The Family of $M^{II}_3(Te^{IV}O_3)_2(OH)_2$ (M = Mg, Mn, Co, Ni) Compounds—Prone to Inclusion of Foreign Components into Large Hexagonal Channels

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Supplementary material

Tables

Table S1. Data collection and refinement details of related $M^{II}_3(TeO_3)_2(OH)_2$-type compounds

Empirical formula	$Co_3H_2O_8Te_2$	$Co_3H_{1.76}O_{8.24}S_{0.12}Te_2$	$Cl_{0.18}H_{1.82}Mn_3\ O_{7.82}Te_2$	$H_{1.70}Mn_3O_{8.30}S_{0.15}Te_2$
Cryst. Chem. Formula	$Co_3(TeO_3)_2(OH)_{1.5}$-$(OH)_{0.5}$	$Co_3(TeO_3)_2(OH)_{1.5}\{(SO_4)_{0.12}(OH)_{0.26}\}$	$Mn_3(TeO_3)_2(OH)_{1.5}\{Cl_{0.18}(OH)_{0.32}\}$	$Mn_3(TeO_3)_2(OH)_{1.5}\{(SO_4)_{0.15}(OH)_{0.20}\}$
Obtained from batch	2	1	8	7
M_r	562.01	569.45	553.43	559.34
Temp. / °C	23	23	23	23
Cryst. dim./ mm³	0.10×0.01×0.01	0.10×0.015×0.015	0.22×0.03×0.03	0.11×0.02×0.02
Cryst. colour	pink	purple	light-yellow	light-yellow
Cryst. form	needle	needle	bar	bar
Space group, No.	$P6_3mc$, 186	$P6_3mc$, 186	$P6_3mc$, 186	$P6_3mc$, 186
Formula units Z	4	4	4	4
a / Å	13.0907(4)	13.1102(7)	13.4364(6)	13.4509(4)
c / Å	5.02810(10)	5.0179(4)	5.1738(3)	5.1410(2)
V / Å³	746.21(5)	746.91(10)	808.92(9)	805.53(6)
μ / mm⁻¹	14.265	14.290	11.749	11.784
X-ray density / g·cm⁻³	5.003	5.064	4.544	4.612
ϑ_{min}-ϑ_{max} / °	4.434 - 29.978	3.108 - 29.987	3.032 - 36.297	3.029 - 34.991
h	−18 - 10	-18 − 12	−22 − 17	-20 - 21
k	−14 − 18	−18 − 18	−17 − 22	−21 - 13
l	−7 -7	−7 - 7	−8 - 8	−8 - 8
Measured refl.	11516	12497	10713	19118
Independent refl.	811	813	1442	1300
Observed refl. ($I>2\sigma(I)$)	788	721	1412	1245
R_i	0.0479	0.0837	0.0248	0.0443
T_{min}; T_{max}	0.2398; 0.8669	0.3185; 0.4554	0.5169; 0.7231	0.2816; 0.3604
No. of parameters	50	41	54	63
Flack parameter [22, 23]	0.04(5) using 342 quotients	0.02(12)	0.00(5) using 635 quotients	0.01(2) using 547 quotients
$R1$ ($F^2>2\sigma(F^2)$)	0.0235	0.0318	0.0172	0.0134

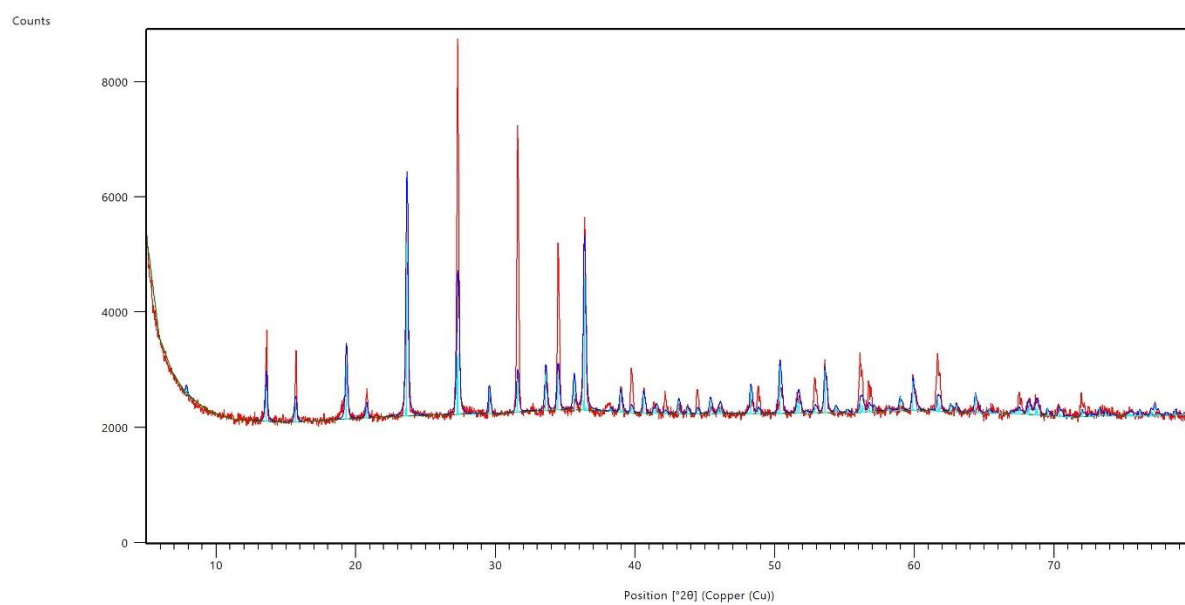|				
$wR2(F^2$ all)	0.0630	0.0749	0.0442	0.0273
GOF	1.096	1.028	1.092	1.025
CSD-deposition code	2203362	2203361	2203364	2203366

Single-crystal measurements of samples from batches 1, 2 and 7 were performed on a STOE Stadivari diffractometer equipped with an Anton Paar Primux 50 MoK_α microsource and a DECTRIS EIGER® 2 R 1M CdTe detector. The instrument software was X-Area [X-Area, version 2.0, STOE & Cie GmbH, Darmstadt, Germany, 2021], for absorption LANA was used.

Table S2. Selected interatomic distances / Å in the crystal structures of of related $M^{II}_3(TeO_3)_2(OH)_2$-type compounds

|	$Co_3(TeO_3)_2(OH)_{1.5\text{-}}(OH)_{0.5}$	$Co_3(TeO_3)_2(OH)_{1.5\text{-}}\{(SO_4)_{0.12}(OH)_{0.26}\}$	$Mn_3(TeO_3)_2(OH)_{1.5\text{-}}\{Cl_{0.18}(OH)_{0.32}\}$	$Mn_3(TeO_3)_2(OH)_{1.5\text{-}}\{(SO_4)_{0.15}(OH)_{0.20}\}$
*M*1—O2	2.039(5)	2.032(8)	2.137(3)	2.121(2)
*M*1—O1	2.104(4)	2.110(6)	2.149(2)	2.1365(18)
*M*1—O3	2.074(5)	2.078(8)	2.179(3)	2.171(2)
*M*1—O2	2.071(5)	2.074(7)	2.228(3)	2.218(2)
*M*1—O4	2.168(6)	2.162(8)	2.237(3)	2.220(2)
*M*1—O4	2.205(5)	2.219(8)	2.335(3)	2.336(2)
Te1—O2 (2x)	1.889(5)	1.891(7)	1.875(2)	1.874(2)
Te1—O1	1.909(8)	1.903(11)	1.890(4)	1.888(3(
Te2—O3 (3x)	1.859(7)	1.859(10)	1.847(4)	1.854(3)

Figures

Batch 1
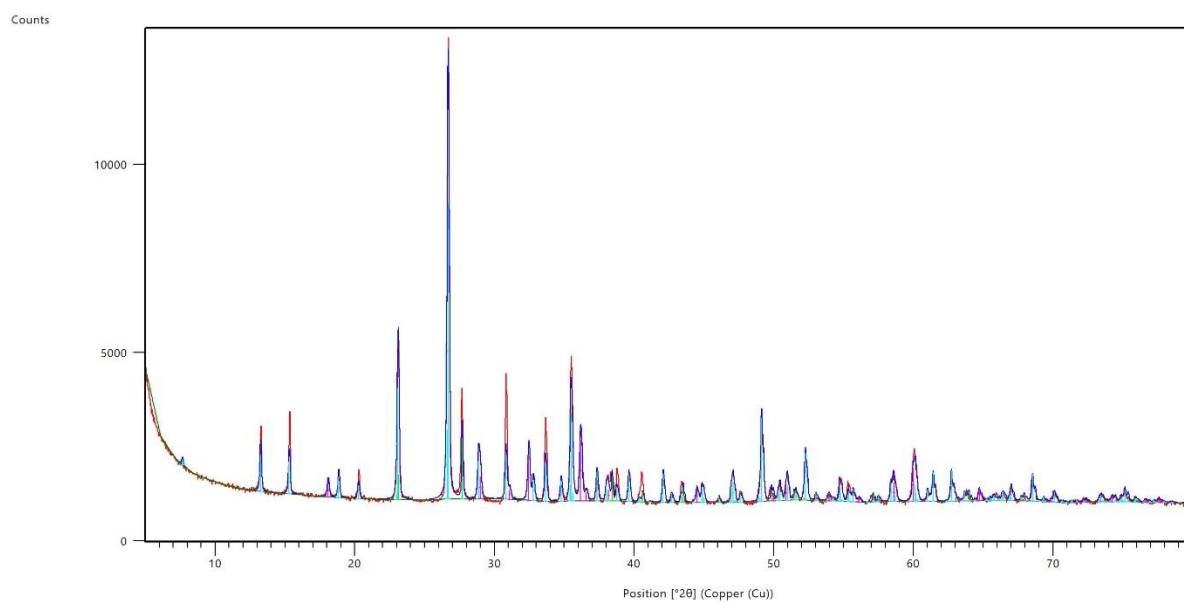

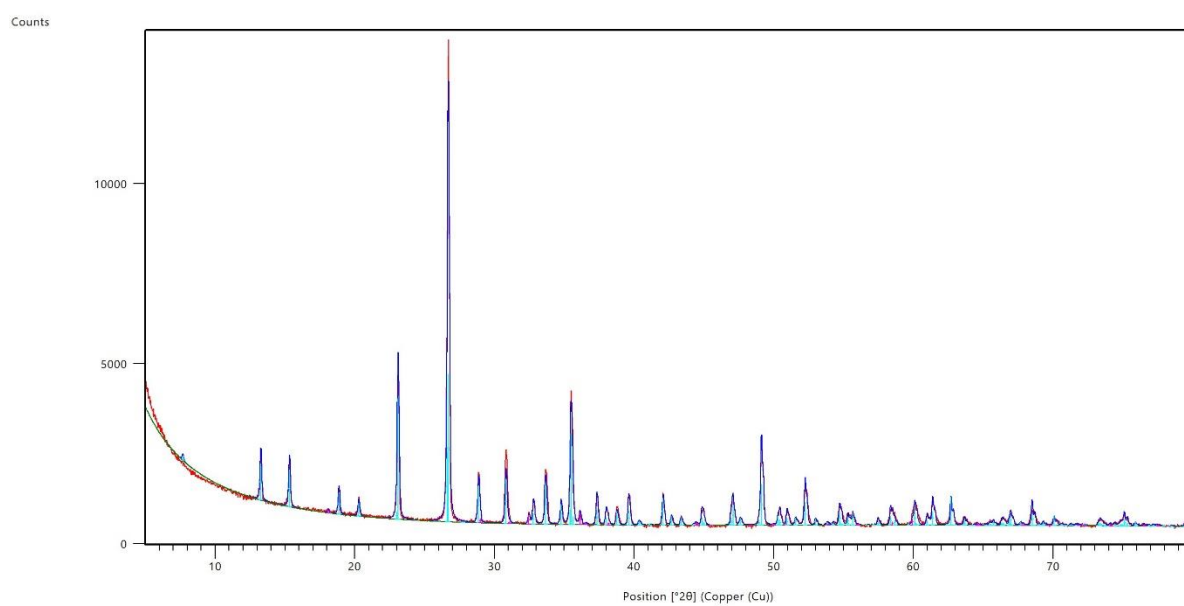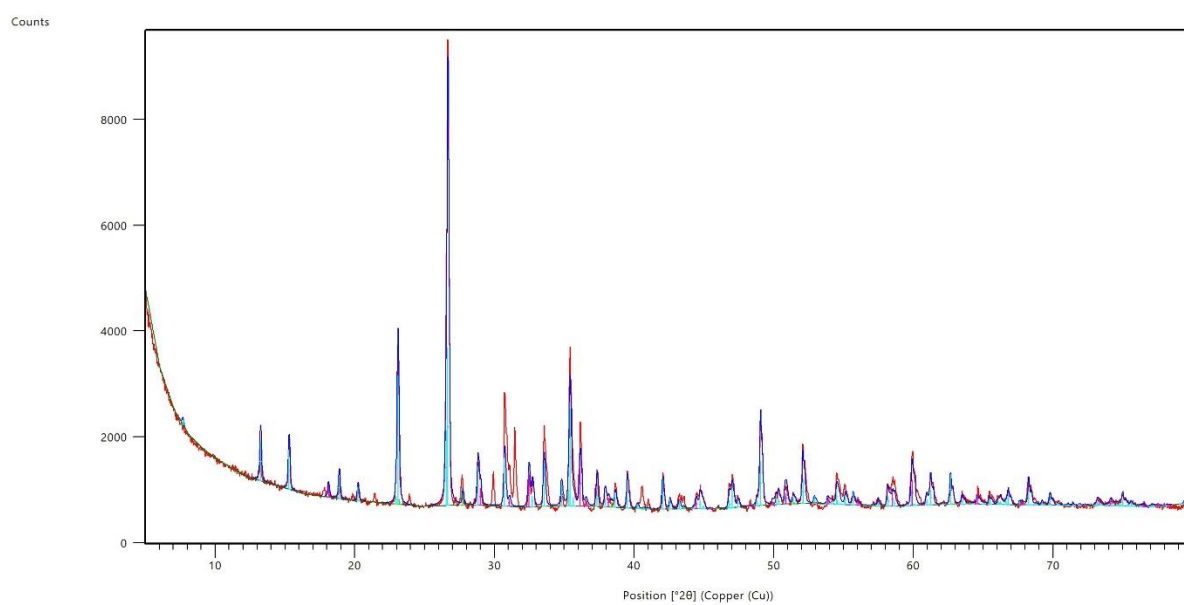Batch 1 heated at 210 °C
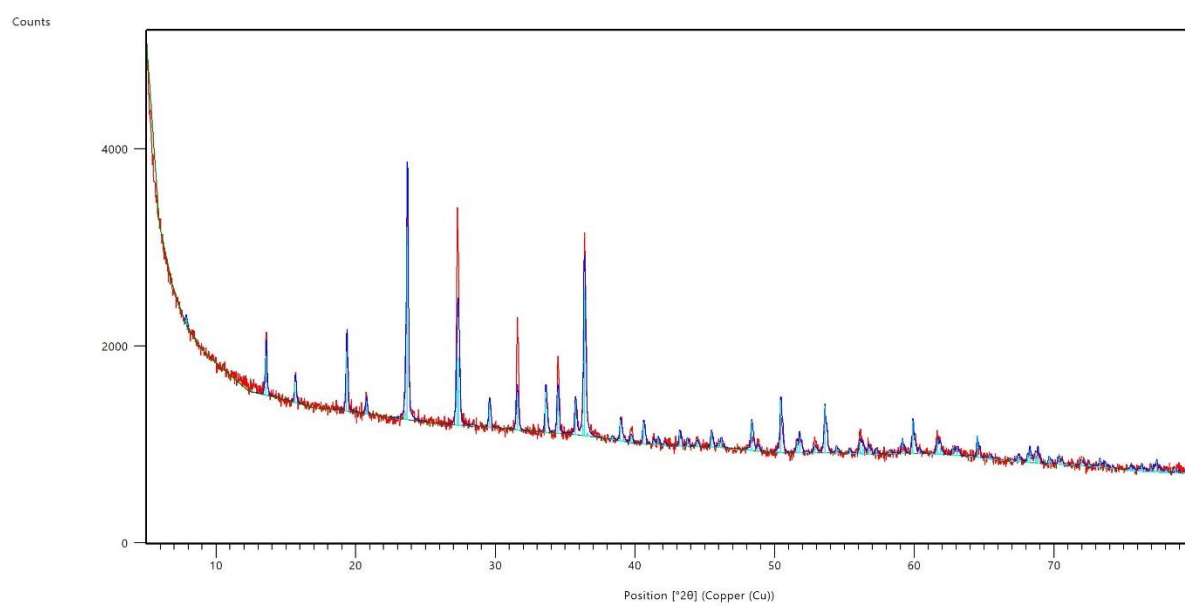
Batch 2
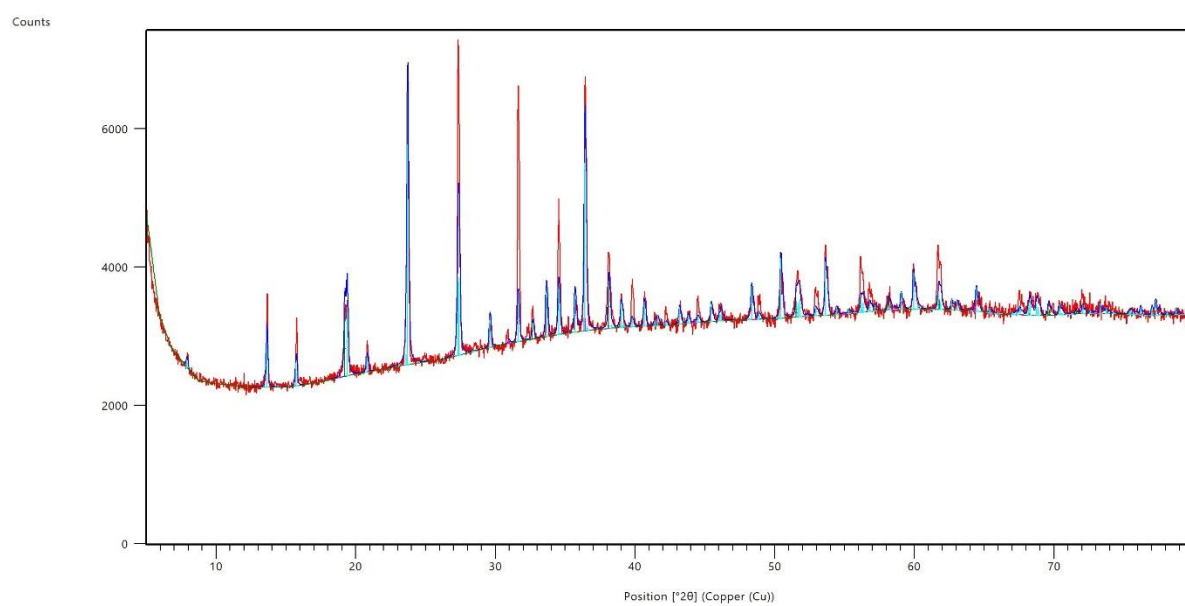
Batch 2 heated at 210 °C
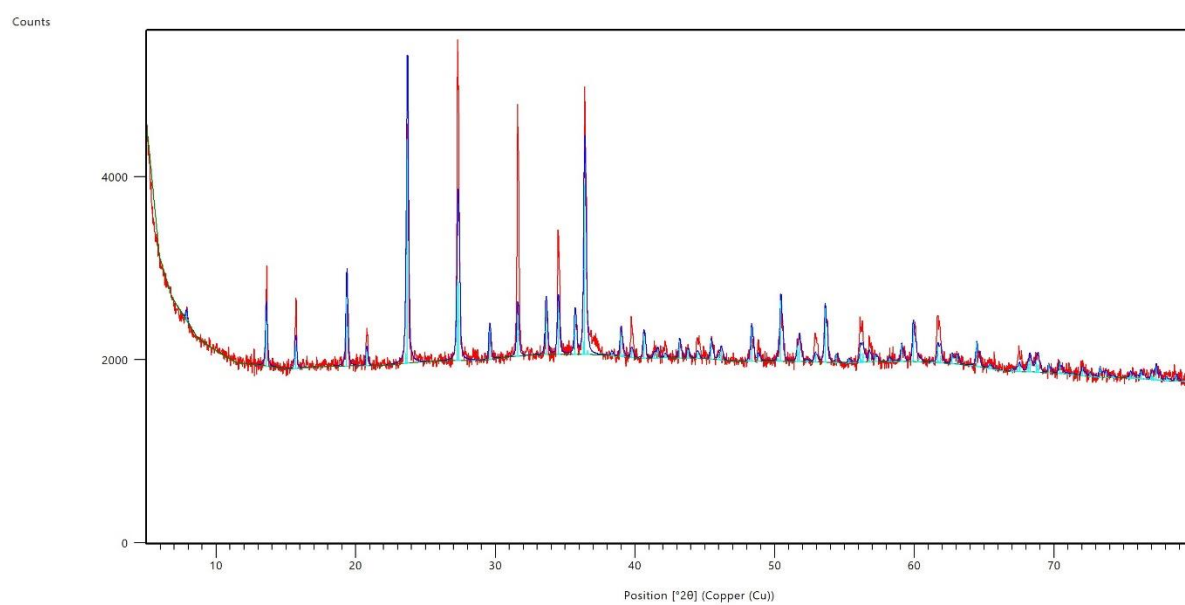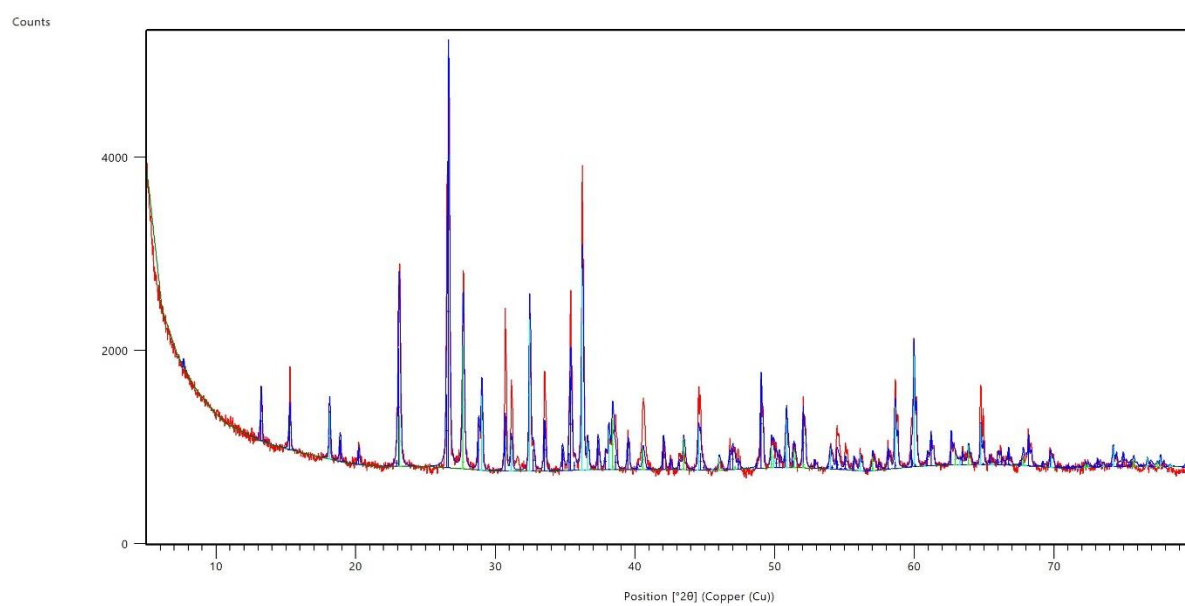
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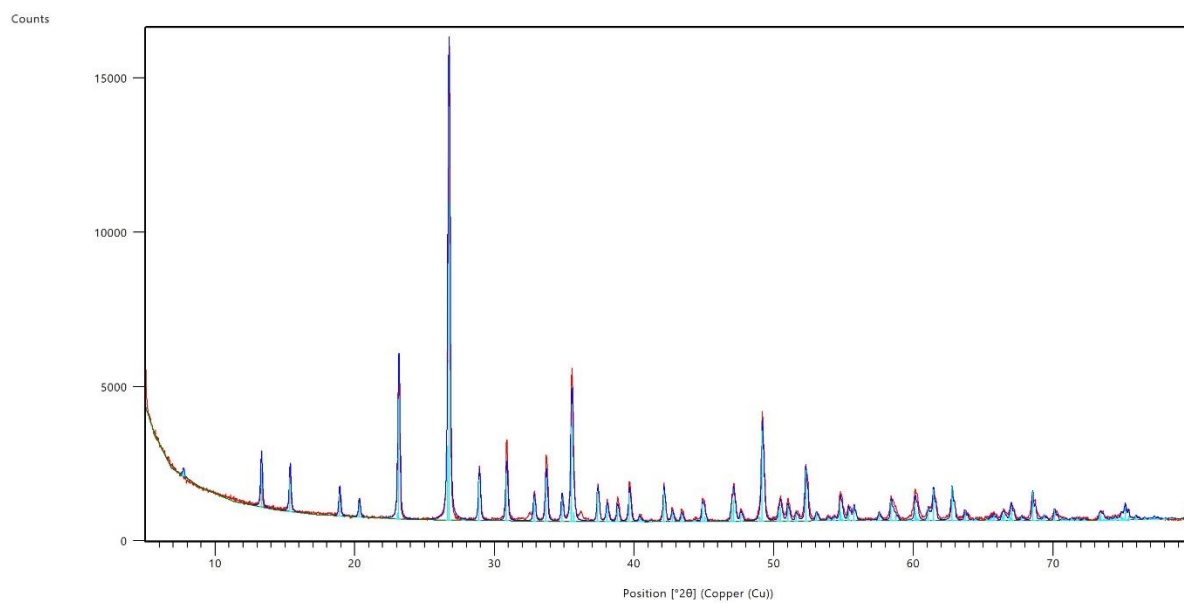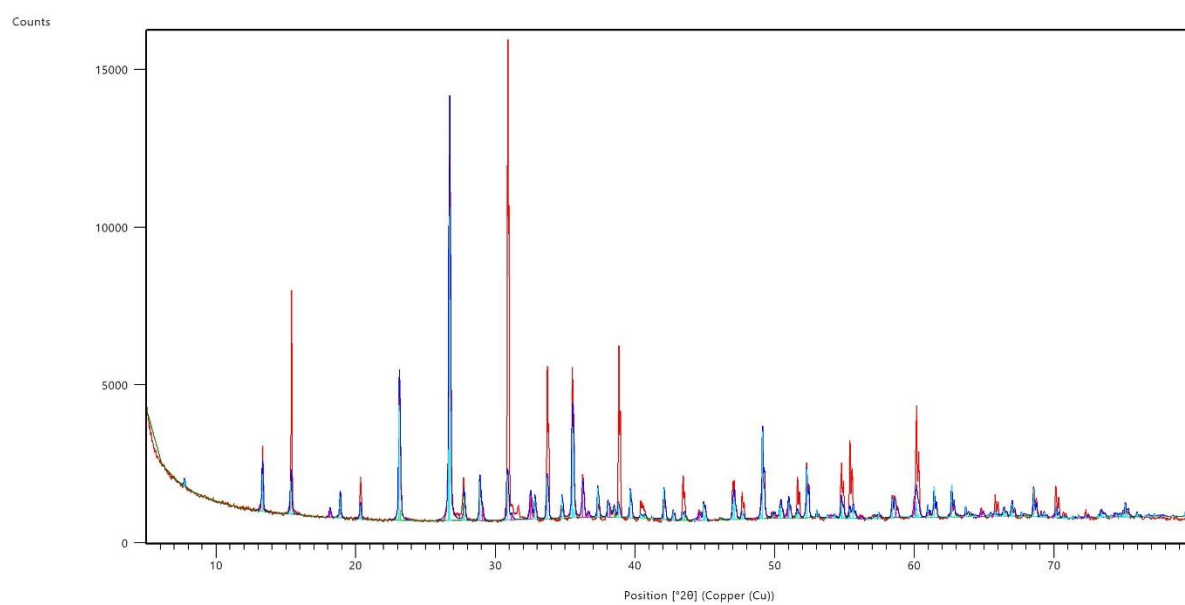

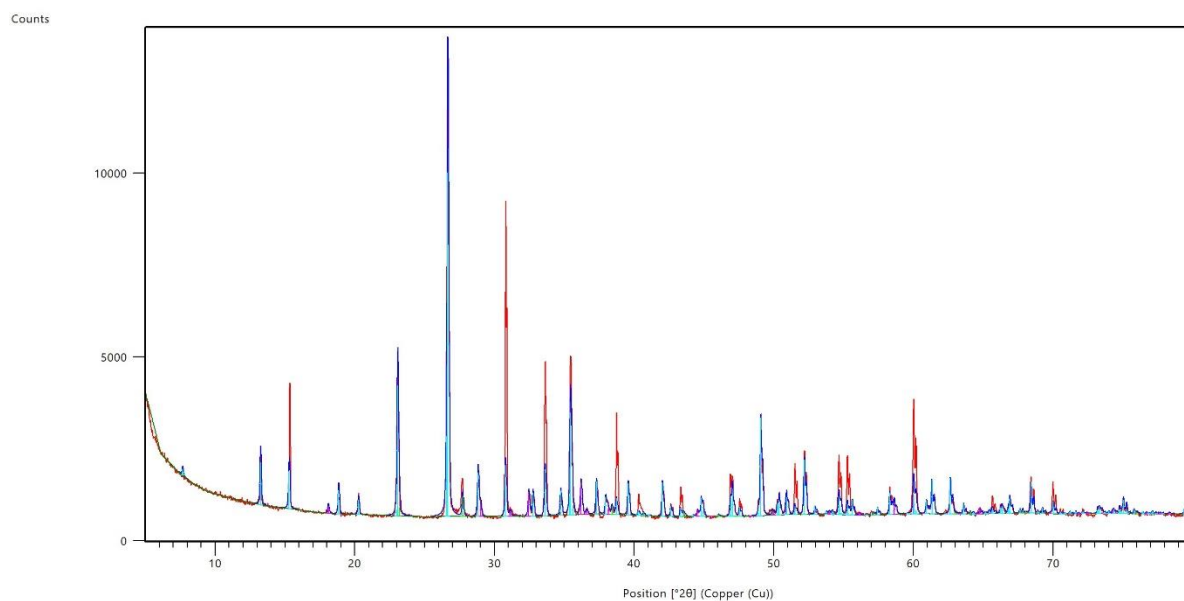## Batch 4

Batch 5

Batch 6

Batch 7

Batch 8

Batch 9

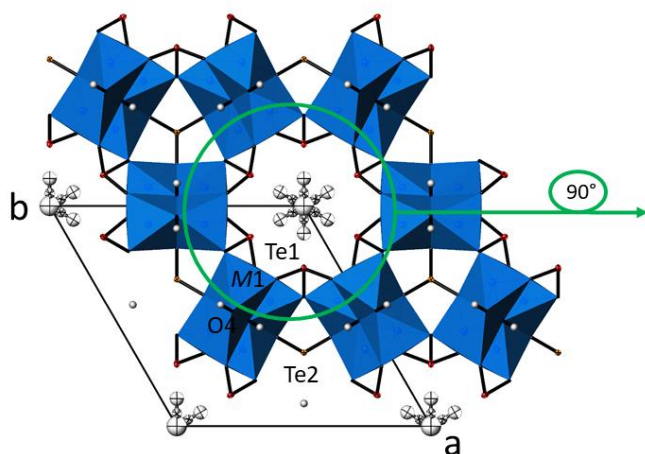**Figure S1**. PXRD measurements of the different batches. Red lines indicate measured intensities. Contributions of $M^{II}_3(TeO_3)_2(OH)_2$-type phases is indicated in turquoise, additional phases for batch 2 are Co_3O_4, $Co(OH)_2$ (dark green), and for batches 4-9 are Mn_3O_4 (pink), Te (light green).
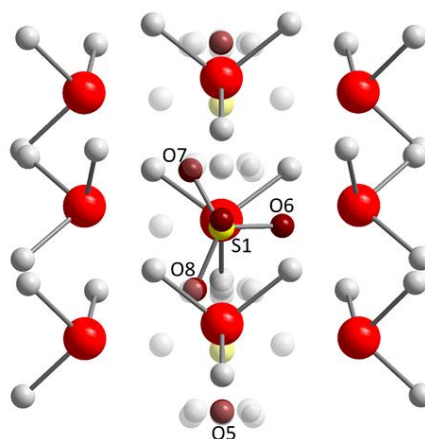
Figure S2. (**a**) Crystal structure of $Mn_3(TeO_3)_2(OH)_{1.5}\{(SO_4)_{0.15}(OH)_{0.20}\}$ with further disorder modelling of the sulfate group in the hexagonal channels. Displacement ellipsoids are drawn at the 90% probability level (isotropic for O5 and the sulfate group; anisotropic for all other atoms). (**b**) The content of the hexagonal channel with surrounding [Te1O_3] units, and the O5 atom and the sulfate group in the centre.