Supporting Information for

Anhydrous copper tellurite-disulfate $Cu_3TeO_3(SO_4)_2$ featuring coexistence of spin singlets and long-range antiferromagnetic order

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Fig. S1. Comparison of PXRD pattern from prepared $Cu_3TeO_3(SO_4)_2$ sample (upper panel and calculated one from the single crystal data (lower panel)

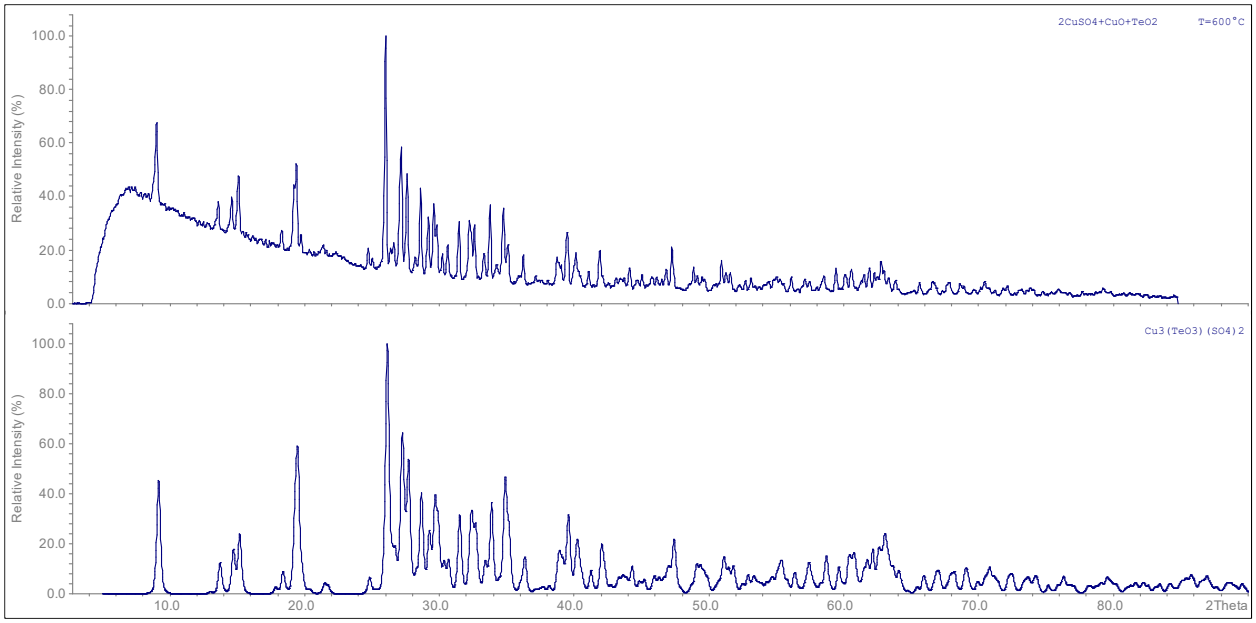

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Cu_3TeO_3(SO_4)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U(eq)
Te(1)	3076(1)	7121(1)	6405(1)	8(1)
Cu(1)	8456(1)	8242(1)	5393(1)	9(1)
Cu(2)	5882(1)	8482(1)	3040(1)	10(1)

Cu(3)	2891(1)	7701(1)	-510(1)	9(1)
S(1)	1781(1)	6178(1)	2912(1)	9(1)
S(2)	7484(1)	7370(1)	186(1)	8(1)
O(1)	3663(4)	8685(3)	7453(2)	10(1)
O(2)	1287(4)	8945(3)	5527(2)	11(1)
O(3)	5690(3)	7958(3)	4989(2)	10(1)
O(4)	3579(4)	6453(3)	3546(2)	11(1)
O(5)	1726(4)	4067(3)	2992(2)	12(1)
O(6)	-343(4)	6753(3)	3691(2)	13(1)
O(7)	2261(4)	7344(3)	1472(2)	11(1)
O(8)	6850(4)	5355(3)	998(2)	12(1)
O(9)	7240(4)	8665(3)	1137(2)	11(1)
O(10)	9807(4)	7546(3)	-649(2)	13(1)
O(11)	6073(4)	8122(3)	-773(2)	12(1)

Table S2. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cu_3TeO_3(SO_4)_2$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Te(1)	8(1)	8(1)	8(1)	-2(1)	-2(1)	0(1)
Cu(1)	8(1)	8(1)	11(1)	-2(1)	-4(1)	-1(1)
Cu(2)	14(1)	10(1)	7(1)	-3(1)	-2(1)	-3(1)
Cu(3)	8(1)	11(1)	7(1)	-2(1)	-2(1)	0(1)
S(1)	9(1)	9(1)	8(1)	-2(1)	-1(1)	-1(1)
S(2)	8(1)	9(1)	8(1)	-3(1)	-2(1)	1(1)
O(1)	12(1)	9(1)	10(1)	-3(1)	-3(1)	-1(1)
O(2)	10(1)	8(1)	15(1)	0(1)	-7(1)	0(1)
O(3)	9(1)	12(1)	8(1)	-2(1)	-2(1)	0(1)
O(4)	13(1)	10(1)	9(1)	0(1)	-4(1)	-4(1)
O(5)	14(1)	9(1)	13(1)	-2(1)	-6(1)	-1(1)
O(6)	10(1)	16(1)	12(1)	-5(1)	0(1)	0(1)
O(7)	13(1)	11(1)	7(1)	0(1)	-2(1)	0(1)
O(8)	15(1)	8(1)	12(1)	-2(1)	-3(1)	0(1)
O(9)	14(1)	10(1)	11(1)	-5(1)	-2(1)	-2(1)
O(10)	9(1)	18(1)	12(1)	-7(1)	-2(1)	2(1)
O(11)	10(1)	15(1)	10(1)	-2(1)	-4(1)	1(1)