Supplementary Information

1. Characterisation

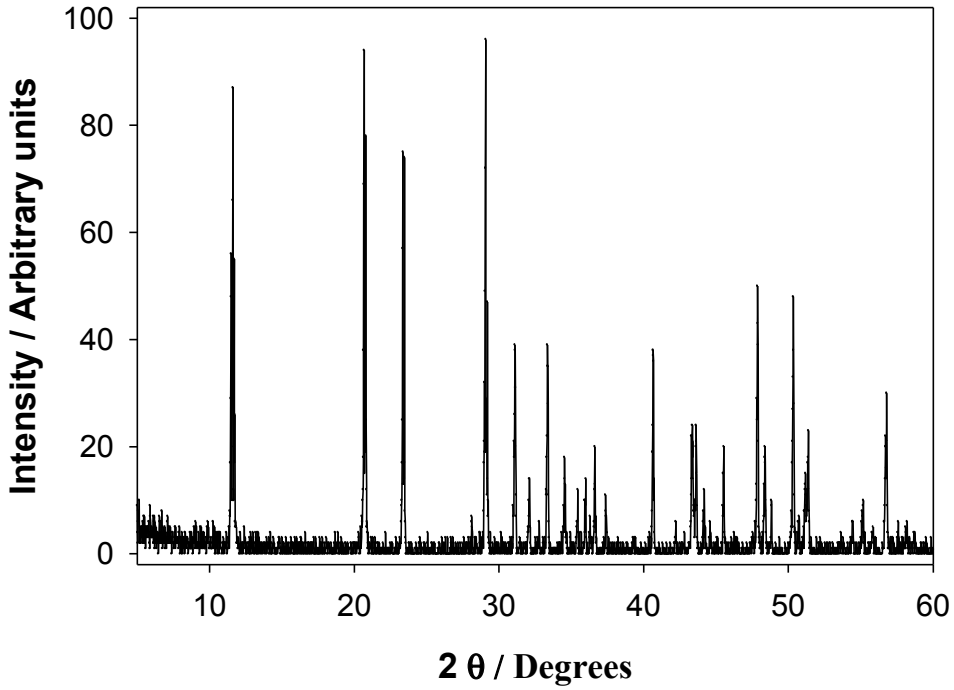

Figure S1. Powder X-ray diffraction pattern of as-bought synthetic $CaSO_4.2H_2O$.

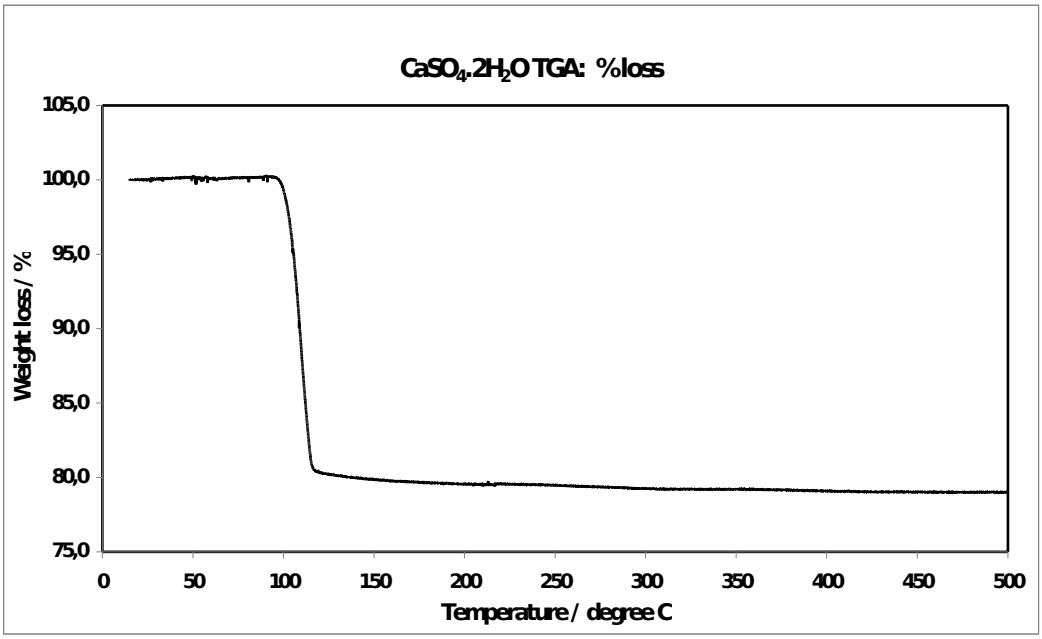

Figure S2. TGA of $CaSO_4.2H_2O$ from room temperature to 500 ℃ with a heating rate of 1 °min^{-1}. The theoretical weight loss is 20.927 % with the removal of the two waters of crystallisation and this compares very well with the observed weight loss of 20.973 %.

2. Rietveld Profile fits
    a. I 2/a model

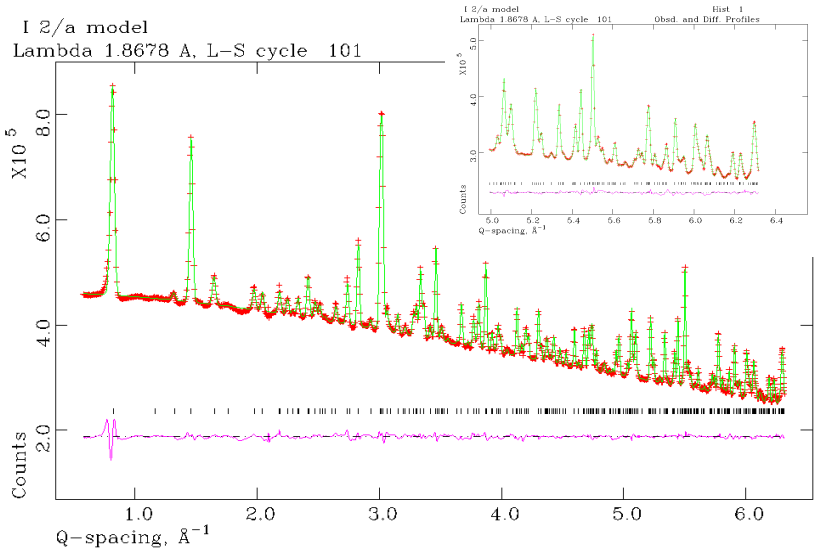

Figure S3. Final Rietveld refinement profile for the 1.87 Å incident wavelength data for the 9mm sample can of gypsum. The observed data are crosses, the calculated pattern a solid line, the tick marks show the allowed reflections and the lower solid line is the difference plot; R_{wp} = 1.78%, R_p = 0.92% and R_{F**2} = 4.78% for 273 observations. The inset shows the higher Q-space region.

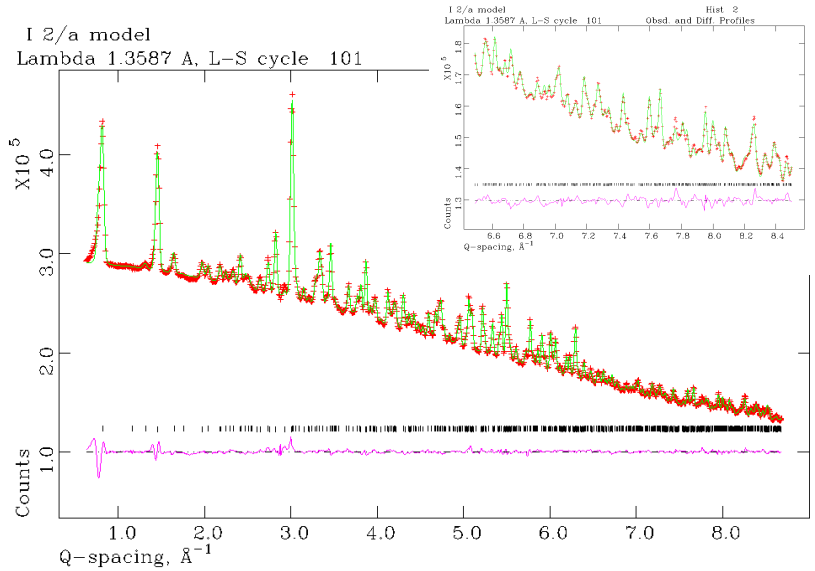

Figure S4. Final Rietveld refinement profile for the 1.36 Å incident wavelength data for the 9mm sample can of gypsum. The observed data are crosses, the calculated pattern a solid line, the tick marks show the allowed reflections and the lower solid line is the difference plot; R_{wp} = 1.63%, R_p = 0.85% and R_{F**2} = 6.53% for 696 observations. The inset shows the higher Q-space region.

b. C 2/c model

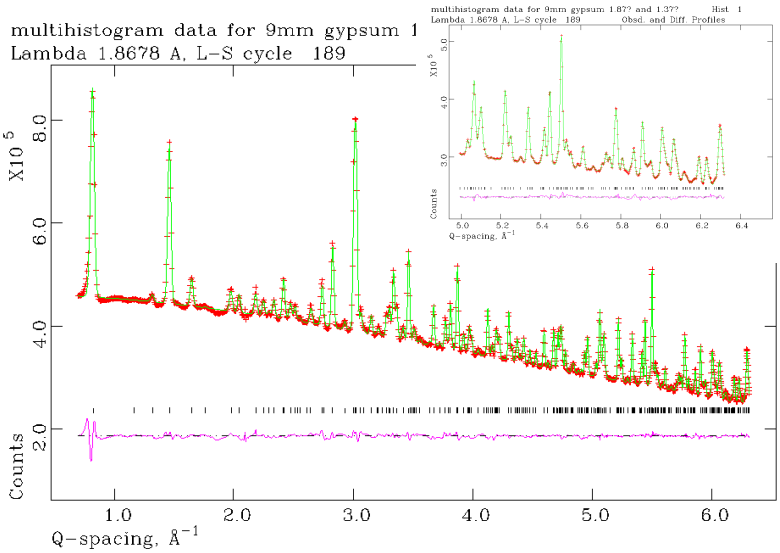

Figure S5. Final Rietveld refinement profile for the 1.87 Å incident wavelength data for the 9mm sample can of gypsum. The observed data are crosses, the calculated pattern a solid line, the tick marks show the allowed reflections and the lower solid line is the difference plot; R_{wp} = 1.78%, R_p = 0.92% and $R_{F^{**}2}$ = 4.77% for 273 observations. The inset shows the higher Q-space region.

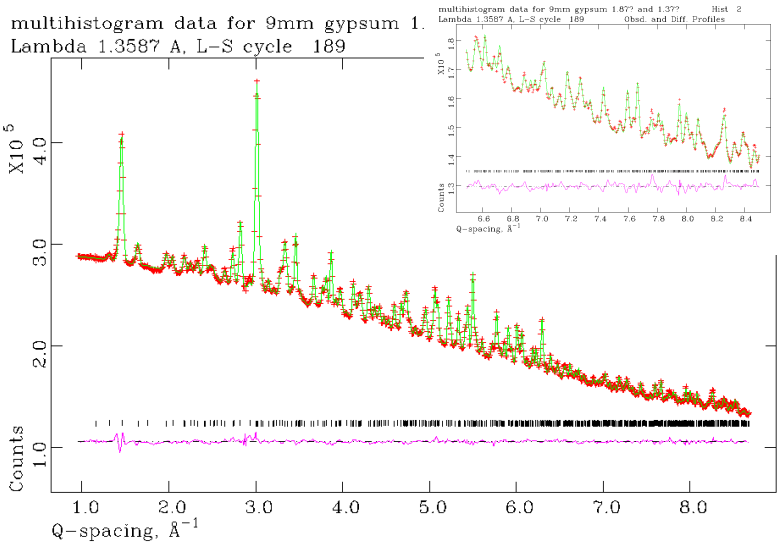

Figure S6. Final Rietveld refinement profile for the 1.36 Å incident wavelength data for the 9mm sample can of gypsum. The observed data are crosses, the calculated pattern a solid line, the tick marks show the allowed reflections and the lower solid line is the difference plot; R_{wp} = 0.97%, R_p = 0.60% and $R_{F^{**}2}$ = 6.19% for 698 observations. The inset shows the higher Q-space region.

3. Bond length and angle data
    a. I 2/a model

Atomic data

CA1	0.5000000(0)	0.07872(29)	0.2500000(0)	2(010)	CA	1 1.000(0)
S2	0.0000000(0)	0.0775(4)	0.7500000(0)	2(010)	S	2 1.000(0)
O3	0.9649(4)	0.13261(16)	0.5519(4)	1	O	3 1.000(0)
O4	0.7572(4)	0.02286(17)	0.6674(4)	1	O	4 1.000(0)
O5	0.3808(6)	0.18264(20)	0.4569(5)	1	O	5 1.000(0)
H6	0.2486(9)	0.15985(28)	0.5068(9)	1	H	6 1.000(0)
H7	0.4067(10)	0.2419(4)	0.4937(10)	1	H	7 1.000(0)

Bond lengths

Vector	Length	Optr Cell	Neighbor atom coordinates		
CA1_CA1	4.050(5)	-1 1 0 0	0.50000	-0.07872	-0.25000
CA1_CA1	4.050(5)	-1 1 0 1	0.50000	-0.07872	0.75000
CA1_S2	3.14368(9)	1 0 0-1	0.00000	0.07749	-0.25000
CA1_S2	3.14368(9)	1 1 0 0	1.00000	0.07749	0.75000
CA1_O3	2.5624(30)	1 0 0 0	0.96487	0.13261	0.55187
CA1_O3	2.5624(30)	2 1 0 0	0.03513	0.13261	-0.05187
CA1_O4	2.5471(24)	1 0 0 0	0.75722	0.02286	0.66738
CA1_O4	2.5471(24)	2 1 0 0	0.24278	0.02286	-0.16738
CA1_O4	2.359(4)	-1 1 0 1	0.24278	-0.02286	0.33262
CA1_O4	2.359(4)	-2 0 0 0	0.75722	-0.02286	0.16738
CA1_O5	2.379(5)	1 0 0 0	0.38080	0.18264	0.45695
CA1_O5	2.379(5)	2 1 0 0	0.61920	0.18264	0.04305
CA1_H6	2.942(5)	1 0 0 0	0.24863	0.15985	0.50679
CA1_H6	2.942(5)	2 1 0 0	0.75137	0.15985	-0.00679
CA1_H7	3.127(7)	1 0 0 0	0.40666	0.24186	0.49369
CA1_H7	3.127(7)	2 1 0 0	0.59334	0.24186	0.00631
S2_O3	1.473(4)	1-1 0 0	-0.03513	0.13261	0.55187
S2_O3	1.473(4)	2 1 0 1	0.03513	0.13261	0.94813
S2_O4	1.474(4)	1-1 0 0	-0.24278	0.02286	0.66738
S2_O4	1.474(4)	2 1 0 1	0.24278	0.02286	0.83262
O3_H6	1.819(5)	1 1 0 0	1.24863	0.15985	0.50679
O3_H7	1.945(6)	-102 0 0 0	0.90666	0.25814	0.49369
O5_H6	1.011(6)	1 0 0 0	0.24863	0.15985	0.50679
O5_H7	0.926(8)	1 0 0 0	0.40666	0.24186	0.49369
H6_H7	1.563(7)	1 0 0 0	0.40666	0.24186	0.49369

Bond Angles

Angle	Degrees	atom 1 loc	atom 3 loc
O3_S2_O3	110.6(4)	1-1 0 0	2 1 0 1
O3_S2_O4	106.75(12)	1-1 0 0	1-1 0 0
O3_S2_O4	110.70(14)	1-1 0 0	2 1 0 1
O3_S2_O4	110.70(14)	2 1 0 1	1-1 0 0
O3_S2_O4	106.75(12)	2 1 0 1	2 1 0 1
O4_S2_O4	111.4(4)	1-1 0 0	2 1 0 1
H6_O5_H7	107.5(5)	1 0 0 0	1 0 0 0

b. C 2/c model

Atomic data

CA1	0.5000000(0)	0.07853(27)	0.7500000(0)	2(010)	CA	1 1.000(0)
S2	0.0000000(0)	0.0774(4)	0.7500000(0)	2(010)	S	2 1.000(0)
O3	0.0353(4)	0.13258(14)	0.5871(4)	1	O	3 1.000(0)
O4	0.2426(4)	0.02279(15)	0.9101(4)	1	O	4 1.000(0)
O5	0.6191(5)	0.18253(18)	0.0763(5)	1	O	5 1.000(0)
H6	0.7512(8)	0.16020(26)	0.2578(8)	1	H	6 1.000(0)
H7	0.5936(9)	0.24203(34)	0.0872(9)	1	H	7 1.000(0)

Bond lengths

Vector	Length	Optr Cell	Neighbor atom coordinates		
CA1_CA1	4.046(5)	-1 1 0 1	0.50000	-0.07853	0.25000
CA1_CA1	4.046(5)	-1 1 0 2	0.50000	-0.07853	1.25000
CA1_S2	3.14350(8)	1 0 0 0	0.00000	0.07737	0.75000
CA1_S2	3.14350(8)	1 1 0 0	1.00000	0.07737	0.75000
CA1_O3	2.5623(27)	1 0 0 0	0.03530	0.13258	0.58711
CA1_O3	2.5623(27)	2 1 0 1	0.96470	0.13258	0.91289
CA1_O4	2.5467(22)	1 0 0 0	0.24263	0.02279	0.91008
CA1_O4	2.5467(22)	2 1 0 1	0.75737	0.02279	0.58992
CA1_O4	2.3570(34)	-1 1 0 2	0.75737	-0.02279	1.08992
CA1_O4	2.3570(34)	-2 0 0 0	0.24263	-0.02279	0.41008
CA1_O5	2.380(4)	1 0 0 1	0.61910	0.18253	1.07627
CA1_O5	2.380(4)	2 1 0 0	0.38090	0.18253	0.42373
CA1_H6	2.944(5)	1 0 0 1	0.75122	0.16020	1.25779
CA1_H6	2.944(5)	2 1 0 0	0.24878	0.16020	0.24221
CA1_H7	3.131(6)	1 0 0 1	0.59363	0.24203	1.08721
CA1_H7	3.131(6)	2 1 0 0	0.40637	0.24203	0.41279
S2_O3	1.474(4)	1 0 0 0	0.03530	0.13258	0.58711
S2_O3	1.474(4)	2 0 0 1	-0.03530	0.13258	0.91289
S2_O4	1.473(4)	1 0 0 0	0.24263	0.02279	0.91008
S2_O4	1.473(4)	2 0 0 1	-0.24263	0.02279	0.58992
O3_H6	1.823(5)	1-1 0 0	-0.24878	0.16020	0.25779
O3_H7	1.943(6)	-102-1 0 1	0.09363	0.25797	0.58721
O5_H6	1.007(6)	1 0 0 0	0.75122	0.16020	0.25779
O5_H7	0.929(7)	1 0 0 0	0.59363	0.24203	0.08721
H6_H7	1.559(7)	1 0 0 0	0.59363	0.24203	0.08721

Bond Angles

Angle	Degrees	atom 1 loc	atom 3 loc
O3_S2_O3	110.5(4)	1 0 0 0	2 0 0 1
O3_S2_O4	106.74(11)	1 0 0 0	1 0 0 0
O3_S2_O4	110.74(12)	1 0 0 0	2 0 0 1
O3_S2_O4	110.74(12)	2 0 0 1	1 0 0 0
O3_S2_O4	106.74(11)	2 0 0 1	2 0 0 1
O4_S2_O4	111.4(4)	1 0 0 0	2 0 0 1
H6_O5_H7	107.2(5)	1 0 0 0	1 0 0 0