Supporting Information

Two New Tellurite Compounds $ACu_3Te_2O_8$ (A = Ca, Cd) with Ferromagnetic Spin-1/2 Kagomé Layers

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Experimental details

Single crystals of $ACu_3Te_2O_8$ (A = Ca, Cd) were synthesized by a conventional hydrothermal method. For $CaCu_3Te_2O_8$, a mixture includes 0.6 mmol CuO (macklin, 99.9%, 0.0477 g), 1.15 mmol K_2TeO_3 (macklin, 99.5%, 0.2919 g), 0.3 mmol $CaCO_3$ (aladdin, 99%, 0.0300 g), and 3 mL deionized water. For $CdCu_3Te_2O_8$, a mixture includes 0.6 mmol CuO (macklin, 99.9%, 0.0477 g), 1.2 mmol K_2TeO_3 (macklin, 99.5%, 0.3046 g), 0.45 mmol $CdCO_3$ (aladdin, 97%, 0.0776 g), and 1.5 mL deionized water. Such mixtures were separately sealed in autoclaves equipped with a Teflon liner (28 mL). The autoclaves were then put into a furnace and heated at 270 °C for 4 days under autogenous pressure respectively, followed by slowly cooling to room temperature at a rate of ~ 4 °C h^{-1} for 2 days. The black block-shaped crystals of $CaCu_3Te_2O_8$ and $CdCu_3Te_2O_8$ (Figure S1) were selected by manual under a microscope and washed several times using deionized water and ethanol (99%), and further dried at 60 ℃ for 2 h. The powdered samples for various physical measurements were prepared by crushing single crystals, which were confirmed to have a high purity by powder X-ray diffraction (XRD) (Figure S2) and the EDS element analysis (Figure S3).

Small crystals of both compounds were selected and mounted on glassy fibers for single-crystal XRD measurements. Data collection was performed on a Rigaku Mercury CCD diffractometer equipped with a graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 100 K. The data sets were corrected for Lorentz and polarization factors as well as for the absorption by Multiscan method. The structure was solved by direct methods and refined by Olex-2 software [1] All non-hydrogen atoms were refined with anisotropic thermal parameters. The final refined structural parameters were checked by the PLATON program [2]. Crystallographic data and structural refinement details are summarized in Table S1. The detailed structural parameters can be seen in Tables S2-S5.

Magnetic and specific heat measurements were performed using a commercial Quantum Design Physical Property Measurement System (PPMS). Samples of $CaCu_3Te_2O_8$ (12.80 mg) and $CdCu_3Te_2O_8$ (12.80 mg) were placed in a gel capsule

sample holder which was suspended in a plastic drinking straw. Magnetic susceptibility was measured at 0.1 T from 300 to 2 K (temperature scan of 5 K/min). Isothermal magnetization was measured at 2 K in applied field from 0 to 5 T (field scan of 0.1 T/step). Specific heat data was obtained from 2 to 150 K under zero field using a relaxation method.

[1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.

[2] A. L. Spek, *J. Appl. Crystallogr.*, 2003, **36**, 7-13.

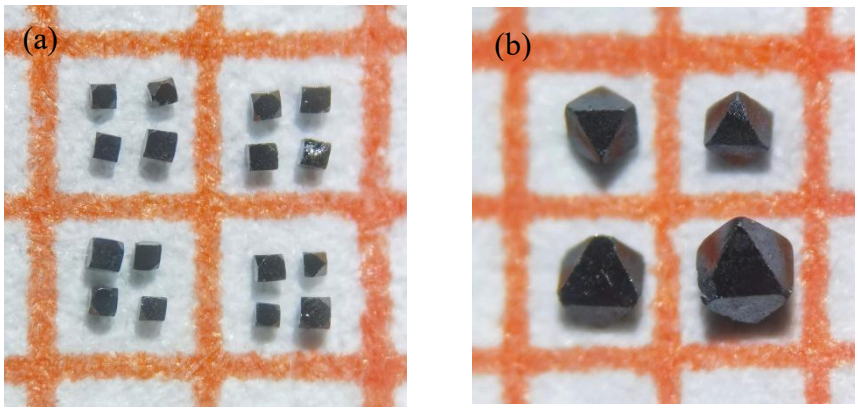


Figure S1 The grown crystals of (a) $CaCu_3Te_2O_8$ and (b) $CdCu_3Te_2O_8$.

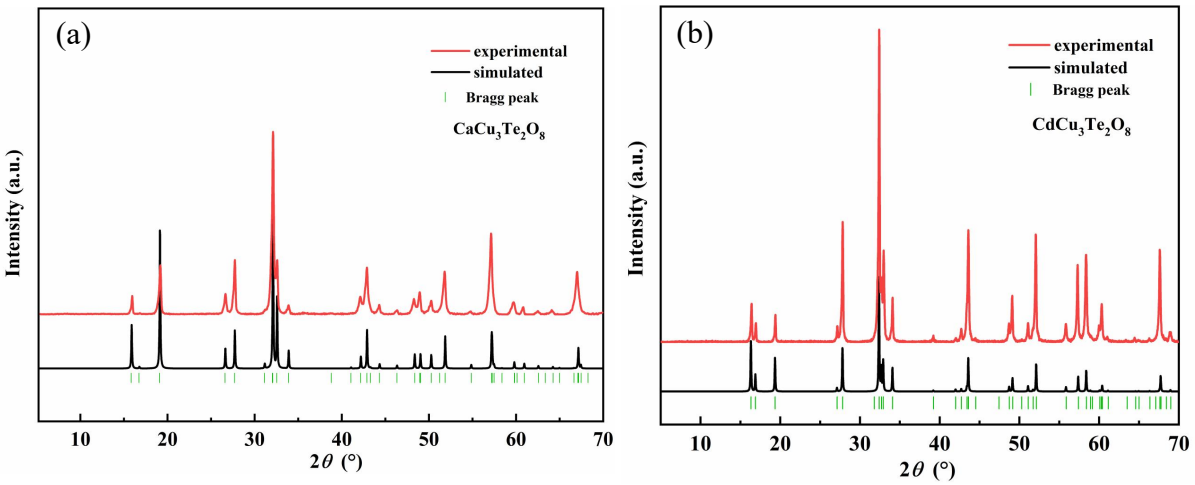


Figure S2 The powder XRD patterns of (a) $CaCu_3Te_2O_8$ and (b) $CdCu_3Te_2O_8$.

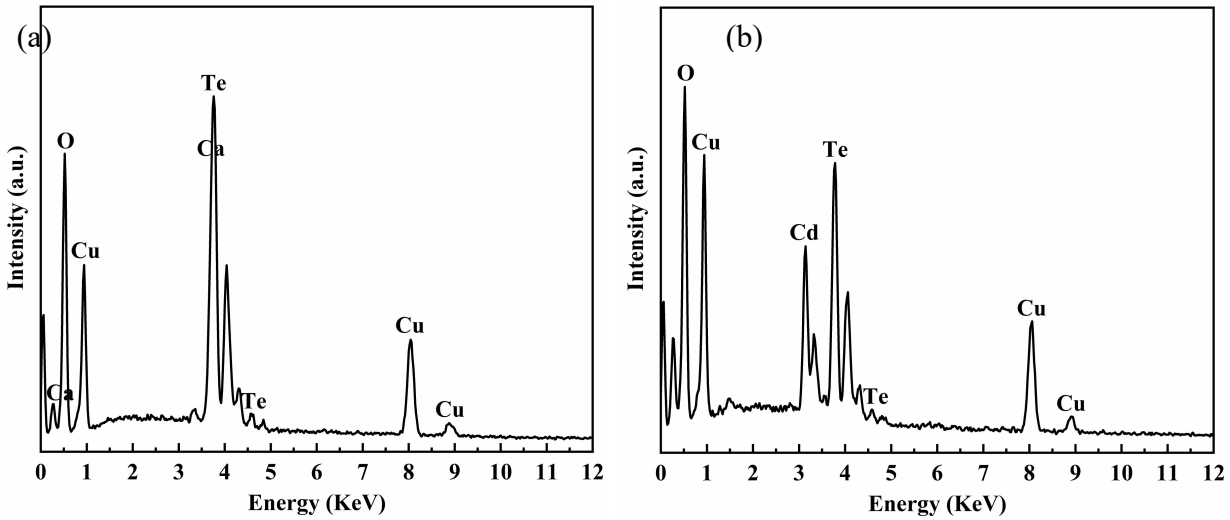
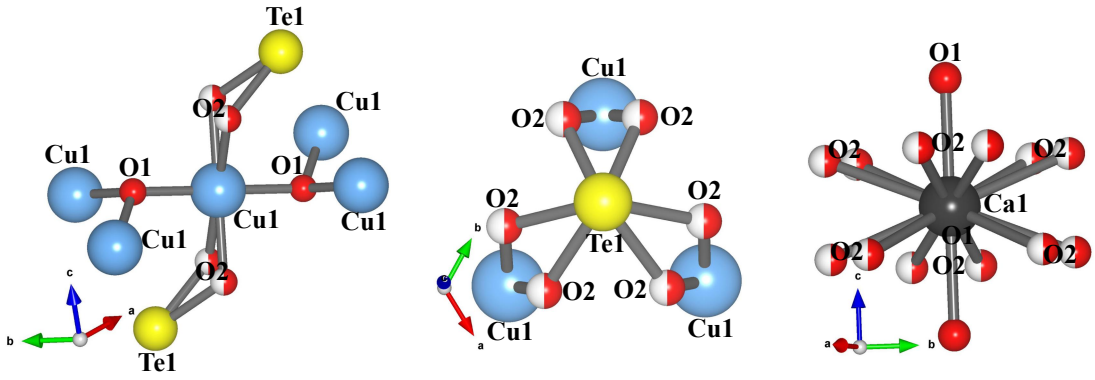


Figure S3 The energy-dispersive spectrometry (EDS) elemental analyses of (a) $CaCu_3Te_2O_8$ and (b) $CdCu_3Te_2O_8$.



(a) (b) (c)

Figure S4 Views of the coordination environments of (a) Cu, (b) Te, and (c) Ca atoms in the structure.

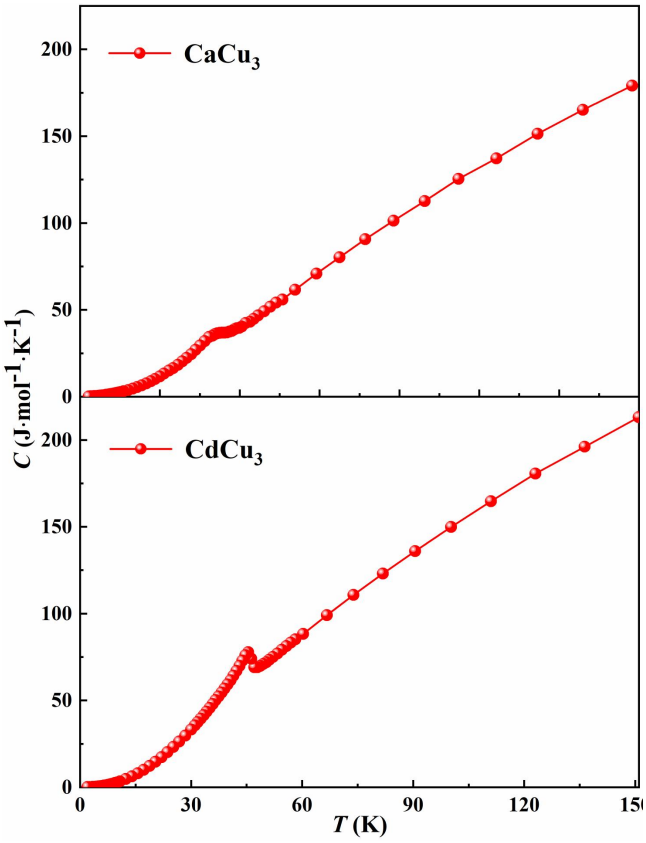


Figure S5 Specific heat of $ACu_3Te_2O_8$ (A = Ca, Cd) measured at 0 T.

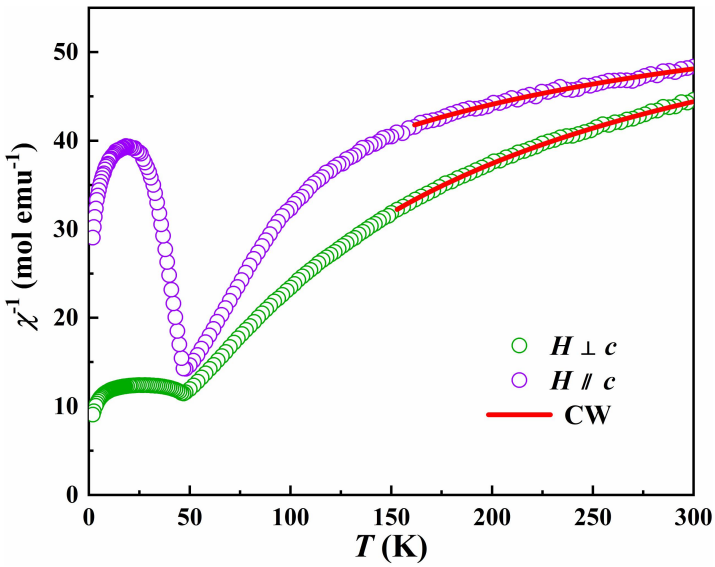


Figure S6 Temperature-dependence of reciprocal magnetic susceptibilities (χ^{-1}) for $CdCu_3Te_2O_8$ with the applied field (H) parallel and perpendicular to the c-axis, in which the red solid line is a fit of Curie–Weiss law.

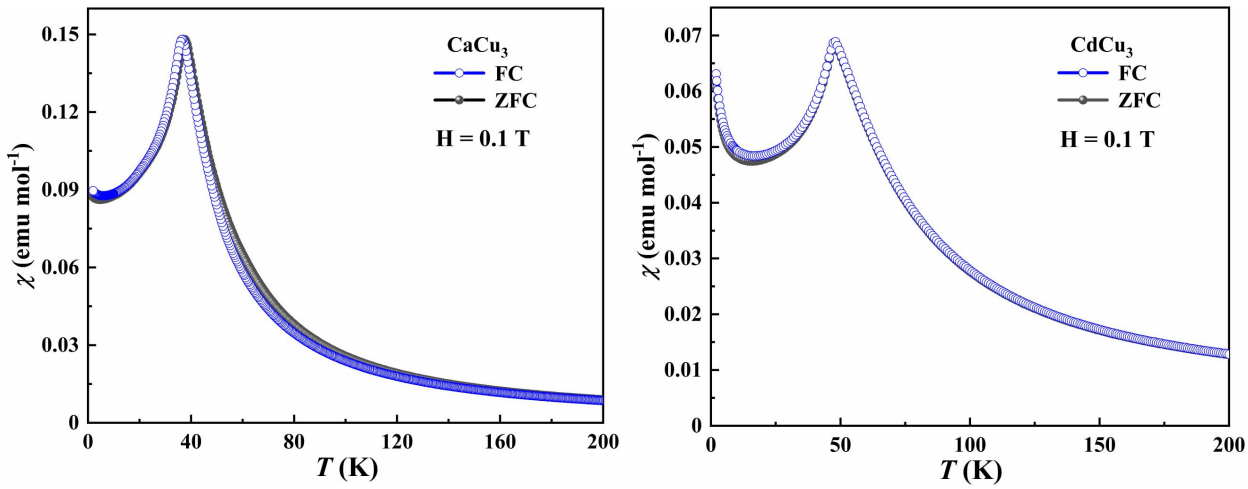


Figure S7 FC and ZFC susceptibilities of $ACu_3Te_2O_8$ (A= Ca, Cd) measured at 0.1 T.

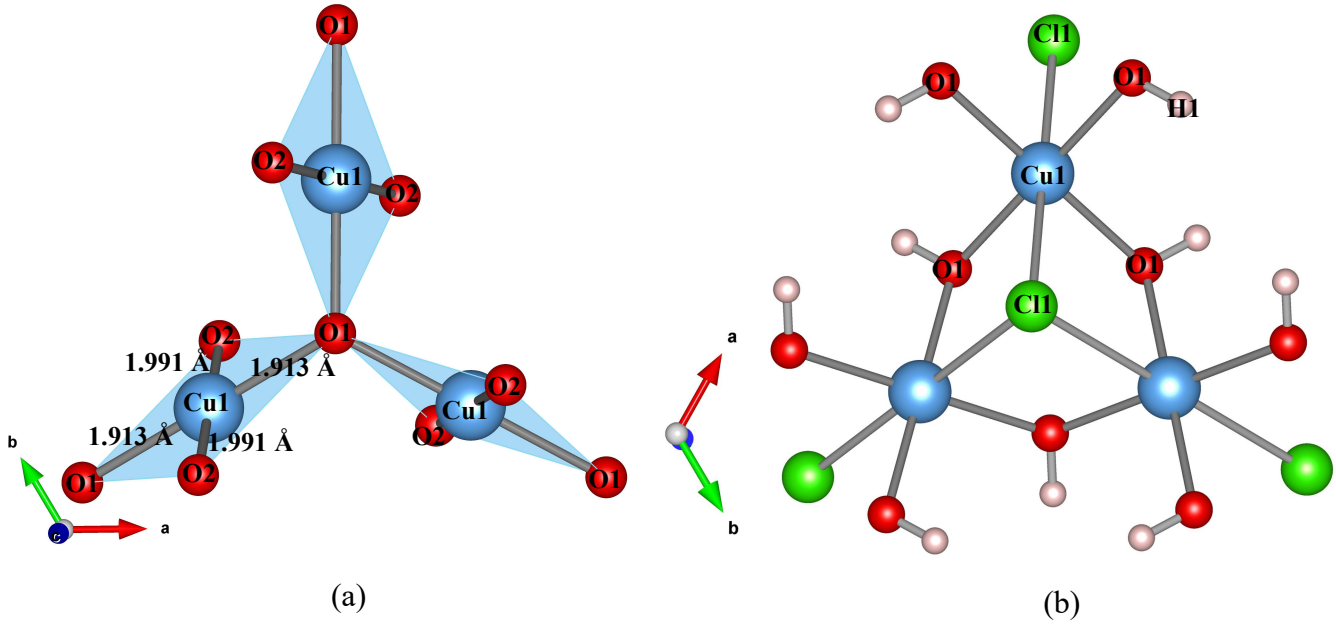


Figure S8 The linkages of magnetic Cu^{2+} ions of (a) $ACu_3Te_2O_8$ (A = Ca, Cd) and (b) $Zn_xCu_{4-x}(OH)_6Cl_2$ ($0 \leqslant x \leqslant 1$), where one of the two equivalent O2 sites is shown in $ACu_3Te_2O_8$.

Table S1. Crystal Data and Structure Refinements for $ACu_3Te_2O_8$ (A = Ca, Cd)

formula	$CaCu_3Te_2O_8$	$CdCu_3Te_2O_8$
Fw	613.9	686.22
T (K)	100	100
λ (Å)	0.71073	0.71073
space group	R-3m	R-3m
a (Å)	6.4391(3)	6.4227(12)
c (Å)	16.7324(8)	16.340(4)
V (Å3)	600.81(6)	583.8(3)
Z	3	3
D_{calcd} (g cm^{-3})	5.090	5.856
μ (mm^{-1})	15.684	18.141
GOF on F^2	1.296	1.161
R1, wR2 [$I > 2\sigma(I)$][a]	0.0311, 0.0732	0.0358, 0.0745
R1, wR2 (all data)	0.0313, 0.0733	0.0391, 0.0756

[a] $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$, and $wR2 = \{\sum w[(F_o)^2 - (F_c)^2]^2 / \sum w[(F_o)^2]^2\}^{1/2}$

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $ACu_3Te_2O_8$ (A = Ca, Cd). U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor

Atom	***x***	***y***	***z***	**U(eq)**
Te1	3333.33	6666.67	5008.4(5)	7.2(3)
Cu1	1666.67	3333.33	3333.33	10.0(4)
Ca1	0	0	5000	10.7(8)
O1	0	0	3605(6)	8(2)
O2	1018(16)	3937(15)	4448(4)	10.0(16)

Atom	**x**	**y**	**z**	**U(eq)**
Te1	3333.33	6666.67	5037.7(7)	4.2(4)
Cd1	3333.33	6666.67	1666.67	4.9(5)
Cu1	1666.67	3333.33	3333.33	4.8(5)
O1	3333.33	6666.67	3033(8)	6(3)
O2	975(19)	4030(20)	4430(6)	7(2)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for $ACu_3Te_2O_8$ (A = Ca, Cd). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te1	5.7(4)	5.7(4)	10.3(5)	0	0	2.8(2)
Cu1	9.0(6)	7.6(8)	13.0(7)	-0.3(5)	-0.2(3)	3.8(4)
Ca1	9.9(13)	9.9(13)	12.1(19)	0	0	5.0(6)
O1	10(3)	10(3)	3(4)	0	0	5.0(16)
O2	8(4)	6(4)	13(4)	-2(3)	-1(3)	1(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te1	4.6(5)	4.6(5)	3.5(6)	0	0	2.3(2)
Cd1	5.9(6)	5.9(6)	3.0(8)	0	0	3.0(3)
Cu1	5.9(7)	4.6(10)	3.3(8)	1.5(7)	0.8(4)	2.3(5)
O1	8(4)	8(4)	3(6)	0	0	4(2)
O2	7(2)	7(2)	7(2)	-0.8(10)	0.4(10)	3.5(13)

Table S4 Selected bond lengths [Å] and bond angles for $CaCu_3Te_2O_8$

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Te1-O2[3]	1.890(8)	Ca1-O1[11]	2.335(10)
Te1-O2[4]	1.890(8)	Ca1-O1	2.335(10)
Te1-O2[5]	1.890(8)	Ca1-O2[12]	2.460(8)
Te1-O2[6]	1.890(8)	Ca1-O2[13]	2.460(8)
Te1-O2[7]	1.890(8)	Ca1-O2[14]	2.460(8)
Te1-O2	1.890(8)	Ca1-O2[15]	2.460(8)
Cu1-O1[9]	1.913(2)	Ca1-O2[16]	2.460(8)
Cu1-O1	1.913(2)	Ca1-O2[17]	2.460(8)
Cu1-O2	1.991(8)	Ca1-O2[18]	2.460(8)

Cu1-O2[7]	1.991(8)	Ca1-O2[19]	2.460(8)
Cu1-O2[9]	1.991(8)	Ca1-O2[20]	2.460(8)
Cu1-O2[10]	1.991(8)	Ca1-O2[7]	2.460(8)

[1]+X,1+Y,+Z; [2]1+X,1+Y,+Z; [3]1-Y,1+X-Y,+Z; [4]1-Y,1-X,+Z; [5]+Y-X,1-X,+Z; [6]+X,1+X-Y,+Z; [7]+Y-X,+Y,+Z; [8]1/3+X,2/3+Y,-1/3+Z; [9]1/3-X,2/3-Y,2/3-Z; [10]1/3-Y+X,2/3-Y,2/3-Z; [11]-X,-Y,1-Z; [12]-Y+X,+X,1-Z; [13]-X,-X+Y,1-Z; [14]+Y,-X+Y,1-Z; [15]-Y+X,-Y,1-Z; [16]-Y,-X,+Z; [17]-Y,+X-Y,+Z; [18]+Y-X,-X,+Z; [19]+Y,+X,1-Z; [20]+X,+X-Y,+Z

Atom-Atom-Atom	**Angle/°**	**Atom-Atom-Atom**	**Angle/°**
O2[3]-Te1-O2[5]	118.5(5)	O1[11]-Ca1-O2[18]	67.93(18)
O2[3]-Te1-O2[6]	37.8(5)	O2[16]-Ca1-O2[19]	180.0(3)
O2[4]-Te1-O2	118.5(5)	O2[16]-Ca1-O2[18]	73.25(19)
O2[5]-Te1-O2	97.5(3)	O2[16]-Ca1-O2[14]	106.75(19)
O2[6]-Te1-O2	97.5(3)	O2[18]-Ca1-O2[14]	73.25(19)
O2[6]-Te1-O2[4]	64.8(5)	O2[12]-Ca1-O2[18]	127.7(4)
O2[7]-Te1-O2[5]	64.8(5)	O2[16]-Ca1-O2[12]	99.1(4)
O2[6]-Te1-O2[5]	97.5(3)	O2[15]-Ca1-O2[13]	180.0(3)
O2[3]-Te1-O2[4]	97.5(3)	O2[16]-Ca1-O2[17]	80.9(4)
O2[4]-Te1-O2[7]	97.5(3)	O2[15]-Ca1-O2[18]	80.9(4)
O2[3]-Te1-O2[7]	97.5(3)	O2[17]-Ca1-O2[20]	151.2(4)
O2[4]-Te1-O2[5]	37.8(5)	O2[19]-Ca1-O2[15]	28.8(4)
O2[7]-Te1-O2	37.8(5)	O2[19]-Ca1-O2[17]	99.1(4)
O2[6]-Te1-O2[7]	118.5(5)	O2[13]-Ca1-O2[12]	73.25(19)
O2[3]-Te1-O2	64.8(5)	O2[13]-Ca1-O2[14]	127.7(4)
O1-Cu1-O1[9]	180	O2[16]-Ca1-O2[15]	151.2(4)
O1[9]-Cu1-O2	93.3(4)	O2[15]-Ca1-O2[17]	73.25(19)
O1-Cu1-O2[10]	93.3(4)	O2[19]-Ca1-O2[18]	106.75(19)
O1-Cu1-O2[9]	93.3(4)	O2[19]-Ca1-O2[20]	106.75(19)
O1-Cu1-O2	86.7(4)	O2[13]-Ca1-O2[18]	99.1(4)
O1[9]-Cu1-O2[7]	93.3(4)	O2[13]-Ca1-O2[17]	106.75(19)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1^{9}-Cu1-O2^{10}	86.7(4)	O2^{17}-Ca1-O2^{18}	52.3(4)
O1-Cu1-O2^{7}	86.7(4)	O2^{7}-Ca1-O2^{18}	180
O1^{9}-Cu1-O2^{9}	86.7(4)	O2^{13}-Ca1-O2^{7}	80.9(4)
O2^{10}-Cu1-O2	144.2(5)	O2^{12}-Ca1-O2^{17}	180
O2^{9}-Cu1-O2^{10}	35.8(5)	O2^{12}-Ca1-O2^{7}	52.3(4)
O2^{9}-Cu1-O2	180	O2^{19}-Ca1-O2^{14}	73.25(19)
O2^{10}-Cu1-O2^{7}	180.0(6)	O2^{17}-Ca1-O2^{7}	127.7(4)
O2^{9}-Cu1-O2^{7}	144.2(5)	O2^{16}-Ca1-O2^{13}	28.8(4)
O2-Cu1-O2^{7}	35.8(5)	O2^{7}-Ca1-O2^{14}	106.75(19)
O1^{11}-Ca1-O1	180	O2^{17}-Ca1-O2^{14}	28.8(4)
O1^{11}-Ca1-O2^{12}	67.93(18)	O2^{19}-Ca1-O2^{12}	80.9(4)
O1^{11}-Ca1-O2^{13}	112.07(17)	O2^{19}-Ca1-O2^{13}	151.2(4)
O1^{11}-Ca1-O2^{14}	112.07(18)	O2^{16}-Ca1-O2^{20}	73.25(19)
O1-Ca1-O2^{15}	112.07(17)	O2^{15}-Ca1-O2^{12}	106.75(19)
O1^{11}-Ca1-O2^{7}	112.07(18)	O2^{15}-Ca1-O2^{20}	127.7(4)
O1-Ca1-O2^{13}	67.93(17)	O2^{16}-Ca1-O2^{7}	106.75(19)
O1^{11}-Ca1-O2^{16}	112.07(17)	O2^{12}-Ca1-O2^{20}	28.8(4)
O1-Ca1-O2^{12}	112.07(18)	O2^{13}-Ca1-O2^{20}	52.3(4)
O1^{11}-Ca1-O2^{17}	112.07(18)	O2^{7}-Ca1-O2^{20}	73.25(19)
O1-Ca1-O2^{7}	67.93(18)	O2^{19}-Ca1-O2^{7}	73.25(19)
O1-Ca1-O2^{16}	67.93(17)	O2^{14}-Ca1-O2^{20}	180
O1-Ca1-O2^{18}	112.07(18)	O2^{18}-Ca1-O2^{20}	106.75(19)
O1^{11}-Ca1-O2^{19}	67.93(17)	O2^{15}-Ca1-O2^{14}	52.3(4)
O1-Ca1-O2^{14}	67.93(17)	O2^{15}-Ca1-O2^{7}	99.1(4)
O1^{11}-Ca1-O2^{20}	67.93(17)	O2^{12}-Ca1-O2^{14}	151.2(4)
O1-Ca1-O2^{20}	112.07(18)	Cu1^{17}-O1-Cu1^{13}	114.6(2)
O1-Ca1-O2^{19}	112.07(17)	Cu1^{17}-O1-Cu1	114.6(2)
O1^{11}-Ca1-O2^{15}	67.93(17)	Cu1^{13}-O1-Cu1	114.6(2)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Ca1-O2[17]	67.93(18)	-	-

[1]+X,1+Y,+Z; [2]1+X,1+Y,+Z; [3]+X,1+X-Y,+Z; [4]1-Y,1-X,+Z; [5]1-Y,1+X-Y,+Z; [6]+Y-X,1-X,+Z; [7]+Y-X,+Y,+Z; [8]1/3+X,2/3+Y,-1/3+Z; [9]1/3-X,2/3-Y,2/3-Z; [10]1/3-Y+X,2/3-Y,2/3-Z; [11]-X,-Y,1-Z; [12]+Y,-X+Y,1-Z; [13]+Y-X,-X,+Z; [14]-Y,-X,+Z; [15]-Y+X,+X,1-Z; [16]+X,+X-Y,+Z; [17]-Y,+X-Y,+Z; [18]-Y+X,-Y,1-Z; [19]-X,-X+Y,1-Z; [20]+Y,+X,1-Z

Table S5 Selected bond lengths [Å] and bond angles for $CdCu_3Te_2O_8$

Atom-Atom	Length/Å	Atom-Atom	Length/Å
Te1-O2[1]	1.892(11)	Cd1-O2[11]	2.518(11)
Te1-O2	1.892(11)	Cd1-O2[12]	2.518(11)
Te1-O2[2]	1.892(11)	Cd1-O2[13]	2.518(11)
Te1-O2[3]	1.892(11)	Cd1-O2[14]	2.518(11)
Te1-O2[4]	1.892(11)	Cd1-O2[15]	2.518(11)
Te1-O2[5]	1.892(11)	Cd1-O2[16]	2.518(11)
Cd1-O1	2.233(13)	Cu1-O1	1.918(3)
Cd1-O1[6]	2.233(13)	Cu1-O1[12]	1.918(3)
Cd1-O2[7]	2.518(11)	Cu1-O2[9]	1.952(10)
Cd1-O2[8]	2.518(11)	Cu1-O2[12]	1.952(10)
Cd1-O2[9]	2.518(11)	Cu1-O2[4]	1.952(10)
Cd1-O2[10]	2.518(11)	Cu1-O2	1.952(10)

[1]+X,1+X-Y,+Z; [2]1-Y,1-X,+Z; [3]1-Y,1+X-Y,+Z; [4]+Y-X,+Y,+Z; [5]+Y-X,1-X,+Z; [6]2/3-X,4/3-Y,1/3-Z; [7]1/3-Y,2/3-X,-1/3+Z; [8]1/3+Y,2/3-X+Y,2/3-Z; [9]1/3-Y+X,2/3-Y,2/3-Z; [10]1/3+X,2/3+Y,-1/3+Z; [11]1/3-Y,2/3+X-Y,-1/3+Z; [12]1/3-X,2/3-Y,2/3-Z; [13]1/3-X,2/3-X+Y,2/3-Z; [14]1/3-Y+X,2/3+X,2/3-Z; [15]1/3+Y-X,2/3+Y,-1/3+Z; [16]1/3+Y,2/3+X,2/3-Z

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O2[1]-Te1-O2[2]	41.4(7)	O2[13]-Cd1-O2[16]	129.3(5)
O2-Te1-O2[3]	41.4(6)	O2[9]-Cd1-O2[7]	149.2(5)
O2-Te1-O2[4]	95.0(4)	O2[15]-Cd1-O2[9]	107.2(2)
O2[5]-Te1-O2[3]	95.0(4)	O2[15]-Cd1-O2[7]	100.6(5)

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
$O2^{2}$-Te1-$O2^{4}$	95.0(4)	$O2^{14}$-Cd1-$O2^{9}$	180
$O2^{5}$-Te1-$O2^{4}$	41.4(6)	$O2^{13}$-Cd1-$O2^{14}$	72.8(2)
$O2^{2}$-Te1-$O2^{3}$	115.9(6)	$O2^{10}$-Cd1-$O2^{15}$	30.8(5)
$O2^{1}$-Te1-$O2^{5}$	95.0(4)	$O2^{11}$-Cd1-$O2^{9}$	79.4(5)
$O2^{2}$-Te1-O2	95.0(4)	$O2^{10}$-Cd1-$O2^{12}$	100.6(5)
$O2^{1}$-Te1-$O2^{4}$	115.9(6)	$O2^{16}$-Cd1-$O2^{14}$	149.2(5)
$O2^{5}$-Te1-O2	115.9(6)	$O2^{13}$-Cd1-$O2^{12}$	180
$O2^{2}$-Te1-$O2^{5}$	59.3(7)	$O2^{15}$-Cd1-$O2^{12}$	72.8(2)
$O2^{1}$-Te1-$O2^{3}$	95.0(4)	$O2^{8}$-Cd1-$O2^{12}$	30.8(5)
$O2^{3}$-Te1-$O2^{4}$	59.3(7)	$O2^{8}$-Cd1-$O2^{14}$	79.4(5)
$O2^{1}$-Te1-O2	59.3(7)	$O2^{11}$-Cd1-$O2^{12}$	149.2(5)
O1-Cd1-$O1^{6}$	180	$O2^{14}$-Cd1-$O2^{12}$	107.2(2)
O1-Cd1-$O2^{7}$	111.7(2)	$O2^{15}$-Cd1-$O2^{8}$	50.7(5)
$O1^{6}$-Cd1-$O2^{8}$	68.3(2)	$O2^{10}$-Cd1-$O2^{16}$	107.2(2)
O1-Cd1-$O2^{9}$	68.3(2)	$O2^{10}$-Cd1-$O2^{7}$	72.8(2)
$O1^{6}$-Cd1-$O2^{10}$	111.7(2)	$O2^{13}$-Cd1-$O2^{8}$	149.2(5)
O1-Cd1-$O2^{11}$	68.3(2)	$O2^{13}$-Cd1-$O2^{7}$	50.7(5)
$O1^{6}$-Cd1-$O2^{11}$	111.7(2)	$O2^{16}$-Cd1-$O2^{7}$	180
O1-Cd1-$O2^{12}$	111.7(2)	$O2^{16}$-Cd1-$O2^{8}$	72.8(2)
$O1^{6}$-Cd1-$O2^{7}$	68.3(2)	$O2^{10}$-Cd1-$O2^{13}$	79.4(5)
O1-Cd1-$O2^{13}$	68.3(2)	$O2^{11}$-Cd1-$O2^{7}$	72.8(2)
O1-Cd1-$O2^{14}$	111.7(2)	$O2^{9}$-Cd1-$O2^{12}$	72.8(2)
$O1^{6}$-Cd1-$O2^{13}$	111.7(2)	$O2^{12}$-Cd1-$O2^{7}$	129.3(5)
O1-Cd1-$O2^{15}$	68.3(2)	$O2^{10}$-Cd1-$O2^{8}$	72.8(2)
O1-Cd1-$O2^{16}$	68.3(2)	$O2^{10}$-Cd1-$O2^{9}$	129.3(5)
$O1^{6}$-Cd1-$O2^{9}$	111.7(2)	$O2^{8}$-Cd1-$O2^{7}$	107.2(2)
$O1^{6}$-Cd1-$O2^{16}$	111.7(2)	$O2^{15}$-Cd1-$O2^{16}$	79.4(5)
$O1^{6}$-Cd1-$O2^{15}$	111.7(2)	O1-Cu1-$O1^{9}$	180

Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O1-Cd1-O2[10]	68.3(2)	O1[9]-Cu1-O2	87.6(5)
O1[6]-Cd1-O2[12]	68.3(2)	O1-Cu1-O2[16]	87.6(5)
O1-Cd1-O2[8]	111.7(2)	O1[9]-Cu1-O2[16]	92.4(5)
O1[6]-Cd1-O2[14]	68.3(2)	O1[9]-Cu1-O2[9]	92.4(5)
O2[13]-Cd1-O2[9]	107.2(2)	O1-Cu1-O2[3]	92.4(5)
O2[15]-Cd1-O2[13]	107.2(2)	O1-Cu1-O2	92.4(5)
O2[16]-Cd1-O2[11]	107.2(2)	O1-Cu1-O2[9]	87.6(5)
O2[16]-Cd1-O2[9]	30.8(5)	O1[9]-Cu1-O2[3]	87.6(5)
O2[15]-Cd1-O2[11]	129.3(5)	O2[16]-Cu1-O2	140.0(6)
O2[10]-Cd1-O2[14]	50.7(5)	O2[16]-Cu1-O2[3]	180
O2[14]-Cd1-O2[11]	100.6(5)	O2-Cu1-O2[3]	40.0(6)
O2[15]-Cd1-O2[14]	72.8(2)	O2[9]-Cu1-O2	180
O2[10]-Cd1-O2[11]	107.2(2)	O2[9]-Cu1-O2[3]	140.0(6)
O2[8]-Cd1-O2[9]	100.6(5)	O2[9]-Cu1-O2[16]	40.0(6)
O2[13]-Cd1-O2[11]	30.8(5)	Cu1[2]-O1-Cu1	113.7(3)
O2[14]-Cd1-O2[7]	30.8(5)	Cu1[2]-O1-Cu1[4]	113.7(3)
O2[8]-Cd1-O2[11]	180	Cu1-O1-Cu1[4]	113.7(3)
O2[16]-Cd1-O2[12]	50.7(5)		

[1]+X,1+X-Y,+Z; [2]+Y-X,1-X,+Z; [3]+Y-X,+Y,+Z; [4]1-Y,1+X-Y,+Z; [5]1-Y,1-X,+Z; [6]2/3-X,4/3-Y,1/3-Z; [7]1/3+Y-X,2/3+Y,-1/3+Z; [8]1/3-Y,2/3-X,-1/3+Z; [9]1/3-X,2/3-Y,2/3-Z; [10]1/3-X,2/3-X+Y,2/3-Z; [11]1/3+Y,2/3+X,2/3-Z; [12]1/3-Y,2/3+X-Y,-1/3+Z; [13]1/3+Y,2/3-X+Y,2/3-Z; [14]1/3+X,2/3+Y,-1/3+Z; [15]1/3-Y+X,2/3+X,2/3-Z; [16]1/3-Y+X,2/3-Y,2/3-Z; [17]-1/3+X,-2/3+Y,1/3+Z

Table S6 A comparison between $ACu_3Te_2O_8$ (A = Ca, Cd) and $Zn_xCu_{4-x}(OH)_6Cl_2$ ($0 \leq x \leq 1$)

	Herbertsmithite $ZnCu_3(OH)_6Cl_2$	**Kapellasite $ZnCu_3(OH)_6Cl_2$**	**$CaCu_3Te_2O_8$**	**$CdCu_3Te_2O_8$**
Space group	R-3m	P-3m1	R-3m	R-3m
The location of nonmagnetic cations	Between the layers	Within the layers	Between the layers	Between the layers
Cu-O-Cu	Connected via edge-sharing	Connected via edge-sharing	Connected via corner-sharing	Connected via corner-sharing
Cu^{2+} Coordination (Å)	Cu-O, 1.982 (4×); Cu-Cl, 2.769 (2×)	Cu-O, 1.974 (4×); Cu-Cl, 2.762 (2×)	Cu-O, 1.913 (2×), 1.991 (2×)	Cu-O, 1.918 (2×), 1.952 (2×)
d_{Cu-Cu}(Å)	3.417	3.165	3.219	3.211
$d_{interlayer}$ (Å)	5.089	5.702	5.879	5.754
∠Cu-O-Cu(deg)	118.9	105.54	114.54	113.7