

Inorg. Chem., 1996, 35(13), 3836-3838, DOI:10.1021/ic951641b

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Formula	CsTh ₂ Te ₆
Formula mass (amu)	1362.59
Space group	D_{2b}^{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
$\rho_{\rm c} (\rm g \ \rm cm^{-3})$	6.719
T of data collection (K) ^b	113(2)
Crystal shape	Needle $(0.36 \times 0.08 \times 0.01 \text{ mm})$ bounded by $\{100\}$.
· ·	{010}, {001}
Crystal volume (mm ³)	2.88 x 10 ⁻⁴
Radiation	$\lambda(MoK\alpha_1) = 0.7093$
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)	$3.24 \le \theta \le 29.90$
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	$\pm h, \pm k, \pm l$ (2° $\leq 2\theta \leq 23^{\circ}$),
	$\pm h$, $\pm k$, $\pm \ell$ (23° $\leq 2\theta \leq 60^{\circ}$)
No. of data collected	2191
No. of unique data, including	
$0 \ge F_{\rho}^2 \ge -3\sigma(F_{\rho}^2)$	593
Raverage	0.0909
No. of variables	19
$R_{\rm w}(F^2)$ (all data)	0.102
R (on F for $F_{\rho}^2 > 2\sigma(F_{\rho}^2)$	0.049
Error in observation of unit weight (e^2)	1.30

Table SI. Crystal Data and Intensity Collection Details for CsTh₂Te₆.

a.

Obtained from a refinement with the constraints $\alpha = \beta = \gamma = 90^{\circ}$. The low-temperature system is based on a design by Huffman.²³ b.

The analytical method, as employed in the Northwestern absorption program AGNOST, c. was used for the absorption correction.²⁴

d. The diffractometer was operated with the use of the Indiana University PCPS system.³² 0.009(2)

0.0100(5)

0.0094(9)

0.0096(6)

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Cs

 \mathbf{Th}

Te(1)

Te(2)

0.018(2)

0.0063(5) 0.0070(8)

0.0086(6)

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3

0.000

0.000

Table SII. Anisotropic displacement parameters $(Å^2)$ for CsTh ₂ Te ₆ . The anisotropic displacement factor exponent takes the form: -2 π^2 [$h^2 a^{*2}$ U11 + + 2 h k a* b* U12]							
atom	U11	U22	U33	U23	U1 3	U12	

0.019(2)

0.0050(5)

0.0043(8) 0.0104(6)

0.000

0.000

0.000

-0.0010(5)

0.000

0.000

0.000

0.000

Table	SII.	Anisotr	opic	disp	laceme	ent pa:	ramet	ers (1	Ų) f	lor	$CsTh_2Te_6$.
The an	isotrop	bic disp	lacem	ent	factor	expo	nent	takes	the	for	rm:
$-2 \pi^2$	$[h^2 a^{*2}]$	'U11 +	+	2 h	k a*	b* Ū12	2 1				

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Table SIII.	Bond lengths	s (Å)	and angles	(deg.)	for	$CsTh_2Te_6.$
$\begin{array}{c} Cs - Cs \# 1 \\ Cs - Cs \# 2 \\ Cs - Te(2) \# 3 \\ Cs - Te(2) \# 4 \\ Cs - Te(2) \# 5 \\ Cs - Te(2) \# 6 \\ Cs - Te(2) \# 6 \\ Cs - Te(2) \# 8 \\ Cs - Te(2) \# 8 \\ Cs - Te(2) \# 9 \\ Cs - Te(2) \# 10 \\ Cs - Cs \# 11 \\ Cs - Cs \# 12 \\ Th - Te(1) \# 7 \\ Th - Te(1) \# 7 \\ Th - Te(1) \# 8 \\ Th - Te(2) \# 10 \\ Th - Te(1) \# 1 \\ Th - Te(1) \# 1 \\ Th - Te(1) \# 1 \\ Th - Te(1) - Th \# 1 \\ Te(2) - Te(2) \# 1 \\ Te(2) - Te(2) \# 1 \\ Te(2) - Te(2) \# 1 \\ Te(2) - Th \# 1 \\ Te(2) - Cs \# 3 \\ Te(2) - Cs \# 1 \\ Te(2) - Cs \# 1 \\ \end{array}$	-5		3.074(2) 3.074(2) 3.817(4) 3.817(4) 3.817(4) 3.817(4) 3.929(4) 3.929(4) 3.929(4) 3.929(4) 4.367(2) 4.367(2) 4.367(2) 3.164(2) 3.201(2) 3.201(2) 3.201(2) 3.264(2) 3.264(2) 3.164(2) 3.164(2) 3.292(4) 3.201(2) 3.201(2) 3.201(2) 3.201(2) 3.264(2) 3.264(2) 3.264(2) 3.264(2) 3.264(2) 3.292(4) 3.292(4) 3.929(4) 3.929(4)			
Cs#1-Cs-Cs#2 Cs#1-Cs-Te(2) Cs#2-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Te(2)#3-Cs-Te(2) Te(2)#3-Cs-Te(2) Te(2)#4-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#4-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Te(2)#3-Cs-Te(2) Te(2)#3-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#4-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#4-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#4-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3-Cs-Te(2) Cs#2-Cs-Te(2) Te(2)#3	#3 #4 #4 #4 #4 #4 #2 #4 #2 #5 #46 (2) #6 (2) #6 (2) #6 (2) #6 (2) #6 (2) #6 (2) #7 #(2) #7 (2) #7 (3) #7 (3) #8 (2) #8 (2) #8 (2) #8		73.8(3) 16.3(2) 68.56(11) 16.3(2) 68.56(11) 69.79(8) 68.56(11) 16.3(2) 47.73(6) 88.97(10) 47.73(6) 69.79(8) 10.4(2) 64.70(12) 33.26(3) 92.84(4) 78.18(9) 11.33(4) 10.4(2) 64.70(12) 92.84(4) 78.18(9) 11.33(4) 10.3(2) 11.33(4) 11.33(4)			

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Table SIII. Bond lengths	(A) and angles	(deg.)	for CsTh
Cs-Cs#1 Cs-Cs#2 Cs-Te(2)#3 Cs-Te(2)#4 Cs-Te(2)#5 Cs-Te(2)#7 Cs-Te(2)#8 Cs-Te(2)#9 Cs-Te(2)#9 Cs-Te(2)#9 Cs-Te(2)#10 Cs-Cs#12 Th-Te(1)#7 Th-Te(1)#8 Th-Te(2)#7 Th-Te(2)#7 Th-Te(2)#7 Th-Te(2)#9 Th-Te(2)#9 Th-Te(1)#1 Th-Te(1)#2 Te(1)-Th#13 Te(1)-Th#14 Te(1)-Th#14 Te(2)-Te(2)#16 Te(2)-Cs#4 Te(2)-Cs#13	3.074(2) 3.074(2) 3.817(4) 3.817(4) 3.817(4) 3.929(4) 3.929(4) 3.929(4) 3.929(4) 4.367(2) 4.367(2) 3.164(2) 3.164(2) 3.201(2) 3.201(2) 3.201(2) 3.201(2) 3.201(2) 3.264(2) 3.164(2) 3.264(2) 3.264(2) 3.264(2) 3.264(2) 3.264(2) 3.264(2) 3.201(2) 3.201(2) 3.264(2) 3.292(4) 3.201(2) 3.20		
Cs#1-Cs-Cs#2 $Cs#1-Cs-Te(2)#3$ $Cs#2-Cs-Te(2)#4$ $Cs#2-Cs-Te(2)#4$ $Cs#2-Cs-Te(2)#4$ $Cs#1-Cs-Te(2)#5$ $Cs#2-Cs-Te(2)#5$ $Te(2)#3-Cs-Te(2)#5$ $Cs#2-Cs-Te(2)#5$ $Cs#1-Cs-Te(2)#6$ $Te(2)#3-Cs-Te(2)#6$ $Te(2)#3-Cs-Te(2)#6$ $Te(2)#3-Cs-Te(2)#6$ $Te(2)#3-Cs-Te(2)#6$ $Te(2)#3-Cs-Te(2)#6$ $Te(2)#4-Cs-Te(2)#6$ $Te(2)#4-Cs-Te(2)#6$ $Cs#1-Cs-Te(2)#7$ $Te(2)#3-Cs-Te(2)#7$ $Te(2)#3-Cs-Te(2)#7$ $Te(2)#4-Cs-Te(2)#7$ $Te(2)#3-Cs-Te(2)#7$ $Te(2)#4-Cs-Te(2)#7$ $Te(2)#4-Cs-Te(2)#7$ $Te(2)#6-Cs-Te(2)#7$ $Te(2)#6-Cs-Te(2)#7$ $Cs#1-Cs-Te(2)#8$ $Cs#2-Cs-Te(2)#8$ $Te(2)#4-Cs-Te(2)#8$ $Te(2)#4-Cs-Te(2)#8$	173.8(3) $116.3(2)$ $68.56(11)$ $116.3(2)$ $68.56(11)$ $69.79(8)$ $68.56(11)$ $116.3(2)$ $47.73(6)$ $88.97(10)$ $68.56(11)$ $116.3(2)$ $88.97(10)$ $47.73(6)$ $69.79(8)$ $110.4(2)$ $64.70(12)$ $133.26(3)$ $92.84(4)$ $178.18(9)$ $111.33(4)$ $110.4(2)$ $64.70(12)$ $92.84(4)$ $178.18(9)$ $111.33(4)$ $110.4(2)$ $64.70(12)$ $92.84(4)$ $133.26(3)$ $111.33(4)$ $133.26(3)$ $111.33(4)$		

Table	SIII.	Bond	lengths	(Å)	anđ	angles	(deg.)	for	$CsTh_2Te_6$.
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Te	
me i	e(2)#6-Cs-Te(2)#8
- 1 (H)	(2) #7 - Cs - Te(2) #8
Cat	1 - C = T = (2) # 9
Car	2 - 2 = 2 = 12(2) + 2
CS	2-CS-Te(2)#9
Te (2)#3-Cs-Te(2)#9
Te (2)#4-Cs-Te(2)#9
Te	2) #5-Cs-Te(2) #9
Tel	(2) # 6 - C = -T + (2) # 9
Te i	(2) # 0 C3 Ie(2) # 0
Ter	(2) = 7 - (2) = 10 (2) = 9
Te	2)#8-Cs-Te(2)#9
Cst	1-Cs-Te(2)#10
Cst	2-Cs-Te(2)#10
Tel	2)#3-Cs-Te(2)#10
To	2) # 1 = C = T = (2) # 10
	$(2) \# = C_{2} \# = (2) \# = 0$
Tet	(2) = 5 - CS - Te(2) = 10
'I'e (2)#6-Cs-Te(2)#10
Te (2)#7-Cs-Te(2)#10
Te (2)#8-Cs-Te(2)#10
Te (2) #9 - Cs - Te(2) #10
Cat	1-Cs-Cs#11
Cat	2 - Ca - Ca + 11
C 3 ft	2) 40 Carta 2) 40 Carta
Te (
Te (2)#4-Cs-Cs#11
Te (2)#5-Cs-Cs#11
Te (2)#6-Cs-Cs#11
Te (2)#7-Cs-Cs#11
Tel	2) #8-Cs-Cs#11
To	2) #9 - Ca - Ca #11
me	2) + 3 - CS - CS + 11
Tet	
Csł	1-Cs-Cs#12
Csł	2-Cs-Cs#12
Te (2)#3-Cs-Cs#12
Tel	2) #4 - Cs - Cs #12
Tel	$2) \pm 5 - Ca - Ca \pm 12$
me	2) + 5 - C = C = + 12
Tet	
Te (
	2)#/-CS-CS#12
Te (2)#7-CS-CS#12 2)#8-Cs-Cs#12
Te (Te (2)#7-CS-CS#12 2)#8-Cs-Cs#12 2)#9-Cs-Cs#12
Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12
Te (Te (Te (Csi	2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12
Te (Te (Te (Cs#	2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-CD-CS(1)#8
Te (Te (Te (Cs# Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(1)#8
Te (Te (Te (Cs# Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8
Te (Te (Te (Cs# Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8
Te (Te (Te (Cs # Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8 1)#7-Th-Te(2)#7
Te (Te (Te (Te (Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8 1)#7-Th-Te(2)#7 1)#8-Th-Te(2)#7
Te (Te (Te (Cs # Te (Te (Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 11-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8 1)#8-Th-Te(2)#7 1)#8-Th-Te(2)#7 2)#8-Th-Te(2)#7
Te (Te (Te (Cs ii Te (Te (Te (Te (Te (2) #7-CS-CS#12 2) #8-CS-CS#12 2) #9-CS-CS#12 2) #10-CS-CS#12 11-CS-CS#12 1) #7-Th-Te(1) #8 1) #7-Th-Te(2) #8 1) #8-Th-Te(2) #8 1) #8-Th-Te(2) #7 1) #8-Th-Te(2) #7 2) #8-Th-Te(2) #7 1) #7-Th-Te(2) #10
Te (Te (Cs # Te (Te (Te (Te (Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8 1)#7-Th-Te(2)#7 1)#8-Th-Te(2)#7 2)#8-Th-Te(2)#7 1)#8-Th-Te(2)#10 1)#8-Th-Te(2)#10
Te (Te (Cs # Te (Te (Te (Te (Te (Te (Te (Te (2)#7-CS-CS#12 2)#8-CS-CS#12 2)#9-CS-CS#12 2)#10-CS-CS#12 1)#7-Th-Te(1)#8 1)#7-Th-Te(2)#8 1)#8-Th-Te(2)#8 1)#8-Th-Te(2)#7 1)#8-Th-Te(2)#7 2)#8-Th-Te(2)#7 1)#7-Th-Te(2)#10 1)#8-Th-Te(2)#10 2)#8-Th-Te(2)#10
Te (Te (Te (Te (Te (Te (Te (Te (2) #7-CS-CS#12 2) #8-CS-CS#12 2) #9-CS-CS#12 2) #10-CS-CS#12 11-CS-CS#12 1) #7-Th-Te(1) #8 1) #7-Th-Te(2) #8 1) #8-Th-Te(2) #8 1) #8-Th-Te(2) #7 1) #8-Th-Te(2) #7 2) #8-Th-Te(2) #7 1) #7-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10
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Te (Te (Te (Te (Te (Te (Te (Te (2) #7-CS-CS#12 2) #8-CS-CS#12 2) #9-CS-CS#12 11-CS-CS#12 1) #7-Th-Te(1) #8 1) #7-Th-Te(2) #8 1) #8-Th-Te(2) #8 1) #8-Th-Te(2) #7 1) #8-Th-Te(2) #7 2) #8-Th-Te(2) #7 1) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #7-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #9 1) #8-Th-Te(2) #9 2) #8-Th-Te(2) #9 2) #8-Th-Te(2) #9
Te() Te() CS#() CTe() Te() Te() Te() Te() Te() Te() Te()	2) #7-CS-CS#12 2) #8-CS-CS#12 2) #9-CS-CS#12 2) #10-CS-CS#12 11-CS-CS#12 1) #7-Th-Te(1) #8 1) #7-Th-Te(2) #8 1) #8-Th-Te(2) #8 1) #8-Th-Te(2) #7 1) #8-Th-Te(2) #7 2) #8-Th-Te(2) #7 1) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #10 2) #8-Th-Te(2) #9 1) #8-Th-Te(2) #9 2) #8-Th-Te(2) #9 2) #8-Th-Te(2) #9 2) #7-Th-Te(2) #9 2) #7-Th-Te(2) #9 2) #7-Th-Te(2) #9
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178.18(9) 67.51(8) 6 4 .70(12)	
110.4(2) 178.18(9) 111.33(4)	
133.26(3) 92.84(4) 45.70(6) 85.36(10)	
64.70(12) 110.4(2) 111.33(4)	
178.18(9) 92.84(4) 133.26(3) 85.36(10)	
45.70(6) 67.51(8) 90.0	
90.0 55.10(4) 124.90(4)	
124.90(4) 123.76(4) 56.24(4)	
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55.10(4) 124.90(4) 55.11(4)	
56.24(4) 123.76(4)	
56.24(4) 123.76(4) 180.0(2)	
87.29(7) 150.70(3)	
86.01(4) 86.01(4)	
150.70(3) 86.03(5)	
86.01(4)	
112.66(6) 86 01(4)	
150.70(3) 112.66(6)	
56.94(6) 86.03(5)	
75.77(3) 75.77(3)	
129.55(3) 129.55(3) 74.02(4)	
74.93(4) 75.77(3)	

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Te(1)#8-Th-Te(1)#2 Te(2)#8-Th-Te(1)#2 Te(2)#7-Th-Te(1)#2 Te(2)#10-Th-Te(1)#2 Te(2)#9-Th-Te(1)#2 Te(1)#1-Th-Te(1)#2 Te(1)#7-Th-Cs Te(1)#8-Th-Cs Te(2)#8-Th-Cs Te(2)#7-Th-Cs	$\begin{array}{c} 75.77(3) \\ 74.93(4) \\ 74.93(4) \\ 129.55(3) \\ 129.55(3) \\ 140.27(8) \\ 136.36(3) \\ 136.36(3) \\ 56.33(3) \\ 56.33(3) \\ 56.33(3) \end{array}$
Te (2) #10-Th-Cs Te (2) #9-Th-Cs Te (1) #1-Th-Cs Te (1) #2-Th-Cs Th#13-Te (1) -Th#14 Th#13-Te (1) -Th#14 Th#14-Te (1) -Th#1 Th#13-Te (1) -Th#2 Th#14-Te (1) -Th#2	56.33(3) 56.33(3) 109.86(4) 109.86(4) 87.29(7) 104.23(3) 104.23(3) 104.23(3)
Th#1-Te(1) -Th#2 Te(2)#15-Te(2)-Te(2)#16 Te(2)#15-Te(2)-Th#14 Te(2)#16-Te(2)-Th#14 Te(2)#16-Te(2)-Th#13 Te(2)#16-Te(2)-Th#13 Th#14-Te(2)-Th#13 Te(2)#15-Te(2)-Cs#3	$140.27(8) \\ 140.27(8) \\ 180.00(10) \\ 61.53(3) \\ 118.47(3) \\ 61.53(3) \\ 118.47(3) \\ 86.03(5) \\ 113.87(3)$
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)
W= (2) #15 W= (2) - Cs#4	67.15(2)
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)
Tb#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