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Supporting information for article:

Crystallography relevant to Mars and Galilean icy moons: Crystal behavior of kieserite-type monohydrate sulfates at extraterrestrial conditions down to 15 Kelvin

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Figure S1. Relative unit cell dimensions of kieserite-type compounds $M^{2+}\text{SO}_4\cdot\text{H}_2\text{O}$ ($M^{2+} = \text{Mg, Fe, Co, Ni}$) as a function of temperature (upper right plot) and pressure (lower left plot, data from Meusburger *et al.*, 2019, 2020, Ende *et al.*, 2020, and Wildner *et al.*, 2021). Note that the plot referring to temperature is scaled to 500%. Linear regression lines are shown to guide the eye. For errors see the underlying structural data in Tables S1 and S2 and in the references cited above.

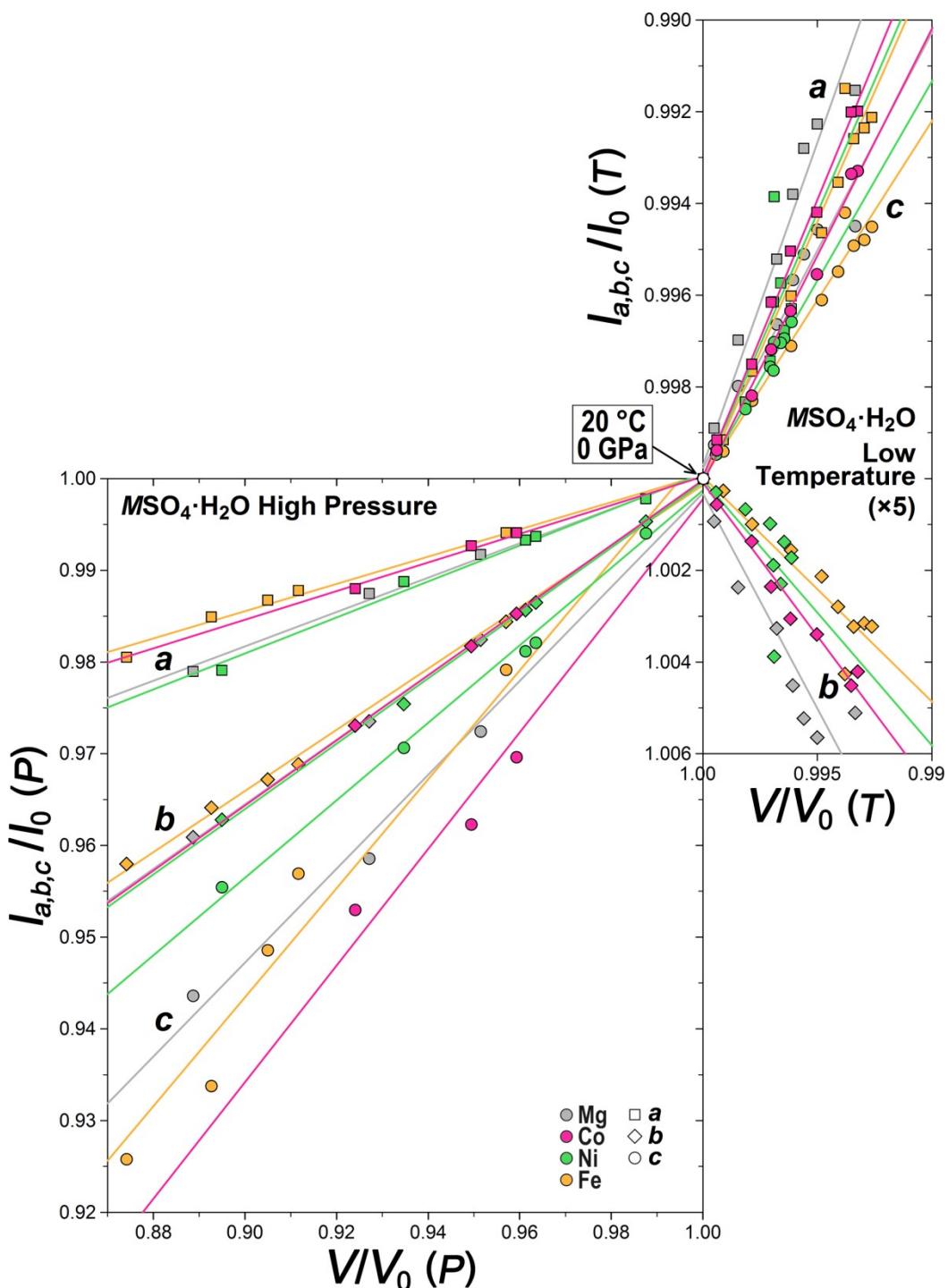


Table S1. Selected crystal data and details of the data collections and structure refinements for kieserite-type compounds $M^{2+}\text{SO}_4\cdot\text{H}_2\text{O}$ ($M^{2+} = \text{Mg, Fe, Co, Ni}$) between 15 and 313 K.

MgSO₄·H₂O	T (K)	313	273	233	193	153	113	30	15
<i>a</i> (Å) ^a		6.9227(3)	6.9070(3)	6.8937(3)	6.8815(3)	6.8717(3)	6.8648(3)	6.8560(9)	6.8611(6)
<i>b</i> (Å) ^a		7.6212(3)	7.6356(3)	7.6466(3)	7.6534(3)	7.6629(3)	7.6684(3)	7.6675(8)	7.6716(6)
<i>c</i> (Å) ^a		7.6488(3)	7.6373(3)	7.6275(3)	7.6172(3)	7.6098(3)	7.6055(3)	7.6008(10)	7.6014(7)
β (°) ^a		118.11(1)	118.02(1)	117.94(1)	117.88(1)	117.83(1)	117.79(1)	117.82(2)	117.79(1)
<i>V</i> (Å ³)		355.94(2)	355.57(2)	355.20(2)	354.60(2)	354.35(3)	354.18(3)	353.38(7)	353.97(5)
μ (mm ⁻¹)		0.97	0.97	0.97	0.97	0.97	0.97	0.97	0.97
<i>D</i> _{calc} (g cm ⁻³)		2.582	2.585	2.588	2.592	2.594	2.595	2.601	2.597
Total number of reflections		10441	10423	10356	10428	10369	10307	1112	1294
Intensity data for unit cell		6121	6673	6681	6649	6917	7061	762	886
Unique hkl's		1103	1101	1100	1098	1098	1097	410	422
<i>R</i> _i (%)		2.09	1.87	1.94	1.96	1.87	1.84	7.12	2.30
<i>F</i> _o > 4σ(<i>F</i> _o)		1049	1058	1050	1047	1049	1054	352	381
wR2 [for all <i>F</i> _o ²] (%)		4.84	4.57	4.45	4.48	4.38	4.26	12.67	5.77
weighting parameter a, b ^b		0.020, 0.22	0.020, 0.17	0.019, 0.19	0.020, 0.18	0.019, 0.18	0.018, 0.21	0.078, 0.00	0.026, 0.47
R1 [for <i>F</i> _o > 4σ(<i>F</i> _o)] (%)		1.72	1.57	1.51	1.56	1.51	1.48	5.05	2.30
R1 [for all <i>F</i> _o] (%)		1.85	1.66	1.63	1.67	1.60	1.56	5.88	2.66
Goodness of fit		1.180	1.211	1.200	1.202	1.232	1.207	1.051	1.112
Extinction coefficient		0.004(2)	0.005(2)	0.005(2)	0.004(2)	0.005(2)	0.006(2)	0.132(18)	0.077(5)
Δρ _{max, min} (e ⁻ Å ⁻³)		0.47, -0.37	0.52, -0.37	0.52, -0.41	0.49, -0.37	0.48, -0.41	0.46, -0.40	0.82, -0.96	0.41, -0.50

^a lattice parameters are corrected to comply with respective data from Nonius Kappa CCD room temperature measurement (see Experimental section).

^b $w = 1 / [\sigma^2(F_o^2) + (axP)^2 + b \times P]$; $P = \{\text{max of } (0 \text{ or } F_o^2)\} + 2F_c^2\} / 3$.

FeSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	75	60	45	15*
<i>a</i> (Å) ^a		7.0923(5)	7.0802(3)	7.0696(3)	7.0580(3)	7.0482(3)	7.0404(3)	7.0337(9)	7.0320(8)	7.0304(8)	7.0259(11)
<i>b</i> (Å) ^a		7.5523(5)	7.5565(4)	7.5620(3)	7.5663(3)	7.5706(4)	7.5756(4)	7.5789(7)	7.5783(6)	7.5789(6)	7.5867(11)
<i>c</i> (Å) ^a		7.7848(5)	7.7755(4)	7.7669(3)	7.7576(3)	7.7498(4)	7.7450(4)	7.7406(9)	7.7396(8)	7.7374(8)	7.7350(11)
β (°) ^a		118.65(1)	118.58(1)	118.52(1)	118.45(1)	118.40(1)	118.37(1)	118.33(2)	118.33(1)	118.31(1)	118.20(2)
<i>V</i> (Å ³)		365.93(7)	365.31(5)	364.85(5)	364.23(5)	363.74(5)	363.48(5)	363.23(7)	363.06(6)	362.94(6)	363.37(9)
μ (mm ⁻¹)		4.58	4.58	4.59	4.60	4.60	4.61	4.61	4.61	4.61	
<i>D</i> _{calc} (gcm ⁻³)		3.084	3.090	3.094	3.099	3.103	3.105	3.107	3.109	3.110	
Total number of reflections		10941	10880	10878	10851	10827	10783	1255	1248	1250	
Intensity data for unit cell		7887	8198	8419	8498	8632	8607	995	998	997	297
Unique hkl's		1139	1137	1133	1131	1130	1128	445	442	442	
<i>R</i> _i (%)		3.64	3.20	3.06	2.60	2.33	2.30	1.90	2.06	1.99	
<i>F</i> _o > 4σ(<i>F</i> _o)		1115	1117	1117	1112	1118	1118	425	423	425	
wR2 [for all <i>F</i> _o ²] (%)		3.79	3.60	3.53	3.38	3.32	3.22	5.16	4.36	4.25	
weighting parameter a, b ^b		0.018, 0.15	0.018, 0.17	0.017, 0.17	0.015, 0.20	0.014, 0.24	0.013, 0.24	0.029, 0.14	0.020, 0.31	0.021, 0.34	
R1 [for <i>F</i> _o > 4σ(<i>F</i> _o)] (%)		1.46	1.37	1.32	1.28	1.28	1.27	1.87	1.77	1.72	
R1 [for all <i>F</i> _o] (%)		1.50	1.40	1.34	1.31	1.30	1.29	2.00	1.88	1.77	
Goodness of fit		1.128	1.101	1.146	1.168	1.182	1.193	1.120	1.094	1.121	
Extinction coefficient		0.209(4)	0.231(4)	0.079(2)	0.033(1)	0.022(1)	0.042(1)	0.035(2)	0.033(2)	0.035(2)	
Δρ _{max, min} (e ⁻ Å ⁻³)		0.51, -0.71	0.51, -0.83	0.55, -0.54	0.49, -0.52	0.55, -0.50	0.68, -0.44	0.62, -0.55	0.51, -0.44	0.54, -0.47	

* only lattice parameters, no structure refinement

^a lattice parameters are corrected to comply with respective data from Nonius Kappa CCD room temperature measurement (see Experimental section).

^b $w = 1 / [\sigma^2(F_o^2) + (axP)^2 + bxP]$; $P = \{\text{max of } (0 \text{ or } F_o^2)\} + 2F_c^2\} / 3$.

CoSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	30	15
<i>a</i> (Å) ^a		6.9765(4)	6.9641(4)	6.9526(4)	6.9432(4)	6.9354(4)	6.9295(4)	6.9142(10)	6.9143(10)
<i>b</i> (Å) ^a		7.5904(4)	7.5990(4)	7.6051(4)	7.6126(4)	7.6179(4)	7.6205(5)	7.6267(8)	7.6290(8)
<i>c</i> (Å) ^a		7.6373(4)	7.6275(4)	7.6184(4)	7.6107(4)	7.6043(4)	7.5982(5)	7.5810(10)	7.5815(10)
β (°) ^a		118.62(1)	118.55(1)	118.50(1)	118.44(1)	118.40(1)	118.38(1)	118.18(2)	118.19(2)
<i>V</i> (Å ³)		355.03(5)	354.56(5)	354.02(5)	353.72(5)	353.42(5)	353.01(6)	352.38(9)	352.48(9)
μ (mm ⁻¹)		5.30	5.31	5.32	5.32	5.33	5.33	5.34	5.34
<i>D</i> _{calc} (gcm ⁻³)		3.237	3.241	3.246	3.249	3.251	3.255	3.261	3.260
Total number of reflections		11992	11964	11947	11894	11922	10933	1297	1289
Intensity data for unit cell		9143	9270	9349	9419	9452	8741	777	769
Unique hkl's		1105	1103	1101	1098	1098	1095	432	428
<i>R</i> _i (%)		1.97	1.94	1.97	1.98	1.97	1.85	3.36	4.88
<i>F</i> _o > 4σ(<i>F</i> _o)		1094	1095	1095	1089	1089	1086	386	383
wR2 [for all <i>F</i> _o ²] (%)		3.30	3.19	3.19	2.99	2.95	2.84	6.17	6.50
weighting parameter a, b ^b		0.014, 0.20	0.013, 0.26	0.013, 0.28	0.012, 0.28	0.011, 0.32	0.010, 0.32	0.022, 0.85	0.021, 0.36
R1 [for <i>F</i> _o > 4σ(<i>F</i> _o)] (%)		1.22	1.21	1.22	1.17	1.18	1.16	2.85	2.69
R1 [for all <i>F</i> _o] (%)		1.24	1.24	1.23	1.19	1.20	1.18	3.37	3.31
Goodness of fit		1.207	1.160	1.161	1.135	1.139	1.147	1.113	1.146
Extinction coefficient		0.024(1)	0.023(1)	0.022(1)	0.021(1)	0.018(1)	0.022(1)	0.020(2)	0.020(2)
Δρ _{max, min} (e ⁻ Å ⁻³)		0.44, -0.41	0.47, -0.42	0.47, -0.41	0.48, -0.46	0.52, -0.48	0.50, -0.43	0.80, -0.80	0.83, -0.71

^a lattice parameters are corrected to comply with respective data from Nonius Kappa CCD room temperature measurement (see Experimental section).

^b $w = 1 / [\sigma^2(F_o^2) + (a \times P)^2 + b \times P]$; $P = \{[\max \text{ of } (0 \text{ or } F_o^2)] + 2F_c^2\} / 3$.

NiSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	75	45	15
<i>a</i> (Å) ^a		6.8332(4)	6.8252(4)	6.8176(5)	6.8115(7)	6.8069(8)	6.8037(9)	6.8027(9)	6.7999(8)	6.7870(11)
<i>b</i> (Å) ^a		7.6026(5)	7.6070(4)	7.6098(5)	7.6122(8)	7.6152(9)	7.6178(10)	7.6191(7)	7.6222(6)	7.6342(9)
<i>c</i> (Å) ^a		7.4669(4)	7.4587(4)	7.4513(5)	7.4444(8)	7.4398(9)	7.4371(10)	7.4450(10)	7.4405(9)	7.4404(12)
β (°) ^a		117.78(1)	117.72(1)	117.68(1)	117.63(1)	117.60(1)	117.58(1)	117.61(2)	117.58(2)	117.51(2)
<i>V</i> (Å ³)		343.21(6)	342.79(5)	342.35(7)	341.98(10)	341.77(12)	341.66(13)	341.93(7)	341.82(6)	341.92(9)
μ (mm ⁻¹)		6.14	6.14	6.15	6.16	6.16	6.16	6.16	6.16	6.14
<i>D</i> _{calc} (gem ⁻³)		3.344	3.348	3.352	3.356	3.358	3.359	3.356	3.358	3.345
Total number of reflections		11484	11574	11529	11491	11529	11115	1293	1304	1207
Intensity data for unit cell		8005	8253	8459	8457	8648	8497	991	1003	903
Unique hkl's		1068	1064	1064	1063	1062	1061	424	422	430
<i>R</i> _i (%)		2.47	2.40	2.35	2.32	2.27	2.35	2.72	2.27	3.63
<i>F</i> _o > 4σ(<i>F</i> _o)		1034	1031	1033	1036	1034	1034	395	400	398
wR2 [for all <i>F</i> _o ²] (%)		4.19	4.11	4.37	4.20	4.13	4.22	5.21	5.13	6.61
weighting parameters a, b ^b		0.021, 0.33	0.021, 0.34	0.023, 0.40	0.021, 0.47	0.021, 0.48	0.021, 0.53	0.026, 0.00	0.029, 0.09	0.035, 0.00
R1 [for <i>F</i> _o > 4σ(<i>F</i> _o)] (%)		1.59	1.54	1.63	1.60	1.55	1.61	2.09	1.99	2.60
R1 [for all <i>F</i> _o] (%)		1.66	1.62	1.72	1.67	1.61	1.66	2.27	2.12	2.80
Goodness of fit		1.133	1.127	1.128	1.118	1.110	1.123	1.120	1.106	1.107
Extinction coefficient		0.027(1)	0.025(1)	0.022(1)	0.022(1)	0.020(1)	0.019(1)	0.041(2)	0.043(3)	0.033(3)
Δρ _{max, min} (e ⁻ Å ⁻³)		0.71, -0.61	0.67, -0.68	0.85, -0.68	0.80, -0.72	0.78, -0.68	0.82, -0.67	0.44, -0.50	0.55, -0.61	0.88, -0.66

^a lattice parameters are corrected to comply with respective data from Nonius Kappa CCD room temperature measurement (see Experimental section).

^b $w = 1 / [\sigma^2(F_o^2) + (axP)^2 + bxP]$; $P = \{[\max \text{ of } (0 \text{ or } F_o^2)] + 2F_c^2\} / 3$.

Table S2. Final atomic parameters for kieserite-type compounds $M^{2+}\text{SO}_4\cdot\text{H}_2\text{O}$ ($M^{2+} = \text{Mg, Fe, Co, Ni}$) between 15 and 313 K.**MgSO₄·H₂O**

15 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.0038(3)	0.0035(4)	0.0038(5)	0.0049(4)	0.0000(3)	0.0025(3)	0.0005(3)
S	0	0.15743(8)	0.25	0.0030(2)	0.0030(3)	0.0029(4)	0.0037(3)	0	0.0022(2)	0
O1	0.17523(19)	0.04823(17)	0.39724(17)	0.0049(3)	0.0040(6)	0.0042(7)	0.0062(6)	0.0010(5)	0.0022(5)	0.0011(5)
O2	0.09598(19)	0.27005(17)	0.15141(18)	0.0048(3)	0.0042(6)	0.0041(7)	0.0069(6)	0.0000(5)	0.0034(5)	0.0012(5)
O3	0	0.6334(3)	0.25	0.0049(4)	0.0037(9)	0.0040(9)	0.0065(9)	0	0.0020(7)	0
H	0.101(4)	0.700(4)	0.288(4)	0.021(7)*						
30 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.0057(5)	0.0047(8)	0.0041(9)	0.0093(8)	-0.0002(5)	0.0042(6)	0.0002(5)
S	0	0.15735(13)	0.25	0.0046(5)	0.0037(7)	0.0021(7)	0.0084(7)	0	0.0032(5)	0
O1	0.1756(3)	0.0480(3)	0.3969(3)	0.0073(6)	0.0060(11)	0.0068(13)	0.0096(11)	-0.0001(8)	0.0040(9)	0.0012(8)
O2	0.0959(3)	0.2699(3)	0.1514(3)	0.0070(6)	0.0049(11)	0.0047(12)	0.0123(10)	0.0005(8)	0.0047(9)	0.0010(8)
O3	0	0.6338(4)	0.25	0.0062(8)	0.0039(16)	0.0050(16)	0.0087(16)	0	0.0023(13)	0
H	0.094(7)	0.690(7)	0.284(6)	0.013(11)*						
113 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.00431(6)	0.00388(11)	0.00445(11)	0.00431(10)	-0.00022(8)	0.00167(8)	0.00014(8)
S	0	0.15710(2)	0.25	0.00337(5)	0.00268(7)	0.00342(7)	0.00377(7)	0	0.00131(5)	0
O1	0.17522(7)	0.04770(6)	0.39686(6)	0.00648(7)	0.00418(14)	0.00732(15)	0.00704(14)	0.00193(11)	0.00186(11)	0.00289(11)
O2	0.09574(7)	0.26975(5)	0.15109(6)	0.00597(7)	0.00588(15)	0.00573(14)	0.00753(14)	0.00023(11)	0.00417(12)	0.00206(11)
O3	0	0.63384(8)	0.25	0.00572(9)	0.0051(2)	0.00623(19)	0.00593(19)	0	0.00259(16)	0
H	0.106(2)	0.6987(18)	0.290(2)	0.019(3)*						
153 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.00490(6)	0.00441(11)	0.00511(11)	0.00489(11)	-0.00030(8)	0.00194(8)	0.00018(8)
S	0	0.15678(2)	0.25	0.00394(5)	0.00310(7)	0.00392(7)	0.00449(7)	0	0.00152(5)	0
O1	0.17528(7)	0.04724(6)	0.39649(6)	0.00764(7)	0.00485(14)	0.00865(15)	0.00845(15)	0.00234(11)	0.00228(12)	0.00359(12)
O2	0.09519(7)	0.26939(5)	0.15082(6)	0.00695(7)	0.00680(15)	0.00652(14)	0.00900(15)	0.00050(11)	0.00491(12)	0.00257(11)
O3	0	0.63402(8)	0.25	0.00651(9)	0.0059(2)	0.0072(2)	0.0065(2)	0	0.00297(16)	0
H	0.105(2)	0.6999(18)	0.290(2)	0.019(3)*						
193 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.00566(6)	0.00494(11)	0.00595(11)	0.00571(11)	-0.00034(8)	0.00217(9)	0.00024(8)
S	0	0.15635(2)	0.25	0.00461(5)	0.00351(7)	0.00455(7)	0.00540(7)	0	0.00177(5)	0
O1	0.17541(7)	0.04664(6)	0.39602(7)	0.00910(8)	0.00578(15)	0.01021(16)	0.01016(16)	0.00271(12)	0.00276(13)	0.00436(13)
O2	0.09440(7)	0.26900(6)	0.15044(7)	0.00824(7)	0.00810(16)	0.00758(15)	0.01082(16)	0.00065(12)	0.00592(13)	0.00323(12)
O3	0	0.63431(8)	0.25	0.00757(9)	0.0070(2)	0.0083(2)	0.0075(2)	0	0.00343(17)	0
H	0.104(2)	0.7003(18)	0.291(2)	0.022(3)*						
233 K	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0	0.5	0	0.00652(6)	0.00574(11)	0.00680(11)	0.00652(11)	-0.00039(8)	0.00244(9)	0.00034(8)
S	0	0.15586(2)	0.25	0.00530(5)	0.00400(7)	0.00518(7)	0.00623(7)	0	0.00198(5)	0

O1	0.17551(7)	0.04607(6)	0.39547(7)	0.01054(8)	0.00642(15)	0.01185(17)	0.01192(17)	0.00311(13)	0.00312(13)	0.00518(13)
O2	0.09346(7)	0.26857(6)	0.15003(7)	0.00955(8)	0.00931(17)	0.00875(16)	0.01258(17)	0.00087(12)	0.00678(14)	0.00375(12)
O3	0	0.63464(8)	0.25	0.00867(10)	0.0082(2)	0.0095(2)	0.0084(2)	0	0.00396(18)	0
H	0.103(2)	0.7020(18)	0.291(2)	0.024(3)*						

273 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Mg	0	0.5	0	0.00746(6)	0.00655(12)	0.00777(12)	0.00747(11)	-0.00039(8)	0.00280(9)	0.00049(8)
S	0	0.15529(2)	0.25	0.00604(5)	0.00453(7)	0.00592(7)	0.00710(7)	0	0.00226(5)	0
O1	0.17569(7)	0.04536(7)	0.39486(7)	0.01209(8)	0.00720(16)	0.01384(18)	0.01366(17)	0.00361(13)	0.00358(13)	0.00604(14)
O2	0.09235(8)	0.26806(6)	0.14957(7)	0.01101(8)	0.01084(17)	0.01001(16)	0.01447(17)	0.00112(12)	0.00785(14)	0.00436(13)
O3	0	0.63497(9)	0.25	0.00991(10)	0.0095(2)	0.0108(2)	0.0096(2)	0	0.00462(18)	0
H	0.104(2)	0.7024(18)	0.293(2)	0.025(3)*						

313 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Mg	0	0.5	0	0.00852(7)	0.00750(13)	0.00876(13)	0.00858(13)	-0.00057(9)	0.00319(10)	0.00055(9)
S	0	0.15461(3)	0.25	0.00684(5)	0.00519(8)	0.00655(8)	0.00819(8)	0	0.00267(6)	0
O1	0.17585(8)	0.04442(7)	0.39411(8)	0.01380(9)	0.00842(18)	0.0155(2)	0.0157(2)	0.00412(15)	0.00418(15)	0.00690(16)
O2	0.09120(9)	0.26743(7)	0.14908(8)	0.01257(9)	0.0126(2)	0.01123(18)	0.0167(2)	0.00131(14)	0.00915(17)	0.00498(15)
O3	0	0.63534(10)	0.25	0.01125(11)	0.0110(3)	0.0123(3)	0.0110(2)	0	0.0056(2)	0
H	0.103(2)	0.703(2)	0.293(2)	0.028(4)*						

FeSO₄·H₂O

45 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00235(16)	0.0025(2)	0.0022(2)	0.0022(2)	0.00025(12)	0.00098(16)	0.00075(11)
S	0	0.15535(7)	0.25	0.00229(17)	0.0019(3)	0.0024(3)	0.0026(3)	0	0.0011(2)	0
O1	0.1683(2)	0.04564(17)	0.40068(17)	0.0046(3)	0.0036(7)	0.0049(6)	0.0045(5)	0.0010(5)	0.0013(5)	0.0008(5)
O2	0.10045(19)	0.27064(15)	0.15967(16)	0.0044(3)	0.0038(7)	0.0042(6)	0.0052(5)	0.0002(5)	0.0023(5)	0.0017(4)
O3	0	0.6435(2)	0.25	0.0045(4)	0.0036(10)	0.0045(9)	0.0056(8)	0	0.0024(7)	0
H	0.101(4)	0.715(3)	0.290(3)	0.020(6)*						
60 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00233(16)	0.0024(2)	0.0018(2)	0.0024(2)	0.00016(13)	0.00083(17)	0.00064(12)
S	0	0.15520(8)	0.25	0.00232(18)	0.0020(3)	0.0020(3)	0.0030(3)	0	0.0012(2)	0
O1	0.1684(2)	0.04575(18)	0.40074(19)	0.0050(3)	0.0038(7)	0.0051(6)	0.0055(6)	0.0007(5)	0.0018(5)	0.0012(5)
O2	0.1003(2)	0.27048(16)	0.15946(17)	0.0043(3)	0.0037(7)	0.0041(7)	0.0056(6)	0.0005(5)	0.0028(5)	0.0020(5)
O3	0	0.6434(3)	0.25	0.0043(4)	0.0034(10)	0.0044(9)	0.0046(9)	0	0.0015(8)	0
H	0.102(4)	0.711(3)	0.294(3)	0.012(6)*						
75 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00280(18)	0.0025(3)	0.0027(3)	0.0028(2)	0.00005(13)	0.00097(18)	0.00058(12)
S	0	0.15532(8)	0.25	0.0027(2)	0.0021(4)	0.0026(3)	0.0030(3)	0	0.0010(3)	0
O1	0.1686(2)	0.0458(2)	0.40091(19)	0.0052(3)	0.0039(7)	0.0047(7)	0.0060(6)	0.0012(6)	0.0016(5)	0.0018(5)
O2	0.1002(2)	0.27064(17)	0.15934(18)	0.0049(3)	0.0041(7)	0.0047(7)	0.0062(6)	0.0005(5)	0.0027(5)	0.0020(5)
O3	0	0.6434(3)	0.25	0.0046(4)	0.0039(10)	0.0050(10)	0.0046(9)	0	0.0017(8)	0
H	0.098(4)	0.712(3)	0.291(3)	0.011(6)*						
113 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00387(4)	0.00364(5)	0.00378(5)	0.00416(5)	0.00003(3)	0.00182(4)	0.00046(3)
S	0	0.15512(2)	0.25	0.00351(4)	0.00283(7)	0.00326(7)	0.00436(7)	0	0.00162(5)	0
O1	0.16853(7)	0.04497(6)	0.40047(7)	0.00700(7)	0.00455(14)	0.00773(16)	0.00792(15)	0.00210(12)	0.00231(12)	0.00347(12)
O2	0.09991(7)	0.27015(6)	0.15910(6)	0.00624(7)	0.00607(15)	0.00564(15)	0.00832(15)	0.00030(11)	0.00450(13)	0.00221(12)
O3	0	0.64381(8)	0.25	0.00616(9)	0.0060(2)	0.0064(2)	0.0064(2)	0	0.00316(17)	0
H	0.109(2)	0.712(2)	0.292(2)	0.021(3)*						
153 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00477(4)	0.00440(5)	0.00465(5)	0.00517(5)	0.00000(3)	0.00221(4)	0.00056(3)
S	0	0.15482(2)	0.25	0.00421(4)	0.00323(7)	0.00388(7)	0.00537(7)	0	0.00192(5)	0
O1	0.16858(7)	0.04450(7)	0.40013(7)	0.00847(7)	0.00528(15)	0.00941(17)	0.00988(16)	0.00255(13)	0.00292(13)	0.00441(13)
O2	0.09931(7)	0.26982(6)	0.15882(7)	0.00747(7)	0.00714(15)	0.00668(15)	0.01017(16)	0.00053(12)	0.00539(13)	0.00284(12)
O3	0	0.64402(9)	0.25	0.00722(9)	0.0070(2)	0.0074(2)	0.0076(2)	0	0.00373(18)	0
H	0.107(2)	0.716(2)	0.294(2)	0.025(4)*						
193 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe	0	0.5	0	0.00582(4)	0.00531(5)	0.00572(5)	0.00630(5)	-0.00003(3)	0.00266(4)	0.00064(3)
S	0	0.15447(2)	0.25	0.00507(4)	0.00382(7)	0.00462(7)	0.00651(7)	0	0.00225(5)	0
O1	0.16874(7)	0.04405(7)	0.39968(7)	0.01016(8)	0.00629(15)	0.01111(17)	0.01199(17)	0.00299(13)	0.00347(13)	0.00538(14)
O2	0.09854(7)	0.26941(6)	0.15838(7)	0.00889(7)	0.00832(15)	0.00798(15)	0.01216(17)	0.00074(12)	0.00633(13)	0.00344(13)
O3	0	0.64418(9)	0.25	0.00850(9)	0.0084(2)	0.0088(2)	0.0087(2)	0	0.00439(18)	0

H	0.108(2)	0.716(2)	0.294(2)	0.028(4)*							
233 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Fe	0	0.5	0	0.00700(4)	0.00634(5)	0.00685(6)	0.00754(6)	-0.00004(3)	0.00310(4)	0.00074(3)	
S	0	0.15406(2)	0.25	0.00601(4)	0.00456(7)	0.00540(7)	0.00768(7)	0	0.00260(5)	0	
O1	0.16893(7)	0.04355(7)	0.39918(7)	0.01200(8)	0.00723(15)	0.01321(18)	0.01418(18)	0.00356(14)	0.00400(13)	0.00646(15)	
O2	0.09766(7)	0.26893(6)	0.15794(7)	0.01060(8)	0.01009(16)	0.00930(16)	0.01444(18)	0.00102(12)	0.00749(14)	0.00417(13)	
O3	0	0.64450(9)	0.25	0.00989(10)	0.0099(2)	0.0102(2)	0.0099(2)	0	0.00501(18)	0	
H	0.105(3)	0.718(2)	0.295(2)	0.034(4)*							
273 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Fe	0	0.5	0	0.00810(4)	0.00734(6)	0.00813(6)	0.00863(6)	-0.00008(3)	0.00365(4)	0.00083(3)	
S	0	0.15360(2)	0.25	0.00688(5)	0.00523(7)	0.00633(7)	0.00873(7)	0	0.00305(5)	0	
O1	0.16920(7)	0.04295(7)	0.39860(8)	0.01391(8)	0.00844(16)	0.01536(19)	0.01643(19)	0.00421(14)	0.00475(14)	0.00751(16)	
O2	0.09661(7)	0.26840(6)	0.15737(7)	0.01223(8)	0.01166(16)	0.01093(17)	0.01664(19)	0.00136(13)	0.00882(15)	0.00494(14)	
O3	0	0.64461(9)	0.25	0.01132(10)	0.0115(2)	0.0120(2)	0.0110(2)	0	0.00587(19)	0	
H	0.106(3)	0.718(2)	0.296(2)	0.037(4)*							
313 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Fe	0	0.5	0	0.00928(5)	0.00841(6)	0.00935(6)	0.00991(6)	-0.00014(3)	0.00425(4)	0.00092(3)	
S	0	0.15309(3)	0.25	0.00781(5)	0.00596(7)	0.00716(8)	0.00993(8)	0	0.00352(6)	0	
O1	0.16949(8)	0.04222(8)	0.39797(8)	0.01594(9)	0.00969(17)	0.0176(2)	0.0190(2)	0.00462(16)	0.00563(15)	0.00856(17)	
O2	0.09559(8)	0.26774(7)	0.15682(8)	0.01397(9)	0.01329(18)	0.01247(18)	0.0190(2)	0.00163(14)	0.01008(16)	0.00557(15)	
O3	0	0.64483(10)	0.25	0.01298(11)	0.0133(2)	0.0137(3)	0.0127(2)	0	0.0069(2)	0	
H	0.107(3)	0.722(3)	0.297(2)	0.040(4)*							

CoSO₄·H₂O

15 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.0041(2)	0.0045(3)	0.0025(4)	0.0049(4)	-0.0002(2)	0.0019(3)	0.0002(2)
S	0	0.15579(15)	0.25	0.0042(3)	0.0046(5)	0.0026(6)	0.0050(5)	0	0.0019(4)	0
O1	0.1722(3)	0.0452(3)	0.4025(3)	0.0051(5)	0.0045(10)	0.0025(11)	0.0079(10)	0.0013(9)	0.0026(9)	0.0003(9)
O2	0.1006(3)	0.2687(3)	0.1558(3)	0.0058(5)	0.0060(10)	0.0034(12)	0.0084(10)	0.0003(9)	0.0036(9)	0.0019(8)
O3	0	0.6373(5)	0.25	0.0068(7)	0.0042(15)	0.0062(18)	0.0088(16)	0	0.0021(14)	0
H	0.100(5)	0.697(5)	0.293(5)	0.008(10)*						
30 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.0039(2)	0.0043(3)	0.0028(4)	0.0042(4)	-0.0003(2)	0.0017(3)	0.0002(2)
S	0	0.15584(15)	0.25	0.0041(3)	0.0050(5)	0.0026(6)	0.0052(5)	0	0.0028(4)	0
O1	0.1720(3)	0.0451(3)	0.4027(3)	0.0056(5)	0.0048(10)	0.0049(12)	0.0071(10)	0.0006(9)	0.0027(9)	0.0009(8)
O2	0.1005(3)	0.2688(3)	0.1559(3)	0.0056(5)	0.0065(10)	0.0039(12)	0.0069(10)	0.0001(9)	0.0037(9)	0.0012(8)
O3	0	0.6368(4)	0.25	0.0056(7)	0.0058(15)	0.0043(17)	0.0074(15)	0	0.0037(14)	0
H	0.104(6)	0.695(7)	0.291(6)	0.029(13)*						
113 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.00327(3)	0.00299(5)	0.00348(5)	0.00344(5)	-0.00003(3)	0.00161(3)	0.00024(3)
S	0	0.15532(2)	0.25	0.00313(4)	0.00255(7)	0.00322(7)	0.00371(7)	0	0.00155(5)	0
O1	0.17207(7)	0.04480(6)	0.40193(7)	0.00652(7)	0.00425(14)	0.00740(16)	0.00727(16)	0.00203(12)	0.00220(13)	0.00341(13)
O2	0.09983(7)	0.26818(6)	0.15527(7)	0.00564(7)	0.00567(15)	0.00528(15)	0.00750(16)	0.00047(12)	0.00437(13)	0.00230(12)
O3	0	0.63777(8)	0.25	0.00535(9)	0.0051(2)	0.0057(2)	0.0055(2)	0	0.00273(17)	0
H	0.110(2)	0.704(2)	0.294(2)	0.022(3)*						
153 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.00391(3)	0.00381(5)	0.00393(5)	0.00408(5)	-0.00008(3)	0.00195(3)	0.00027(3)
S	0	0.15498(3)	0.25	0.00364(4)	0.00310(7)	0.00347(7)	0.00437(7)	0	0.00180(5)	0
O1	0.17219(7)	0.04444(7)	0.40161(7)	0.00767(7)	0.00509(15)	0.00865(17)	0.00855(16)	0.00232(13)	0.00265(13)	0.00426(13)
O2	0.09929(7)	0.26795(6)	0.15505(7)	0.00672(7)	0.00699(16)	0.00600(16)	0.00904(16)	0.00071(12)	0.00532(13)	0.00279(12)
O3	0	0.63789(9)	0.25	0.00618(9)	0.0061(2)	0.0065(2)	0.0063(2)	0	0.00327(17)	0
H	0.110(2)	0.705(2)	0.293(2)	0.019(3)*						
193 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.00474(3)	0.00454(5)	0.00472(5)	0.00503(5)	-0.00008(3)	0.00235(3)	0.00034(3)
S	0	0.15468(2)	0.25	0.00432(4)	0.00356(7)	0.00404(7)	0.00533(7)	0	0.00210(5)	0
O1	0.17231(7)	0.04404(7)	0.40123(7)	0.00913(7)	0.00576(15)	0.01036(18)	0.01044(17)	0.00267(13)	0.00319(13)	0.00513(14)
O2	0.09866(7)	0.26764(6)	0.15475(7)	0.00793(7)	0.00812(16)	0.00695(16)	0.01093(16)	0.00101(12)	0.00634(13)	0.00341(13)
O3	0	0.63806(9)	0.25	0.00719(9)	0.0071(2)	0.0076(2)	0.0072(2)	0	0.00371(17)	0
H	0.110(2)	0.705(2)	0.294(2)	0.020(3)*						
233 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co	0	0.5	0	0.00568(4)	0.00537(5)	0.00567(5)	0.00604(5)	-0.00009(3)	0.00275(4)	0.00038(3)
S	0	0.15433(3)	0.25	0.00510(4)	0.00412(7)	0.00475(7)	0.00634(7)	0	0.00242(5)	0
O1	0.17242(8)	0.04355(7)	0.40080(8)	0.01078(8)	0.00670(16)	0.01221(19)	0.01247(18)	0.00322(14)	0.00380(14)	0.00609(15)
O2	0.09802(8)	0.26722(6)	0.15443(7)	0.00931(8)	0.00939(17)	0.00810(17)	0.01282(18)	0.00123(13)	0.00722(15)	0.00394(14)
O3	0	0.63819(9)	0.25	0.00832(10)	0.0083(2)	0.0087(2)	0.0083(2)	0	0.00431(19)	0

H	0.103(2)	0.704(2)	0.294(2)	0.026(4)*							
273 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Co	0	0.5	0	0.00667(4)	0.00626(5)	0.00668(5)	0.00709(5)	-0.00011(3)	0.00322(4)	0.00044(3)	
S	0	0.15394(3)	0.25	0.00590(4)	0.00478(7)	0.00550(7)	0.00729(7)	0	0.00277(5)	0	
O1	0.17252(8)	0.04305(8)	0.40031(8)	0.01245(8)	0.00762(16)	0.0141(2)	0.01452(19)	0.00368(15)	0.00439(15)	0.00713(16)	
O2	0.09729(8)	0.26680(7)	0.15409(8)	0.01077(8)	0.01087(17)	0.00944(17)	0.01480(19)	0.00154(14)	0.00840(15)	0.00458(14)	
O3	0	0.63844(9)	0.25	0.00956(10)	0.0095(2)	0.0102(2)	0.0096(2)	0	0.00499(19)	0	
H	0.102(2)	0.703(2)	0.294(2)	0.028(4)*							
313 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Co	0	0.5	0	0.00773(4)	0.00722(5)	0.00778(5)	0.00821(5)	-0.00010(3)	0.00373(4)	0.00052(3)	
S	0	0.15349(3)	0.25	0.00676(4)	0.00542(7)	0.00632(7)	0.00835(7)	0	0.00315(5)	0	
O1	0.17268(8)	0.04243(8)	0.39981(8)	0.01420(9)	0.00875(17)	0.0160(2)	0.0166(2)	0.00400(15)	0.00506(15)	0.00796(17)	
O2	0.09640(8)	0.26637(7)	0.15370(8)	0.01236(8)	0.01246(18)	0.01089(18)	0.01701(19)	0.00190(14)	0.00970(16)	0.00524(15)	
O3	0	0.63871(10)	0.25	0.01098(10)	0.0112(2)	0.0117(3)	0.0108(2)	0	0.0058(2)	0	
H	0.101(2)	0.704(2)	0.295(2)	0.031(4)*							

NiSO₄·H₂O

15 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.0077(2)	0.0073(3)	0.0069(3)	0.0093(3)	-0.00018(16)	0.0041(2)	-0.00008(14)
S	0	0.15772(12)	0.25	0.0078(3)	0.0075(5)	0.0072(5)	0.0092(5)	0	0.0041(4)	0
O1	0.1727(3)	0.0480(3)	0.4050(3)	0.0101(4)	0.0091(11)	0.0093(9)	0.0118(9)	-0.0003(8)	0.0047(8)	0.0013(7)
O2	0.1051(3)	0.2710(3)	0.1556(2)	0.0085(4)	0.0088(10)	0.0082(9)	0.0100(9)	-0.0003(7)	0.0056(7)	0.0009(7)
O3	0	0.6302(4)	0.25	0.0100(6)	0.0086(15)	0.0099(13)	0.0110(13)	0	0.0040(11)	0
H	0.113(6)	0.696(5)	0.296(5)	0.014(9)*						
45 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.00160(19)	0.0011(3)	0.0023(3)	0.0017(3)	-0.00009(11)	0.00086(19)	-0.00006(11)
S	0	0.15779(9)	0.25	0.0018(2)	0.0010(4)	0.0022(4)	0.0023(4)	0	0.0009(3)	0
O1	0.1727(2)	0.0479(2)	0.4051(2)	0.0036(3)	0.0020(7)	0.0049(7)	0.0039(8)	0.0010(6)	0.0015(6)	0.0015(6)
O2	0.1052(2)	0.2713(2)	0.1554(2)	0.0035(3)	0.0028(7)	0.0043(7)	0.0038(7)	-0.0001(5)	0.0018(6)	0.0013(5)
O3	0	0.6308(3)	0.25	0.0035(4)	0.0014(10)	0.0044(10)	0.0036(11)	0	0.0003(9)	0
H	0.109(4)	0.691(4)	0.299(4)	0.012(7)*						
75 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.0026(2)	0.0017(3)	0.0030(3)	0.0031(3)	-0.00013(12)	0.0011(2)	-0.00009(13)
S	0	0.15780(10)	0.25	0.0028(2)	0.0018(4)	0.0031(4)	0.0037(4)	0	0.0015(3)	0
O1	0.1724(2)	0.0479(2)	0.4049(2)	0.0047(4)	0.0031(8)	0.0049(7)	0.0054(8)	0.0008(6)	0.0015(7)	0.0012(6)
O2	0.1051(2)	0.2709(2)	0.1556(2)	0.0046(4)	0.0037(7)	0.0044(8)	0.0063(8)	0.0004(6)	0.0028(6)	0.0011(6)
O3	0	0.6304(3)	0.25	0.0046(5)	0.0024(11)	0.0055(11)	0.0061(12)	0	0.0022(10)	0
H	0.099(4)	0.698(4)	0.299(5)	0.024(9)*						
113 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.00292(5)	0.00272(6)	0.00320(7)	0.00283(6)	-0.00010(4)	0.00127(5)	0.00010(3)
S	0	0.15763(4)	0.25	0.00284(5)	0.00228(9)	0.00297(10)	0.00321(9)	0	0.00121(7)	0
O1	0.17257(10)	0.04772(9)	0.40473(9)	0.00604(10)	0.0039(2)	0.0070(2)	0.0067(2)	0.00183(17)	0.00202(17)	0.00315(17)
O2	0.10507(10)	0.27108(8)	0.15552(9)	0.00506(9)	0.0051(2)	0.0047(2)	0.0067(2)	0.00031(16)	0.00378(17)	0.00181(16)
O3	0	0.63055(12)	0.25	0.00491(12)	0.0042(3)	0.0056(3)	0.0050(3)	0	0.0022(2)	0
H	0.109(3)	0.695(3)	0.294(3)	0.020(5)*						
153 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.00357(5)	0.00321(6)	0.00392(7)	0.00349(6)	-0.00011(3)	0.00146(4)	0.00013(3)
S	0	0.15750(3)	0.25	0.00344(5)	0.00269(9)	0.00365(9)	0.00388(9)	0	0.00144(7)	0
O1	0.17263(10)	0.04756(9)	0.40448(9)	0.00712(10)	0.0044(2)	0.0084(2)	0.0080(2)	0.00214(17)	0.00232(17)	0.00384(17)
O2	0.10474(10)	0.27084(8)	0.15537(9)	0.00604(9)	0.0058(2)	0.0057(2)	0.0079(2)	0.00046(16)	0.00435(17)	0.00231(16)
O3	0	0.63067(11)	0.25	0.00555(12)	0.0050(3)	0.0062(3)	0.0054(3)	0	0.0024(2)	0
H	0.109(3)	0.695(3)	0.294(3)	0.018(5)*						
193 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Ni	0	0.5	0	0.00428(5)	0.00390(6)	0.00468(7)	0.00412(6)	-0.00014(4)	0.00173(5)	0.00016(3)
S	0	0.15727(3)	0.25	0.00404(5)	0.00314(9)	0.00423(10)	0.00453(9)	0	0.00159(7)	0
O1	0.17262(10)	0.04732(9)	0.40413(10)	0.00843(10)	0.0052(2)	0.0100(2)	0.0094(2)	0.00250(18)	0.00281(18)	0.00463(18)
O2	0.10428(10)	0.27059(8)	0.15519(9)	0.00703(9)	0.0067(2)	0.0066(2)	0.0094(2)	0.00068(16)	0.00512(18)	0.00264(16)
O3	0	0.63077(12)	0.25	0.00631(12)	0.0060(3)	0.0070(3)	0.0061(3)	0	0.0029(2)	0

H	0.109(3)	0.695(3)	0.294(3)	0.020(5)*							
233 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Ni	0	0.5	0	0.00492(5)	0.00440(7)	0.00540(7)	0.00470(7)	-0.00017(4)	0.00190(5)	0.00020(3)	
S	0	0.15705(3)	0.25	0.00453(6)	0.00342(9)	0.00469(10)	0.00518(9)	0	0.00173(7)	0	
O1	0.17277(10)	0.04702(10)	0.40390(10)	0.00962(11)	0.0057(2)	0.0114(3)	0.0109(2)	0.00282(19)	0.00316(18)	0.00550(19)	
O2	0.10392(10)	0.27036(8)	0.15499(10)	0.00809(10)	0.0077(2)	0.0077(2)	0.0107(2)	0.00093(17)	0.00581(18)	0.00324(17)	
O3	0	0.63099(12)	0.25	0.00704(12)	0.0064(3)	0.0078(3)	0.0069(3)	0	0.0031(2)	0	
H	0.109(3)	0.695(3)	0.296(3)	0.018(4)*							
273 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Ni	0	0.5	0	0.00577(5)	0.00521(6)	0.00627(7)	0.00552(6)	-0.00020(3)	0.00223(4)	0.00023(3)	
S	0	0.15681(3)	0.25	0.00527(5)	0.00403(9)	0.00542(9)	0.00597(9)	0	0.00201(7)	0	
O1	0.17279(10)	0.04668(9)	0.40353(10)	0.01106(10)	0.0065(2)	0.0132(3)	0.0125(2)	0.00321(18)	0.00356(18)	0.00631(19)	
O2	0.10339(10)	0.27006(8)	0.15477(9)	0.00926(10)	0.0089(2)	0.0086(2)	0.0122(2)	0.00120(16)	0.00657(18)	0.00377(17)	
O3	0	0.63108(12)	0.25	0.00810(12)	0.0076(3)	0.0092(3)	0.0076(3)	0	0.0037(2)	0	
H	0.108(3)	0.695(2)	0.294(3)	0.020(4)*							
313 K	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³	
Ni	0	0.5	0	0.00653(5)	0.00586(6)	0.00709(7)	0.00627(6)	-0.00018(4)	0.00251(5)	0.00029(3)	
S	0	0.15651(3)	0.25	0.00591(5)	0.00440(9)	0.00604(9)	0.00675(9)	0	0.00215(7)	0	
O1	0.17290(10)	0.04625(10)	0.40317(10)	0.01253(11)	0.0073(2)	0.0148(3)	0.0144(2)	0.00359(19)	0.00413(19)	0.0072(2)	
O2	0.10276(10)	0.26975(8)	0.15448(10)	0.01045(10)	0.0100(2)	0.0096(2)	0.0141(2)	0.00137(17)	0.00752(19)	0.00425(17)	
O3	0	0.63132(12)	0.25	0.00908(13)	0.0085(3)	0.0103(3)	0.0087(3)	0	0.0043(2)	0	
H	0.107(3)	0.696(3)	0.294(3)	0.023(5)*							

Table S3. Selected bond distances (\AA) and angles ($^\circ$) for kieserite-type compounds $M^{2+}\text{SO}_4\cdot\text{H}_2\text{O}$ ($M^{2+} = \text{Mg, Fe, Co, Ni}$) between 15 and 313 K. Respective room-temperature data for $M = \text{Mg}$ and Co are given by Bechtold & Wildner (2016), for $M = \text{Fe}$ by Talla & Wildner (2019), and for $M = \text{Ni}$ by Talla *et al.* (2020). Note: S–O bond lengths are not corrected for thermal motion.

MgSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	30	15
Mg–O1 (2 \times)		2.0232(6)	2.0230(6)	2.0229(6)	2.0222(5)	2.0222(5)	2.0222(5)	2.0170(21)	2.0223(12)
Mg–O2 (2 \times)		2.0401(5)	2.0405(5)	2.0409(5)	2.0407(5)	2.0413(5)	2.0410(5)	2.0403(22)	2.0405(13)
Mg–O3 (2 \times)		2.1726(4)	2.1697(4)	2.1671(4)	2.1640(4)	2.1619(4)	2.1607(4)	2.1596(17)	2.1583(9)
<Mg–O>		2.0786	2.0777	2.0770	2.0756	2.0751	2.0746	2.0723	2.0737
S–O1 (2 \times)		1.4621(5)	1.4628(5)	1.4634(5)	1.4640(5)	1.4643(5)	1.4647(5)	1.4647(22)	1.4647(13)
S–O2 (2 \times)		1.4809(5)	1.4820(5)	1.4832(5)	1.4837(5)	1.4843(4)	1.4849(4)	1.4826(22)	1.4838(12)
<S–O>		1.4715	1.4724	1.4733	1.4739	1.4743	1.4748	1.4737	1.4743
Mg–O1–S		140.38(4)	140.26(3)	140.12(3)	140.00(3)	139.91(3)	139.84(3)	139.96(14)	139.81(8)
Mg–O2–S		134.44(3)	134.16(3)	133.87(3)	133.63(3)	133.44(3)	133.32(3)	133.34(12)	133.30(7)
Mg–O3–Mg		123.32(4)	123.28(3)	123.27(3)	123.28(3)	123.28(3)	123.28(3)	123.26(16)	123.40(9)
O3 \cdots O2		2.7495(7)	2.7422(6)	2.7353(6)	2.7292(6)	2.7246(6)	2.7216(5)	2.7183(24)	2.7218(14)

FeSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	75	60	45
Fe–O1 (2 \times)		2.1076(6)	2.1085(6)	2.1095(6)	2.1093(6)	2.1093(6)	2.1088(5)	2.1085(15)	2.1090(14)	2.1093(13)
Fe–O2 (2 \times)		2.0575(5)	2.0560(5)	2.0558(5)	2.0551(5)	2.0547(5)	2.0546(5)	2.0530(13)	2.0543(12)	2.0540(11)
Fe–O3 (2 \times)		2.2325(4)	2.2299(4)	2.2281(4)	2.2252(4)	2.2232(4)	2.2217(4)	2.2195(10)	2.2192(10)	2.2193(9)
<Fe–O>		2.1325	2.1315	2.1311	2.1299	2.1291	2.1284	2.1270	2.1275	2.1275
S–O1 (2 \times)		1.4647(5)	1.4646(5)	1.4649(5)	1.4652(5)	1.4656(5)	1.4657(5)	1.4645(15)	1.4630(14)	1.4635(13)
S–O2 (2 \times)		1.4856(5)	1.4868(5)	1.4879(5)	1.4887(5)	1.4892(5)	1.4901(5)	1.4908(13)	1.4903(12)	1.4896(11)
<S–O>		1.4752	1.4757	1.4764	1.4770	1.4774	1.4779	1.4777	1.4767	1.4766
Fe–O1–S		136.72(3)	136.55(3)	136.37(3)	136.22(3)	136.09(3)	136.04(3)	136.10(8)	136.08(8)	136.03(7)
Fe–O2–S		133.54(3)	133.30(3)	133.02(3)	132.79(3)	132.61(3)	132.45(3)	132.45(8)	132.42(8)	132.41(7)
Fe–O3–Fe		121.33(3)	121.32(3)	121.26(3)	121.28(3)	121.26(3)	121.27(3)	121.35(9)	121.36(9)	121.29(8)
O3 \cdots O2		2.7603(7)	2.7537(6)	2.7469(6)	2.7409(6)	2.7356(6)	2.7316(6)	2.7307(15)	2.7292(15)	2.7285(14)

CoSO₄·H₂O	<i>T</i> (K)	313	273	233	193	153	113	30	15
Co—O1 (2×)		2.0567(6)	2.0564(6)	2.0556(6)	2.0555(6)	2.0555(6)	2.0557(5)	2.0559(21)	2.0540(22)
Co—O2 (2×)		2.0540(5)	2.0541(5)	2.0537(5)	2.0535(5)	2.0535(5)	2.0531(5)	2.0523(22)	2.0533(22)
Co—O3 (2×)		2.1804(4)	2.1778(4)	2.1753(4)	2.1736(4)	2.1720(4)	2.1704(4)	2.1633(17)	2.1654(17)
<Co—O>		2.0970	2.0961	2.0949	2.0942	2.0937	2.0931	2.0905	2.0909
S—O1 (2×)		1.4665(5)	1.4667(5)	1.4672(5)	1.4676(5)	1.4679(5)	1.4680(5)	1.4719(22)	1.4715(22)
S—O2 (2×)		1.4836(5)	1.4845(5)	1.4850(5)	1.4857(5)	1.4863(5)	1.4865(5)	1.4841(22)	1.4850(21)
<S—O>		1.4751	1.4756	1.4761	1.4767	1.4771	1.4773	1.4780	1.4783
Co—O1—S		136.98(3)	136.87(3)	136.76(3)	136.66(3)	136.57(3)	136.47(3)	136.29(14)	136.45(14)
Co—O2—S		132.83(3)	132.61(3)	132.44(3)	132.30(3)	132.15(3)	131.98(3)	131.88(13)	131.82(12)
Co—O3—S		122.25(3)	122.23(3)	122.22(3)	122.17(3)	122.15(3)	122.14(3)	122.35(16)	122.16(17)
O ₃ ···O ₂		2.7248(7)	2.7186(7)	2.7134(7)	2.7091(6)	2.7051(6)	2.7015(6)	2.7010(25)	2.6980(24)

Ni(SO₄)·H₂O	<i>T</i> (K)	313	273	233	193	153	113	75	45	15
Ni—O1 (2×)		2.0338(7)	2.0338(7)	2.0332(7)	2.0336(7)	2.0334(7)	2.0336(7)	2.0345(15)	2.0320(14)	2.0295(21)
Ni—O2 (2×)		2.0329(6)	2.0328(6)	2.0321(7)	2.0317(6)	2.0313(6)	2.0309(6)	2.0325(16)	2.0305(15)	2.0355(19)
Ni—O3 (2×)		2.1169(5)	2.1145(5)	2.1127(5)	2.1106(5)	2.1094(5)	2.1085(5)	2.1097(11)	2.1106(10)	2.1088(14)
<Ni—O>		2.0612	2.0604	2.0593	2.0586	2.0580	2.0577	2.0589	2.0577	2.0579
S—O1 (2×)		1.4654(7)	1.4654(6)	1.4659(7)	1.4657(7)	1.4668(6)	1.4672(7)	1.4670(16)	1.4687(15)	1.4685(21)
S—O2 (2×)		1.4865(6)	1.4869(6)	1.4874(6)	1.4872(6)	1.4879(6)	1.4888(6)	1.4879(16)	1.4905(15)	1.4877(18)
<S—O>		1.4760	1.47615	1.4767	1.47645	1.4774	1.4780	1.4775	1.4796	1.4781
Ni—O1—S		136.82(4)	136.75(4)	136.69(4)	136.63(4)	136.55(4)	136.47(4)	136.35(11)	136.42(10)	136.43(12)
Ni—O2—S		130.95(4)	130.79(4)	130.66(4)	130.57(4)	130.45(4)	130.38(4)	130.37(9)	130.35(9)	130.48(12)
Ni—O3—S		123.72(4)	123.73(4)	123.70(4)	123.72(4)	123.71(4)	123.72(4)	123.83(11)	123.60(10)	123.78(14)
O ₃ ···O ₂		2.6796(8)	2.6760(8)	2.6725(8)	2.6706(8)	2.6681(8)	2.6667(8)	2.6662(17)	2.6640(17)	2.6630(22)