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Disordered amorphous calcium carbonate from direct precipitation

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Supplementary Figures

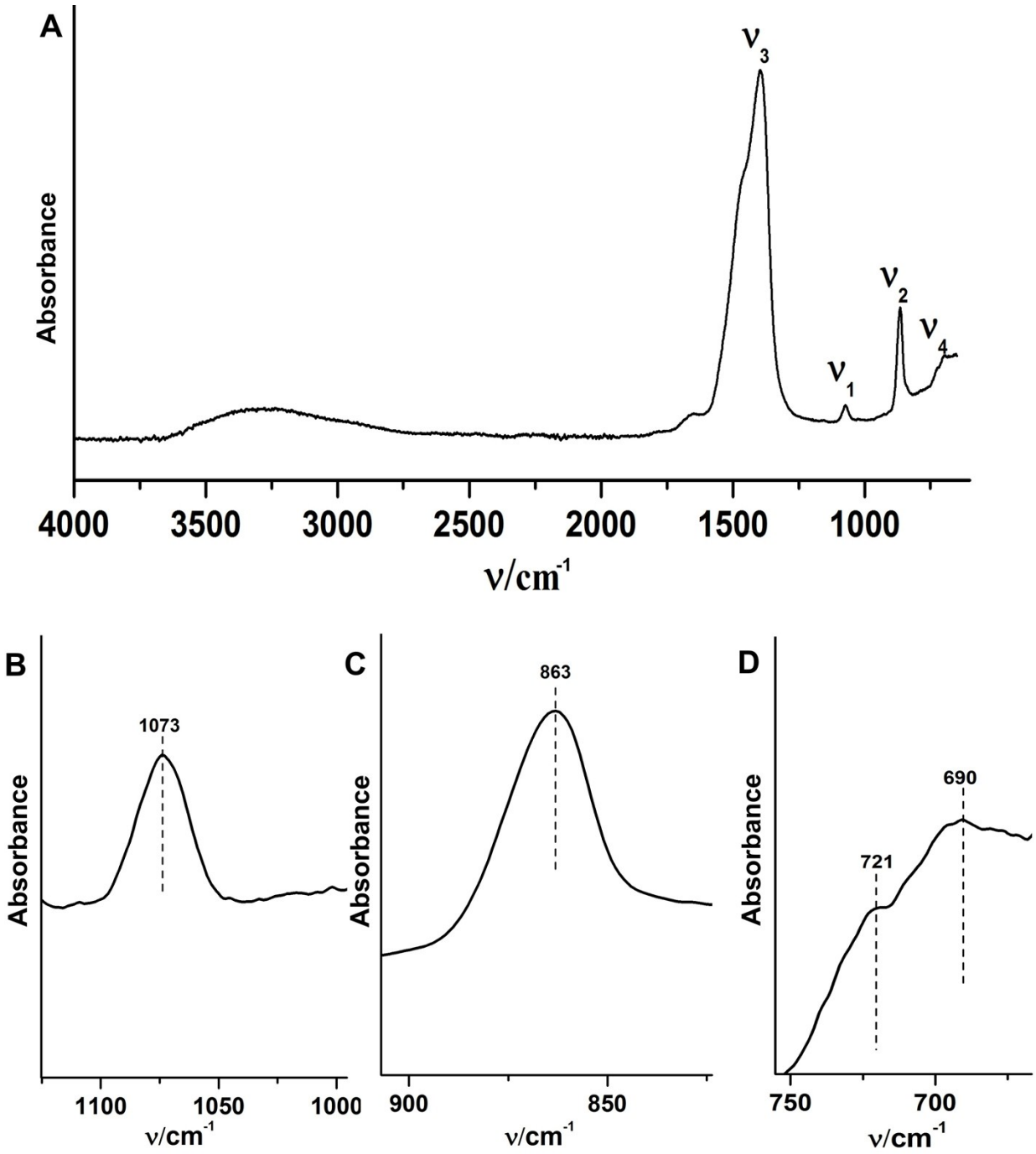

Fig. S1: ATR spectrum of the ACC of this work. (A) The overview of the full spectral range, and spectral regions of the (B) ν_1 band, (C) ν_2 band, and (D) ν_4 band.

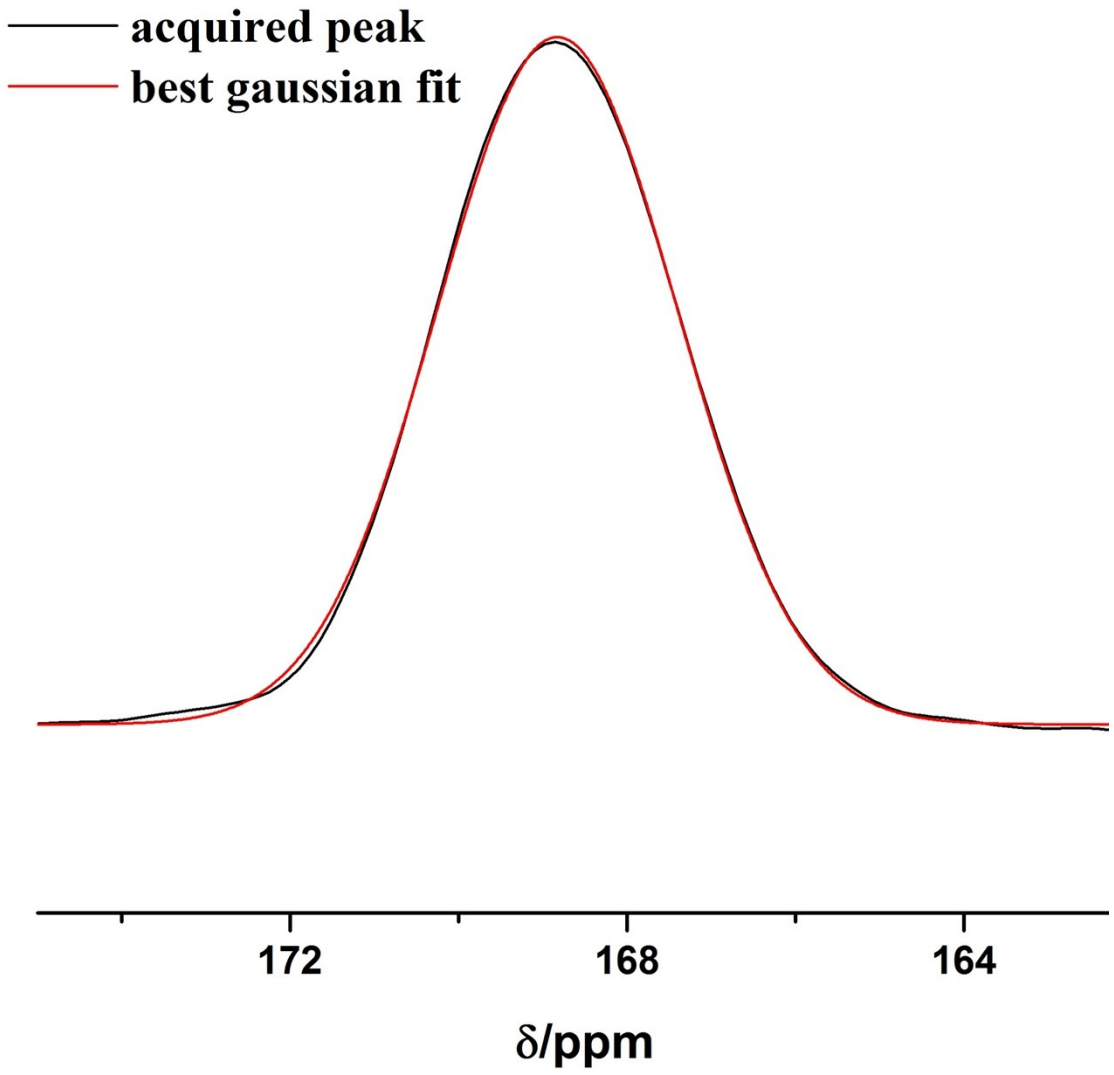

Fig S2: ^{13}C MAS-NMR spectrum of the precipitated ACC (black trace) together with a Gaussian fit (red).

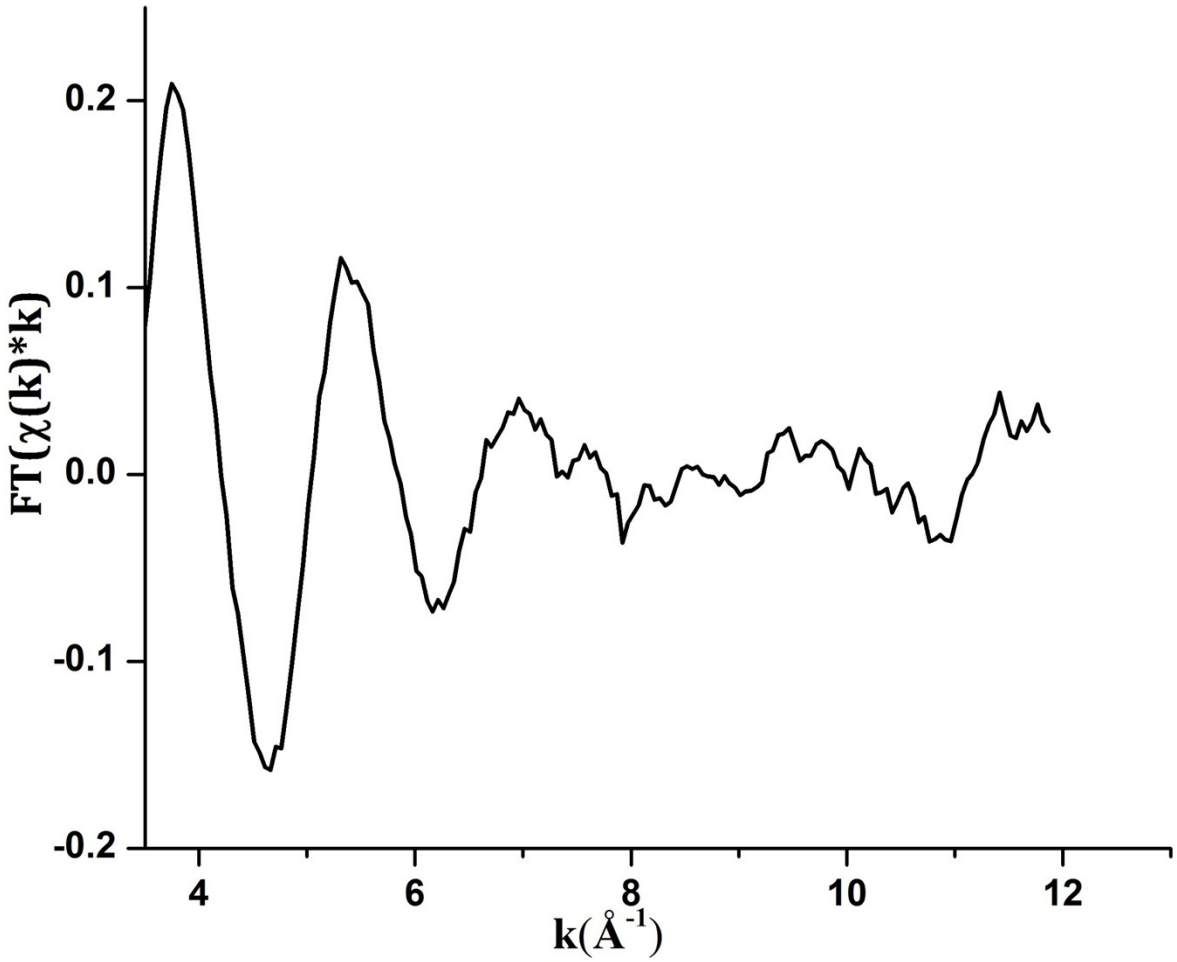

Fig S3: Calcium *K*-edge EXAFS for the ACC of this work plotted in *k*-space.

Table S1: ATR/FT-IR band positions of obtained ACC in this work in comparison with those of some other additive-free ACCs.[1-3]

Sample	ν_1	ν_2	ν_3	ν_4
ACC in this work	1073	863	1395, 1464	690, 721
pc-ACC	1074	862	1392, 1462	694, 723
pv-ACC	1026,1071	864	1392, 1462	697,721
Ethanolic ACC	1075	864	1417,1471	613, 693
Freeze-dried ACC	1130	868	1406,1473	NA

Table S2: The chemical shift together with full width at half maximum (FWHM) of unstructured ACC together with crystalline polymorphs (calcite and vaterite). The data in the parentheses represent those, which are achieved from best Gaussian fit of the acquired NMR peak of unstructured ACC of this work.

Sample	δ/ppm	FWHM/ppm
Unstructured ACC	168.85 (168.83)	3.4 (3.34)
Calcite	168.7	0.25
Vaterite	170.7; 169.5	0.46; 0.69

Table S3: Comparison between EXAFS data for synthetic ACCs,[2, 4, 5] biogenic ACCs,[6-13] and crystalline polymorphs[9, 14] with those of the ACC of this work. The data are arranged based on ascending values of the first-shell distance R. CN is the coordination number within that shell, σ the Debye-Waller factor.

Sample	CN	R/Å	σ^2 (x10^3)/Å^2	Ref.
plant cystoliths ACC	2.3	2.20	5	12
lobster carapace ACC	1.9	2.23	5	7
calcite	6	2.34	9	9
plant cystoliths ACC	2	2.35	17	12
pc-ACC	2	2.36	20 ± 10	2
rough woodlouse cuticula (with calcite) ACC	5.1 6.6	2.37 2.37	10 12	10
vaterite	6	2.37	7	9
sea tulip spicules ACC	7.4	2.37	9	8
rough woodlouse sternal deposits ACC	3.8	2.38	14	11
pv-ACC	2	2.39	20 ± 10	2
Synthetic ACCs	6.4 5.7 5.3	2.39 2.40 2.41	11.1 11.6 10.7	4
Gastrolith ACC	5.8	2.41	8	13
Synthetic ACCs	6.1 6.7	2.41 2.41	10 9	5
monohydrocalcite	8.2	2.42	14	14
plant cystoliths ACC	2 2	2.43 2.44	29 34	12
ACC in this work	**5.1 ± 0.7**	**2.440 ± 0.015**	**7.3 ± 2.7**	-
snail larval shells ACC	9	2.44	31	6
aragonite	9	2.47	33	9

References

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