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Article

Mg/Ca Ratios in Synthetic Low-Magnesium Calcite: An Experimental Investigation

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Supplementary Materials:

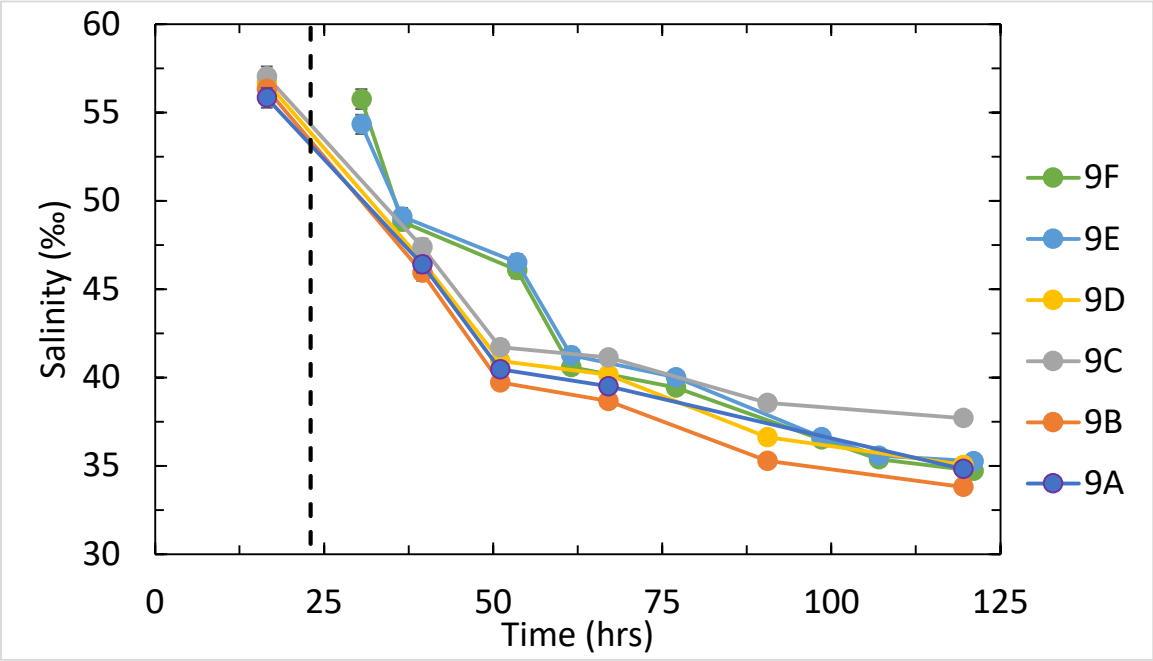


Figure S1. Graphical representation of salinity plotted against time for experiments 9A through 9F (pH during precipitation was 6-7). Analytical uncertainty is ± 1.0%. The vertical dashed line is included to indicate the observed onset of crystallization at approximately 24 hours.

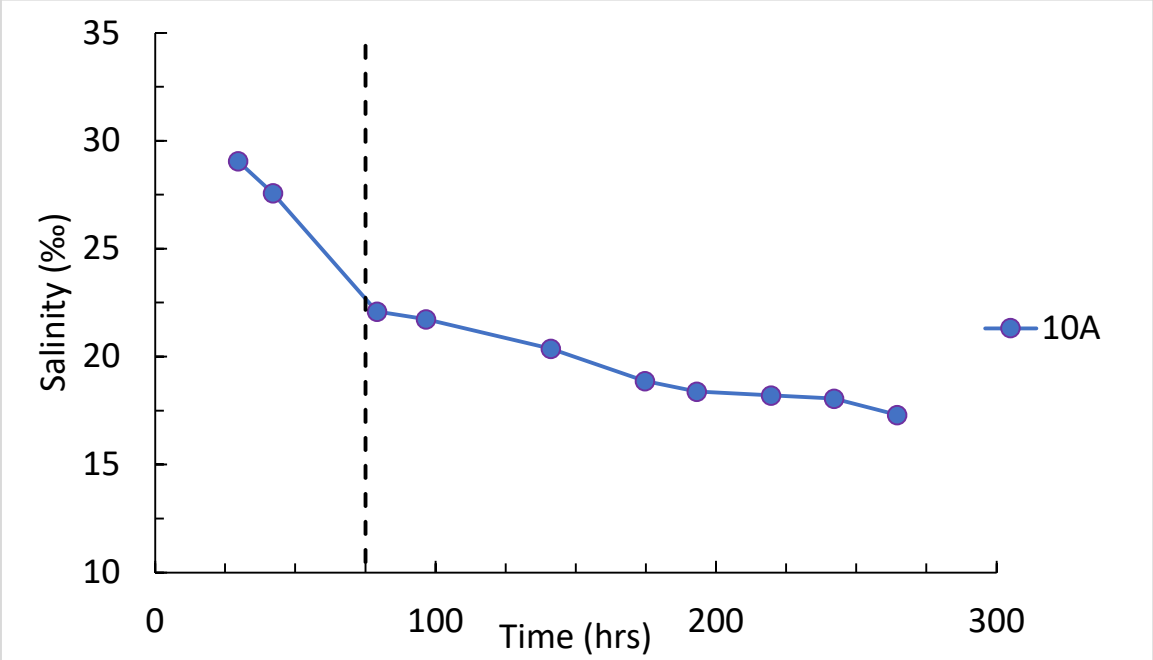


Figure S2. Graphical representation of salinity plotted against time for experiments 10A (pH during precipitation was 7.75-8.25). Analytical uncertainty is ± 1.0%. The vertical dashed line is included to indicate the observed onset of crystallization at approximately 75 hours.

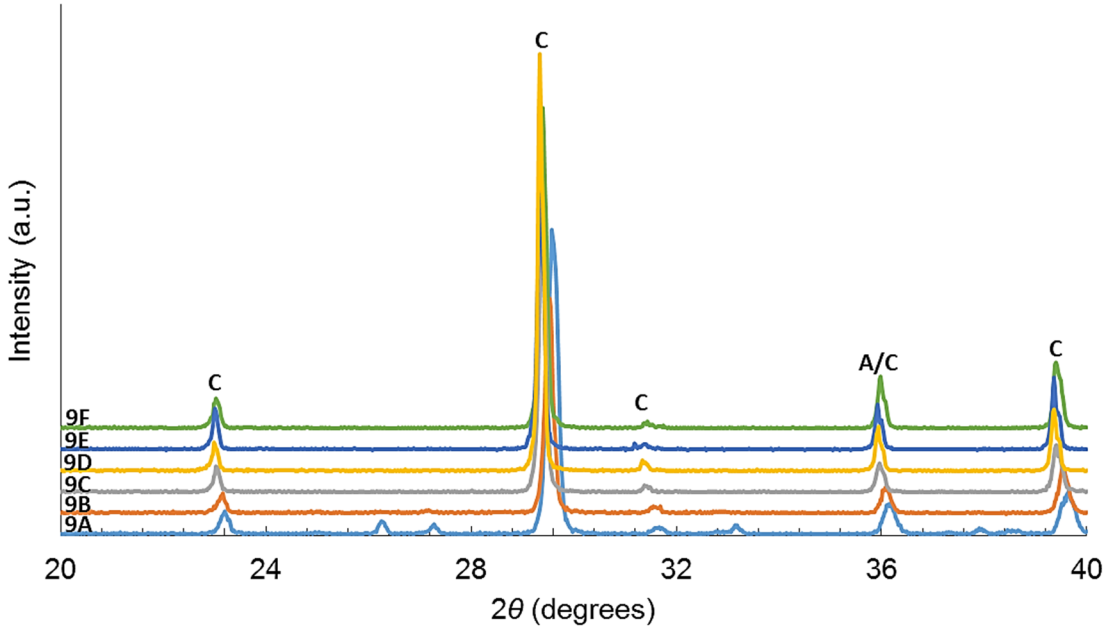


Figure S3. Series 9. Powdered X-ray diffraction scans with Cu-Kα radiation of different calcium carbonate polymorphs. C = calcite and A/C indicates the position of the peak that is representative of both calcite and aragonite. The experiment which corresponds to the diffraction pattern is noted along the y-axis of the plot. The slight shift observed for the major peaks of each scan may be due to instrument drift from reoccurring use or slight variations in the Mg content.

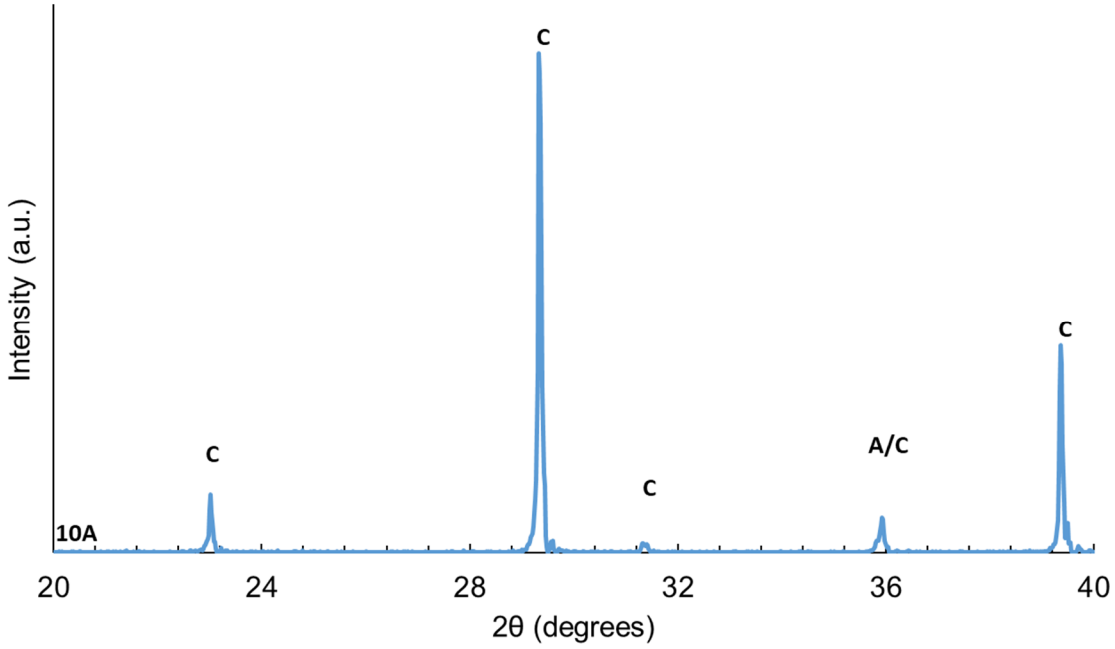


Figure S4. Series 10. Powdered X-ray diffraction scans with Cu-Kα radiation of different calcium carbonate polymorphs. C = calcite and A/C indicates the position of the peak that is representative of both calcite and aragonite. The experiment which corresponds to the diffraction pattern is noted along the y-axis of the plot. The slight shift observed for the major peaks of each scan may be due to instrument drift from reoccurring use or slight variations in the Mg content.

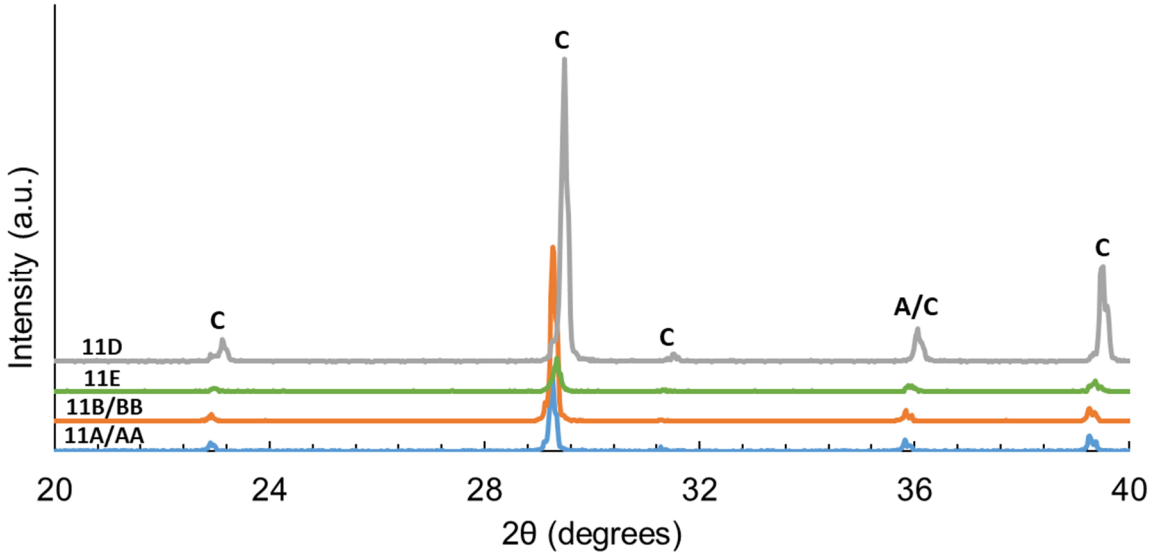


Figure S5. Series 11. Powdered X-ray diffraction scans with Cu-Kα radiation of different calcium carbonate polymorphs. C = calcite and A/C indicates the position of the peak that is representative of both calcite and aragonite. The experiment which corresponds to the diffraction pattern is noted along the y-axis of the plot. The slight shift observed for the major peaks of each scan may be due to instrument drift from reoccurring use or slight variations in the Mg content.

Table S1. Compiled data documenting time of sample collection in hrs, measured pH value, salinity, and LS-AAS data for Mg and Ca (ppm) and Mg/Ca ratios (mmol/mol).

Sample Id	Time (hrs)	pH	Salinity	Mg (ppm)	Ca (ppm)	Mg/Ca (mmol/mol)

9A-11-13	16.5	6.62	55.84	1270.586409	571.8208806	3663.992795
9A-11-14	51	6.89	40.47	1049.526358	405.1853237	4271.201487
9A-11-15	67	6.93	39.51	915.3840244	354.4773856	4258.191711
9A-11-16	90.5	6.88		872.2304969	324.0401485	4438.567822
9A-11-17	119.5	6.88	34.83	1141.940044	686.2723767	2743.829996
9B-11-13	16.5	6.56	56.34	710.3045106	892.2538839	1312.703191
9B-11-14	51	6.77	39.72	757.5093778	1267.662381	985.3597696
9B-11-15	67	6.77	38.68	669.2791897	1070.156619	1031.265276
9B-11-16	90.5	6.82	35.28	669.7941519	394.4260088	2800.181757
9B-11-17	119.5	6.94	33.81	625.5074038	332.4083097	3102.922997
9C-11-13	16.5	6.35	57.05	566.9900781	1179.764814	792.483877
9C-11-14	51	6.61	41.72	332.2189688	1707.823775	320.7685538
9C-11-15	67	6.72	41.13	235.9104063	968.1028766	401.8241211
9C-11-16	90.5	7.04	38.56	322.2691094	522.9239672	1016.226573
9C-11-17	119.5	7	37.71	188.2877969	669.1460453	463.9932619
9D-11-12	0	5.96		74.53735875	3330.00387	36.90962873
9D-11-13	16.5	6.06	56.73	55.8164325	2475.446727	37.18081509
9D-11-14	51	6.31	40.94	42.071955	2105.941343	32.94252151
9D-11-15	67	6.3	41.13	36.76738875	1523.385821	39.79818748
9D-11-16	90.5	6.37	38.56	38.0251725	1754.36811	35.74052142
9D-11-17	119.5	6.38	37.71	26.38611563	1744.094866	24.94685329
9E-11-18	0	6.38		272.3800588	4179.511811	107.4632988
9E-11-19	30.5	6.35	54.34	142.6885788	2339.559387	100.5693293
9E-11-20	61.5	6.46	41.27	164.2805331	1737.540109	155.9055876
9E-11-21	77	6.46	40.02	171.6525434	2112.288697	134.0007976
9E-11-22	107	6.48	35.58	154.4977706	2017.994431	126.2445589
9E-11-23	121	6.48	35.27	136.2599063	1444.978098	155.4952893
9F-11-18	0	6.13		629.2199925	2993.538038	346.5996723
9F-11-19	30.5	6.46	55.76	538.6869056	1800.741612	493.2821882
9F-11-20	61.5	6.61	40.6	439.8323944	1524.991696	475.5871911
9F-11-21	77	6.63	39.43	394.5157219	1371.803811	474.2231221
9F-11-22	107	6.65	35.38	353.6104069	1623.053044	359.2549328
9F-11-23	121	6.56	34.73	346.2915638	1328.927615	429.6857992
10A-11-26	0	7.73		16.29994166	167.5173731	160.448851
10A-11-27	29.5	8.16	29.07	12.02741432	118.0720023	167.9715613
10A-11-28	42	8.28	27.58	10.20971628	98.73881597	170.504629
10A-11-29	79	8.02	22.09	10.56576023	86.80878769	200.7000475
10A-11-30	96.5	7.87	21.74	7.68305355	81.77721522	154.9215946
10A-12-2	141	7.98	20.37	8.954192898	64.95981511	227.2961509
10A-12-3	174.5	7.92	18.87	5.181376358	68.98455809	123.8521837
10A-12-4	193	7.97	18.39	7.148987633	67.90562827	173.5997876
10A-12-5	219.5	8.05	18.2	7.305147258	71.21194303	169.1556681
10A-12-6	242	7.96	18.06	7.086523783	65.10401575	179.4881936
11A_1	0	7.96		0.149	6.485	37.88669341

11A_2	18	6.71	0.265	15.852	27.56590314
11A_3	29	6.4	0.274	20.161	22.4103639
11A_4	44	6.23	0.344	27.392	20.70833181
11AA_1	5	6.67	0.332	22.324	24.52316303
11AA_2	23.5	6.5	0.338	24.779	22.4927906
11AA_3	29.5	6.5	0.336	24.032	23.05471605
11AA_4	45	6.51	0.31	22.945	22.27840257
11B_1	0	8.3	0.235	8.354	46.3856671
11B_2	18	6.78	0.207	9.358	36.47520321
11B_3	29	6.51	0.226	13.864	26.88006441
11B_4	44	6.56	0.298	17.659	27.82662741
11BB_1	5	7.1	0.259	12.809	33.34225387
11BB_2	23.5	6.87	0.272	9.227	48.60923641
11BB_3	29.5	6.82	0.271	8.568	52.15551626
11BB_4	45	6.84	0.269	7.18	61.77862689
11D_1	16.5	6.73	2.245	7.492	494.1160855
11D_2	42	6.48	4.141	21.484	317.8341088
11D_3	66	6.35	5.325	28.343	309.8019955
11D_4	88	6.42	7.071	36.152	322.5216882
11D_5	113.5	6.45	7.694	41.897	302.8165943
11E_1	16.5	7.01	1.928	5.623	565.3916126
11E_2	42	6.71	3.287	8.881	610.3068572
11E_3	66	6.61	3.535	9.989	583.5496602
11E_4	88	6.61	3.861	10.37	613.9478188
11E_5	113.5	6.61	5.143	24.144	351.2511198
11F_1	16.5	8.84	1.068	0.755	2332.570166
11F_2	42	7.23	3.254	3.866	1387.92537
11F_3	66	6.94	5.203	8.257	1039.063183
11F_4	88	7.46	4.598	1.739	4359.93285
11F_5	113.5	7.85	1.605	0.035	75616.6456