Supporting Information for

Wealth from waste: Blue mussels (*Mylitus edulis*) offer up a sustainable source of natural and synthetic nacre

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Analyte (LOD)	Untreated (Mixer Mill) ^a	220 °C, 48 h (Mixer Mill)	Untreated (Mortar & Pestle) ^b	220 °C,48 h (Mortar & Pestle) ^b
Li (0.001)	1.588	1.242	0.873	0.994
Ca (0.182)	353442.0	386784.4	345618.0	367614.3
Cl (4.031)	4572.6	1861.50	619.25	553.31
Cr (0.004)	7.526	3.132	1.770	1.191
Fe (0.142)	3434.395	112.692	<80.2	<99.91
Mn (0.001)	37.547	1.699	1.222	2.011
Co (0.000)	< 0.15	< 0.16	< 0.13	< 0.15
Cu (0.004)	158.99	188.603	157.654	164.724
As (0.001)	0.445	0.456	0.155	< 0.41
Sr (0.0003)	809.453	894.522	798.713	827.754
Ag (0.0002)	<0.15	<0.14	<0.12	< 0.15
Cd (0.000)	< 0.29	< 0.29	< 0.25	< 0.31
Hg (0.000)	< 0.15	< 0.15	< 0.13	< 0.16
Pb (0.000)	0.462	0.117	0.117	< 0.08
Ba (0.0001)	11.972	3.738	1.960	1.725

Table S1: Selected ICP-MS analytes for untreated blue mussel shells and mussel shells heated at 220 °C for 48 h. Units are in ppm.

^a Mussel shells were ground in a mixer mill equipped in a 65 mL stainless steel vial with two quarter inch stainless steel balls for 12 min. ^bMussel shells were ground using a mortar and pestle.



Fig. S1 Infrared spectra of untreated mussel shells (green) and mussel shells heated to 160 °C (blue), 200 °C (red) and 225 °C (black) for 48 h.



Fig. S2 Infrared spectra of optical calcite sourced from Mexico (orange) and reagent grade calcium carbonate from Sigma Aldrich (teal). Neither samples underwent heat treatment.



Fig. S3 Powder XRD diffractograms for untreated mussel shells (green) and mussel shells heated to 160 °C (blue), 200 °C (red) and 225 °C (black) for 48 h.



Fig. S4 Infrared spectra for whole mussel shells heated at 220 °C for 48 h (black) and the resulting outer prismatic calcite layer (pink) and inner nacreous aragonite layer (purple) of the shell that cleanly separate as a result of heating.



Fig. S5 Infrared spectra of blue mussel, Mytilus edulis, (black) and eastern oyster, Crassostrea virginica, (burgundy) shells treated at 220 °C for 48 h.



Fig. S6 SEM micrographs of A) the cross section of untreated blue mussel shells shows the outer prismatic calcite layer separated from the inner nacreous aragonite layer by the myostracum (denoted by a star), B) cross section of the inner nacreous layer that results from heating the blue mussel shell to 220 °C for 48 h, C) the back side of the inner nacreous layer of blue mussel shell, and D) the inside of the outer layer of the blue mussel shell (where it separates from the inner nacreous layer) that clearly shows some of the myostracum attached.



Fig. S7 Normalized 600 MHz¹H NMR spectra of untreated blue mussel shells that were ground with a mortar and pestle. 3.2 mm zirconia rotor and spinning at 20 kHz with a relaxation delay of 2 s. 16 scans. This spectrum shows the deconvolution of peaks where the pink lines (that correspond to the zirconia rotor that is shown in Figure S7) are not part of the signal from the organic matrix in the blue mussel shell.



Fig. S8 Normalized 600 MHz ¹H NMR spectra of empty 3.2 mm zirconia rotor. Spinning at 20 kHz with a relaxation delay of 2 s. 16 scans



Fig. S9 ¹³C CP MAS NMR spectra of the inner nacreous layer of blue mussel (teal) that is a result of heating the shells to 220 °C for 48 h and untreated mussel shells (purple). Acquisition of the two spectra had the same experimental conditions. 3.2 mm zirconia rotor spinning at 20 kHz with a contact time of 1 ms. Proton decoupling level of 100 kHz and a relaxation delay of 1 s. Hartmann-Hahn rf was matched to 62.5 kHz. 16k scans.



Fig. S10 ¹³C DE MAS NMR of the inner nacreous layer of blue mussel shells ground with a mortar and pestle. 3.2 mm zirconia rotor. Spinning at 20 kHz with a proton decoupling level of 100 kHz and a relaxation delay of 320 s. 60 scans.



Fig. S11 ¹³C DE MAS NMR of the outer prismatic layer of blue mussel shells ground with a mortar and pestle. 3.2 mm zirconia rotor. Spinning at 20 kHz with a proton decoupling level of 100 kHz and a relaxation delay of 10 s. 8k scans.



Fig. S12 Thermogravimetric analysis of untreated blue mussel shells.



Fig. S13 Thermogravimetric analysis of blue mussel shells that have been heated to 220 °C for 48 h.



Fig. S14 Thermogravimetric analysis of the outer layer of blue mussel shells.



Fig. S15 Thermogravimetric analysis of the inner layer of blue mussel shells.



Fig. S16 Infrared spectra of blue mussels treated from 450 °C (green), 550 °C (blue), 650 °C (pink) and 750 °C (purple) for 2 h.



Fig. S17 SEM micrographs of A) the inner layer of blue mussel shell after heating to 450 °C, B) the outer layer of blue mussel shell after heating to 450 °C, C) the inner layer of blue mussel shell after heating to 550 °C, D) the outer layer of blue mussel shell after heating to 550 °C, E) the inner layer of blue mussel shell after heating to 650 °C and F) the inner layer of blue mussel shell after heating to 650 °C. Shells were heated for 2 h at their respective temperatures.



Fig. S18 Normalized 600 MHz ¹H NMR spectra of freeze-dried blue mussel meat. 3.2 mm zirconia rotor and spinning at 20 kHz with a relaxation delay of 5 s. 4 scans.



Fig. S19 ¹³C CP MAS NMR of freeze-dried blue mussel (Mytilus edulis) meat. 3.2 mm zirconia rotor spinning at 20 kHz with a contact time of 2 ms. Proton decoupling level of 100 kHz and a relaxation delay of 3 s. Hartmann-Hahn rf was matched to 62.5 kHz. 1k scans.



Fig. S20 Representative SEM micrographs of synthetic CaCO₃ products. A) calcite, B) vaterite, C) aragonite, D) mixture of calcite, aragonite and vaterite, E) vaterite with a unique formation, similar to nacre and F) zoomed in region of vaterite.



Fig. S21 Powder XRD diffractograms for synthetic CaCO₃ products from reaction conditions 0.8 M CaCl₂ and Na₂CO₃ (black), 0.8 M CaCl₂ and Na₂CO₃ with the addition of mussel protein hydrolysate (purple) and 0.8 M CaCl₂ and Na₂CO₃ with the addition of mussel protein hydrolysate and mussel shells for seeding nacre (pink). Identification of polymorphs denoted by blue triangles for aragonite, red squares for calcite and green circles for vaterite.



Fig. S22 Examples of colour and texture of dyed nacre and its use in UV cure gel nail enhancements.

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Cald	cite											
CaC	:0 3											
					— Powder F	Pattern (C	alculated)					
Radi	ation: Cu (Ka1)		λ:	1.54059 Å		Filter:					
Calib	pration:			2	9 : 119.246°		Lines: 51	Ē.	RI	R: 2.99		
Refe	rence: Cal	culated fro	m CSD#	141 in MD	I-500.csd @1:	2/19/07						
					11mi		- 11					
			au.	2.2	011	Cell Dat	a()	21 - 121	121	2007030200		
Crys	tal System:	Hexagon	al	S	.G: R-3c (16	7)	Z	2: 6	P.3	S: hR10		
Lattic	ce Constan	ts: 4.9890), 4.9890	, 17.0620 (A) <90.00°, 90	0.00°, 120).00°>					
Volu	me: 367.8		Density:	2.711	Mwt:		F	=(30):				
Refe	rence: Act	a Cryst 10	(1957) 5	67-570, Sa	ass R L, Vidal	e R, Dono	hue J, See	also PDF :	5-586.			
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	30°	40*		50°	60°	70*	80°	90°		100°	110°	120
#	Angle	d(Å)	1%(f)	(hkl)	2π/d	#	Angle	d(Å)	1%(f)	(hkl)	2π/d	
1	23.056	3.8545	18.4	(012)	1.6301	27	82.100	1.1729	0.5	(0,1,14)	5.3568	
2	29.401	3.0355	100.0	(104)	2.0699	28	83.779	1.1537	6.6	(134)	5.4463	
3	31.433	2.8437	2.0	(006)	2.2095	29	84.813	1.1422	3.5	(226)	5.5009	
4	35.973	2.4945	12.0	(110)	2.5188	30	86.459	1.1246	0.7	(1,2,11)	5.5868	
	39.412	2.2844	24.8	(113)	2.7504	31	93.053	1.0615	1.4	(2,0,14)	5.9194	
5 6	43 163	20042				32	04 724	1 0471	4.4	(404)	6 0006	
6 7	43.163	2.0942	6.7	(024)	3.2602	32	94.724 95.009	1.0471	4.4	(404) (318)	6.0006 6.0143	
5 6 7 8	43.163 47.118 47.504	2.0942 1.9272 1.9124	6.7 21.7	(202) (024) (018)	3.2602 3.2854	32 33 34	94.724 95.009 96.151	1.0471 1.0447 1.0353	4.4 5.0 2.3	(404) (318) (1.0.16)	6.0006 6.0143 6.0689	
5 6 7 8 9	43.163 47.118 47.504 48.506	2.0942 1.9272 1.9124 1.8752	6.7 21.7 29.3	(202) (024) (018) (116)	3.2602 3.2854 3.3506	32 33 34 35	94.724 95.009 96.151 96.195	1.0471 1.0447 1.0353 1.0349	4.4 5.0 2.3 0.7	(404) (318) (1,0,16) (1,1,15)	6.0006 6.0143 6.0689 6.0710	
5 6 7 8 9 10	43.163 47.118 47.504 48.506 56.569	2.0942 1.9272 1.9124 1.8752 1.6256	6.7 21.7 29.3 4.2	(202) (024) (018) (116) (211)	3.2602 3.2854 3.3506 3.8651	32 33 34 35 36	94.724 95.009 96.151 96.195 97.696	1.0471 1.0447 1.0353 1.0349 1.0230	4.4 5.0 2.3 0.7 0.5	(404) (318) (1,0,16) (1,1,15) (2,1,13)	6.0006 6.0143 6.0689 6.0710 6.1418	
5 6 7 8 9 10 11	43.163 47.118 47.504 48.506 56.569 57.405	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039	6.7 21.7 29.3 4.2 13.4	(202) (024) (018) (116) (211) (122)	3.2602 3.2854 3.3506 3.8651 3.9174	32 33 34 35 36 37	94.724 95.009 96.151 96.195 97.696 99.157	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118	4.4 5.0 2.3 0.7 0.5 5.1	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098	
5 6 7 8 9 10 11 12	43.163 47.118 47.504 48.506 56.569 57.405 58.077	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869	6.7 21.7 29.3 4.2 13.4 1.6	(202) (024) (018) (116) (211) (122) (1,0,10)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593	32 33 34 35 36 37 38	94.724 95.009 96.151 96.195 97.696 99.157 102.235	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895	4.4 5.0 2.3 0.7 0.5 5.1 0.6	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496	
6 7 8 9 10 11 12 13	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8	(202) (024) (018) (116) (211) (122) (1,0,10) (214)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199	32 33 34 35 36 37 38 39	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815	
5 6 7 8 9 10 11 12 13 14	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177	6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (412)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399	32 33 34 35 36 37 38 39 40	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (421)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4020	
5 6 7 8 9 10 11 12 13 14 15 16	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.957	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094	6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654	32 33 34 35 36 37 38 39 40 41	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4073 6.4330	
5 6 7 8 9 10 11 12 13 14 15 16	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.658	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.2654	32 33 34 35 36 37 38 39 40 41 41 42	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9806 0.9767 0.9655 0.9635	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (0,48)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3496 6.3815 6.4073 6.4330 6.5078 6.5078	
5 6 7 8 9 10 11 12 13 14 15 16 17 18	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0012)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191	32 33 34 35 36 37 38 39 40 41 41 42 43 44	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7 3.8	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0216)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5204 6.5708	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4402 1.4218 1.3567	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313	32 33 34 35 36 37 38 39 40 41 41 42 43 44	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5078 6.5204 6.5708 6.6009	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926	32 33 34 35 36 37 38 39 40 41 41 42 43 44 45 46	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5078 6.5204 6.5708 6.6009 6.6642	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241 72.896	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390 1.2966	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2 3.9	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10) (128)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926 4.8459	32 33 34 35 36 37 38 39 40 41 41 42 43 44 45 46 47	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571 110.478	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428 0.9376	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7 1.8	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410) (2,2,12)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5204 6.5708 6.6009 6.6642 6.7012	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241 72.896 73.673	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390 1.2966 1.2848	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2 3.9 0.9	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10) (128) (306)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926 4.8459 4.8903	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571 110.478 114.053	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428 0.9376 0.9182	4.4 5.0 2.3 0.7 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7 1.8 0.5	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410) (2,2,12) (327)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5204 6.5708 6.6009 6.6642 6.7012 6.8430	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241 72.896 73.673 76.281	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390 1.2966 1.2848 1.2473	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2 3.9 0.9 1.6	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10) (128) (306) (220)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926 4.8459 4.8903 5.0376	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49	94.724 95.009 96.151 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571 110.478 114.053 117.952	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428 0.9376 0.9182 0.8989	4.4 5.0 2.3 0.7 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7 1.8 0.5 1.8	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410) (2,2,12) (327) (238)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5204 6.5708 6.5204 6.5708 6.6009 6.6642 6.7012 6.8430 6.9900	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241 72.896 73.673 76.281 77.157	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390 1.2966 1.2848 1.2473 1.2353	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2 3.9 0.9 1.6 2.9	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10) (128) (306) (220) (1,1,12)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926 4.8459 4.8903 5.0376 5.0865	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571 110.478 114.053 117.952 118.798	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428 0.9376 0.9182 0.8989 0.8949	4.4 5.0 2.3 0.7 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7 1.8 0.5 1.8 1.8	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410) (2,2,12) (327) (238) (416)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3815 6.4073 6.4330 6.5078 6.5204 6.5708 6.5009 6.6642 6.7012 6.8430 6.9900 7.0209	
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25	43.163 47.118 47.504 48.506 56.569 57.405 58.077 60.674 60.999 61.374 63.057 64.668 65.607 69.191 70.241 72.896 73.673 76.281 77.157 80.951	2.0942 1.9272 1.9124 1.8752 1.6256 1.6039 1.5869 1.5251 1.5177 1.5094 1.4730 1.4402 1.4218 1.3567 1.3390 1.2966 1.2848 1.2473 1.2353 1.1867	21.0 6.7 21.7 29.3 4.2 13.4 1.6 6.8 3.1 3.7 2.6 8.6 4.7 1.7 3.2 3.9 0.9 1.6 2.9 0.9	(202) (024) (018) (116) (211) (122) (1,0,10) (214) (208) (119) (125) (300) (0,0,12) (217) (0,2,10) (128) (306) (220) (1,1,12) (312)	3.2602 3.2854 3.3506 3.8651 3.9174 3.9593 4.1199 4.1399 4.1628 4.2654 4.3627 4.4191 4.6313 4.6926 4.8459 4.8903 5.0376 5.0865 5.2948	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51	94.724 95.009 96.151 96.195 97.696 99.157 102.235 102.952 103.536 104.121 105.846 106.142 107.329 108.044 109.571 110.478 114.053 117.952 118.798 119.246	1.0471 1.0447 1.0353 1.0349 1.0230 1.0118 0.9895 0.9846 0.9806 0.9767 0.9655 0.9636 0.9562 0.9519 0.9428 0.9376 0.9182 0.8989 0.8949 0.8929	4.4 5.0 2.3 0.7 0.5 5.1 0.6 2.4 0.6 2.2 1.7 3.8 0.9 0.5 3.7 1.8 0.5 1.8 1.8 2.0	(404) (318) (1,0,16) (1,1,15) (2,1,13) (0,3,12) (321) (232) (1,3,10) (1,2,14) (324) (048) (0,2,16) (235) (410) (2,2,12) (327) (238) (416) (2,1,16)	6.0006 6.0143 6.0689 6.0710 6.1418 6.2098 6.3496 6.3496 6.3496 6.3496 6.4073 6.4330 6.5078 6.5204 6.5708 6.5009 6.6642 6.7012 6.8430 6.9900 7.0209 7.0371	

Fig. S23 Phase information for calcite. For powder XRD comparison and identification purposes. See reference in the image.

Ara	aonite												
~~~	gointe												
Cat	.03				Den de a Des		01	Different	and a d				
		CREEK CV			Powder Pal	ttern (QM:	Star	, Diffracto	meter) —				
Rad	iation: Cu	ιΚα1			λ: 1.5405	98 A		Filter:		0	CAS#: 1479	91-73-2	
Cali	bration: I	nternal (Si)	1		<b>20</b> : 89.41	1°		Lines: 8	32	F	RIR: 1.00		
Refe	erence: K	eller, L., R	ask, J., E	Buseck, P.,	Arizona St	tate Univ.,	Tem	npe, AZ, U	SA., ICDE	Grant-ir	n-Aid (1989	)	
					- Unit Ce	ll Data (Po	owde	r Diffractio	on)				
-	tal Svetor	n: Orthort	ombic		S.G. Pmg	m (62)			7. 4		S. 0P20		
orya	co Constr	nto: 4.06	22 7 060	0 5 7420	(A) -00.00	00 000 000 0	00.00	n°>	2. 4	1	. <b>G.</b> 0120		
Latu	Ce Consta	4.50.	23, 7.900	0, 5.7459	(M) ~90.00	, 90.00 , 3	90.00	- 0	E(20) 0/	00 0 (0 0)	240.24/0		
	ime: 227	1	Densit	V: 2.950	IVI	wt: 100.0	19		F(30): 24	20.6 (0.00	J40,34/0)		
rete	sience: J	aroscn, D.,	neger, (	a., ischen	naks Mine	rai. Petrog	jr. IVII	u., v35 p1	21 (1990)	5			
			I.										mi
			11	1 1	11								
			L	M		A.M.	~	00.			~~~~	~ ~~	~ ~
20°		30°		10°		1. 50°	~	 60°	~~~	~ 70°	<u>محممہ</u> 80	~~~	
20° #	Angle	d(Å)	I%(f)	40°	2π/d	M.	~ #		 d(A)	70°		2π/d	
20° #	Angle 21.075	d(Å) 4.2120	I%(f) 3.0	(h k l) (1 1 0)	2π/d 1.4917	M.	~ # 23	60° Angle 50.229	d(A) 1.8149	70° 1%(f) 20.0	( h k l) ( 1 3 2)	2π/d 3.4620	
20° # 1 2	Angle 21.075 22.296	d(A) 4.2120 3.9840	I%(f) 3.0 1.0	40° (h k l) (1 1 0) (0 2 0)	2π/d 1.4917 1.5771	1. 50°	# 23 24	60° Angle 50.229 51.917	d(Å) 1.8149 1.7598	70° 1%(f) 20.0 3.0	( h k l) ( 1 3 2) ( 1 4 1)	2π/d 3.4620 3.5704	<u>90°</u>
20° # 1 2	Angle 21.075 22.296 26.212	d(A) 4.2120 3.9840 3.3970	1%(f) 3.0 1.0 100.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1)	2π/d 1.4917 1.5771 1.8496	1. 50°	# 23 24 25	60° Angle 50.229 51.917 52.455	d(A) 1.8149 1.7598 1.7430	70° 1%(f) 20.0 3.0 25.0	(h k l) (1 3 2) (1 4 1) (1 1 3)	2π/d 3.4620 3.5704 3.6048	
20° # 1 2 3 4	Angle 21.075 22.296 26.212 27.216	d(Å) 4.2120 3.9840 3.3970 3.2740	1%(f) 3.0 1.0 100.0 50.0	4b° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1)	2π/d 1.4917 1.5771 1.8496 1.9191	<u>M</u> ,	# 23 24 25 26	60° Angle 50.229 51.917 52.455 52.913	d(Å) 1.8149 1.7598 1.7430 1.7290	70° 1%(f) 20.0 3.0 25.0 12.0	(h kl) (1 3 2) (1 4 1) (1 1 3) (2 3 1)	2π/d 3.4620 3.5704 3.6048 3.6340	~~ <u>9</u> å°
20° # 1 2 3 4 5	Angle 21.075 22.296 26.212 27.216 31.115 22.241	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7220	1%(f) 3.0 1.0 100.0 50.0 6.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 0 2) (1 2 1)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2000	A.M.	# 23 24 25 26 27 28	60° Angle 50.229 51.917 52.455 52.913 53.022 52.042	d(A) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6024	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0	(h kl) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 2.6005	<u>90°</u>
^{20°} # 1 2 3 4 5 6 7	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 0 2) (1 2 1) (0 1 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254	50°	# 23 24 25 26 27 28 29	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144	d(A) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6984 1.6369	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385	90°
20° # 1 2 3 4 5 6 7 8	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0	40° (h kl) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325	1. 50°	# 23 24 25 26 27 28 29 30	Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403	d(A) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6984 1.6369 1.6369	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8385	<u></u>
^{20°} # 1 2 3 4 5 6 7 8 9	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0	(h kl) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061		# 23 24 25 26 27 28 29 30 31	Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790	d(A) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6984 1.6369 1.6300 1.6198	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8385 3.8547 3.8790	∽~~ġġ••
20° # 1 2 3 4 5 6 7 8 9 10	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0	(h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478	50°	# 23 24 25 26 27 28 29 30 31 32	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8385 3.8547 3.8790 4.0308	<u></u>
20° # 1 2 3 4 5 6 7 8 9 10 11	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 14.0 45.0 25.0	(h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828	<u>, M</u> ,	# 23 24 25 26 27 28 29 30 31 32 33	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914	9 ⁰ *
20° # 1 2 3 4 5 6 7 8 9 10 11 12	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966	1. M.	# 23 24 25 26 27 28 29 30 31 32 33 34	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357 1.4993	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 2.0 4.0	(h kl) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907	9 ⁰ *
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.3300 2.1900	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 25.0 12.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690	1. M.	# 23 24 25 26 27 28 29 30 31 32 33 33 34 35	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.301	d(Å) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5557 1.4993 1.4891	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0	(h kl) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195	<u>90</u> *
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.3420 2.3300 2.1900 2.1680	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 12.0 2.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981	50°	# 23 24 25 26 27 28 29 30 31 32 33 34 35 36	60° 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.301 62.898	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5588 1.5357 1.4993 1.4891 1.4764	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0 2.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195 4.2557	90°*
^{20°} # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 6	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.264 37.884 38.405 38.610 41.187 41.624 42.866	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.1900 2.1680 2.1080	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 12.0 2.0 2.0 2.0 2.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 2) (1 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1) (2 2 0) (1 3 1) (2 2 0) (2 1 2) (2 1 2) (1 3 1) (2 2 0) (2 1 2) (2 1 2) (2 1 2) (2 1 2) (1 2 2) (2 1 2) (1 2 2) (1 3 1) (2 2 0) (1 2 2) (2 1 2) (1 2 1) (1 2 2) (2 2 1) (1 2 1) (1 2 2) (2 2 1) (1 3 1) (2 2 0) (2 2 1) (1 3 1) (2 2 0) (2 2 1) (1 3 0) (2 2 0) (2 2 0) (2 2 1) (1 3 0) (2 2 0)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981 2.9806	1. M.	# 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37	60° 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.301 62.898 63.338	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5588 1.5587 1.4993 1.4891 1.4764 1.4764	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 1.0	(h kl) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1) (1 5 1) (1 5 1)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824	90°*
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624 42.866 42.866 42.866	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3730 2.3300 2.1900 2.1680 2.1080 2.1080	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 12.0 2.0 20.0 20.0 20.0 25.0	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 0 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1) (2 2 0) (1 2 2) (1 2 1) (1 2 2) (1 2 1) (1 2 2) (1 2 2) (1 2 1) (1 2 2) (2 2 1) (1 2 2) (1 2 1) (1 2 2) (2 2 1) (1 2 2) (1 2 2) (1 2 1) (1 2 2) (2 2 1) (1 2 2) (1 2 2) (1 2 2) (2 2 2) (1 2 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981 2.9806 2.9806 2.9806 2.9806	50°	# 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 36	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.301 62.898 63.338 64.880	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5588 1.5557 1.4993 1.4891 1.4764 1.4672 1.4360	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0 2.0 4.0 1.0 2.0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1) (1 5 1) (0 0 4)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824 4.3755	90°*
20° # 1 2 3 4 5 6 7 8 9 10 11 2 3 4 5 6 7 8 9 10 11 2 3 14 15 16 17 17 17 10 10 10 10 10 10 10 10 10 10 10 10 10	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624 42.866 42.866 45.853	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.1080 2.1080 2.1080 1.9774 1.9502	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 12.0 2.0 20.0 20.0 20.0 55.0 12.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 2 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1) (2 2 0) (1 2 2) (1 2 2) (2 2 1) (1 2 2) (2 2 2) (2 2 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981 2.9806 2.9806 3.1775 3.2224	J.M.	# 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39	60° Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.898 63.338 64.880 65.855	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357 1.4993 1.4891 1.4764 1.4672 1.4360 1.4167	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 4.0 2.0 4.0 2.0 4.0 1.0 2.0 4.0 1.0 2.0 4.0 2.0 2.0 4.0 2.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 2.0 3.0 2.0 2.0 3.0 2.0 2.0 3.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1) (1 5 1) (0 0 4) (2 2 3) (0 2 4)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824 4.3755 4.4351	90°*
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# 1234 567 8910 112 13 14 15 16 17 18 19 20	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624 42.866 42.866 42.865 346.535 48.319 48.444	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.1900 2.1680 2.1080 2.1080 1.9774 1.9500 1.8821 1.8775	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 12.0 20.0 20.0 55.0 1.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.0 25.	40° (h k l) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 2 1) (1 2 1) (0 2 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1) (2 2 0) (1 2 2) (2 2 1) (0 3 2) (0 4 1) (2 0 2)	2π/d 1.4917 1.5771 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6328 2.6966 2.8690 2.8981 2.9806 2.9806 3.1775 3.2221 3.3384 3.3466	50°	# 23 24 25 26 27 28 29 30 31 32 33 33 33 33 33 33 33 33 33 33 33 34 35 36 37 38 39 40 41 42	Angle 50.229 51.917 52.455 53.942 56.144 56.403 56.790 59.229 60.211 61.831 62.301 62.898 63.338 64.880 65.875 66.059 66.191	d(A) 1.8149 1.7598 1.7430 1.7290 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357 1.4993 1.4891 1.4764 1.4764 1.4764 1.4167 1.4132 1.4107 1.400	70° 70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0 2.0 4.0 1.0 2.0 4.0 1.0 3.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 2.0 3.0 3.0 2.0 3.0 3.0 2.0 3.0 3.0 2.0 3.0 3.0 2.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (1 5 1) (0 0 4) (2 2 3) (0 1 4) (3 1 2) (3 3 0)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824 4.3755 4.4351 4.4461 4.4539 4.4752	90°*
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624 42.866 42.866 45.853 46.535 48.319 48.444 48.885	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.1900 2.1680 2.1080 2.1080 1.9774 1.9500 1.8821 1.8775 1.8616	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 12.0 20.0 20.0 20.0 20.0 25.0 1.0 25.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.	40° (h kl) (1 1 0) (0 2 0) (1 1 1) (0 2 1) (0 2 1) (0 2 2) (1 2 1) (0 1 2) (2 0 0) (0 3 1) (1 1 2) (1 3 0) (0 2 2) (2 1 1) (1 3 1) (2 2 0) (1 2 2) (2 2 1) (0 3 2) (0 4 1) (2 0 2) (0 1 3)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981 2.9806 3.1775 3.2221 3.3384 3.3466 3.3752	50°	# 23 24 25 26 27 28 29 30 31 32 33 33 33 33 33 33 33 33 33 34 35 36 37 38 39 40 41 42 43	Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 60.211 61.831 62.301 62.898 63.338 64.880 65.875 66.059 66.191 66.548 67.838	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357 1.4993 1.4891 1.4764 1.4672 1.4360 1.4167 1.4132 1.4107 1.4132 1.4107 1.4040 1.3804	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0 2.0 4.0 1.0 3.0 4.0 1.0 3.0 4.0 3.0 0 0 3.0 0 0 0 0 0 0 0 0 0 0 0 0 0	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1) (1 5 1) (0 0 4) (2 2 3) (0 1 4) (3 1 2) (3 3 0) (0 4 3)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824 4.3755 4.4351 4.4461 4.4539 4.4752 4.5517	90 ⁺
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 9 20 21 22	Angle 21.075 22.296 26.212 27.216 31.115 32.741 33.128 36.176 37.264 37.884 38.405 38.610 41.187 41.624 42.866 42.866 45.853 46.535 48.319 48.444 48.885 49.859	d(A) 4.2120 3.9840 3.3970 3.2740 2.8720 2.7330 2.7020 2.4810 2.4110 2.3730 2.3420 2.3300 2.1900 2.1680 2.1080 2.1080 1.9774 1.9500 1.8821 1.8775 1.8616 1.8275	1%(f) 3.0 1.0 100.0 50.0 6.0 9.0 60.0 40.0 14.0 45.0 25.0 25.0 12.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20.0 20	40°     (h k l)     (1 1 0)     (0 2 0)     (1 1 1)     (0 2 0)     (1 1 1)     (0 2 0)     (1 1 1)     (0 2 1)     (0 0 2)     (1 2 1)     (0 1 2)     (2 0 0)     (0 3 1)     (1 1 2)     (1 3 0)     (0 2 2)     (2 1 1)     (1 3 1)     (2 2 0)     (0 3 2)     (0 4 1)     (2 0 2)     (0 1 3)     (2 1 2)	2π/d 1.4917 1.5771 1.8496 1.9191 2.1877 2.2990 2.3254 2.5325 2.6061 2.6478 2.6828 2.6966 2.8690 2.8981 2.9806 3.1775 3.2221 3.3384 3.3466 3.3752 3.4381	50°	# 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44	Angle 50.229 51.917 52.455 52.913 53.022 53.942 56.144 56.403 56.790 60.211 61.831 62.301 62.898 63.338 64.880 65.875 66.059 66.191 66.548 67.838 68.635	d(A) 1.8149 1.7598 1.7430 1.7257 1.6984 1.6369 1.6300 1.6198 1.5588 1.5357 1.4993 1.4891 1.4764 1.4672 1.4360 1.4167 1.4132 1.4107 1.4132 1.4107 1.4040 1.3804 1.3663	70° 1%(f) 20.0 3.0 25.0 12.0 16.0 2.0 3.0 1.0 2.0 4.0 2.0 4.0 1.0 2.0 4.0 1.0 3.0 4.0 1.0 2.0 4.0 3.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 4.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2	(h k l) (1 3 2) (1 4 1) (1 1 3) (2 3 1) (0 2 3) (2 2 2) (0 4 2) (1 2 3) (3 1 0) (3 1 1) (0 5 1) (2 4 1) (2 1 3) (3 2 1) (1 5 1) (0 0 4) (2 2 3) (0 1 4) (3 1 2) (3 3 0) (0 4 3) (2 4 2)	2π/d 3.4620 3.5704 3.6048 3.6340 3.6409 3.6995 3.8385 3.8547 3.8790 4.0308 4.0308 4.0914 4.1907 4.2195 4.2557 4.2824 4.3755 4.4351 4.4461 4.4539 4.4752 4.5517 4.5987	90 ⁺

*Fig. S24 Phase information for aragonite. For powder XRD comparison and identification purposes. See reference in the image.* 

vare	rite										
CaC	<b>O</b> 3										
	aros 202	one.	P	Powder Pat	tern (QM: In	idexed, Del	bye-Scherre	er, Film/Vis	ual) —		122121
Radia	ation: CuK	a		λ:	1.5418 A		Filter: Ni		C/	AS#: 13701	-58-1
Calib	ration: Inte	ernal (Si)		2	9; 115.641		Lines: 33	9	RI	R;	
Refe	rence: Ro	use, R., De	ept. of Ge	eological S	ciences, Uni	iv. of Michig	jan, Ann Ar	bor, MI, US	SA., Priva	ate Commu	inication (1980)
					U	nit Cell Dat	a()				
Cryst	al System:	Hexagon	al	S	.G: P63/mn	nc (194)	2	Z: 12	P.:	S: hP60	
Lattic	e Constant	ts: 7.1473	3, 7.1473	, 16.9170 (	Å) <90.00°,	90.00°, 120	<"00.00">				
Volur	ne: 748.4		Density:	2.665	Mwt:	100.09	F	F(30): 4.2	(0.046,1	56/0)	
Refe	rence: Ibid	ł	0					8 S -			
	1		1								Yunna (())
1			1		1						
20°		ļ	mell 40°		1		U	بسب		100°	<u>, , , , , , , , , , , , , , , , , , , </u>
20°		d(A)	40°	50°	60° 2π/d		Angle	<b>ــــــــــــــــــــــــــــــــــــ</b>	90°	100°	<u>λ</u> 110° 2π/d
20° #	30 Angle 21.005	d(Å) 4.2260	40° 1%(f) 25.0	5b° (h k l) (0 0 4)	2π/d 1.4868		Angle 71.969	d(Å)	90° 1%(f) 20.0	100° ( h k l) (1,1,12)	<u>Λ</u> 110° 2π/d 4.7927
20° # 1 2	30 Angle 21.005 24.900	d(Å) 4.2260 3.5730	40° 1%(f) 25.0 60.0	50° (h k l) (0 0 4) (1 1 0)	2π/d 1.4868 1.7585	70° # 23 24	Angle 71.969 73.595	d(Å) 1.3110 1.2860	90° 1%(f) 20.0 20.0	100° ( h k l) (1,1,12) ( 4 1 4)	<u>Λ</u> 110° 2π/d 4.7927 4.8858
↓ 20° # 1 2 3	Angle 21.005 24.900 27.047	d(A) 4.2260 3.5730 3.2940	40° 1%(f) 25.0 60.0 100.0	(h k l) (0 0 4) (1 1 0) (1 1 2)	2π/d 1.4868 1.7585 1.9075	70° # 23 24 25	Angle 71.969 73.595 80.678	d(Å) 1.3110 1.2860 1.1900	1%(f) 20.0 20.0 5.0	100° ( h k l) (1,1,12) ( 4 1 4) ( 3 3 0)	<u>110</u> 2π/d 4.7927 4.8858 5.2800
20° # 1 2 3 4	Angle 21.005 24.900 27.047 32.778	d(A) 4.2260 3.5730 3.2940 2.7300	40° 1%(f) 25.0 60.0 100.0 90.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4)	2π/d 1.4868 1.7585 1.9075 2.3015	70° # 23 24 25 26	Angle 71.969 73.595 80.678 82.956	d(Å) 1.3110 1.2860 1.1900 1.1630	90° 1%(f) 20.0 20.0 5.0 5.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12)	2π/d 4.7927 4.8858 5.2800 5.4026
20° # 1 2 3 4 5	Angle 21.005 24.900 27.047 32.778 38.818 20.450	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2320	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.724	70° # 23 24 25 26 27 27	Angle 71.969 73.595 80.678 82.956 84.468	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460	1%(f) 20.0 20.0 5.0 5.0 10.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 4)	<u>110°</u> 2π/d 4.7927 4.8858 5.2800 5.4026 5.4827 5.4827
# 1 2 3 4 5 6 7	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120	1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 5.0	50° (h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405	70° # 23 24 25 26 27 28 27 28	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1380	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2 2 12)	<u>110°</u> 2π/d 4.7927 4.8858 5.2800 5.4026 5.4827 5.5213 5.6556
20° # 1 2 3 4 5 6 7 8	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 5.0 2.0 5.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075	70° # 23 24 25 26 27 28 29 30	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1090 1.0570	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 5.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0 0 16)	2π/d 4.7927 4.8858 5.2800 5.4026 5.4827 5.5213 5.6656 5.9444
20° # 1 2 3 4 5 6 7 8 9	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130	1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 5.0 2.0 2.0 2.0	50 ² (h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736	70° # 23 24 25 26 27 28 29 30 31	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1090 1.0570 1.0320	1%(f) 20.0 20.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0	700° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0)	<u>110°</u> 2π/d 4.7927 4.8858 5.2800 5.4026 5.4827 5.5213 5.6656 5.9444 6.0884
20° # 1 2 3 4 5 6 7 8 9 10	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 2.0 20.0 60.0	50° (h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8) (3 0 0)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457	70° # 23 24 25 26 27 28 29 30 31 31 32	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1090 1.0570 1.0320 1.0140	1%(f) 20.0 20.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0	tóp*     (h k l)     (1,1,12)     (4 1 4)     (3 3 0)     (3,0,12)     (3 3 4)     (4 1 8)     (2,2,12)     (0,0,16)     (6 0 0)     (1,1,16)	Λ     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964
20° # 1 2 3 4 5 6 7 8 9 10 11	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 5.0 2.0 2.0 2.0 20.0 60.0 30.0	50° (hkl) (004) (110) (112) (114) (211) (205) (116) (213) (008) (300) (304)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890	70° # 23 24 25 26 27 28 29 30 31 32 33	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1090 1.0570 1.0320 1.0140 1.0020	1%(f) 20.0 20.0 5.0 10.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0	ndo*     (h k l)     (1,1,12)     (4 1 4)     (3 3 0)     (3,0,12)     (3 3 4)     (4 1 8)     (2,2,12)     (0,0,16)     (6 0 0)     (1,1,16)     (6 0 4)	Λ     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706
20° # 1 2 3 4 5 6 6 7 8 9 10 11 12	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8200	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0	50° (hkl) (004) (110) (112) (114) (211) (205) (116) (213) (008) (300) (304) (118)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9075 2.9736 3.0457 3.3890 3.4523	70° # 23 24 25 26 27 28 29 30 31 32 33 34	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.0900 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 0.0	A     100°     (1,1,12)     (414)     (330)     (3,0,12)     (334)     (418)     (2,2,12)     (0,0,16)     (600)     (1,1,16)     (624)     (520)	Λ     2π/d     4.7927     4.8858     5.2800     5.4026     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8200 1.7880	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 2.0 2.0 60.0 30.0 70.0 5.0	50° (hkl) (004) (110) (112) (114) (211) (205) (116) (213) (008) (300) (304) (118) (220)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141	70° # 23 24 25 26 27 28 29 30 31 32 33 34 35	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1460 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0	A     100°     (1,1,12)     (414)     (330)     (3,0,12)     (334)     (418)     (2,2,12)     (0,0,16)     (600)     (1,1,16)     (520)     (4,1,12)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8540 1.8200 1.7880 1.7500	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904	70° # 23 24 25 26 27 28 29 30 31 32 33 34 35 36	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1460 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 2.0	A     100°     (h k l)     (1,1,12)     (4 1 4)     (3 3 0)     (3,0,12)     (3 3 4)     (4 1 8)     (2,2,12)     (0,0,16)     (6 0 0)     (1,1,16)     (6 0 4)     (5 2 0)     (4,1,12)     (5 2 4)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117
20° # 1 2 3 4 5 6 6 7 8 9 10 11 12 13 14 15	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8200 1.7880 1.7500 1.6460	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 70.0 5.0 30.0 70.0 5.0 30.0 5.0 30.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172	70° # 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939 109.888	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1090 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9410	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0	A     100°     (1,1,12)     (414)     (330)     (3,0,12)     (334)     (418)     (2,2,12)     (0,0,16)     (600)     (1,1,16)     (520)     (4,1,12)     (524)     (3,0,16)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8200 1.7880 1.7500 1.6460 1.5402	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 0)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694	70° # 23 24 25 26 27 28 29 30 31 31 32 33 34 35 36 37 38	200 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939 109.888 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1630 1.1460 1.1380 1.0900 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9101 0.9101	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0 2.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0) (1,1,16) (6 0 4) (5 2 0) (4,1,12) (5 2 4) (3,0,16) (3,3,12) (2 2,16)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771     6.9038     0.9032
20° # 1 2 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854 61.345 62.950	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8200 1.7880 1.7500 1.6460 1.5440 1.5100 1.4772	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 5.0 30.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 30.0 7.0 5.0 2.0 5.0 30.0 7.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 5.0 5.0 5.0 2.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 1 1) (2 1 3) (1 1 6) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 6) (3 0 8)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694 4.1611 4.2540	70° # 23 24 25 26 27 28 29 30 31 31 32 33 34 35 36 37 38 39	202 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939 109.888 115.641 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1460 1.0320 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9410 0.9101 0.9101	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0 2.0 2.0	100°     (h k l)     (1,1,12)     (4 1 4)     (3 3 0)     (3,0,12)     (3 3 4)     (4 1 8)     (2,2,12)     (0,0,16)     (6 0 0)     (1,1,16)     (6 0 4)     (5 2 0)     (4,1,12)     (5 2 4)     (3,0,16)     (3,3,12)     (2,2,16)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771     6.9038
20° # 1 2 3 4 5 6 6 7 8 9 10 11 12 13 14 15 16 17 18 19	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854 61.345 62.869 66.070	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8540 1.7500 1.6460 1.5440 1.5100 1.4130	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 30.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 5.0 2.0 3.0 5.0 2.0 3.0 5.0 2.0 3.0 5.0 2.0 3.0 5.0 2.0 3.0 5.0 2.0 3.0 5.0 5.0 2.0 3.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 1 3) (2 1 3) (1 1 6) (2 1 3) (0 0 8) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 6) (3 0 8) (0 0 13)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694 4.1611 4.2540 4.4467	70° # 23 24 25 26 27 28 29 30 31 31 32 33 34 35 36 37 38 39	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939 109.888 115.641 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1460 1.0570 1.0570 1.0320 1.0140 1.020 0.9909 0.9749 0.9649 0.9410 0.9101 0.9101	1%(f) 20.0 20.0 5.0 5.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0 2.0 2.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0) (1,1,16) (6 0 4) (5 2 0) (4,1,12) (5 2 4) (3,0,16) (3,3,12) (2,2,16)	Λ     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4827     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771     6.9038
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854 61.345 62.869 66.070 68.653	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8540 1.8200 1.7500 1.6460 1.5440 1.5100 1.4770 1.4130 1.3650	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 5.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 0 5) (1 1 6) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 6) (3 0 8) (0,0,12) (2 2 8)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694 4.1611 4.2540 4.4467 4.5997	70° # 23 24 25 26 27 28 29 30 31 31 32 33 34 35 36 37 38 39	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 96.561 98.868 100.485 102.041 104.395 105.939 109.888 115.641 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1460 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9410 0.9101 0.9101	1%(f) 20.0 20.0 5.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0 2.0 2.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0) (1,1,16) (6 0 4) (5 2 0) (4,1,12) (5 2 4) (3,0,16) (3,3,12) (2,2,16)	2π/d     4.7927     4.8858     5.2800     5.4026     5.427     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771     6.9038
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854 61.345 62.869 66.070 68.653 69.524	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8540 1.8200 1.7880 1.7500 1.6460 1.5440 1.5100 1.4770 1.4130 1.3660 1.3510	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 5.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 6) (3 0 8) (0,0,12) (2 2 8) (4 1 0)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694 4.1611 4.2540 4.4467 4.5997 4.6508	70° # 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 93.564 98.868 100.485 102.041 104.395 105.939 109.888 115.641 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1380 1.1400 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9410 0.9101 0.9101	1%(f) 20.0 5.0 5.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 0.0 5.0 0.0 0.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0) (1,1,16) (6 0 4) (5 2 0) (4,1,12) (5 2 4) (3,0,16) (3,3,12) (2,2,16)	2π/d     110°     2π/d     4.7927     4.8858     5.2800     5.4026     5.4026     5.427     5.5213     5.6656     5.9444     6.0884     6.1964     6.2706     6.3409     6.4450     6.5117     6.6771     6.9038     6.9038
20° # 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	30 Angle 21.005 24.900 27.047 32.778 38.818 39.456 40.759 41.765 42.760 43.849 49.099 50.079 51.038 52.229 55.807 59.854 61.345 62.869 66.070 68.653 69.524 70.480	d(A) 4.2260 3.5730 3.2940 2.7300 2.3180 2.2820 2.2120 2.1610 2.1130 2.0630 1.8540 1.8540 1.8200 1.7880 1.7500 1.6460 1.5440 1.5100 1.4770 1.4130 1.3660 1.3510 1.3350	40° 1%(f) 25.0 60.0 100.0 90.0 5.0 2.0 2.0 20.0 60.0 30.0 70.0 5.0 2.0 30.0 70.0 5.0 2.0 30.0 70.0 5.0 2.0 30.0 70.0 5.0 2.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0 10.0	(h k l) (0 0 4) (1 1 0) (1 1 2) (1 1 4) (2 1 1) (2 1 3) (0 0 8) (3 0 0) (3 0 4) (1 1 8) (2 2 0) (2 2 2) (2 2 4) (4 0 1) (2 2 6) (3 0 8) (0,0,12) (2 2 8) (4 1 0) (4 1 2)	2π/d 1.4868 1.7585 1.9075 2.3015 2.7106 2.7534 2.8405 2.9075 2.9736 3.0457 3.3890 3.4523 3.5141 3.5904 3.8172 4.0694 4.1611 4.2540 4.4467 4.5997 4.6508 4.7065	70° # 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39	80 Angle 71.969 73.595 80.678 82.956 84.468 85.201 87.988 93.564 93.564 98.868 100.485 102.041 104.395 105.939 109.888 115.641	d(A) 1.3110 1.2860 1.1900 1.1630 1.1460 1.1460 1.1380 1.0570 1.0570 1.0320 1.0140 1.0020 0.9909 0.9749 0.9649 0.9410 0.9101 0.9101	1%(f) 20.0 5.0 5.0 10.0 10.0 10.0 5.0 0.0 5.0 0.0 5.0 2.0 10.0 2.0 2.0	100° (h k l) (1,1,12) (4 1 4) (3 3 0) (3,0,12) (3 3 4) (4 1 8) (2,2,12) (0,0,16) (6 0 0) (1,1,16) (6 0 4) (5 2 0) (4,1,12) (5 2 4) (3,0,16) (3,3,12) (2,2,16)	110°   2π/d   4.7927   4.8858   5.2800   5.4026   5.5213   5.6656   5.9444   6.0884   6.1964   6.2706   6.3409   6.4450   6.5117   6.6771   6.9038   6.9038

*Fig. S25 Phase information for vaterite. For powder XRD comparison and identification purposes. See reference in the image.*