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Table SI. Crystal Data and Intensity Collection Details for $CsTh_2Te_6$.

Formula	$CsTh_2Te_6$
Formula mass (amu)	1362.59
Space group	D_{2h}^{17}–*Cmcm*
a (Å)	4.367(2)[a]
b (Å)	25.119(10)
c (Å)	6.140(3)
V (Å^3)	673.5(5)
Z	2
ρ_c (g cm^{-3})	6.719
T of data collection (K)[b]	113(2)
Crystal shape	Needle (0.36 x 0.08 x 0.01 mm) bounded by {100}, {010}, {001}
Crystal volume (mm^3)	2.88 x 10^{-4}
Radiation	λ(Mo*K*α_1) = 0.7093
Linear absorption coefficient (cm^{-1})	374
Transmission factors[c]	0.369 - 0.710
Detector aperture (mm)	6.5 x 6.5, 32 cm from crystal
Scan type	$\theta - 2\theta$
Scan speed (deg min^{-1})	2
Scan range (deg)	−1.2 to +1.1
θ limits (deg)	$3.24 \leq \theta \leq 29.90$
Background counts[d]	12 sec at each end of scan
Weighting scheme	$w^{-1} = \sigma^2(F_o^2)+(0.04 \times F_o^2)^2$
Data collected	$\pm h, \pm k, \pm \ell$ ($2° \leq 2\theta \leq 23°$), $\pm h, +k, \pm \ell$ ($23° \leq 2\theta \leq 60°$)
No. of data collected	2191
No. of unique data, including $0 \geq F_o^2 \geq -3\sigma(F_o^2)$	593
$R_{average}$	0.0909
No. of variables	19
$R_w(F^2)$ (all data)	0.102
R (on *F* for $F_o^2 > 2\sigma(F_o^2)$	0.049
Error in observation of unit weight (e^2)	1.30

a. Obtained from a refinement with the constraints $\alpha = \beta = \gamma = 90°$.
b. The low-temperature system is based on a design by Huffman.[23]
c. The analytical method, as employed in the Northwestern absorption program AGNOST, was used for the absorption correction.[24]
d. The diffractometer was operated with the use of the Indiana University PCPS system.[32]

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Table SII. Anisotropic displacement parameters ($Å^2$) for $CsTh_2Te_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

atom	U11	U22	U33	U23	U13	U12
Cs	0.018(2)	0.009(2)	0.019(2)	0.000	0.000	0.000
Th	0.0063(5)	0.0100(5)	0.0050(5)	0.000	0.000	0.000
Te(1)	0.0070(8)	0.0094(9)	0.0043(8)	0.000	0.000	0.000
Te(2)	0.0086(6)	0.0096(6)	0.0104(6)	-0.0010(5)	0.000	0.000

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Table SIII. Bond lengths (Å) and angles (deg.) for $CsTh_2Te_6$.

Cs-Cs#1	3.074(2)
Cs-Cs#2	3.074(2)
Cs-Te(2)#3	3.817(4)
Cs-Te(2)#4	3.817(4)
Cs-Te(2)#5	3.817(4)
Cs-Te(2)#6	3.817(4)
Cs-Te(2)#7	3.929(4)
Cs-Te(2)#8	3.929(4)
Cs-Te(2)#9	3.929(4)
Cs-Te(2)#10	3.929(4)
Cs-Cs#11	4.367(2)
Cs-Cs#12	4.367(2)
Th-Te(1)#7	3.164(2)
Th-Te(1)#8	3.164(2)
Th-Te(2)#8	3.201(2)
Th-Te(2)#7	3.201(2)
Th-Te(2)#10	3.201(2)
Th-Te(2)#9	3.201(2)
Th-Te(1)#1	3.264(2)
Th-Te(1)#2	3.264(2)
Te(1)-Th#13	3.164(2)
Te(1)-Th#14	3.164(2)
Te(1)-Th#1	3.264(2)
Te(1)-Th#2	3.264(2)
Te(2)-Te(2)#15	3.052(3)
Te(2)-Te(2)#16	3.088(3)
Te(2)-Th#14	3.201(2)
Te(2)-Th#13	3.201(2)
Te(2)-Cs#3	3.817(4)
Te(2)-Cs#4	3.817(4)
Te(2)-Cs#13	3.929(4)
Te(2)-Cs#14	3.929(4)
Cs#1-Cs-Cs#2	173.8(3)
Cs#1-Cs-Te(2)#3	116.3(2)
Cs#2-Cs-Te(2)#3	68.56(11)
Cs#1-Cs-Te(2)#4	116.3(2)
Cs#2-Cs-Te(2)#4	68.56(11)
Te(2)#3-Cs-Te(2)#4	69.79(8)
Cs#1-Cs-Te(2)#5	68.56(11)
Cs#2-Cs-Te(2)#5	116.3(2)
Te(2)#3-Cs-Te(2)#5	47.73(6)
Te(2)#4-Cs-Te(2)#5	88.97(10)
Cs#1-Cs-Te(2)#6	68.56(11)
Cs#2-Cs-Te(2)#6	116.3(2)
Te(2)#3-Cs-Te(2)#6	88.97(10)
Te(2)#4-Cs-Te(2)#6	47.73(6)
Te(2)#5-Cs-Te(2)#6	69.79(8)
Cs#1-Cs-Te(2)#7	110.4(2)
Cs#2-Cs-Te(2)#7	64.70(12)
Te(2)#3-Cs-Te(2)#7	133.26(3)
Te(2)#4-Cs-Te(2)#7	92.84(4)
Te(2)#5-Cs-Te(2)#7	178.18(9)
Te(2)#6-Cs-Te(2)#7	111.33(4)
Cs#1-Cs-Te(2)#8	110.4(2)
Cs#2-Cs-Te(2)#8	64.70(12)
Te(2)#3-Cs-Te(2)#8	92.84(4)
Te(2)#4-Cs-Te(2)#8	133.26(3)
Te(2)#5-Cs-Te(2)#8	111.33(4)

Table SIII. Bond lengths (Å) and angles (deg.) for $CsTh_2Te_6$.

Cs-Cs#1	3.074(2)
Cs-Cs#2	3.074(2)
Cs-Te(2)#3	3.817(4)
Cs-Te(2)#4	3.817(4)
Cs-Te(2)#5	3.817(4)
Cs-Te(2)#6	3.817(4)
Cs-Te(2)#7	3.929(4)
Cs-Te(2)#8	3.929(4)
Cs-Te(2)#9	3.929(4)
Cs-Te(2)#10	3.929(4)
Cs-Cs#11	4.367(2)
Cs-Cs#12	4.367(2)
Th-Te(1)#7	3.164(2)
Th-Te(1)#8	3.164(2)
Th-Te(2)#8	3.201(2)
Th-Te(2)#7	3.201(2)
Th-Te(2)#10	3.201(2)
Th-Te(2)#9	3.201(2)
Th-Te(1)#1	3.264(2)
Th-Te(1)#2	3.264(2)
Te(1)-Th#13	3.164(2)
Te(1)-Th#14	3.164(2)
Te(1)-Th#1	3.264(2)
Te(1)-Th#2	3.264(2)
Te(2)-Te(2)#15	3.052(3)
Te(2)-Te(2)#16	3.088(3)
Te(2)-Th#14	3.201(2)
Te(2)-Th#13	3.201(2)
Te(2)-Cs#3	3.817(4)
Te(2)-Cs#4	3.817(4)
Te(2)-Cs#13	3.929(4)
Te(2)-Cs#14	3.929(4)
Cs#1-Cs-Cs#2	173.8(3)
Cs#1-Cs-Te(2)#3	116.3(2)
Cs#2-Cs-Te(2)#3	68.56(11)
Cs#1-Cs-Te(2)#4	116.3(2)
Cs#2-Cs-Te(2)#4	68.56(11)
Te(2)#3-Cs-Te(2)#4	69.79(8)
Cs#1-Cs-Te(2)#5	68.56(11)
Cs#2-Cs-Te(2)#5	116.3(2)
Te(2)#3-Cs-Te(2)#5	47.73(6)
Te(2)#4-Cs-Te(2)#5	88.97(10)
Cs#1-Cs-Te(2)#6	68.56(11)
Cs#2-Cs-Te(2)#6	116.3(2)
Te(2)#3-Cs-Te(2)#6	88.97(10)
Te(2)#4-Cs-Te(2)#6	47.73(6)
Te(2)#5-Cs-Te(2)#6	69.79(8)
Cs#1-Cs-Te(2)#7	110.4(2)
Cs#2-Cs-Te(2)#7	64.70(12)
Te(2)#3-Cs-Te(2)#7	133.26(3)
Te(2)#4-Cs-Te(2)#7	92.84(4)
Te(2)#5-Cs-Te(2)#7	178.18(9)
Te(2)#6-Cs-Te(2)#7	111.33(4)
Cs#1-Cs-Te(2)#8	110.4(2)
Cs#2-Cs-Te(2)#8	64.70(12)
Te(2)#3-Cs-Te(2)#8	92.84(4)
Te(2)#4-Cs-Te(2)#8	133.26(3)
Te(2)#5-Cs-Te(2)#8	111.33(4)

Te(2)#6-Cs-Te(2)#8	178.18(9)
Te(2)#7-Cs-Te(2)#8	67.51(8)
Cs#1-Cs-Te(2)#9	64.70(12)
Cs#2-Cs-Te(2)#9	110.4(2)
Te(2)#3-Cs-Te(2)#9	178.18(9)
Te(2)#4-Cs-Te(2)#9	111.33(4)
Te(2)#5-Cs-Te(2)#9	133.26(3)
Te(2)#6-Cs-Te(2)#9	92.84(4)
Te(2)#7-Cs-Te(2)#9	45.70(6)
Te(2)#8-Cs-Te(2)#9	85.36(10)
Cs#1-Cs-Te(2)#10	64.70(12)
Cs#2-Cs-Te(2)#10	110.4(2)
Te(2)#3-Cs-Te(2)#10	111.33(4)
Te(2)#4-Cs-Te(2)#10	178.18(9)
Te(2)#5-Cs-Te(2)#10	92.84(4)
Te(2)#6-Cs-Te(2)#10	133.26(3)
Te(2)#7-Cs-Te(2)#10	85.36(10)
Te(2)#8-Cs-Te(2)#10	45.70(6)
Te(2)#9-Cs-Te(2)#10	67.51(8)
Cs#1-Cs-Cs#11	90.0
Cs#2-Cs-Cs#11	90.0
Te(2)#3-Cs-Cs#11	55.10(4)
Te(2)#4-Cs-Cs#11	124.90(4)
Te(2)#5-Cs-Cs#11	55.11(4)
Te(2)#6-Cs-Cs#11	124.90(4)
Te(2)#7-Cs-Cs#11	123.76(4)
Te(2)#8-Cs-Cs#11	56.24(4)
Te(2)#9-Cs-Cs#11	123.76(4)
Te(2)#10-Cs-Cs#11	56.24(4)
Cs#1-Cs-Cs#12	90.0
Cs#2-Cs-Cs#12	90.0
Te(2)#3-Cs-Cs#12	124.90(4)
Te(2)#4-Cs-Cs#12	55.10(4)
Te(2)#5-Cs-Cs#12	124.90(4)
Te(2)#6-Cs-Cs#12	55.11(4)
Te(2)#7-Cs-Cs#12	56.24(4)
Te(2)#8-Cs-Cs#12	123.76(4)
Te(2)#9-Cs-Cs#12	56.24(4)
Te(2)#10-Cs-Cs#12	123.76(4)
Cs#11-Cs-Cs#12	180.0(2)
Te(1)#7-Th-Te(1)#8	87.29(7)
Te(1)#7-Th-Te(2)#8	150.70(3)
Te(1)#8-Th-Te(2)#8	86.01(4)
Te(1)#7-Th-Te(2)#7	86.01(4)
Te(1)#8-Th-Te(2)#7	150.70(3)
Te(2)#8-Th-Te(2)#7	86.03(5)
Te(1)#7-Th-Te(2)#10	150.70(3)
Te(1)#8-Th-Te(2)#10	86.01(4)
Te(2)#8-Th-Te(2)#10	56.94(6)
Te(2)#7-Th-Te(2)#10	112.66(6)
Te(1)#7-Th-Te(2)#9	86.01(4)
Te(1)#8-Th-Te(2)#9	150.70(3)
Te(2)#8-Th-Te(2)#9	112.66(6)
Te(2)#7-Th-Te(2)#9	56.94(6)
Te(2)#10-Th-Te(2)#9	86.03(5)
Te(1)#7-Th-Te(1)#1	75.77(3)
Te(1)#8-Th-Te(1)#1	75.77(3)
Te(2)#8-Th-Te(1)#1	129.55(3)
Te(2)#7-Th-Te(1)#1	129.55(3)
Te(2)#10-Th-Te(1)#1	74.93(4)
Te(2)#9-Th-Te(1)#1	74.93(4)
Te(1)#7-Th-Te(1)#2	75.77(3)

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Te(1)#8-Th-Te(1)#2	75.77(3)
Te(2)#8-Th-Te(1)#2	74.93(4)
Te(2)#7-Th-Te(1)#2	74.93(4)
Te(2)#10-Th-Te(1)#2	129.55(3)
Te(2)#9-Th-Te(1)#2	129.55(3)
Te(1)#1-Th-Te(1)#2	140.27(8)
Te(1)#7-Th-Cs	136.36(3)
Te(1)#8-Th-Cs	136.36(3)
Te(2)#8-Th-Cs	56.33(3)
Te(2)#7-Th-Cs	56.33(3)
Te(2)#10-Th-Cs	56.33(3)
Te(2)#9-Th-Cs	56.33(3)
Te(1)#1-Th-Cs	109.86(4)
Te(1)#2-Th-Cs	109.86(4)
Th#13-Te(1)-Th#14	87.29(7)
Th#13-Te(1)-Th#1	104.23(3)
Th#14-Te(1)-Th#1	104.23(3)
Th#13-Te(1)-Th#2	104.23(3)
Th#14-Te(1)-Th#2	104.23(3)
Th#1-Te(1)-Th#2	140.27(8)
Te(2)#15-Te(2)-Te(2)#16	180.00(10)
Te(2)#15-Te(2)-Th#14	61.53(3)
Te(2)#16-Te(2)-Th#14	118.47(3)
Te(2)#15-Te(2)-Th#13	61.53(3)
Te(2)#16-Te(2)-Th#13	118.47(3)
Th#14-Te(2)-Th#13	86.03(5)
Te(2)#15-Te(2)-Cs#3	113.87(3)
Te(2)#16-Te(2)-Cs#3	66.13(3)
Th#14-Te(2)-Cs#3	168.15(6)
Th#13-Te(2)-Cs#3	101.43(5)
Te(2)#15-Te(2)-Cs#4	113.87(3)
Te(2)#16-Te(2)-Cs#4	66.13(3)
Th#14-Te(2)-Cs#4	101.43(5)
Th#13-Te(2)-Cs#4	168.15(6)
Cs#3-Te(2)-Cs#4	69.79(8)
Te(2)#15-Te(2)-Cs#13	67.15(3)
Te(2)#16-Te(2)-Cs#13	112.85(3)
Th#14-Te(2)-Cs#13	126.98(5)
Th#13-Te(2)-Cs#13	80.99(6)
Cs#3-Te(2)-Cs#13	46.74(3)
Cs#4-Te(2)-Cs#13	87.16(4)
Te(2)#15-Te(2)-Cs#14	67.15(3)
Te(2)#16-Te(2)-Cs#14	112.85(3)
Th#14-Te(2)-Cs#14	80.99(6)
Th#13-Te(2)-Cs#14	126.98(5)
Cs#3-Te(2)-Cs#14	87.16(4)
Cs#4-Te(2)-Cs#14	46.74(3)
Cs#13-Te(2)-Cs#14	67.52(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1 #2 -x,-y+1,-z #3 -x-1/2,-y+1/2,-z
#4 -x+1/2,-y+1/2,-z #5 -x-1/2,-y+1/2,z+1/2
#6 -x+1/2,-y+1/2,z+1/2 #7 x+1/2,y+1/2,z
#8 x-1/2,y+1/2,z #9 x+1/2,y+1/2,-z+1/2
#10 x-1/2,y+1/2,-z+1/2 #11 x-1,y,z #12 x+1,y,z
#13 x-1/2,y-1/2,z #14 x+1/2,y-1/2,z #15 x,y,-z+1/2
#16 x,y,-z-1/2