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Table 1. Crystal data and structure refinement for cz028s, $[Tl(ONep)]_4$, **4**.

Identification code	cz028s
Empirical formula	C20 H44 O4 Tl4
Formula weight	1166.03
Temperature	168(2) K
Wavelength	0.71073 Å
Crystal system	cubic
Space group	P-43n
Unit cell dimensions	a = 18.1390(12) Å _= 90°.
	b = 18.1390(12) Å _= 90°.
	c = 18.1390(12) Å _ = 90°.
Volume	5968.2(7) $Å^3$
Z	8
Density (calculated)	2.595 Mg/m^3
Absorption coefficient	21.553 mm^{-1}
F(000)	4160
Theta range for data collection	1.59 to 23.25∞.
Index ranges	-20<=h<=19, -15<=k<=20, -20<=l<=20
Reflections collected	25533
Independent reflections	1449 [R(int) = 0.0807]
Completeness to theta = 23.25∞	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1449 / 3 / 34
Goodness-of-fit on F^2	1.306
Final R indices [I>2sigma(I)]	R1 = 0.0682, wR2 = 0.2015
R indices (all data)	R1 = 0.1049, wR2 = 0.2215
Absolute structure parameter	0.52(13)
Largest diff. peak and hole	1.884 and -2.174 $e·Å^{-3}$

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3)

for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tl(1)	768(1)	4301(1)	1772(1)	100(1)
Tl(2)	-730(1)	730(1)	730(1)	102(1)
O(1)	586(9)	5643(9)	1873(9)	84(5)
C(1)	1285(9)	5933(18)	1714(15)	260(30)
C(2)	1367(12)	6441(12)	1091(12)	57(7)
C(3)	1190(40)	6030(30)	352(11)	480(60)
C(4)	1992(16)	6850(20)	990(20)	390(50)
C(5)	740(20)	7079(18)	1180(40)	390(50)
O(2)	617(12)	617(12)	617(12)	102(12)
C(6)	959(11)	728(13)	1454(4)	16(10)
C(7)	1290(20)	1492(16)	1520(16)	54(19)
C(8)	1322(18)	880(20)	2098(9)	125(19)
C(9)	1670(30)	1610(30)	2250(20)	210(70)

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Table 3. Bond lengths [Å] and angles [°] for **4**.

Tl(1)-O(1)	2.463(15)
Tl(1)-O(1)#1	2.464(17)
Tl(1)-O(1)#2	2.475(17)
Tl(1)-Tl(1)#3	3.750(2)
Tl(1)-Tl(1)#2	3.750(2)
Tl(1)-Tl(1)#1	3.766(3)
Tl(2)-O(2)#4	2.460(18)
Tl(2)-O(2)#5	2.460(18)
Tl(2)-O(2)	2.460(18)
Tl(2)-Tl(2)#6	3.746(4)
Tl(2)-Tl(2)#4	3.746(4)
Tl(2)-Tl(2)#5	3.746(4)
O(1)-C(1)	1.4023
O(1)-Tl(1)#1	2.464(17)
O(1)-Tl(1)#3	2.475(17)
C(1)-C(2)	1.4668
C(2)-C(4)	1.3693
C(2)-C(3)	1.5692
C(2)-C(5)	1.6323
O(2)-C(6)#7	1.65(3)
O(2)-C(6)	1.65(2)
O(2)-C(6)#8	1.65(2)
O(2)-Tl(2)#4	2.460(18)
O(2)-Tl(2)#5	2.460(18)
C(6)-C(8)	1.3694
C(6)-C(7)#8	1.44(2)
C(6)-C(7)	1.5136
C(6)-C(6)#7	1.65(3)
C(6)-C(6)#8	1.65(4)
C(6)-C(7)#7	1.76(4)
C(7)-C(7)#7	0.56(10)
C(7)-C(7)#8	0.56(8)
C(7)-C(8)#7	1.37(3)
C(7)-C(6)#7	1.438(16)

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C(7)-C(9)#7	1.52(2)
C(7)-C(9)	1.5090
C(7)-C(8)	1.5320
C(7)-C(6)#8	1.757(18)
C(7)-C(9)#8	1.78(6)
C(7)-C(8)#8	1.90(4)
C(8)-C(7)#8	1.37(5)
C(8)-C(9)	1.4996
C(8)-C(7)#7	1.90(6)
C(9)-C(9)#7	1.56(7)
C(9)-C(9)#8	1.56(6)
C(9)-C(7)#8	1.516(17)
C(9)-C(7)#7	1.78(5)

O(1)-Tl(1)-O(1)#1	79.7(6)
O(1)-Tl(1)-O(1)#2	80.3(6)
O(1)#1-Tl(1)-O(1)#2	80.3(6)
O(1)-Tl(1)-Tl(1)#3	40.7(4)
O(1)#1-Tl(1)-Tl(1)#3	83.4(4)
O(1)#2-Tl(1)-Tl(1)#3	40.5(4)
O(1)-Tl(1)-Tl(1)#2	83.4(4)
O(1)#1-Tl(1)-Tl(1)#2	40.7(4)
O(1)#2-Tl(1)-Tl(1)#2	40.5(4)
Tl(1)#3-Tl(1)-Tl(1)#2	60.28(5)
O(1)-Tl(1)-Tl(1)#1	40.2(4)
O(1)#1-Tl(1)-Tl(1)#1	40.2(4)
O(1)#2-Tl(1)-Tl(1)#1	82.9(4)
Tl(1)#3-Tl(1)-Tl(1)#1	59.86(2)
Tl(1)#2-Tl(1)-Tl(1)#1	59.86(2)
O(2)#4-Tl(2)-O(2)#5	80.0(12)
O(2)#4-Tl(2)-O(2)	80.0(12)
O(2)#5-Tl(2)-O(2)	80.0(12)
O(2)#4-Tl(2)-Tl(2)#6	40.4(5)
O(2)#5-Tl(2)-Tl(2)#6	40.4(5)
O(2)-Tl(2)-Tl(2)#6	83.2(8)
O(2)#4-Tl(2)-Tl(2)#4	40.4(5)

O(2)#5-Tl(2)-Tl(2)#4	83.2(8)
O(2)-Tl(2)-Tl(2)#4	40.4(5)
Tl(2)#6-Tl(2)-Tl(2)#4	60.0
O(2)#4-Tl(2)-Tl(2)#5	83.2(8)
O(2)#5-Tl(2)-Tl(2)#5	40.4(5)
O(2)-Tl(2)-Tl(2)#5	40.4(5)
Tl(2)#6-Tl(2)-Tl(2)#5	60.0
Tl(2)#4-Tl(2)-Tl(2)#5	60.0
C(1)-O(1)-Tl(1)	103.5(15)
C(1)-O(1)-Tl(1)#1	150.5(9)
Tl(1)-O(1)-Tl(1)#1	99.7(6)
C(1)-O(1)-Tl(1)#3	95.5(13)
Tl(1)-O(1)-Tl(1)#3	98.8(6)
Tl(1)#1-O(1)-Tl(1)#3	98.8(6)
O(1)-C(1)-C(2)	119.0
C(4)-C(2)-C(1)	122.1
C(4)-C(2)-C(3)	108.0
C(1)-C(2)-C(3)	109.7
C(4)-C(2)-C(5)	101.9
C(1)-C(2)-C(5)	107.2
C(3)-C(2)-C(5)	106.7
C(6)#7-O(2)-C(6)	59.8(16)
C(6)#7-O(2)-C(6)#8	59.8(8)
C(6)-O(2)-C(6)#8	59.8(14)
C(6)#7-O(2)-Tl(2)	90.8(3)
C(6)-O(2)-Tl(2)	106.6(9)
C(6)#8-O(2)-Tl(2)	150.5(9)
C(6)#7-O(2)-Tl(2)#4	106.6(13)
C(6)-O(2)-Tl(2)#4	150.5(13)
C(6)#8-O(2)-Tl(2)#4	90.8(14)
Tl(2)-O(2)-Tl(2)#4	99.1(10)
C(6)#7-O(2)-Tl(2)#5	150.5(16)
C(6)-O(2)-Tl(2)#5	90.8(8)
C(6)#8-O(2)-Tl(2)#5	106.6(10)
Tl(2)-O(2)-Tl(2)#5	99.1(10)
Tl(2)#4-O(2)-Tl(2)#5	99.1(10)

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C(8)-C(6)-C(7)#8	58.5(19)
C(8)-C(6)-C(7)	64.0
C(7)#8-C(6)-C(7)	22(3)
C(8)-C(6)-C(6)#7	115.4(7)
C(7)#8-C(6)-C(6)#7	69(2)
C(7)-C(6)-C(6)#7	53.9(3)
C(8)-C(6)-C(6)#8	111.7(6)
C(7)#8-C(6)-C(6)#8	58.3(12)
C(7)-C(6)-C(6)#8	67.4(10)
C(6)#7-C(6)-C(6)#8	60.0(7)
C(8)-C(6)-O(2)	171.63(12)
C(7)#8-C(6)-O(2)	113.4(18)
C(7)-C(6)-O(2)	109.4(5)
C(6)#7-C(6)-O(2)	60.1(12)
C(6)#8-C(6)-O(2)	60.1(6)
C(8)-C(6)-C(7)#7	73.7(13)
C(7)#8-C(6)-C(7)#7	17(2)
C(7)-C(6)-C(7)#7	18(3)
C(6)#7-C(6)-C(7)#7	52.7(8)
C(6)#8-C(6)-C(7)#7	50(2)
O(2)-C(6)-C(7)#7	98.6(15)
C(7)#7-C(7)-C(7)#8	60.0(4)
C(7)#7-C(7)-C(8)#7	95(4)
C(7)#8-C(7)-C(8)#7	155(4)
C(7)#7-C(7)-C(6)#7	87(2)
C(7)#8-C(7)-C(6)#7	115.7(9)
C(8)#7-C(7)-C(6)#7	58.2(10)
C(7)#7-C(7)-C(9)#7	79(5)
C(7)#8-C(7)-C(9)#7	109(4)
C(8)#7-C(7)-C(9)#7	62.3(18)
C(6)#7-C(7)-C(9)#7	117(2)
C(7)#7-C(7)-C(9)	110(2)
C(7)#8-C(7)-C(9)	80(2)
C(8)#7-C(7)-C(9)	111(3)
C(6)#7-C(7)-C(9)	162(3)
C(9)#7-C(7)-C(9)	62(3)

C(7)#7-C(7)-C(6)	106(3)
C(7)#8-C(7)-C(6)	72(3)
C(8)#7-C(7)-C(6)	120.0(17)
C(6)#7-C(7)-C(6)	67.8(9)
C(9)#7-C(7)-C(6)	174(5)
C(9)-C(7)-C(6)	112.5
C(7)#7-C(7)-C(8)	123(5)
C(7)#8-C(7)-C(8)	63(5)
C(8)#7-C(7)-C(8)	141(5)
C(6)#7-C(7)-C(8)	118.6(16)
C(9)#7-C(7)-C(8)	121(3)
C(9)-C(7)-C(8)	59.1
C(6)-C(7)-C(8)	53.4
C(7)#7-C(7)-C(6)#8	47.5(9)
C(7)#8-C(7)-C(6)#8	55.8(15)
C(8)#7-C(7)-C(6)#8	109(2)
C(6)#7-C(7)-C(6)#8	61.1(9)
C(9)#7-C(7)-C(6)#8	125(5)
C(9)-C(7)-C(6)#8	135.6(15)
C(6)-C(7)-C(6)#8	59.9(14)
C(8)-C(7)-C(6)#8	99(2)
C(7)#7-C(7)-C(9)#8	53.8(8)
C(7)#8-C(7)-C(9)#8	53(3)
C(8)#7-C(7)-C(9)#8	114(2)
C(6)#7-C(7)-C(9)#8	140.0(19)
C(9)#7-C(7)-C(9)#8	55.7(14)
C(9)-C(7)-C(9)#8	55.8(18)
C(6)-C(7)-C(9)#8	124(4)
C(8)-C(7)-C(9)#8	92(4)
C(6)#8-C(7)-C(9)#8	91(2)
C(7)#7-C(7)-C(8)#8	18(2)
C(7)#8-C(7)-C(8)#8	42(2)
C(8)#7-C(7)-C(8)#8	113(2)
C(6)#7-C(7)-C(8)#8	96.0(14)
C(9)#7-C(7)-C(8)#8	88(5)
C(9)-C(7)-C(8)#8	101.6(16)

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C(6)-C(7)-C(8)#8	96(2)
C(8)-C(7)-C(8)#8	106(3)
C(6)#8-C(7)-C(8)#8	43.8(6)
C(9)#8-C(7)-C(8)#8	48.0(16)
C(7)#8-C(8)-C(6)	63.2(4)
C(7)#8-C(8)-C(9)	63.5(8)
C(6)-C(8)-C(9)	122.3
C(7)#8-C(8)-C(7)	21(3)
C(6)-C(8)-C(7)	62.6
C(9)-C(8)-C(7)	59.7
C(7)#8-C(8)-C(7)#7	7.1(17)
C(6)-C(8)-C(7)#7	62.56(17)
C(9)-C(8)-C(7)#7	61.8(7)
C(7)-C(8)-C(7)#7	14(3)
C(9)#7-C(9)-C(9)#8	60.0(18)
C(9)#7-C(9)-C(7)#8	70.7(16)
C(9)#8-C(9)-C(7)#8	58.8(11)
C(9)#7-C(9)-C(8)	120.4(6)
C(9)#8-C(9)-C(8)	102(2)
C(7)#8-C(9)-C(8)	54(2)
C(9)#7-C(9)-C(7)	59.2(8)
C(9)#8-C(9)-C(7)	71(2)
C(7)#8-C(9)-C(7)	21(3)
C(8)-C(9)-C(7)	61.2
C(9)#7-C(9)-C(7)#7	53(3)
C(9)#8-C(9)-C(7)#7	53.6(10)
C(7)#8-C(9)-C(7)#7	17(2)
C(8)-C(9)-C(7)#7	70.2(10)
C(7)-C(9)-C(7)#7	17(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,z #2 y-1/2,-x+1/2,-z+1/2 #3 -y+1/2,x+1/2,-z+1/2

#4 -x,y,-z #5 -x,-y,z #6 x,-y,-z #7 y,z,x

#8 z,x,y

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Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tl(1)	98(1)	88(1)	115(1)	-28(1)	37(1)	16(1)
Tl(2)	102(1)	102(1)	102(1)	-25(1)	25(1)	25(1)

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Table 1. Crystal data and structure refinement for $[Tl(DMP)]_\infty$, **5**.

Identification code	cz024s
Empirical formula	C8 H9 O Tl
Formula weight	325.52
Temperature	168(2) K
Wavelength	0.71073 Å
Crystal system, space group	Rhombohedral, R3c
Unit cell dimensions	a = 25.2686(18) Å alpha = 90°. b = 25.2686(18) Å beta = 90°. c = 6.6317(7) Å gamma = 120°.
Volume	3667.1(5) Å^3
Z, Calculated density	18, 2.653 Mg/m^3
Absorption coefficient	19.747 mm^-1
F(000)	2628
Crystal size	0.2mm x 0.3mm x 0.5mm
Theta range for data collection	1.61 to 28.14 deg.
Limiting indices	-33<=h<=24, -31<=k<=32, -8<=l<=8
Reflections collected / unique	7296 / 1867 [R(int) = 0.0384]
Completeness to theta = 28.14	96.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1867 / 1 / 93
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0221, wR2 = 0.0514
R indices (all data)	R1 = 0.0235, wR2 = 0.0520
Absolute structure parameter	0.008(16)
Largest diff. peak and hole	1.014 and -1.102 e.Å^-3

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Table S5.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Tl(1)	7131(1)	5475(1)	8726(1)	37(1)
O(1)	7457(2)	5445(2)	5047(6)	38(1)
C(1)	6981(3)	5372(3)	3949(12)	31(1)
C(2)	6507(3)	4777(3)	3425(9)	35(1)
C(3)	5999(3)	4711(3)	2394(11)	37(2)
C(4)	5938(3)	5204(3)	1895(11)	38(2)
C(5)	6404(3)	5786(3)	2374(10)	34(1)
C(6)	6931(3)	5884(3)	3383(9)	32(1)
C(8)	7431(4)	6507(3)	3895(14)	49(2)
C(7)	6577(4)	4232(4)	3930(13)	52(2)

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Table S5.3. Bond lengths [Å] and angles [°] for **5**.

Tl(1)-O(1)#1	2.372(4)
Tl(1)-O(1)	2.589(4)
O(1)-C(1)	1.339(8)
O(1)-Tl(1)#2	2.372(4)
C(1)-C(6)	1.411(10)
C(1)-C(2)	1.419(9)
C(2)-C(3)	1.389(9)
C(2)-C(7)	1.512(10)
C(3)-C(4)	1.370(10)
C(4)-C(5)	1.385(10)
C(5)-C(6)	1.397(8)
C(6)-C(8)	1.483(10)
O(1)#1-Tl(1)-O(1)	92.16(8)
C(1)-O(1)-Tl(1)#2	125.0(4)
C(1)-O(1)-Tl(1)	103.8(4)
Tl(1)#2-O(1)-Tl(1)	131.09(18)
O(1)-C(1)-C(6)	120.3(6)
O(1)-C(1)-C(2)	120.2(6)
C(6)-C(1)-C(2)	119.5(6)
C(3)-C(2)-C(1)	119.1(6)
C(3)-C(2)-C(7)	121.4(7)
C(1)-C(2)-C(7)	119.4(6)
C(4)-C(3)-C(2)	121.8(6)
C(3)-C(4)-C(5)	119.2(6)
C(4)-C(5)-C(6)	121.8(6)
C(5)-C(6)-C(1)	118.6(6)
C(5)-C(6)-C(8)	121.9(7)
C(1)-C(6)-C(8)	119.5(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+y+1,y,z+1/2 #2 -x+y+1,y,z-1/2

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Table S5.4. Anisotropic displacement parameters (Å^2 x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Tl(1)	38(1)	65(1)	21(1)	-1(1)	0(1)	35(1)
O(1)	33(2)	70(3)	21(2)	-3(2)	-5(2)	32(2)
C(1)	25(3)	47(4)	20(3)	-1(3)	2(3)	17(3)
C(2)	37(3)	48(4)	25(3)	6(3)	5(2)	26(3)
C(3)	31(3)	31(3)	36(4)	6(3)	-2(3)	5(3)
C(4)	21(3)	55(4)	35(4)	9(3)	-3(2)	18(3)
C(5)	37(3)	48(4)	28(3)	5(3)	3(3)	29(3)
C(6)	29(3)	43(3)	25(3)	-5(3)	3(2)	18(3)
C(8)	53(4)	41(4)	44(5)	-7(3)	-1(3)	15(4)
C(7)	71(6)	48(4)	43(5)	6(3)	-5(4)	34(4)

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Table S5.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(3)	5685	4313	2025	45
H(4)	5581	5148	1229	45
H(5)	6365	6128	2007	41
H(8A)	7355	6811	3245	74
H(8B)	7822	6558	3419	74
H(8C)	7448	6563	5360	74
H(7A)	6182	3856	3768	78
H(7B)	6716	4264	5328	78
H(7C)	6877	4221	3022	78

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Table S6.1. Crystal data and structure refinement for $[Tl(DIP)]_\infty$, **6**.

Identification code	cz026s
Empirical formula	$C_{12}H_{17}OTl$
Formula weight	381.63
Temperature	168(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 9.5104(17) Å alpha = 90°
	b = 6.5998(12) Å beta = 102.591(2)°
	c = 20.268(4) Å gamma = 90°
Volume	1241.5(4) Å^3
Z, Calculated density	4, 2.042 Mg/m^3
Absorption coefficient	12.978 mm^-1
F(000)	712
Crystal size	0.2mm x 0.3mm x 0.7mm
Theta range for data collection	2.06 to 28.16°
Limiting indices	-12<=h<=10, -8<=k<=7, -25<=l<=26
Reflections collected / unique	7598 / 2831 [R(int) = 0.1057]
Completeness to theta = 28.16	92.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2831 / 0 / 131
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1879
R indices (all data)	R1 = 0.0808, wR2 = 0.2000
Largest diff. peak and hole	3.904 and -4.070 e.Å^-3

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Table S6.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **6**. U(eq) is defined as one third of the trace of the Orthogonalized Uij tensor.

	x	y	z	U(eq)
Tl(1)	11657(1)	4500(1)	2697(1)	30(1)
C(2)	12861(11)	9656(16)	3197(5)	23(2)
C(1)	11946(10)	9334(14)	2549(5)	17(2)
C(6)	12374(12)	10232(15)	1977(5)	21(2)
C(4)	14563(10)	11590(18)	2703(6)	30(2)
C(3)	14164(12)	10763(16)	3257(6)	26(2)
C(5)	13647(11)	11318(16)	2070(5)	25(2)
O(1)	10784(7)	8199(10)	2467(4)	23(1)
C(10)	11412(14)	9880(20)	1271(6)	31(3)
C(7)	12421(14)	8840(20)	3830(6)	35(3)
C(9)	11970(30)	10580(20)	4232(8)	62(5)
C(11)	11895(15)	7870(20)	985(6)	42(3)
C(8)	13582(15)	7600(30)	4265(6)	53(4)
C(12)	11450(18)	11570(30)	779(7)	57(4)

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Table S6.3. Bond lengths [Å] and angles [°] for **6**.

Tl(1)-O(1)#1	2.429(7)
Tl(1)-O(1)	2.588(7)
C(2)-C(3)	1.421(15)
C(2)-C(1)	1.424(14)
C(2)-C(7)	1.531(14)
C(1)-O(1)	1.316(12)
C(1)-C(6)	1.438(14)
C(6)-C(5)	1.384(15)
C(6)-C(10)	1.539(16)
C(4)-C(3)	1.375(17)
C(4)-C(5)	1.396(15)
O(1)-Tl(1)#2	2.429(7)
C(10)-C(12)	1.500(19)
C(10)-C(11)	1.555(18)
C(7)-C(8)	1.497(18)
C(7)-C(9)	1.522(19)
O(1)#1-Tl(1)-O(1)	92.83(13)
C(3)-C(2)-C(1)	120.1(10)
C(3)-C(2)-C(7)	120.1(10)
C(1)-C(2)-C(7)	119.8(10)
O(1)-C(1)-C(2)	122.0(9)
O(1)-C(1)-C(6)	120.7(9)
C(2)-C(1)-C(6)	117.3(9)
C(5)-C(6)-C(1)	119.8(9)
C(5)-C(6)-C(10)	122.0(10)
C(1)-C(6)-C(10)	118.2(10)
C(3)-C(4)-C(5)	118.2(10)
C(4)-C(3)-C(2)	121.6(10)
C(6)-C(5)-C(4)	122.9(10)
C(1)-O(1)-Tl(1)#2	124.6(6)
C(1)-O(1)-Tl(1)	106.7(5)
Tl(1)#2-O(1)-Tl(1)	128.1(3)
C(12)-C(10)-C(6)	114.3(12)
C(12)-C(10)-C(11)	109.4(12)
C(6)-C(10)-C(11)	108.1(9)
C(8)-C(7)-C(9)	110.8(13)
C(8)-C(7)-C(2)	112.6(10)
C(9)-C(7)-C(2)	110.2(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y-1/2,-z+1/2 #2 -x+2,y+1/2,-z+1/2

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Table S6.4. Anisotropic displacement parameters (Å^2 x 10^3) for **6**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Tl(1)	20(1)	19(1)	52(1)	-2(1)	12(1)	1(1)
C(2)	17(5)	25(6)	30(5)	0(4)	11(4)	1(4)
C(1)	7(4)	18(5)	26(4)	-2(4)	3(4)	4(3)
C(6)	22(5)	14(5)	28(5)	1(4)	4(4)	6(4)
C(4)	3(4)	30(6)	52(6)	-5(5)	-1(4)	3(4)
C(3)	20(5)	18(5)	34(5)	-5(4)	-3(4)	-4(4)
C(5)	26(5)	18(5)	31(5)	7(4)	9(4)	1(4)
O(1)	20(4)	11(3)	40(4)	-2(3)	11(3)	-4(3)
C(10)	30(6)	35(6)	27(5)	7(5)	-1(5)	10(5)
C(7)	40(7)	34(7)	34(6)	1(5)	16(5)	1(5)
C(9)	92(15)	60(12)	51(9)	4(7)	51(10)	3(9)
C(11)	51(8)	36(7)	35(6)	-12(5)	-1(6)	3(6)
C(8)	48(8)	73(11)	40(7)	32(7)	13(6)	5(8)
C(12)	65(10)	57(10)	42(7)	21(7)	-6(7)	-12(8)

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Table S6.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **6**.

	x	y	z	U(eq)
H(4)	15437	12326	2749	36
H(3)	14776	10936	3691	31
H(5)	13909	11905	1686	30
H(10)	10396	9714	1321	38
H(7)	11565	7944	3678	42
H(9A)	12715	11626	4307	94
H(9B)	11831	10071	4668	94
H(9C)	11059	11159	3978	94
H(11A)	12902	7993	948	64
H(11B)	11286	7613	537	64
H(11C)	11800	6754	1289	64
H(8A)	13802	6432	4008	80
H(8B)	13255	7136	4665	80
H(8C)	14450	8435	4407	80
H(12A)	11227	12854	975	86
H(12B)	10734	11308	360	86
H(12C)	12411	11643	679	86