

Appendix 1

Crystal data and structure refinement for **8**

Table 1. Crystal data and structure refinement for Zntiof.

Identification code	zntiof_abs	
Empirical formula	C ₄₄ H ₆₀ S ₁₂ Zn ₂	
Formula weight	1104.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 29.1118(19) Å	a = 90°
	b = 6.4571(4) Å	b = 112.5790(10)°
	c = 28.8391(19) Å	g = 90°.
Volume	5005.6(6) Å ³	
Z	4	
Density (calculated)	1.465 Mg/m ³	
Absorption coefficient	1.490 mm ⁻¹	
F(000)	2304	
Crystal size	0.34 x 0.14 x 0.05 mm ³	
Theta range for data collection	2.53 to 26.50°.	
Index ranges	-36<=h<=14, -7<=k<=7, -35<=l<=35	
Reflections collected	12744	
Independent reflections	4712 [R(int) = 0.0354]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.928 and 0.734	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4712 / 0 / 382	
Goodness-of-fit on F ²	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0324, wR2 = 0.0718	
R indices (all data)	R1 = 0.0582, wR2 = 0.0838	
Extinction coefficient	0	
Largest diff. peak and hole	0.272 and -0.401 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Zntiof. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	491(1)	2776(1)	329(1)	47(1)
S(1)	1116(1)	3935(1)	1089(1)	43(1)
S(2)	794(1)	-360(1)	836(1)	48(1)
S(3)	1786(1)	2517(1)	2214(1)	43(1)
S(4)	-359(1)	3361(1)	209(1)	41(1)
S(5)	446(1)	2323(1)	-498(1)	44(1)
S(6)	220(1)	6496(1)	1646(1)	43(1)
C(1)	1141(1)	1401(4)	1259(1)	35(1)
C(2)	1451(1)	749(4)	1761(1)	35(1)
C(3)	1528(1)	-1214(5)	1957(1)	42(1)
C(4)	1847(1)	-1275(5)	2459(1)	42(1)
C(5)	2022(1)	612(4)	2660(1)	38(1)
C(6)	2374(1)	1098(5)	3184(1)	45(1)
C(7)	2367(1)	3315(5)	3355(1)	43(1)
C(8)	2712(1)	3652(5)	3899(1)	47(1)
C(9)	2726(1)	5858(5)	4075(1)	51(1)
C(10)	3058(2)	6189(6)	4618(1)	62(1)
C(11)	3080(2)	8401(8)	4791(2)	83(1)
C(12)	-270(1)	5216(4)	665(1)	36(1)
C(13)	-37(1)	4650(4)	1185(1)	36(1)
C(14)	45(1)	2690(5)	1390(1)	45(1)
C(15)	310(1)	2714(5)	1907(1)	49(1)
C(16)	438(1)	4649(5)	2107(1)	42(1)
C(17)	743(2)	5185(5)	2642(1)	55(1)
C(18)	774(1)	7455(5)	2782(1)	45(1)
C(19)	1104(1)	7831(5)	3329(1)	50(1)
C(20)	1140(1)	10073(5)	3483(1)	53(1)
C(21)	1466(2)	10440(6)	4028(1)	66(1)
C(22)	1486(2)	12655(8)	4195(2)	86(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for Zntiof.

Zn(1)-S(5)	2.3543(8)	C(10)-H(10B)	0.95(4)
Zn(1)-S(1)	2.3697(7)	C(11)-H(11A)	0.93(5)
Zn(1)-S(4)	2.3924(8)	C(11)-H(11B)	0.97(4)
Zn(1)-S(2)	2.4540(8)	C(11)-H(11C)	0.96(4)
Zn(1)-S(4)#1	2.8840(8)	C(12)-C(13)	1.435(4)
S(1)-C(1)	1.701(3)	C(12)-S(5)#1	1.683(3)
S(2)-C(1)	1.690(3)	C(13)-C(14)	1.379(4)
S(3)-C(5)	1.721(3)	C(14)-C(15)	1.391(4)
S(3)-C(2)	1.727(3)	C(14)-H(14)	0.98(3)
S(4)-C(12)	1.723(3)	C(15)-C(16)	1.366(4)
S(5)-C(12)#1	1.683(3)	C(15)-H(15)	0.88(3)
S(6)-C(16)	1.715(3)	C(16)-C(17)	1.497(4)
S(6)-C(13)	1.729(3)	C(17)-C(18)	1.513(4)
C(1)-C(2)	1.444(3)	C(17)-H(17A)	0.98(4)
C(2)-C(3)	1.371(4)	C(17)-H(17B)	0.98(4)
C(3)-C(4)	1.388(4)	C(18)-C(19)	1.519(4)
C(3)-H(3)	0.89(3)	C(18)-H(18A)	0.98(3)
C(4)-C(5)	1.362(4)	C(18)-H(18B)	0.98(3)
C(4)-H(4)	0.90(3)	C(19)-C(20)	1.507(5)
C(5)-C(6)	1.498(4)	C(19)-H(19A)	1.00(3)
C(6)-C(7)	1.517(4)	C(19)-H(19B)	0.94(4)
C(6)-H(6A)	0.95(3)	C(20)-C(21)	1.511(4)
C(6)-H(6B)	0.94(3)	C(20)-H(20A)	0.93(3)
C(7)-C(8)	1.519(4)	C(20)-H(20B)	0.99(4)
C(7)-H(7A)	0.96(3)	C(21)-C(22)	1.503(6)
C(7)-H(7B)	1.00(3)	C(21)-H(21A)	1.10(4)
C(8)-C(9)	1.507(4)	C(21)-H(21B)	0.92(5)
C(8)-H(8A)	1.05(3)	C(22)-H(22A)	0.91(5)
C(8)-H(8B)	0.97(3)	C(22)-H(22B)	0.98(5)
C(9)-C(10)	1.505(4)	C(22)-H(22C)	0.87(5)
C(9)-H(9A)	1.02(3)		
C(9)-H(9B)	0.97(3)	S(5)-Zn(1)-S(1)	134.47(3)
C(10)-C(11)	1.507(6)	S(5)-Zn(1)-S(4)	102.78(3)
C(10)-H(10A)	0.99(4)	S(1)-Zn(1)-S(4)	117.86(3)

S(5)-Zn(1)-S(2)	111.59(3)	C(8)-C(7)-H(7A)	110.1(17)
S(1)-Zn(1)-S(2)	74.74(3)	C(6)-C(7)-H(7B)	108.4(17)
S(4)-Zn(1)-S(2)	109.35(3)	C(8)-C(7)-H(7B)	111.9(17)
S(5)-Zn(1)-S(4)#1	67.62(2)	H(7A)-C(7)-H(7B)	104(2)
S(1)-Zn(1)-S(4)#1	96.96(3)	C(9)-C(8)-C(7)	113.9(3)
S(4)-Zn(1)-S(4)#1	82.43(3)	C(9)-C(8)-H(8A)	109.9(17)
S(2)-Zn(1)-S(4)#1	167.72(3)	C(7)-C(8)-H(8A)	107.5(17)
C(1)-S(1)-Zn(1)	83.99(9)	C(9)-C(8)-H(8B)	113.6(18)
C(1)-S(2)-Zn(1)	81.59(9)	C(7)-C(8)-H(8B)	105.6(19)
C(5)-S(3)-C(2)	92.31(13)	H(8A)-C(8)-H(8B)	106(2)
C(12)-S(4)-Zn(1)	98.94(9)	C(10)-C(9)-C(8)	114.1(3)
C(12)#1-S(5)-Zn(1)	93.72(9)	C(10)-C(9)-H(9A)	108.4(18)
C(16)-S(6)-C(13)	92.21(13)	C(8)-C(9)-H(9A)	110.5(18)
C(2)-C(1)-S(2)	119.9(2)	C(10)-C(9)-H(9B)	106.9(18)
C(2)-C(1)-S(1)	120.67(19)	C(8)-C(9)-H(9B)	112.8(18)
S(2)-C(1)-S(1)	119.44(15)	H(9A)-C(9)-H(9B)	104(2)
C(3)-C(2)-C(1)	128.6(2)	C(9)-C(10)-C(11)	114.2(4)
C(3)-C(2)-S(3)	110.1(2)	C(9)-C(10)-H(10A)	104(2)
C(1)-C(2)-S(3)	121.3(2)	C(11)-C(10)-H(10A)	117(2)
C(2)-C(3)-C(4)	113.2(3)	C(9)-C(10)-H(10B)	108(2)
C(2)-C(3)-H(3)	122(2)	C(11)-C(10)-H(10B)	110(2)
C(4)-C(3)-H(3)	124(2)	H(10A)-C(10)-H(10B)	104(3)
C(5)-C(4)-C(3)	114.2(3)	C(10)-C(11)-H(11A)	116(3)
C(5)-C(4)-H(4)	124(2)	C(10)-C(11)-H(11B)	107(3)
C(3)-C(4)-H(4)	122(2)	H(11A)-C(11)-H(11B)	107(4)
C(4)-C(5)-C(6)	128.1(3)	C(10)-C(11)-H(11C)	113(2)
C(4)-C(5)-S(3)	110.2(2)	H(11A)-C(11)-H(11C)	101(4)
C(6)-C(5)-S(3)	121.8(2)	H(11B)-C(11)-H(11C)	113(4)
C(5)-C(6)-C(7)	115.9(2)	C(13)-C(12)-S(5)#1	120.6(2)
C(5)-C(6)-H(6A)	106.7(17)	C(13)-C(12)-S(4)	119.5(2)
C(7)-C(6)-H(6A)	109.2(18)	S(5)#1-C(12)-S(4)	119.84(15)
C(5)-C(6)-H(6B)	107(2)	C(14)-C(13)-C(12)	128.1(3)
C(7)-C(6)-H(6B)	110(2)	C(14)-C(13)-S(6)	110.4(2)
H(6A)-C(6)-H(6B)	108(3)	C(12)-C(13)-S(6)	121.3(2)
C(6)-C(7)-C(8)	112.6(3)	C(13)-C(14)-C(15)	112.6(3)
C(6)-C(7)-H(7A)	109.5(18)	C(13)-C(14)-H(14)	122.0(19)

C(15)-C(14)-H(14)	125.3(19)	C(20)-C(19)-H(19B)	112(2)
C(16)-C(15)-C(14)	114.3(3)	C(18)-C(19)-H(19B)	109(2)
C(16)-C(15)-H(15)	124.6(19)	H(19A)-C(19)-H(19B)	105(3)
C(14)-C(15)-H(15)	121.1(19)	C(19)-C(20)-C(21)	113.8(3)
C(15)-C(16)-C(17)	127.1(3)	C(19)-C(20)-H(20A)	107(2)
C(15)-C(16)-S(6)	110.5(2)	C(21)-C(20)-H(20A)	109(2)
C(17)-C(16)-S(6)	122.3(2)	C(19)-C(20)-H(20B)	111(2)
C(16)-C(17)-C(18)	116.7(3)	C(21)-C(20)-H(20B)	107(2)
C(16)-C(17)-H(17A)	102(2)	H(20A)-C(20)-H(20B)	109(3)
C(18)-C(17)-H(17A)	108(2)	C(22)-C(21)-C(20)	114.4(4)
C(16)-C(17)-H(17B)	103(2)	C(22)-C(21)-H(21A)	110(2)
C(18)-C(17)-H(17B)	112(2)	C(20)-C(21)-H(21A)	107(2)
H(17A)-C(17)-H(17B)	116(3)	C(22)-C(21)-H(21B)	112(3)
C(17)-C(18)-C(19)	112.3(3)	C(20)-C(21)-H(21B)	107(3)
C(17)-C(18)-H(18A)	105.2(16)	H(21A)-C(21)-H(21B)	106(4)
C(19)-C(18)-H(18A)	111.5(16)	C(21)-C(22)-H(22A)	105(3)
C(17)-C(18)-H(18B)	109.1(17)	C(21)-C(22)-H(22B)	111(3)
C(19)-C(18)-H(18B)	108.5(17)	H(22A)-C(22)-H(22B)	112(5)
H(18A)-C(18)-H(18B)	110(2)	C(21)-C(22)-H(22C)	110(3)
C(20)-C(19)-C(18)	113.9(3)	H(22A)-C(22)-H(22C)	107(4)
C(20)-C(19)-H(19A)	108.8(17)	H(22B)-C(22)-H(22C)	112(4)
C(18)-C(19)-H(19A)	108.2(18)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Zntiof. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	45(1)	57(1)	28(1)	-4(1)	3(1)	6(1)
S(1)	48(1)	35(1)	34(1)	-1(1)	1(1)	-2(1)
S(2)	55(1)	38(1)	34(1)	-7(1)	-1(1)	-3(1)
S(3)	51(1)	33(1)	31(1)	-2(1)	-1(1)	-3(1)
S(4)	44(1)	40(1)	31(1)	-8(1)	6(1)	-3(1)
S(5)	55(1)	40(1)	32(1)	-2(1)	11(1)	9(1)
S(6)	54(1)	37(1)	29(1)	-2(1)	7(1)	1(1)
C(1)	35(1)	34(2)	32(1)	-4(1)	9(1)	0(1)
C(2)	34(1)	36(2)	29(1)	-3(1)	5(1)	0(1)
C(3)	43(2)	36(2)	37(2)	-5(1)	5(1)	-5(1)
C(4)	51(2)	34(2)	36(2)	4(1)	9(1)	0(1)
C(5)	41(1)	39(2)	27(1)	0(1)	5(1)	0(1)
C(6)	48(2)	45(2)	31(2)	-1(1)	2(1)	1(1)
C(7)	44(2)	47(2)	32(2)	-2(1)	6(1)	4(1)
C(8)	51(2)	49(2)	32(2)	-4(1)	6(1)	-1(2)
C(9)	55(2)	51(2)	38(2)	-5(2)	8(2)	0(2)
C(10)	74(2)	58(2)	43(2)	-13(2)	9(2)	1(2)
C(11)	99(4)	69(3)	68(3)	-30(2)	19(3)	-6(3)
C(12)	35(1)	39(2)	32(1)	-7(1)	10(1)	-5(1)
C(13)	38(1)	38(2)	30(1)	-4(1)	10(1)	-2(1)
C(14)	56(2)	40(2)	36(2)	-2(1)	14(1)	-6(1)
C(15)	65(2)	39(2)	38(2)	9(2)	16(2)	2(2)
C(16)	47(2)	45(2)	29(2)	1(1)	9(1)	2(1)
C(17)	66(2)	55(2)	33(2)	-2(2)	8(2)	2(2)
C(18)	45(2)	52(2)	33(2)	-2(1)	10(1)	2(1)
C(19)	57(2)	53(2)	32(2)	-3(2)	7(2)	-1(2)
C(20)	56(2)	54(2)	43(2)	-4(2)	12(2)	4(2)
C(21)	86(3)	60(2)	40(2)	-10(2)	13(2)	-10(2)
C(22)	100(4)	75(3)	73(3)	-31(3)	24(3)	-9(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Zntiof.

	x	y	z	U(eq)
H(3)	1387(11)	-2320(50)	1775(12)	50(9)
H(4)	1922(11)	-2470(50)	2632(11)	53(9)
H(6A)	2699(11)	780(40)	3200(10)	52(9)
H(6B)	2299(12)	190(50)	3400(12)	67(11)
H(7A)	2032(11)	3700(40)	3307(10)	50(8)
H(7B)	2450(10)	4250(50)	3123(11)	55(9)
H(8A)	3068(12)	3180(50)	3936(11)	61(9)
H(8B)	2606(11)	2670(50)	4091(12)	55(10)
H(9A)	2376(12)	6360(50)	4022(12)	64(10)
H(9B)	2833(11)	6820(50)	3880(12)	52(9)
H(10A)	3377(14)	5540(60)	4651(13)	80(12)
H(10B)	2939(12)	5320(60)	4816(13)	74(12)
H(11A)	3295(16)	8650(70)	5122(18)	114(16)
H(11B)	2747(16)	8770(70)	4764(16)	105(16)
H(11C)	3209(14)	9320(60)	4611(14)	79(14)
H(14)	-90(11)	1450(50)	1187(12)	69(10)
H(15)	382(10)	1560(50)	2082(11)	45(8)
H(17A)	1078(14)	4730(60)	2680(13)	86(12)
H(17B)	584(13)	4360(60)	2827(14)	89(13)
H(18A)	429(10)	7880(40)	2708(10)	42(8)
H(18B)	910(10)	8230(40)	2571(11)	49(9)
H(19A)	1445(12)	7310(40)	3387(12)	56(9)
H(19B)	994(13)	7000(50)	3532(14)	75(12)
H(20A)	819(13)	10520(50)	3424(12)	65(10)
H(20B)	1277(12)	10930(60)	3279(13)	77(12)
H(21A)	1841(16)	9910(60)	4082(14)	104(14)
H(21B)	1355(17)	9560(70)	4217(17)	120(18)
H(22A)	1610(18)	13370(80)	3998(18)	120(20)
H(22B)	1160(20)	13150(80)	4160(20)	150(20)
H(22C)	1698(18)	12780(70)	4502(19)	111(18)

Table 6. Torsion angles [°] for Zntiof.

S(5)-Zn(1)-S(1)-C(1)	-108.43(10)	C(3)-C(4)-C(5)-S(3)	-0.3(3)
S(4)-Zn(1)-S(1)-C(1)	101.16(9)	C(2)-S(3)-C(5)-C(4)	0.4(2)
S(2)-Zn(1)-S(1)-C(1)	-2.98(9)	C(2)-S(3)-C(5)-C(6)	179.3(3)
S(4)#1-Zn(1)-S(1)-C(1)	-173.75(9)	C(4)-C(5)-C(6)-C(7)	-159.7(3)
S(5)-Zn(1)-S(2)-C(1)	135.31(9)	S(3)-C(5)-C(6)-C(7)	21.5(4)
S(1)-Zn(1)-S(2)-C(1)	3.01(9)	C(5)-C(6)-C(7)-C(8)	176.6(3)
S(4)-Zn(1)-S(2)-C(1)	-111.67(9)	C(6)-C(7)-C(8)-C(9)	178.0(3)
S(4)#1-Zn(1)-S(2)-C(1)	51.47(16)	C(7)-C(8)-C(9)-C(10)	178.5(3)
S(5)-Zn(1)-S(4)-C(12)	-141.90(10)	C(8)-C(9)-C(10)-C(11)	179.0(4)
S(1)-Zn(1)-S(4)-C(12)	16.91(10)	Zn(1)-S(4)-C(12)-C(13)	-68.6(2)
S(2)-Zn(1)-S(4)-C(12)	99.44(10)	Zn(1)-S(4)-C(12)-S(5)#1	110.40(14)
S(4)#1-Zn(1)-S(4)-C(12)	-76.99(10)	S(5)#1-C(12)-C(13)-C(14)	166.7(2)
S(1)-Zn(1)-S(5)-C(12)#1	-87.05(9)	S(4)-C(12)-C(13)-C(14)	-14.3(4)
S(4)-Zn(1)-S(5)-C(12)#1	66.35(9)	S(5)#1-C(12)-C(13)-S(6)	-17.6(3)
S(2)-Zn(1)-S(5)-C(12)#1	-176.57(9)	S(4)-C(12)-C(13)-S(6)	161.40(15)
S(4)#1-Zn(1)-S(5)-C(12)#1	-9.80(9)	C(16)-S(6)-C(13)-C(14)	0.4(2)
Zn(1)-S(2)-C(1)-C(2)	174.7(2)	C(16)-S(6)-C(13)-C(12)	-176.0(2)
Zn(1)-S(2)-C(1)-S(1)	-4.65(14)	C(12)-C(13)-C(14)-C(15)	175.9(3)
Zn(1)-S(1)-C(1)-C(2)	-174.5(2)	S(6)-C(13)-C(14)-C(15)	-0.1(3)
Zn(1)-S(1)-C(1)-S(2)	4.79(15)	C(13)-C(14)-C(15)-C(16)	-0.3(4)
S(2)-C(1)-C(2)-C(3)	2.9(4)	C(14)-C(15)-C(16)-C(17)	-176.9(3)
S(1)-C(1)-C(2)-C(3)	-177.8(2)	C(14)-C(15)-C(16)-S(6)	0.6(4)
S(2)-C(1)-C(2)-S(3)	-176.61(15)	C(13)-S(6)-C(16)-C(15)	-0.6(2)
S(1)-C(1)-C(2)-S(3)	2.7(3)	C(13)-S(6)-C(16)-C(17)	177.0(3)
C(5)-S(3)-C(2)-C(3)	-0.3(2)	C(15)-C(16)-C(17)-C(18)	-172.1(3)
C(5)-S(3)-C(2)-C(1)	179.2(2)	S(6)-C(16)-C(17)-C(18)	10.7(5)
C(1)-C(2)-C(3)-C(4)	-179.3(3)	C(16)-C(17)-C(18)-C(19)	-178.3(3)
S(3)-C(2)-C(3)-C(4)	0.2(3)	C(17)-C(18)-C(19)-C(20)	-179.3(3)
C(2)-C(3)-C(4)-C(5)	0.0(4)	C(18)-C(19)-C(20)-C(21)	179.7(3)
C(3)-C(4)-C(5)-C(6)	-179.2(3)	C(19)-C(20)-C(21)-C(22)	-177.1(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z