

Table S1. Supplementary information to the manuscript by Majzlan and Michallik (*Mineralogical Magazine*). Listed in the sample ID, the amount of chemicals (deionized water and sulfates of Mg, Fe³⁺, Al, Ni, Zn, and Fe²⁺) used to produce the sample; the temperature of synthesis in °C; the expected and measured stoichiometry at the A site in copiapite according to the general formula AFe₄(SO₄)₆(OH)₂(H₂O)₂₀; the structural type of the phase synthesized: **MG** = structural type **MG**, **AL** = structural type **AL**; **CL** = copiapite-like phase; and the lattice parameters of all phases identified in the samples. The values χ^2 and wR_p describe the goodness of the fit and are defined in the technical manual for GSAS (see Larson and von Dreele 1994). For the samples of the type **MG** and **AL**, these values refer to the results of the Rietveld refinement. For samples of the type **CL**, these values refer to the results of the LeBail refinement.

sample	amount of sulfates weighed out (g)				expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							χ^2 wR_p
	water (mL) T (°C)	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		a	b	c	α	β	γ	V	
HSC-1	1.20 25	0.4779 0	2.0221 0	0	1.000 0	0 0	0	1.017 0	0 0	0	MG	7.3451(4)	18.7936(11)	7.3891(4)	91.369(5)	102.169(4)	98.831(4)	983.58(10)	3.81 0.2826
HSC-2	1.20 25	0.4325 0	2.0675 0	0	0.900 0	0.067 0	0	0.972 0	0.019 0	0	MG	7.3451(4)	18.7940(10)	7.3886(4)	91.373(5)	102.163(4)	98.822(4)	983.60(9)	2.74 0.2486
HSC-3	1.20 25	0.3867 0	2.1133 0	0	0.800 0	0.133 0	0	0.958 0	0.028 0	0	MG	7.3444(4)	18.7921(10)	7.3870(4)	91.364(4)	102.163(4)	98.829(4)	983.16(9)	3.07 0.2581
HSC-4	1.20 25	0.3403 0	2.1597 0	0	0.700 0	0.200 0	0	0.951 0	0.033 0	0	MG	7.3440(5)	18.7912(13)	7.3879(5)	91.370(5)	102.168(4)	98.824(5)	983.17(11)	4.44 0.3037
HSC-5	1.20 25	0.2933 0	2.2067 0	0	0.600 0	0.267 0	0	0.927 0	0.048 0	0	MG	7.3446(4)	18.7911(11)	7.3886(4)	91.375(5)	102.165(4)	98.828(4)	983.34(10)	2.50 0.2350
HSC-6	1.20 25	0.2459 0	2.2541 0	0	0.500 0	0.333 0	0	0.893 0	0.071 0	0	MG	7.3457(5)	18.7943(12)	7.3893(5)	91.371(5)	102.174(4)	98.817(4)	983.75(11)	2.78 0.2494
HSC-7	1.20 25	0.1978 0	2.3022 0	0	0.400 0	0.400 0	0	0.819 0	0.120 0	0	MG	7.3493(9)	18.7995(22)	7.3957(9)	91.406(9)	102.176(8)	98.789(8)	985.38(20)	3.69 0.2865
HSC-8	1.20 25	0.1492 0	2.3508 0	0	0.300 0	0.467 0	0	0.573 0	0.285 0	0	MG AL	7.3440(16) 7.3833(26)	18.791(4) 18.437(6)	7.3965(17) 7.3478(24)	91.433(18) 93.795(29)	102.160(15) 102.294(27)	98.795(15) 99.016(28)	984.4(4) 960.1(6)	3.60 0.2844
HSC-9	1.20 25	0.1001 0	2.3999 0	0	0.200 0	0.533 0	0	0.341 0	0.440 0	0	MG AL	7.338(4) 7.3811(16)	18.746(8) 18.368(5)	7.387(4) 7.3317(16)	91.42(5) 93.901(17)	102.11(4) 102.224(16)	98.72(4) 98.953(17)	980.4(9) 954.4(4)	5.16 0.3358
HSC-10	1.20 25	0.0503 0	2.4497 0	0	0.100 0	0.600 0	0	0.147 0	0.569 0	0	MG AL	7.383(11) 7.3839(10)	18.647(22) 18.3662(28)	7.346(11) 7.3298(10)	91.42(15) 93.922(10)	101.87(12) 102.215(9)	98.72(13) 98.926(10)	976.7(25) 954.47(24)	3.87 0.2996
HSC-11	1.20 25	0 0	2.5000 0	0	0 0	0.667 0	0	0 0	0.667 0	0	AL	7.3871(5)	18.3622(13)	7.3286(4)	93.938(5)	102.208(4)	98.920(4)	954.53(11)	2.86 0.2576
HSC-12	1.20 25	0.4311 0	2.0269 0	0.0420 0	0.900 0	0 0	0.067 0	1.008 0	0 0	0.007 0	MG	7.3450(5)	18.7926(12)	7.3882(5)	91.369(5)	102.164(4)	98.825(5)	983.44(11)	3.18 0.2600
HSC-13	1.20 25	0.3841 0	2.0317 0	0.0842 0	0.800 0	0 0	0.133 0	0.966 0	0 0	0.041 0	MG	7.3466(5)	18.7980(12)	7.3908(5)	91.377(5)	102.166(5)	98.828(5)	984.26(11)	2.39 0.2339
HSC-14	1.20 25	0.3369 0	2.0365 0	0.1266 0	0.700 0	0 0	0.200 0	0.908 0	0 0	0.061 0	MG	7.3467(5)	18.7951(13)	7.3906(5)	91.371(6)	102.177(5)	98.820(5)	984.08(12)	2.64 0.2438
HSC-15	1.20 25	0.2894 0	2.0413 0	0.1692 0	0.600 0	0 0	0.267 0	0.964 0	0 0	0.036 0	MG	7.3509(6)	18.8015(15)	7.3943(6)	91.369(6)	102.184(5)	98.809(6)	985.47(14)	2.91 0.2058
HSC-16	1.20 25	0.2418 0	2.0462 0	0.2120 0	0.500 0	0 0	0.333 0	0.826 0	0.004 0	0.112 0	MG	7.3505(8)	18.8031(19)	7.3970(8)	91.373(8)	102.186(7)	98.815(7)	985.84(18)	3.90 0.2367
HSC-17	1.20 25	0.1939 0	2.0511 0	0.2550 0	0.400 0	0 0	0.400 0	0.756 0	0.013 0	0.149 0	MG	7.3520(11)	18.8040(27)	7.4019(11)	91.397(11)	102.187(10)	98.801(10)	986.75(25)	4.54 0.2535

sample	water (mL) T (°C)	amount of sulfates weighed out (g)			expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							χ^2 wRp
		Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		a	b	c	α	β	γ	V	
HSC-18	1.20 25	0.1458 0	2.0560 0	0.2982 0	0.300 0	0 0	0.467 0	0.662 0	0.043 0	0.182 0	MG	7.3545(18)	18.812(4)	7.4113(18)	91.453(18)	102.211(16)	98.805(16)	988.6(4)	6.52 0.3026
HSC-19	1.20 25	0.0974 0	2.0609 0	0.3417 0	0.200 0	0 0	0.533 0	0.319 0	0.081 0	0.373 0	AL MG	7.3766(20) 7.357(5)	18.253(6) 18.536(11)	7.3296(20) 7.385(6)	93.819(22) 91.20(6)	102.258(19) 101.99(6)	99.144(19) 98.26(6)	947.0(5) 973.5(12)	7.08 0.3155
HSC-20	1.20 25	0.0488 0	2.0659 0	0.3853 0	0.100 0	0 0	0.600 0	0.132 0	0.097 0	0.482 0	AL	7.3760(12)	18.246(3)	7.3279(11)	93.816(12)	102.231(11)	99.153(11)	946.41(27)	5.61 0.2800
HSC-21	1.20 25	0 0	2.0709 0	0.4291 0	0 0	0 0	0.667 0	0 0	0.034 0	0.632 0	AL	7.3853(7)	18.2486(18)	7.3280(6)	93.873(7)	102.221(6)	99.163(6)	947.65(16)	3.99 0.2544
HSC-22	1.20 25	0 0	2.1125 0	0.3875 0	0 0	0.067 0	0.600 0	0 0	0.148 0	0.518 0	AL	7.3835(7)	18.2502(20)	7.3270(7)	93.866(8)	102.221(7)	99.154(7)	947.42(17)	6.41 0.3080
HSC-23	1.20 25	0 0	2.1544 0	0.3456 0	0 0	0.133 0	0.533 0	0 0	0.186 0	0.481 0	AL	7.3856(8)	18.2569(21)	7.3287(8)	93.864(8)	102.216(7)	99.160(7)	948.25(18)	4.47 0.2607
HSC-24	1.20 25	0 0	2.1965 0	0.3035 0	0 0	0.200 0	0.467 0	0 0	0.239 0	0.428 0	AL	7.3860(8)	18.2670(22)	7.3293(8)	93.882(8)	102.214(7)	99.129(8)	948.98(19)	3.72 0.2454
HSC-25	1.20 25	0 0	2.2390 0	0.2610 0	0 0	0.267 0	0.400 0	0 0	0.274 0	0.392 0	AL	7.3857(6)	18.2680(16)	7.3284(6)	93.889(6)	102.214(5)	99.122(5)	948.87(13)	3.21 0.2286
HSC-26	1.20 25	0 0	2.2818 0	0.2182 0	0 0	0.333 0	0.333 0	0 0	0.297 0	0.369 0	AL	7.3865(4)	18.2770(11)	7.3283(4)	93.887(4)	102.209(4)	99.101(4)	949.53(10)	2.57 0.1969
HSC-27	1.20 25	0 0	2.3248 0	0.1752 0	0 0	0.400 0	0.267 0	0 0	0.366 0	0.301 0	AL	7.3869(4)	18.2883(12)	7.3293(4)	93.888(4)	102.212(4)	99.079(4)	950.35(10)	2.39 0.1916
HSC-28	1.20 25	0 0	2.3682 0	0.1318 0	0 0	0.467 0	0.200 0	0 0	0.449 0	0.218 0	AL	7.3885(5)	18.3142(13)	7.3304(4)	93.900(5)	102.217(5)	99.038(5)	952.13(11)	2.62 0.2066
HSC-29	1.20 25	0 0	2.4118 0	0.0882 0	0 0	0.533 0	0.133 0	0 0	0.520 0	0.147 0	AL	7.3880(4)	18.3277(12)	7.3298(4)	93.912(5)	102.213(4)	99.002(4)	952.78(10)	2.71 0.2070
HSC-30A	1.20 25	0 0	2.4557 0	0.0443 0	0 0	0.600 0	0.067 0	0 0	0.595 0	0.072 0	AL	7.3894(5)	18.3546(14)	7.3314(5)	93.919(5)	102.215(5)	98.943(5)	954.73(11)	3.18 0.2238
HSC-30B	1.20 25	0.3900 0	2.0678 0	0.0422 0	0.810 0	0.060 0	0.067 0	1.002 0	0 0	0.005 0	MG	7.3463(4)	18.7948(11)	7.3894(4)	91.365(5)	102.170(4)	98.826(4)	983.87(10)	3.68 0.2269
HSC-31	1.20 25	0.3484 0	2.1091 0	0.0424 0	0.720 0	0.120 0	0.067 0	0.955 0	0 0	0.030 0	MG	7.3467(4)	18.7979(11)	7.3906(4)	91.364(5)	102.169(4)	98.819(4)	984.26(10)	3.29 0.2173
HSC-32	1.20 25	0.3064 0	2.1509 0	0.0427 0	0.630 0	0.180 0	0.067 0	0.914 0	0 0	0.057 0	MG	7.3475(4)	18.7972(11)	7.3911(4)	91.368(5)	102.178(4)	98.819(4)	984.36(10)	3.32 0.2187
HSC-33	1.20 25	0.2640 0	2.1931 0	0.0429 0	0.540 0	0.240 0	0.067 0	0.957 0	0.029 0	0 0	MG	7.3468(4)	18.7958(11)	7.3909(4)	91.371(5)	102.172(4)	98.820(4)	984.18(10)	3.53 0.2228
HSC-34	1.20 25	0.2212 0	2.2357 0	0.0431 0	0.450 0	0.300 0	0.067 0	0.933 0	0.016 0	0.029 0	MG	7.3494(5)	18.8015(13)	7.3928(5)	91.373(5)	102.178(5)	98.815(5)	985.09(12)	3.26 0.2151
HSC-35	1.20 25	0.1779 0	2.2788 0	0.0433 0	0.360 0	0.360 0	0.067 0	0.797 0	0.068 0	0.067 0	AL MG	7.368(6) 7.3495(9)	18.504(12) 18.8005(22)	7.356(5) 7.3981(9)	92.75(6) 91.414(10)	102.58(7) 102.167(9)	98.81(6) 98.813(8)	963.9(12) 985.75(21)	3.72 0.2352
HSC-36	1.20 25	0.1341 0	2.3223 0	0.0436 0	0.270 0	0.420 0	0.067 0	0.499 0	0.334 0	0 0	AL MG	7.3843(19) 7.3429(16)	18.391(5) 18.774(4)	7.3433(18) 7.3961(17)	93.896(20) 91.426(19)	102.260(19) 102.158(16)	99.051(20) 98.786(16)	957.1(4) 983.3(4)	4.22 0.2512
HSC-37	1.20 25	0.0899 0	2.3663 0	0.0438 0	0.180 0	0.480 0	0.067 0	0.300 0	0.467 0	0 0	AL MG	7.3814(10) 7.336(3)	18.3483(27) 18.728(5)	7.3315(10) 7.3879(29)	93.879(10) 91.44(4)	102.232(9) 102.113(28)	99.011(10) 98.68(3)	953.19(23) 979.4(6)	3.50 0.2283

sample	water (mL) T (°C)	amount of sulfates weighed out (g)			expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							χ^2 wRp
		Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		a	b	c	α	β	γ	V	
HSC-38	1.20	0.0452	2.4108	0.0440	0.090	0.540	0.067	0.124	0.584	0	AL	7.3844(6)	18.3442(17)	7.3279(6)	93.910(7)	102.206(6)	98.980(6)	953.03(14)	2.55
	25	0	0	0	0	0	0	0	0	0	MG	7.335(5)	18.502(9)	7.419(5)	91.75(6)	101.86(6)	98.02(5)	973.9(11)	0.1991
HSC-39	1.20	0.3432	2.0722	0.0846	0.711	0.059	0.133	0.874	0.084	0	MG	7.3469(4)	18.7969(10)	7.3902(4)	91.366(4)	102.170(4)	98.822(4)	984.18(9)	3.09
	25	0	0	0	0	0	0	0	0	0								984.18(9)	0.2113
HSC-40	1.20	0.3018	2.1132	0.0851	0.622	0.119	0.133	0.884	0.078	0	MG	7.3479(4)	18.7974(10)	7.3917(4)	91.370(5)	102.172(4)	98.825(4)	984.52(10)	2.88
	25	0	0	0	0	0	0	0	0	0								984.52(10)	0.2054
HSC-41	1.20	0.2600	2.1545	0.0855	0.533	0.178	0.133	0.854	0.098	0	MG	7.3467(4)	18.7977(11)	7.3908(4)	91.364(5)	102.171(4)	98.821(4)	984.27(10)	3.21
	25	0	0	0	0	0	0	0	0	0								984.27(10)	0.2171
HSC-42	1.20	0.2178	2.1963	0.0859	0.444	0.237	0.133	0.718	0.188	0	MG	7.3492(6)	18.8024(15)	7.3956(6)	91.388(7)	102.176(6)	98.816(6)	985.46(14)	3.72
	25	0	0	0	0	0	0	0	0	0								985.46(14)	0.2320
HSC-43	1.20	0.1751	2.2385	0.0864	0.356	0.296	0.133	0.644	0.237	0	AL	7.370(4)	18.464(10)	7.357(4)	92.79(5)	102.61(5)	98.84(5)	961.9(9)	5.22
	25	0	0	0	0	0	0	0	0	0	MG	7.3474(13)	18.799(3)	7.4006(13)	91.436(13)	102.155(12)	98.839(12)	985.68(29)	0.2707
HSC-44	1.20	0.1320	2.2812	0.0868	0.267	0.356	0.133	0.514	0.324	0	AL	7.3834(19)	18.361(5)	7.3427(18)	93.848(21)	102.253(19)	99.087(20)	955.3(4)	4.60
	25	0	0	0	0	0	0	0	0	0	MG	7.3440(19)	18.769(4)	7.3940(20)	91.408(22)	102.147(18)	98.775(19)	983.0(4)	0.2614
HSC-45	1.20	0.0885	2.3242	0.0873	0.178	0.415	0.133	0.324	0.340	0.111	AL	7.3808(10)	18.3189(29)	7.3304(10)	93.859(11)	102.231(10)	99.043(10)	951.38(24)	3.62
	25	0	0	0	0	0	0	0	0	0	MG	7.337(3)	18.690(6)	7.392(3)	91.42(4)	102.09(3)	98.61(3)	978.4(7)	0.2340
HSC-46	1.20	0.0445	2.3678	0.0877	0.089	0.474	0.133	0.144	0.469	0.101	AL	7.3822(7)	18.3251(19)	7.3280(6)	93.898(7)	102.210(6)	99.030(6)	951.62(16)	2.87
	25	0	0	0	0	0	0	0	0	0	MG	7.366(4)	18.456(8)	7.386(4)	90.88(6)	102.08(5)	97.66(5)	972.1(9)	0.2123
HSC-47	1.20	0.2962	2.0765	0.1272	0.613	0.058	0.200	0.971	0	0.028	MG	7.3471(4)	18.7959(10)	7.3907(4)	91.366(4)	102.172(4)	98.824(4)	984.20(9)	3.13
	25	0	0	0	0	0	0	0	0	0								984.20(9)	0.2108
HSC-48	1.20	0.2552	2.1169	0.1279	0.525	0.117	0.200	0.973	0.035	0	MG	7.3459(4)	18.7948(11)	7.3901(4)	91.370(5)	102.172(4)	98.827(4)	983.90(10)	3.59
	25	0	0	0	0	0	0	0	0	0								983.90(10)	0.2268
HSC-49	1.20	0.2137	2.1577	0.1285	0.438	0.175	0.200	0.877	0	0.083	MG	7.3484(7)	18.8001(18)	7.3929(7)	91.388(8)	102.179(6)	98.821(7)	984.85(16)	4.21
	25	0	0	0	0	0	0	0	0	0								984.85(16)	0.2525
HSC-50	1.20	0.1719	2.1990	0.1292	0.350	0.233	0.200	0.647	0	0.235	AL	7.370(4)	18.500(9)	7.355(3)	92.65(4)	102.61(5)	98.83(4)	963.7(9)	4.73
	25	0	0	0	0	0	0	0	0	0	MG	7.3479(13)	18.804(3)	7.3989(13)	91.426(14)	102.156(13)	98.854(12)	985.7(3)	0.2645
HSC-51	1.20	0.1295	2.2406	0.1298	0.263	0.292	0.200	0.489	0.034	0.307	AL	7.3714(18)	18.304(5)	7.3282(17)	93.870(19)	102.208(18)	99.097(18)	949.0(4)	5.33
	25	0	0	0	0	0	0	0	0	0	MG	7.337(3)	18.725(7)	7.379(3)	91.39(4)	102.08(3)	98.79(3)	978.0(7)	0.2797
HSC-52	1.20	0.0868	2.2827	0.1305	0.175	0.350	0.200	0.195	0.260	0.277	AL	7.3828(7)	18.3189(20)	7.3289(7)	93.882(7)	102.215(7)	99.023(7)	951.52(17)	3.09
	25	0	0	0	0	0	0	0	0	0	MG	7.353(4)	18.718(7)	7.384(4)	91.42(5)	102.03(4)	98.71(4)	980.8(8)	0.2182
HSC-53	1.20	0.0436	2.3252	0.1312	0.088	0.408	0.200	0.130	0.177	0.403	AL	7.3777(7)	18.3000(21)	7.3252(7)	93.876(8)	102.206(7)	99.050(7)	949.38(17)	3.77
	25	0	0	0	0	0	0	0	0	0	MG	7.357(4)	18.711(7)	7.390(4)	91.41(5)	102.10(5)	98.64(5)	981.8(9)	0.2424
HSC-54	1.20	0.2493	2.0806	0.1700	0.514	0.057	0.267	0.832	0	0.112	MG	7.3475(5)	18.7981(12)	7.3920(5)	91.369(5)	102.174(4)	98.826(5)	984.52(11)	3.09
	25	0	0	0	0	0	0	0	0	0								984.52(11)	0.2139
HSC-55	1.20	0.2088	2.1203	0.1709	0.429	0.114	0.267	0.866	0.005	0.084	MG	7.3494(8)	18.8005(19)	7.3958(8)	91.384(8)	102.184(7)	98.826(7)	985.34(18)	4.48
	25	0	0	0	0	0	0	0	0	0								985.34(18)	0.2551
HSC-56	1.20	0.1679	2.1604	0.1717	0.343	0.171	0.267	0.666	0	0.222	AL	7.377(4)	18.445(9)	7.353(3)	93.02(4)	102.43(4)	98.82(4)	961.7(8)	5.13
	25	0	0	0	0	0	0	0	0	0	MG	7.3470(14)	18.797(3)	7.3992(15)	91.406(15)	102.188(13)	98.826(13)	985.3(3)	0.2727
HSC-57	1.20	0.1265	2.2009	0.1726	0.257	0.229	0.267	0.356	0	0.432	AL	7.3819(18)	18.302(5)	7.3364(18)	93.864(19)	102.248(18)	99.119(18)	951.1(4)	4.71
	25	0	0	0	0	0	0	0	0	0	MG	7.3383(29)	18.731(6)	7.3941(29)	91.39(3)	102.124(27)	98.728(28)	980.5(6)	0.2716
HSC-58	1.20	0.0848	2.2418	0.1734	0.171	0.286	0.267	0.267	0.216	0.272	AL	7.3799(10)	18.282(3)	7.3293(10)	93.841(11)	102.232(10)	99.101(10)	949.05(25)	4.15
	25	0	0	0	0	0	0	0	0	0	MG	7.344(4)	18.557(7)	7.394(4)	91.39(4)	101.98(4)	98.26(4)	974.0(8)	0.2489

sample	water (mL) T (°C)	amount of sulfates weighed out (g)			expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							χ^2 wRp
		Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		a	b	c	α	β	γ	V	
HSC-84	1.20 75	0.1225 0	2.1305 0.1430	0 0	0.500 0	0 0.500	0 0	0.817 0	0 0.203	0 0	MG	7.3548(13)	18.801(4)	7.3979(13)	91.361(14)	102.183(12)	98.820(12)	986.4(3)	14.33 0.4424
HSC-85	1.20 75	0.1470 0	2.1376 0.1144	0 0	0.600 0	0 0.400	0 0	0.861 0	0 0.141	0 0	MG	7.3520(8)	18.8060(21)	7.3965(8)	91.364(9)	102.178(7)	98.808(8)	986.18(19)	5.08 0.2663
HSC-86	1.20 75	0.1715 0	2.1447 0.0858	0 0	0.700 0	0 0.300	0 0	0.912 0	0 0.100	0 0	MG	7.3504(7)	18.8059(20)	7.3957(7)	91.356(8)	102.159(7)	98.799(7)	985.96(18)	4.74 0.2599
HSC-87	1.20 75	0.1960 0	2.1518 0.0572	0 0	0.800 0	0 0.200	0 0	0.963 0	0 0.044	0 0	MG	7.3512(7)	18.8036(19)	7.3956(7)	91.348(8)	102.181(7)	98.815(7)	985.81(17)	4.63 0.2554
HSC-88	1.20 75	0.2205 0	2.1589 0.0286	0 0	0.900 0	0 0.100	0 0	0.983 0	0 0.023	0 0	MG	7.3509(14)	18.798(4)	7.3962(14)	91.349(15)	102.177(12)	98.818(13)	985.6(3)	10.28 0.3700
HSC-89	1.20 75	0.2450 0	2.1660 0	0 0	0 0	0 1.000	0 0	1.000 0	0 0	0 0	MG	7.3518(14)	18.793(4)	7.3965(14)	91.350(15)	102.191(12)	98.813(13)	985.4(3)	16.52 0.4802
HSC-90	1.20 110	0.4779 0	2.0221 0	0 0	1.000 0	0 0	0 0	not analyzed			MG	7.345(3)	18.786(7)	7.389(3)	91.41(3)	102.15(3)	98.80(3)	983.4(7)	6.80 0.3632
HSC-94	1.20 110	0 0	2.0709 0	0.4291 0	1.000 0	0 0	0.445 0	not analyzed			AL	7.390(4)	18.302(12)	7.324(4)	93.91(5)	102.26(4)	98.93(5)	951.1(9)	1.04 0.0786
HSC-95	1.20 25	0 0	1.9597 0.5403	0 0	0 0	0 1.000	0 0	0 0	0.134 0.799	0 0	MG	7.359(18)	18.69(5)	7.417(15)	91.03(14)	102.25(14)	98.19(15)	985.4(41)	5.22 0.2065
HSC-96	1.20 25	0 0.5304	1.9696 0	0 0	0 1.000	0 0	0 0	0 0.817	0.122 0	0 0	MG	7.411(19)	18.63(6)	7.467(17)	92.30(14)	102.47(13)	96.72(16)	997.7(46)	8.19 0.4038
HSC-97	1.20 25	0 0	1.9738 0	0 0.5262	0 0	0 1.000	0 0	0 0	0.014 0	0 0.980	AL	7.3869(10)	18.5914(27)	7.3586(10)	92.286(10)	102.283(9)	98.282(10)	974.54(23)	4.01 0.2446
HSC-99	1.20 25	0.4289 0.0543	2.0168 0	0 0	0.900 0.100	0 0	0 0	0.975 0.049	0 0	0 0	MG	7.3471(5)	18.7918(13)	7.3896(5)	91.365(6)	102.167(5)	98.829(5)	983.85(12)	2.51 0.2308
HSC-100	1.20 25	0.3803 0.1083	2.0114 0	0 0	0.800 0.200	0 0	0 0	0.937 0.076	0 0	0 0	MG	7.3450(5)	18.7880(14)	7.3896(5)	91.363(6)	102.165(5)	98.839(5)	983.35(13)	2.78 0.2411
HSC-101	1.20 25	0.3319 0.1621	2.0061 0	0 0	0.700 0.300	0 0	0 0	0.864 0.136	0 0	0 0	MG	7.3462(5)	18.7837(13)	7.3891(5)	91.374(6)	102.165(5)	98.838(5)	983.20(12)	2.61 0.2320
HSC-102	1.20 25	0.2837 0.2155	2.0008 0	0 0	0.600 0.400	0 0	0 0	0.761 0.239	0 0	0 0	MG	7.3453(5)	18.7787(14)	7.3876(5)	91.378(6)	102.156(5)	98.841(5)	982.66(12)	2.66 0.2357
HSC-103	1.20 25	0.2358 0.2687	1.9955 0	0 0	0.500 0.500	0 0	0 0	0.787 0.238	0 0	0 0	MG	7.3456(6)	18.7765(15)	7.3877(6)	91.385(6)	102.165(5)	98.848(6)	982.52(14)	2.86 0.2421
HSC-104	1.20 25	0.1881 0.3216	1.9903 0	0 0	0.400 0.600	0 0	0 0	0.665 0.351	0 0	0 0	MG	7.3467(6)	18.7727(15)	7.3875(6)	91.382(7)	102.166(6)	98.845(6)	982.45(14)	2.75 0.2373
HSC-105	1.20 25	0.1407 0.3742	1.9851 0	0 0	0.300 0.700	0 0	0 0	0.547 0.441	0.008 0	0 0	MG	7.3456(6)	18.7633(15)	7.3875(6)	91.401(7)	102.160(5)	98.852(6)	981.80(14)	2.57 0.2332
HSC-106	1.20 25	0.0936 0.4265	1.9799 0	0 0	0.200 0.800	0 0	0 0	0.319 0.681	0 0	0 0	MG	7.3447(7)	18.7400(18)	7.3838(7)	91.405(8)	102.138(7)	98.881(7)	979.96(16)	3.06 0.2497
HSC-107	1.20 25	0.0467 0.4786	1.9747 0	0 0	0.100 0.900	0 0	0 0	0.182 0.818	0 0	0 0	MG	7.3465(7)	18.7282(20)	7.3842(8)	91.438(9)	102.143(7)	98.878(7)	979.59(18)	3.55 0.2678
HSC-108	1.20 25	0.4287 0	2.0157 0.0556	0 0	0.900 0	0 0.100	0 0	0.944 0	0.010 0.040	0 0	MG	7.3459(5)	18.7925(12)	7.3886(5)	91.365(5)	102.160(4)	98.824(5)	983.63(11)	2.91 0.2473

sample	water (mL) T (°C)	amount of sulfates weighed out (g)			expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							χ^2 wRp
		Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		a	b	c	α	β	γ	V	
HSC-109	1.20 25	0.3799 0	2.0093 0.1108	0 0	0.800 0	0 0.200	0 0	0.910 0	0 0.090	0 0	MG	7.3452(5)	18.7924(12)	7.3886(5)	91.383(5)	102.157(4)	98.828(5)	983.52(11)	2.81 0.2449
HSC-110	1.20 25	0.3313 0	2.0030 0.1657	0 0	0.700 0	0 0.300	0 0	0.872 0	0.008 0.116	0 0	MG	7.3463(5)	18.7924(13)	7.3898(5)	91.380(6)	102.164(5)	98.838(5)	983.77(12)	2.43 0.2266
HSC-111	1.20 25	0.2831 0	1.9967 0.2202	0 0	0.600 0	0 0.400	0 0	0.856 0	0 0.151	0 0	MG	7.3472(6)	18.7950(15)	7.3898(6)	91.384(6)	102.169(5)	98.835(5)	984.01(13)	2.27 0.2205
HSC-112	1.20 25	0.2352 0	1.9904 0.2744	0 0	0.500 0	0 0.500	0 0	0.783 0	0.018 0.189	0 0	MG	7.3445(5)	18.7905(12)	7.3878(5)	91.381(5)	102.166(4)	98.834(5)	983.17(11)	2.77 0.2403
HSC-113	1.20 25	0.1876 0	1.9842 0.3282	0 0	0.400 0	0 0.600	0 0	0.690 0	0.014 0.289	0 0	MG	7.3454(5)	18.7917(13)	7.3874(5)	91.384(6)	102.153(5)	98.849(5)	983.29(12)	3.72 0.2472
HSC-114	1.20 25	0.1402 0	1.9780 0.3818	0 0	0.300 0	0 0.700	0 0	0.613 0	0.003 0.383	0 0	MG	7.3465(5)	18.7924(14)	7.3881(5)	91.396(6)	102.154(5)	98.844(5)	983.57(13)	3.41 0.2391
HSC-115	1.20 25	0.0932 0	1.9719 0.4349	0 0	0.200 0	0 0.800	0 0	0.483 0	0.005 0.509	0 0	MG	7.3464(6)	18.7893(17)	7.3878(6)	91.408(7)	102.158(6)	98.851(6)	983.31(15)	3.19 0.2305
HSC-116	1.20 25	0.0465 0	1.9658 0.4878	0 0	0.100 0	0 0.900	0 0	0.265 0	0 0.735	0 0	MG	7.3491(7)	18.7874(20)	7.3891(7)	91.419(8)	102.167(7)	98.869(7)	983.64(18)	3.42 0.2368
HSC-128	1.20 25	0 0	1.9738 0	0 0.5262	0 0	0 1.000	0 0	0 0	0.002 0	0 0.997	AL	7.3858(9)	18.5917(25)	7.3543(8)	92.273(9)	102.274(8)	98.290(9)	973.87(21)	6.56 0.3105
HSC-129	1.20 25	0.4290 0	2.0172 0	0 0.0538	0.900 0	0 0.100	0 0	0.915 0	0.022 0	0 0.053	MG	7.3465(6)	18.7979(14)	7.3903(6)	91.368(6)	102.174(5)	98.827(5)	984.15(13)	6.42 0.2993
HSC-130	1.20 25	0.3804 0	2.0123 0	0 0.1073	0.800 0	0 0.200	0 0	0.895 0	0.007 0	0 0.094	MG	7.3460(5)	18.7970(13)	7.3893(5)	91.362(6)	102.179(4)	98.830(5)	983.88(12)	5.21 0.2740
HSC-131	1.20 25	0.3321 0	2.0074 0	0 0.1605	0.700 0	0 0.300	0 0	0.824 0	0.038 0	0 0.119	MG	7.3457(6)	18.7986(16)	7.3882(6)	91.371(7)	102.173(5)	98.826(6)	983.81(14)	6.92 0.3140
HSC-132	1.20 25	0.2839 0	2.0025 0	0 0.2135	0.600 0	0 0.400	0 0	0.816 0	0.034 0	0 0.133	MG	7.3455(6)	18.7989(14)	7.3886(6)	91.371(6)	102.175(5)	98.827(5)	983.83(13)	4.07 0.2389
HSC-133	1.20 25	0.2360 0	1.9977 0	0 0.2663	0.500 0	0 0.500	0 0	0.722 0	0.052 0	0 0.200	MG	7.3453(5)	18.8021(13)	7.3889(5)	91.366(6)	102.169(5)	98.834(5)	984.03(12)	4.92 0.2653
HSC-134	1.20 25	0.1884 0	1.9929 0	0 0.3187	0.400 0	0 0.600	0 0	0.639 0	0.051 0	0 0.285	MG	7.3463(7)	18.8057(18)	7.3892(7)	91.371(8)	102.176(6)	98.831(7)	984.36(17)	6.28 0.2974
HSC-135	1.20 25	0.1409 0	1.9881 0	0 0.3710	0.300 0	0 0.700	0 0	0.496 0	0.074 0	0 0.392	MG	7.3504(9)	18.8162(24)	7.3934(9)	91.390(10)	102.179(8)	98.813(9)	986.04(22)	6.48 0.3023
HSC-136	1.20 25	0.0937 0	1.9833 0	0 0.4229	0.200 0	0 0.800	0 0	0.355 0	0.087 0	0 0.514	MG	7.3563(13)	18.820(3)	7.3977(13)	91.430(14)	102.225(12)	98.780(12)	987.5(3)	5.96 0.2972
HSC-137	1.20 25	0.0468 0	1.9786 0	0 0.4747	0.100 0	0 0.900	0 0	0.185 0	0.097 0	0 0.670	MG	7.3604(25)	18.779(6)	7.4062(26)	1.468(27)	102.252(23)	98.416(24)	987.9(6)	10.63 0.3963
HSC-138	1.20 25	0 0	1.9831 0	0.0411 0.4758	0 0	0 0.900	0 0	0 0	0 0	0.023 0.966	AL	7.3870(10)	18.5740(27)	7.3537(10)	92.276(10)	102.261(9)	98.279(10)	973.09(23)	4.98 0.2790
HSC-141	1.20 25	0 0	2.0115 0	0.1667 0.3217	0 0	0 0.600	0 0	0 0	0.097 0	0.306 0.395	AL	7.3813(10)	18.2282(28)	7.3260(10)	93.769(10)	102.243(9)	98.959(9)	946.53(23)	5.36 0.2764
HSC-142	1.20 25	0 0	2.0212 0	0.2094 0.2694	0 0	0 0.500	0 0	0 0	0.110 0	0.388 0.253	AL	7.3848(8)	18.2325(22)	7.3259(8)	93.821(8)	102.238(7)	99.053(7)	946.84(18)	5.48 0.2788

sample	amount of sulfates weighed out (g)				expected stoichiometry at the A site			measured stoichiometry at the A site			type	lattice parameters (Å, °) and unit cell volume (Å ³) for one or two phases in the sample, as applicable							
	water (mL) T (°C)	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺	Mg Ni	Fe ³⁺ Zn	Al Fe ²⁺		<i>a</i>	<i>b</i>	<i>c</i>	α	β	γ	<i>V</i>	χ^2 wRp
FAC-2	1.17 75	0 0	2.2416 0	0.1792 0	0 0	0.133 0	0.533 0	0 0	0.076 0	0.590 0	AL	7.3819(9)	18.233(3)	7.3221(9)	93.896(9)	102.208(8)	99.188(9)	945.60(20)	7.62 0.3469
FAC-3	1.17 75	0 0	2.2739 0	0.1568 0	0 0	0.200 0	0.467 0	0 0	0.111 0	0.556 0	AL	7.3843(5)	18.2290(20)	7.3258(5)	93.900(5)	102.212(5)	99.195(5)	946.10(10)	6.37 0.3020
FAC-4	1.17 75	0 0	2.3062 0	0.1344 0	0 0	0.267 0	0.400 0	0 0	0.139 0	0.528 0	AL	7.3847(7)	18.2350(20)	7.3246(7)	93.892(7)	102.210(7)	99.188(7)	946.30(20)	8.20 0.3478
FAC-5	1.17 75	0 0	2.3385 0	0.1120 0	0 0	0.333 0	0.333 0	0 0	0.163 0	0.504 0	AL	7.3847(8)	18.2380(20)	7.3242(8)	93.895(8)	102.213(7)	99.178(7)	946.40(20)	9.27 0.3726
FAC-6	1.17 75	0 0	2.3708 0	0.0896 0	0 0	0.400 0	0.267 0	0 0	0.223 0	0.444 0	AL	7.3837(6)	18.2470(20)	7.3230(6)	93.905(6)	102.209(5)	99.159(6)	946.70(20)	8.96 0.3531
FAC-7	1.17 75	0 0	2.4031 0	0.0672 0	0 0	0.467 0	0.200 0	0 0	0.313 0	0.353 0	AL	7.3857(7)	18.2640(20)	7.3250(7)	93.910(7)	102.214(6)	99.133(7)	948.20(20)	5.66 0.2947
FAC-8	1.17 75	0 0	2.4354 0	0.0448 0	0 0	0.533 0	0.133 0	0 0	0.392 0	0.274 0	AL	7.3846(6)	18.2730(20)	7.3238(6)	93.933(6)	102.201(6)	99.094(6)	948.50(20)	5.25 0.2773
FAC-9	1.17 75	0 0	2.4677 0	0.0224 0	0 0	0.600 0	0.067 0	0 0	0.523 0	0.144 0	AL	7.3868(6)	18.3130(20)	7.3264(6)	93.948(6)	102.211(5)	99.011(5)	951.40(10)	5.60 0.2847
FAC-10	1.17 75	0 0	2.500 0	0 0	0 0	0.667 0	0 0	0 0	0.667 0	0 0	AL	7.3873(2)	18.3560(10)	7.3280(2)	93.963(2)	102.202(2)	98.939(2)	954.1(1)	2.73 0.2012