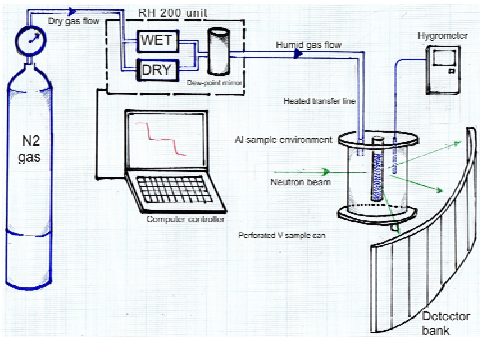

Scheme S1.

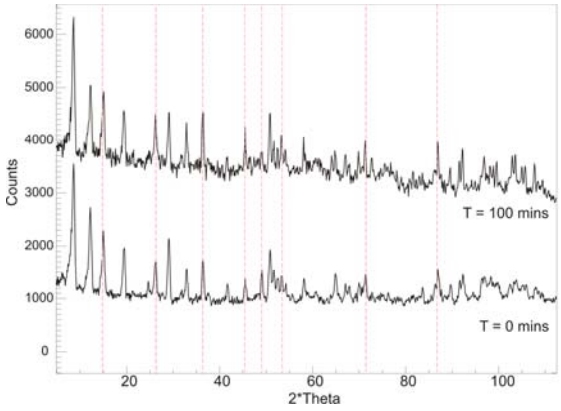

Fig. S1

Supplementary Material (ESI) for Chemical Communications
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Supplementary Table 1:
Fractional atomic coordinates and U_{iso} values for the atoms in the anhydrous $CuSO_4$ structure, as obtained from free refinement against a compiled 30 min NPD data set at $\lambda \sim 1.87$ Å (*Pnma*, $a = 8.3976(1)$ Å, $b = 6.70382(9)$ Å, $c = 4.82443(8)$ Å, $\chi^2 = 6.01$ %, $RF^2 = 2.39$ %).

Atom	x	y	x	U_{iso}
Cu1	0	0	0	0.0048(3)
S1	0.1834(4)	0.25	0.4460(8)	0.0016(8)
O1	0.1289(3)	0.25	0.7366(4)	0.0067(4)
O2	0.3643(2)	0.25	0.4383(3)	0.0061(4)
O3	0.13256(19)	0.06752(15)	0.3091(2)	0.0066(3)

Supplementary Table 2:
Fractional atomic coordinates and U_{iso} values for the atoms in the $CuSO_4.H_2O$ structure, as refined against a compiled 30 min NPD data set at $\lambda \sim 1.87$ Å (*P*-1, $a = 5.0401(6)$ Å, $b = 5.1566(7)$ Å, $c = 7.5691(8)$ Å, $\alpha = 108.39(8)°$, $\beta = 108.992(7)°$, $\gamma = 90.4(1)°$, $\chi^2 = 9.4$ %, $RF^2 = 3.37$ %). The refinement was carried out with soft constraints on the S-O bond lengths.

Atom	x	y	x	U_{iso}
Cu1	0	0	0	0.015(2)
Cu2	0.5	0.5	0.5	0.019(3)
S1	0.6215(19)	0.9269(13)	0.2484(12)	0.008(4)
O1	0.798(2)	0.832(2)	0.1232(18)	0.017(2)
O2	0.3173(18)	0.8316(19)	0.1363(14)	0.010(2)
O3	0.671(2)	0.2312(12)	0.3286(12)	0.009(2)
O4	0.712(2)	0.8058(17)	0.4083(12)	0.012(2)
O5	0.115(2)	0.4391(14)	0.2650(13)	0.002(2)
H1	-0.066(6)	0.482(4)	0.285(4)	0.12(1)
H2	0.171(3)	0.577(3)	0.2170(18)	0.0150(4)

Supplementary Table 3:
Fractional atomic coordinates and U_{iso} values for the atoms in the $CuSO_4.3H_2O$ structure, as refined against a compiled 30 min NPD data set at $\lambda \sim 1.87$ Å (*C*1*c*1, a = 5.5969(8) Å, b = 13.0368(2) Å, c =7.3566(9) Å, β = 97.05(1)°, χ^2 = 9.82 %, RF^2 = 7.38 %). The refinement was carried out with soft constraints on the S-O and O-H bond lengths.

Atom	x	y	x	U_{iso}
Cu1	0.493(4)	0.3653(15)	0.514(3)	0.032(5)
S1	0.276(6)	0.119(3)	0.424(5)	0.16(3)
O1	0.152(5)	0.165(2)	0.250(4)	0.040(8)
O2	0.830(4)	0.304(2)	0.075(3)	0.018(6)
O3	0.487(4)	0.0609(15)	0.389(3)	0.022(6)
O4	0.100(4)	0.9523(16)	0.989(3)	0.008(6)
O5	0.351(3)	0.3647(14)	0.251(2)	0.021(7)
O6	0.686(3)	0.0915(16)	0.084(2)	0.012(6)
O7	0.784(3)	0.3010(16)	0.410(2)	0.004(6)
H1	0.419(8)	0.382(4)	0.139(4)	0.09(2)
H2	0.258(7)	0.302(2)	0.219(6)	0.06(1)
H3	0.638(9)	0.082(3)	0.207(3)	0.06(2)
H4	0.614(6)	0.032(2)	0.015(4)	0.02(1)
H5	0.936(5)	0.324(3)	0.479(4)	0.03(1)
H6	0.799(6)	0.321(3)	0.283(2)	0.04(1)

Supplementary Table 4:
Fractional atomic coordinates and U_{iso} values for the atoms in the $CuSO_4.5H_2O$ structure, as refined against a compiled 30 min NPD data set at $\lambda \sim 1.87$ Å (*P*-1, *a* = 6.1141(5) Å, *b* = 10.7127(9) Å, *c* = 5.9587(5) Å, $\alpha = 82.350(6)°$, $\beta = 107.314(6)°$, $\gamma = 102.589(5)°$, $\chi^2 = 7.68$ %, $RF^2 = 9.54$ %). The refinement was carried out with soft constraints on the S-O and O-H bond lengths. In addition, U_{iso} values of similar atoms in similar bonding environments were constrained to be the same.

Atom	x	y	x	U_{iso}
Cu1	0	0	0	0.014(4)
Cu2	0.5	0.5	0	0.014(4)
S1	0.022(2)	0.2930(14)	0.632(3)	0.02(1)
O1	0.927(3)	0.1545(15)	0.664(3)	0.019(2)
O2	0.255(3)	0.3192(15)	0.805(3)	0.019(2)
O3	0.846(3)	0.3699(16)	0.623(2)	0.019(2)
O4	0.024(3)	0.3030(15)	0.383(3)	0.019(2)
O5	0.812(4)	0.0776(13)	0.145(2)	0.024(2)
O6	0.302(3)	0.1114(13)	0.145(2)	0.024(2)
O7	0.452(2)	0.4174(17)	0.294(2)	0.024(2)
O8	0.749(3)	0.4055(19)	0.007(3)	0.024(2)
O9	0.436(4)	0.1207(19)	0.652(4)	0.024(2)
H1	0.884(4)	0.1403(16)	0.263(3)	0.035(2)
H2	0.726(4)	0.0070(16)	0.225(4)	0.035(2)
H3	0.321(6)	0.2012(15)	0.082(4)	0.035(2)
H4	0.328(5)	0.117(3)	0.314(2)	0.035(2)
H5	0.319(3)	0.385(3)	0.359(4)	0.035(2)
H6	0.588(3)	0.406(3)	0.427(3)	0.035(2)
H7	0.855(6)	0.389(4)	0.924(5)	0.035(2)
H8	0.808(4)	0.368(3)	0.167(3)	0.035(2)
H9	0.597(4)	0.107(4)	0.714(8)	0.035(2)
H10	0.438(6)	0.199(2)	0.722(6)	0.035(2)