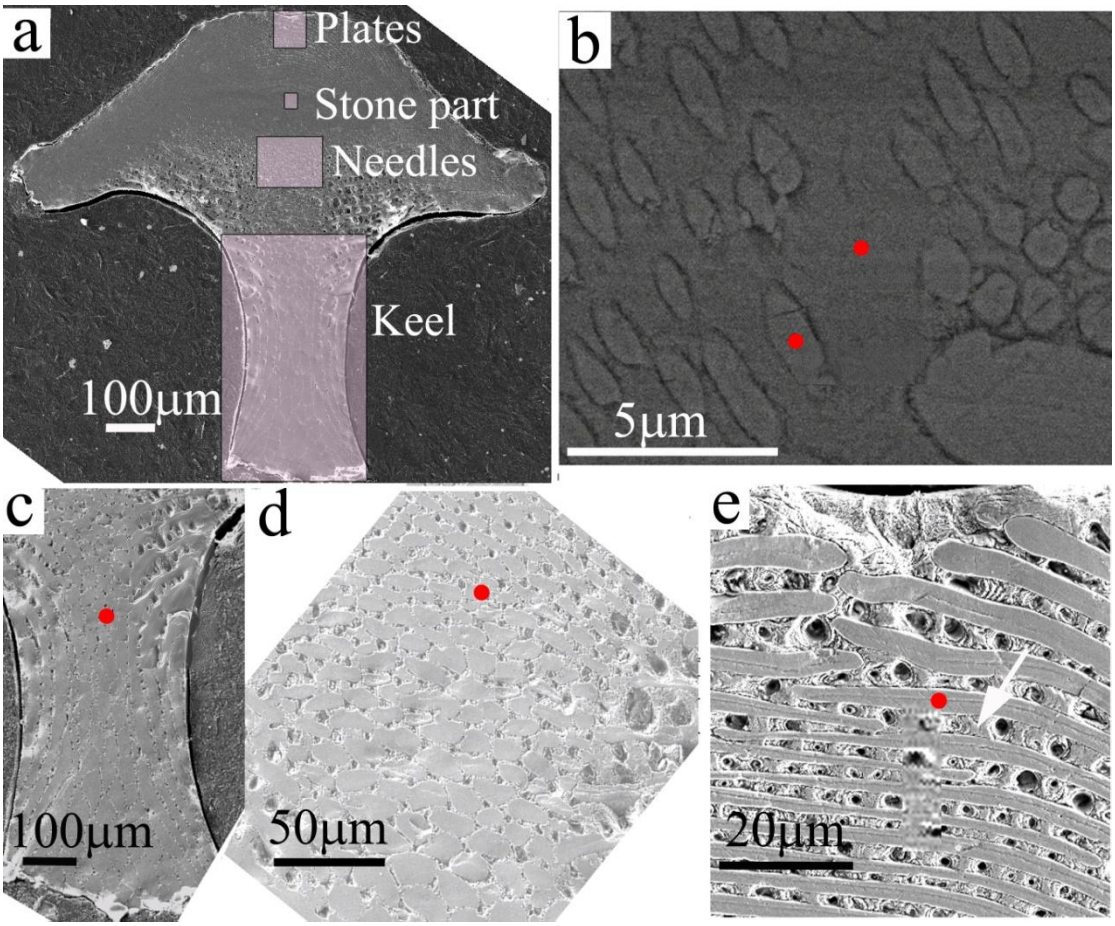

Fig. S4 Scanning electron microscopy (SEM) images of a transverse SUT cross section at the mature end. The red dots indicate in which regions the elemental analysis was done. (a) Overview cross section exhibiting the different regions studied with energy dispersive X-ray spectroscopy (EDS) to determine the local Mg content. The EDS spectra are not shown here. These four regions, stone part, plates, needles and keel are generously consistent with the positions used in the FTIRM measurement shown in Fig. 3-6, S5, and S6. (b) Stone part composed of very high Mg polycrystalline matrix (35-43 mol-% Mg) and single crystalline needles (~10-15 mol-% Mg). (c) Keel (3-4 mol-% Mg). (d) Needles (4-5mol -% Mg). (e) Plates (10-15 mol-% Mg), the white arrow indicating the very high Mg polycrystalline matrix in the plates area.

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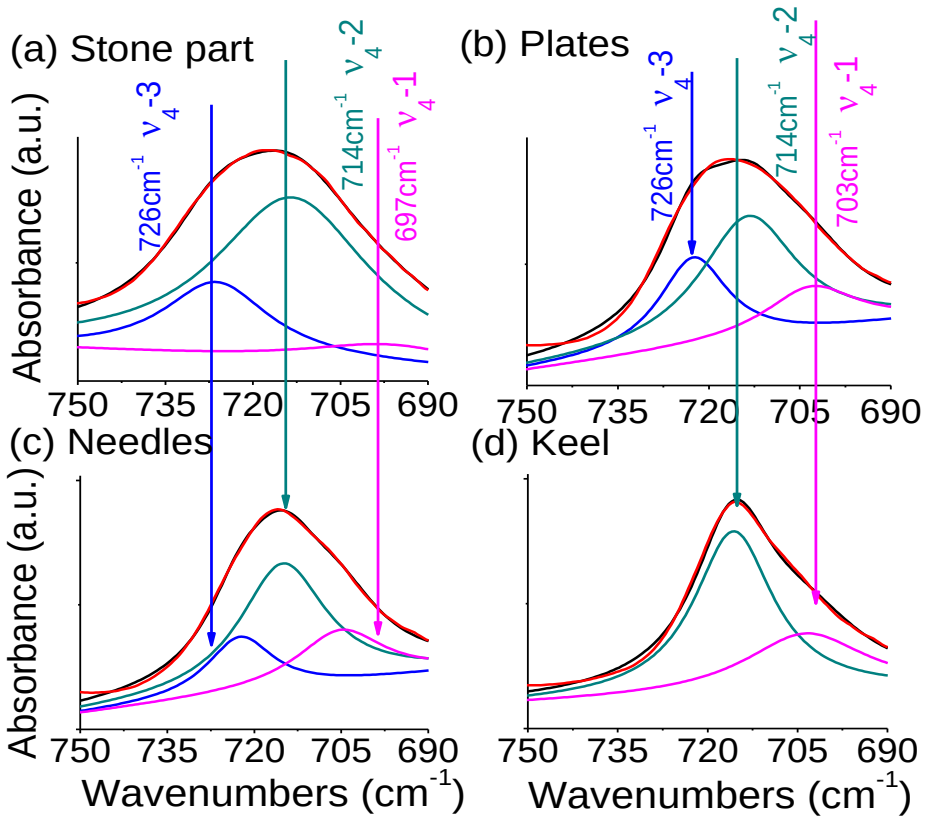

Fig. S5 Lorentzian multi-peak fitting of the ν_4 spectral band of the tFTIRM spectra shown in Fig. 6b and c from different SUT positions. The red curve is the measured spectrum, the black curve corresponds to the result/sum of all single peaks from the multi-peak fit, and the other colours are single Lorentzian peaks.

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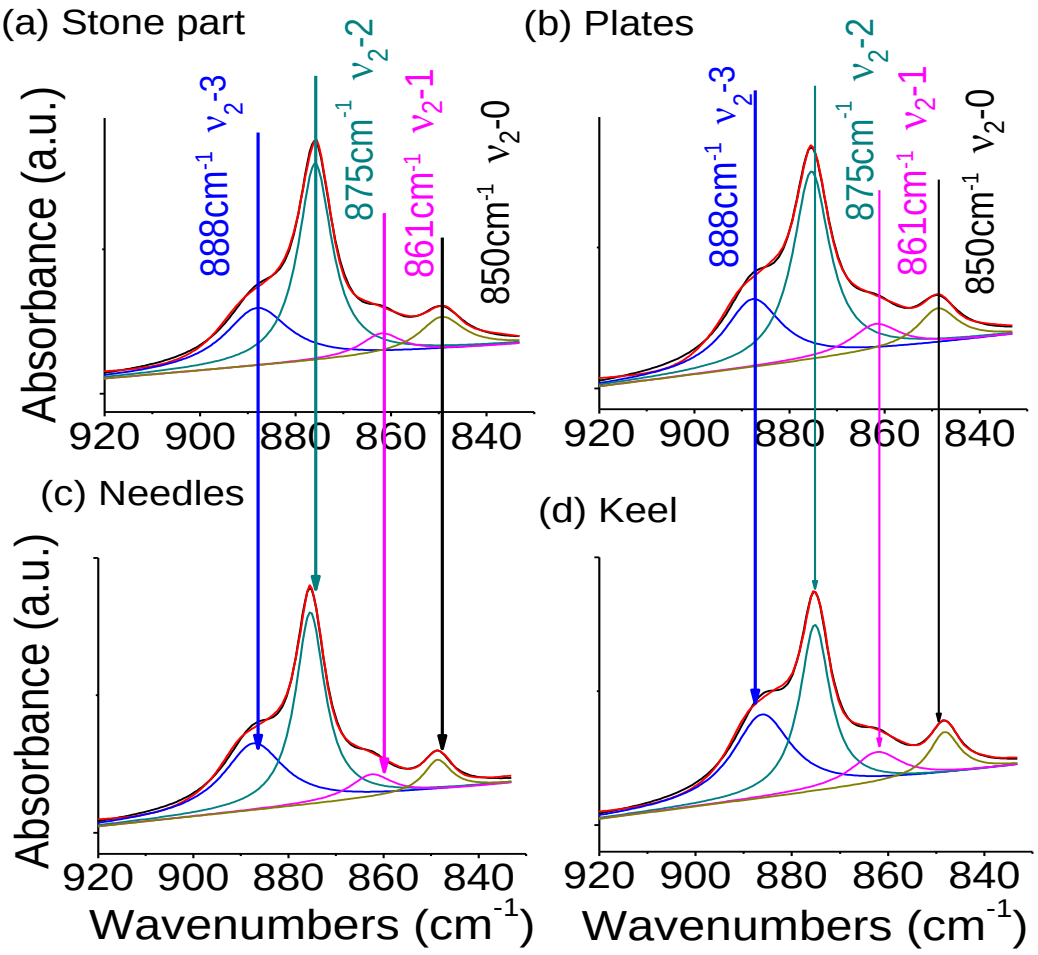

Fig. S6 Lorentzian multi-peak fitting of the ν_2 spectral band of the tFTIRM spectra shown in Fig. 6b and c from different SUT positions. The red curve is the measured spectrum, the black curve corresponds to the result/sum of all single peaks from the multi-peak fit, and the other colours are single Lorentzian peaks.

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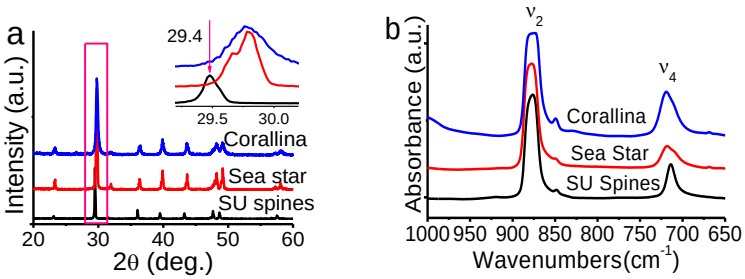

Fig. S7 XRD (a) and tFTIRM spectra (b) of other biogenic Mg calcite minerals: SU spines, corallina, sea star spicules. The inset in (a) shows a close-up of the XRD peaks marked by the red box.

Table S1 Detailed results from the ν_2 and ν_4 multi-peak curve fitting of tFTIRM spectra from other biogenic Mg-containing calcite minerals (SU spines, sea star spicules, and corallina).

	Mg contents SD (±1 mol-%)		**ν_4**			**ν_2**			
			ν_4-1	ν_4-2	ν_4-3	ν_2-0	ν_2-1	ν_2-2	ν_2-3
SU spines	4 mol-%	Peak position (cm^{-1})		714		847		875	882
		FWHM (cm^{-1})		11.6		15.0		10.8	7.5
Sea star spicules	14 mol-%	Peak position (cm^{-1})		710	720	850		875	883
		FWHM (cm^{-1})		19.4	12.9	18.7		11.6	7.6

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Corallina	14mol-%	Peak position (cm^{-1})		712	721	849		873	882
		FWHM (cm^{-1})		18.4	12.4	6.6		12.6	8.2

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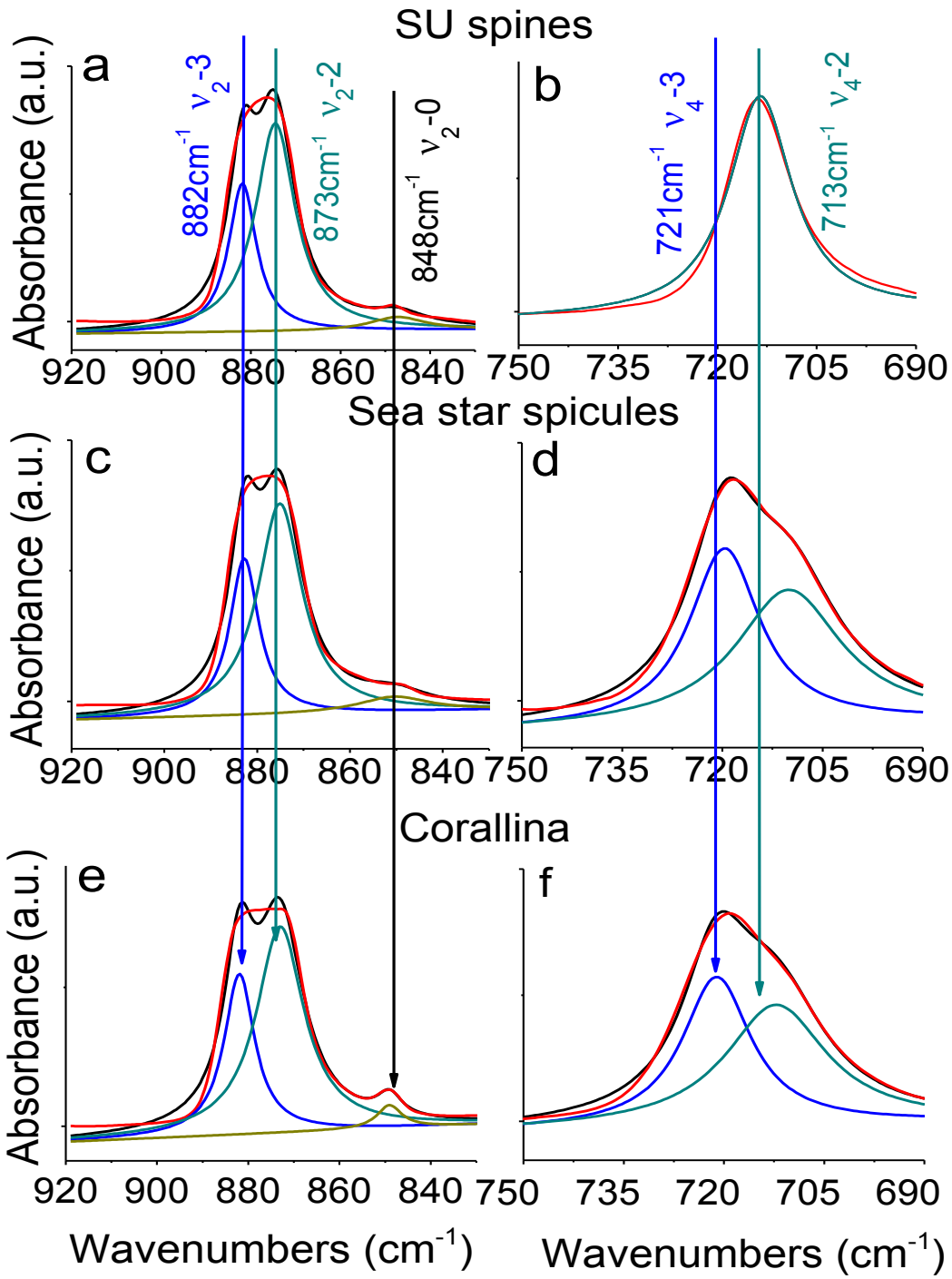

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Fig. S8. Lorentzian multi-peak curve fitting of ν_4 and ν_2 bands of Sea Urchin (SU) spines, corallina, and sea star spicules.