Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Zn(1)	0.64160(6)	0.16340(4)	0.38235(2)	3.678(10)
Zn(2)	0.78561(6)	0.42516(5)	0.32539(3)	4.23(1)
Cl(1)	0.7235(4)	-0.1769(2)	-0.0090(1)	14.19(8)
Cl(2)	0.6944(5)	0.3168(5)	-0.0606(1)	22.7(2)
S(1)	0.8768(1)	0.2114(1)	0.31858(6)	4.13(2)
S(2)	0.9318(2)	0.5822(1)	0.27940(8)	6.81(4)
O(1)	0.6457(4)	0.3368(3)	0.4682(1)	4.53(6)
O(2)	0.4445(3)	0.2011(2)	0.3201(1)	4.24(6)
O(3)	0.5453(3)	0.3842(3)	0.2846(2)	4.73(7)
O(4)	0.7928(4)	0.5077(3)	0.4353(2)	5.22(7)
N(1)	0.7300(4)	0.0765(3)	0.4683(2)	3.67(7)
N(2)	0.5330(4)	-0.0445(3)	0.3426(2)	3.89(7)
C(1)	0.7280(5)	0.4539(4)	0.4823(2)	3.97(9)
C(2)	0.7485(6)	0.5395(4)	0.5627(2)	5.0(1)
C(3)	0.4364(5)	0.2833(4)	0.2809(2)	3.82(8)
C(4)	0.2838(6)	0.2596(5)	0.2263(3)	6.1(1)
C(5)	0.8302(5)	0.1430(4)	0.5308(2)	4.41(9)
C(6)	0.8790(5)	0.0809(5)	0.5840(2)	4.66(10)
C(7)	0.8240(6)	-0.0539(5)	0.5728(3)	5.2(1)
C(8)	0.7245(5)	-0.1262(4)	0.5070(3)	4.9(1)
C(9)	0.6812(4)	-0.0580(4)	0.4556(2)	3.55(8)
C(10)	0.5719(4)	-0.1255(3)	0.3850(2)	3.51(8)
C(11)	0.5093(6)	-0.2631(4)	0.3629(3)	4.9(1)
C(12)	0.4049(6)	-0.3157(4)	0.2984(3)	5.5(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(13)	0.3631(6)	-0.2323(4)	0.2564(2)	5.3(1)
C(14)	0.4321(6)	-0.0981(4)	0.2788(2)	4.9(1)
C(15)	0.8240(5)	0.1006(4)	0.2253(2)	4.23(9)
C(16)	0.8497(8)	-0.0311(5)	0.2108(3)	6.8(1)
C(17)	0.8196(9)	-0.1188(6)	0.1375(4)	8.4(2)
C(18)	0.7631(9)	-0.0729(7)	0.0824(3)	8.3(2)
C(19)	0.7276(10)	0.0606(7)	0.0964(3)	9.2(2)
C(20)	0.7608(8)	0.1442(5)	0.1677(3)	6.9(1)
C(21)	0.8678(7)	0.5119(5)	0.1819(3)	5.8(1)
C(22)	0.7058(7)	0.5091(6)	0.1529(3)	7.1(2)
C(23)	0.6535(10)	0.4532(9)	0.0792(4)	9.7(2)
C(24)	0.760(1)	0.395(1)	0.0333(4)	12.2(3)
C(25)	0.923(1)	0.399(1)	0.0574(5)	13.1(4)
C(26)	0.9770(9)	0.4590(9)	0.1341(4)	9.5(2)
H(1)	0.8667	0.5634	0.5794	5.9977
H(2)	0.6991	0.6190	0.5669	5.9977
H(3)	0.6962	0.4879	0.5933	5.9977
H(4)	0.2250	0.3376	0.2392	7.1845
H(5)	0.3162	0.2483	0.1771	7.1845
H(6)	0.2097	0.1819	0.2288	7.1845
H(7)	0.8685	0.2378	0.5390	5.3591
H(8)	0.9505	0.1309	0.6281	5.6162
H(9)	0.8539	-0.0993	0.6091	6.2035
H(10)	0.6882	-0.2208	0.4980	5.7943

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(11)	0.5379	-0.3202	0.3925	5.8500
H(12)	0.3645	-0.4113	0.2827	6.4906
H(13)	0.2874	-0.2675	0.2120	6.4842
H(14)	0.4061	-0.0400	0.2486	5.9533
H(15)	0.8898	-0.0650	0.2512	8.1823
H(16)	0.8450	-0.2109	0.1285	9.9492
H(17)	0.6809	0.0933	0.0569	11.0210
H(18)	0.7365	0.2357	0.1772	8.2655
H(19)	0.6272	0.5483	0.1855	8.5080
H(20)	0.5391	0.4573	0.0612	11.5790
H(21)	1.0017	0.3533	0.0244	15.9958
H(22)	1.0924	0.4665	0.1524	11.5109

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	0.0595(3)	0.0376(2)	0.0415(2)	0.0022(2)	-0.0019(2)	0.0125(2)
Zn(2)	0.0632(3)	0.0473(3)	0.0477(3)	-0.0047(2)	-0.0019(2)	0.0159(2)
Cl(1)	0.272(3)	0.156(2)	0.074(1)	0.054(2)	-0.005(1)	-0.039(1)
Cl(2)	0.316(4)	0.456(6)	0.058(1)	0.035(4)	0.011(2)	0.028(2)
S(1)	0.0525(6)	0.0541(6)	0.0489(5)	0.0039(4)	-0.0017(4)	0.0146(5)
S(2)	0.0990(9)	0.0740(8)	0.0805(9)	-0.0303(7)	-0.0046(7)	0.0346(7)
O(1)	0.081(2)	0.041(1)	0.047(2)	0.006(1)	0.002(1)	0.008(1)
O(2)	0.056(2)	0.046(1)	0.059(2)	0.003(1)	-0.005(1)	0.019(1)
O(3)	0.059(2)	0.056(2)	0.069(2)	0.001(1)	-0.004(1)	0.029(1)
O(4)	0.095(2)	0.048(2)	0.047(2)	-0.004(1)	0.001(2)	0.007(1)
N(1)	0.054(2)	0.041(2)	0.044(2)	0.008(1)	0.000(1)	0.011(1)
N(2)	0.062(2)	0.037(2)	0.046(2)	0.003(1)	-0.003(1)	0.011(1)
C(1)	0.064(2)	0.041(2)	0.045(2)	0.013(2)	-0.007(2)	0.009(2)
C(2)	0.082(3)	0.054(2)	0.047(2)	0.008(2)	-0.004(2)	0.007(2)
C(3)	0.051(2)	0.050(2)	0.044(2)	0.009(2)	0.000(2)	0.011(2)
C(4)	0.066(3)	0.093(4)	0.073(3)	0.005(3)	-0.014(2)	0.031(3)
C(5)	0.061(2)	0.050(2)	0.053(2)	0.008(2)	-0.005(2)	0.010(2)
C(6)	0.059(2)	0.067(3)	0.051(2)	0.014(2)	-0.004(2)	0.015(2)
C(7)	0.067(3)	0.079(3)	0.064(3)	0.016(2)	-0.002(2)	0.036(2)
C(8)	0.064(3)	0.055(2)	0.074(3)	0.007(2)	-0.005(2)	0.034(2)
C(9)	0.042(2)	0.049(2)	0.050(2)	0.011(2)	0.007(2)	0.021(2)
C(10)	0.049(2)	0.038(2)	0.047(2)	0.006(2)	0.010(2)	0.012(2)
C(11)	0.078(3)	0.041(2)	0.069(3)	0.007(2)	0.002(2)	0.019(2)
C(12)	0.089(3)	0.041(2)	0.069(3)	-0.002(2)	0.000(2)	0.005(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(13)	0.081(3)	0.055(3)	0.054(3)	0.001(2)	-0.002(2)	0.003(2)
C(14)	0.083(3)	0.050(2)	0.050(2)	0.003(2)	-0.009(2)	0.012(2)
C(15)	0.059(2)	0.050(2)	0.050(2)	0.006(2)	0.008(2)	0.012(2)
C(16)	0.124(4)	0.066(3)	0.071(3)	0.025(3)	0.007(3)	0.015(3)
C(17)	0.159(6)	0.064(3)	0.086(4)	0.026(4)	0.012(4)	-0.001(3)
C(18)	0.143(6)	0.098(5)	0.059(3)	0.028(4)	0.004(4)	-0.010(3)
C(19)	0.189(7)	0.112(5)	0.051(3)	0.055(5)	-0.006(4)	0.011(3)
C(20)	0.144(5)	0.069(3)	0.051(3)	0.038(3)	0.003(3)	0.009(2)
C(21)	0.086(3)	0.077(3)	0.071(3)	0.010(3)	0.013(3)	0.046(3)
C(22)	0.090(4)	0.117(5)	0.077(4)	0.023(3)	0.011(3)	0.046(3)
C(23)	0.128(6)	0.176(7)	0.081(4)	0.028(5)	0.003(4)	0.060(5)
C(24)	0.163(9)	0.25(1)	0.063(4)	0.039(8)	0.013(5)	0.062(6)
C(25)	0.179(9)	0.26(1)	0.088(5)	0.080(9)	0.061(6)	0.061(7)
C(26)	0.113(5)	0.177(8)	0.097(5)	0.052(5)	0.030(4)	0.067(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Zn(1)	S(1)	2.347(1)	Zn(1)	O(1)	2.047(3)
Zn(1)	O(2)	2.039(2)	Zn(1)	N(1)	2.153(3)
Zn(1)	N(2)	2.121(3)	Zn(2)	S(1)	2.379(1)
Zn(2)	S(2)	2.254(1)	Zn(2)	O(3)	1.976(3)
Zn(2)	O(4)	1.982(3)	Cl(1)	C(18)	1.735(5)
Cl(2)	C(24)	1.733(8)	S(1)	C(15)	1.794(4)
S(2)	C(21)	1.778(5)	O(1)	C(1)	1.252(4)
O(2)	C(3)	1.259(4)	O(3)	C(3)	1.253(4)
O(4)	C(1)	1.254(5)	N(1)	C(5)	1.337(4)
N(1)	C(9)	1.344(4)	N(2)	C(10)	1.342(4)
N(2)	C(14)	1.338(5)	C(1)	C(2)	1.505(5)
C(3)	C(4)	1.492(5)	C(5)	C(6)	1.375(6)
C(6)	C(7)	1.358(6)	C(7)	C(8)	1.391(6)
C(8)	C(9)	1.379(5)	C(9)	C(10)	1.481(5)
C(10)	C(11)	1.384(5)	C(11)	C(12)	1.360(6)
C(12)	C(13)	1.362(6)	C(13)	C(14)	1.365(6)
C(15)	C(16)	1.355(6)	C(15)	C(20)	1.361(6)
C(16)	C(17)	1.405(7)	C(17)	C(18)	1.316(8)
C(18)	C(19)	1.398(8)	C(19)	C(20)	1.362(7)
C(21)	C(22)	1.368(7)	C(21)	C(26)	1.340(8)
C(22)	C(23)	1.353(8)	C(23)	C(24)	1.32(1)
C(24)	C(25)	1.34(1)	C(25)	C(26)	1.41(1)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.96	C(2)	H(2)	0.94
C(2)	H(3)	0.95	C(4)	H(4)	0.96
C(4)	H(5)	0.94	C(4)	H(6)	0.95
C(5)	H(7)	0.95	C(6)	H(8)	0.95
C(7)	H(9)	0.95	C(8)	H(10)	0.95
C(11)	H(11)	0.94	C(12)	H(12)	0.96
C(13)	H(13)	0.95	C(14)	H(14)	0.95
C(16)	H(15)	0.96	C(17)	H(16)	0.97
C(19)	H(17)	0.96	C(20)	H(18)	0.96
C(22)	H(19)	0.95	C(23)	H(20)	0.97
C(25)	H(21)	0.98	C(26)	H(22)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	Zn(1)	O(1)	104.21(8)	S(1)	Zn(1)	O(2)	103.40(8)
S(1)	Zn(1)	N(1)	106.60(8)	S(1)	Zn(1)	N(2)	111.37(9)
O(1)	Zn(1)	O(2)	94.4(1)	O(1)	Zn(1)	N(1)	85.3(1)
O(1)	Zn(1)	N(2)	143.3(1)	O(2)	Zn(1)	N(1)	149.1(1)
O(2)	Zn(1)	N(2)	86.0(1)	N(1)	Zn(1)	N(2)	76.6(1)
S(1)	Zn(2)	S(2)	121.79(5)	S(1)	Zn(2)	O(3)	106.21(8)
S(1)	Zn(2)	O(4)	102.33(9)	S(2)	Zn(2)	O(3)	111.62(9)
S(2)	Zn(2)	O(4)	106.26(9)	O(3)	Zn(2)	O(4)	107.5(1)
Zn(1)	S(1)	Zn(2)	86.97(4)	Zn(1)	S(1)	C(15)	103.9(1)
Zn(2)	S(1)	C(15)	109.5(1)	Zn(2)	S(2)	C(21)	100.0(2)
Zn(1)	O(1)	C(1)	132.8(3)	Zn(1)	O(2)	C(3)	131.7(2)
Zn(2)	O(3)	C(3)	130.4(2)	Zn(2)	O(4)	C(1)	127.0(2)
Zn(1)	N(1)	C(5)	126.1(2)	Zn(1)	N(1)	C(9)	115.5(2)
C(5)	N(1)	C(9)	118.4(3)	Zn(1)	N(2)	C(10)	116.4(2)
Zn(1)	N(2)	C(14)	124.4(3)	C(10)	N(2)	C(14)	119.2(3)
O(1)	C(1)	O(4)	126.0(4)	O(1)	C(1)	C(2)	117.3(4)
O(4)	C(1)	C(2)	116.7(3)	O(2)	C(3)	O(3)	125.2(3)
O(2)	C(3)	C(4)	117.4(4)	O(3)	C(3)	C(4)	117.4(4)
N(1)	C(5)	C(6)	122.8(4)	C(5)	C(6)	C(7)	118.9(4)
C(6)	C(7)	C(8)	119.3(4)	C(7)	C(8)	C(9)	118.9(4)
N(1)	C(9)	C(8)	121.6(3)	N(1)	C(9)	C(10)	115.6(3)
C(8)	C(9)	C(10)	122.8(3)	N(2)	C(10)	C(9)	116.0(3)
N(2)	C(10)	C(11)	120.4(3)	C(9)	C(10)	C(11)	123.6(3)
C(10)	C(11)	C(12)	119.6(4)	C(11)	C(12)	C(13)	119.6(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(12)	C(13)	C(14)	119.0(4)	N(2)	C(14)	C(13)	122.1(4)
S(1)	C(15)	C(16)	119.3(4)	S(1)	C(15)	C(20)	122.4(3)
C(16)	C(15)	C(20)	118.3(4)	C(15)	C(16)	C(17)	121.0(5)
C(16)	C(17)	C(18)	119.5(5)	Cl(1)	C(18)	C(17)	121.4(5)
Cl(1)	C(18)	C(19)	117.8(5)	C(17)	C(18)	C(19)	120.8(5)
C(18)	C(19)	C(20)	118.5(5)	C(15)	C(20)	C(19)	121.9(5)
S(2)	C(21)	C(22)	121.5(4)	S(2)	C(21)	C(26)	121.0(5)
C(22)	C(21)	C(26)	117.5(5)	C(21)	C(22)	C(23)	122.4(6)
C(22)	C(23)	C(24)	119.4(7)	Cl(2)	C(24)	C(23)	120.4(8)
Cl(2)	C(24)	C(25)	118.4(8)	C(23)	C(24)	C(25)	121.2(8)
C(24)	C(25)	C(26)	118.9(7)	C(21)	C(26)	C(25)	120.4(7)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	109.0	C(1)	C(2)	H(2)	110.2
C(1)	C(2)	H(3)	109.3	H(1)	C(2)	H(2)	109.7
H(1)	C(2)	H(3)	108.6	H(2)	C(2)	H(3)	110.1
C(3)	C(4)	H(4)	108.9	C(3)	C(4)	H(5)	110.3
C(3)	C(4)	H(6)	110.2	H(4)	C(4)	H(5)	108.7
H(4)	C(4)	H(6)	108.5	H(5)	C(4)	H(6)	110.2
N(1)	C(5)	H(7)	118.5	C(6)	C(5)	H(7)	118.7
C(5)	C(6)	H(8)	121.0	C(7)	C(6)	H(8)	120.1
C(6)	C(7)	H(9)	120.8	C(8)	C(7)	H(9)	119.9
C(7)	C(8)	H(10)	119.9	C(9)	C(8)	H(10)	121.2
C(10)	C(11)	H(11)	120.3	C(12)	C(11)	H(11)	120.1
C(11)	C(12)	H(12)	119.2	C(13)	C(12)	H(12)	121.2
C(12)	C(13)	H(13)	120.3	C(14)	C(13)	H(13)	120.7
N(2)	C(14)	H(14)	118.7	C(13)	C(14)	H(14)	119.2
C(15)	C(16)	H(15)	119.5	C(17)	C(16)	H(15)	119.5
C(16)	C(17)	H(16)	119.0	C(18)	C(17)	H(16)	121.5
C(18)	C(19)	H(17)	121.2	C(20)	C(19)	H(17)	120.3
C(15)	C(20)	H(18)	119.6	C(19)	C(20)	H(18)	118.5
C(21)	C(22)	H(19)	119.0	C(23)	C(22)	H(19)	118.6
C(22)	C(23)	H(20)	119.1	C(24)	C(23)	H(20)	121.5
C(24)	C(25)	H(21)	121.7	C(26)	C(25)	H(21)	119.1
C(21)	C(26)	H(22)	118.8	C(25)	C(26)	H(22)	120.7