Supporting Information

Table of Contents

Table S1. Selected bond lengths (Å) and angles (deg) for NTU-1.

Table S2. Selected bond lengths (Å) and angles (deg) for NTU-2.

Table S3. Selected bond lengths (Å) and angles (deg) for NTU-3.

Table S4. Selected bond lengths (Å) and angles (deg) for NTU-4.

Table S1. Selected bond lengths (Å) and angles (deg) for NTU-1.

Bond lengths	(Å)	Bond lengths	(Å)
Zn(1)-N(1)	2.0441(19)	C(9)-C(10)	1.371(4)
Zn(1)-S(1)	2.2595(6)	C(11)-C(16)	1.360(3)
Zn(1)-S(2)	2.3836(6)	C(11)-C(12)	1.410(3)
Zn(1)-S(2)#1	2.3943(5)	C(12)-C(13)	1.355(4)
S(1)-C(1)	1.779(3)	C(13)-C(14)	1.407(4)
S(2)-C(11)	1.774(2)	C(14)-C(15)	1.417(3)
S(2)-Zn(1)#1	2.3943(5)	C(14)-C(17)	1.425(4)
N(1)-C(21)	1.325(3)	C(15)-C(20)	1.407(4)
N(1)-C(25)	1.350(3)	C(15)-C(16)	1.427(3)
C(1)-C(6)	1.357(3)	C(17)-C(18)	1.340(5)
C(1)-C(2)	1.423(3)	C(18)-C(19)	1.403(4)
C(2)-C(3)	1.377(5)	C(19)-C(20)	1.369(4)
C(3)-C(4)	1.396(5)	C(21)-C(22)	1.390(4)
C(4)-C(5)	1.415(3)	C(22)-C(23)	1.404(5)
C(4)-C(7)	1.426(4)	C(23)-C(24)	1.366(4)
C(5)-C(10)	1.394(4)	C(23)-C(26)	1.484(5)
C(5)-C(6)	1.424(3)	C(24)-C(25)	1.363(4)
C(7)-C(8)	1.351(5)	C(26)-C(26)#2	1.059(8)
C(8)-C(9)	1.374(5)		
Bond angles	(deg)	Bond angles	(deg)
N(1)-Zn(1)-S(1)	108.75(5)	C(8)-C(9)-C(10)	120.3(3)
N(1)-Zn(1)-S(2)	105.38(5)	C(9)-C(10)-C(5)	121.2(3)
S(1)-Zn(1)-S(2)	120.46(2)	C(16)-C(11)-C(12)	118.6(2)
N(1)-Zn(1)-S(2)#1	114.66(5)	C(16)-C(11)-S(2)	123.08(15)
S(1)-Zn(1)-S(2)#1	111.60(2)	C(12)-C(11)-S(2)	118.16(18)
S(2)-Zn(1)-S(2)#1	95.699(17)	C(13)-C(12)-C(11)	121.2(2)
C(1)-S(1)-Zn(1)	100.73(6)	C(12)-C(13)-C(14)	121.80(19)
C(11)-S(2)-Zn(1)	105.37(6)	C(13)-C(14)-C(15)	117.8(2)
C(11)-S(2)-Zn(1)#1	117.32(7)	C(13)-C(14)-C(17)	123.5(2)
Zn(1)-S(2)-Zn(1)#1	84.301(17)	C(15)-C(14)-C(17)	118.6(2)

C(21)-N(1)-C(25)	117.1(2)	C(20)-C(15)-C(14)	118.4(2)
C(21)-N(1)-Zn(1)	123.51(16)	C(20)-C(15)-C(16)	122.70(19)
C(25)-N(1)-Zn(1)	119.38(18)	C(14)-C(15)-C(16)	118.9(2)
C(6)-C(1)-C(2)	118.1(2)	C(11)-C(16)-C(15)	121.71(18)
C(6)-C(1)-S(1)	121.69(17)	C(18)-C(17)-C(14)	121.7(2)
C(2)-C(1)-S(1)	120.2(2)	C(17)-C(18)-C(19)	119.5(3)
C(3)-C(2)-C(1)	120.7(3)	C(20)-C(19)-C(18)	121.2(3)
C(2)-C(3)-C(4)	121.6(2)	C(19)-C(20)-C(15)	120.6(2)
C(3)-C(4)-C(5)	118.5(3)	N(1)-C(21)-C(22)	122.4(3)
C(3)-C(4)-C(7)	123.2(3)	C(21)-C(22)-C(23)	119.4(3)
C(5)-C(4)-C(7)	118.3(3)	C(24)-C(23)-C(22)	117.6(3)
C(10)-C(5)-C(4)	118.6(2)	C(24)-C(23)-C(26)	119.2(4)
C(10)-C(5)-C(6)	122.7(2)	C(22)-C(23)-C(26)	123.1(4)
C(4)-C(5)-C(6)	118.8(2)	C(23)-C(24)-C(25)	119.4(3)
C(1)-C(6)-C(5)	122.4(2)	N(1)-C(25)-C(24)	124.1(3)
C(8)-C(7)-C(4)	120.7(3)	C(26)#2-C(26)-C(23)	139.8(11)
C(7)-C(8)-C(9)	120.8(3)		

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

Table S2. Selected bond lengths (Å) and angles (deg) for NTU-2.

Bond lengths	(Å)	Bond lengths	(Å)
Zn(1)-N(1)	2.0603(13)	C(31)-N(2)	1.3367(19)
Zn(1)-N(2)#1	2.0552(12)	C(31)-C(29)	1.377(2)
Zn(1)-S(1)	2.2717(5)	C(30)-C(23)	1.388(2)
Zn(1)-S(3)	2.3668(4)	C(30)-C(15)	1.391(3)
Zn(2)-N(3)	2.0977(12)	C(28)-N(1)	1.336(2)
Zn(2)-S(2)	2.2913(4)	C(28)-C(27)	1.374(2)
Zn(2)-S(4)	2.2963(5)	C(26)-N(2)	1.340(2)
Zn(2)-S(3)	2.4133(4)	C(26)-C(25)	1.378(2)
S(4)-C(24)	1.7628(18)	C(24)-C(21)	1.388(3)
S(3)-C(41)	1.7896(15)	C(24)-C(18)	1.394(3)
S(2)-C(32)	1.7714(18)	C(23)-C(7)	1.389(3)
S(1)-C(30)	1.7795(17)	C(22)-C(20)	1.375(2)
C(42)-C(39)	1.394(2)	C(21)-C(2)	1.390(3)
C(42)-C(34)	1.395(2)	C(20)-N(1)	1.338(2)
C(42)-C(35)	1.4704(19)	C(19)-C(10)	1.387(3)
C(41)-C(11)	1.378(2)	C(18)-C(8)	1.399(4)
C(41)-C(16)	1.377(2)	C(17)-C(12)	1.351(3)
C(40)-C(27)	1.384(3)	C(17)-C(16)	1.393(3)
C(40)-C(22)	1.387(2)	C(15)-C(13)	1.389(3)
C(40)-C(1)	1.461(2)	C(14)-C(13)	1.371(3)
C(39)-C(36)	1.381(2)	C(14)-C(7)	1.371(3)
C(38)-C(25)	1.388(2)	C(12)-C(5)	1.358(3)
C(38)-C(29)	1.390(2)	C(11)-C(5)	1.389(3)
C(38)-C(37)	1.471(2)	C(10)-C(4)	1.357(4)
C(37)-C(35)	1.330(2)	C(9)-C(6)	1.406(4)
C(36)-N(3)	1.3408(19)	C(8)-C(3)	1.363(5)
C(34)-C(33)	1.383(2)	C(6)-C(4)	1.367(4)
C(33)-N(3)	1.3415(19)	C(3)-C(2)	1.370(4)
C(32)-C(9)	1.394(2)	C(1)-C(1)#2	1.330(3)
C(32)-C(19)	1.393(3)	N(2)-Zn(1)#3	2.0552(12)

Bond angles	(deg)	Bond angles	(deg)
N(1)-Zn(1)-N(2)#1	102.57(5)	C(15)-C(30)-S(1)	121.28(14)
N(1)-Zn(1)-S(1)	107.41(4)	C(31)-C(29)-C(38)	119.88(15)
N(2)#1-Zn(1)-S(1)	114.88(4)	N(1)-C(28)-C(27)	122.96(17)
N(1)-Zn(1)-S(3)	109.42(4)	C(40)-C(27)-C(28)	120.15(17)
N(2)#1-Zn(1)-S(3)	105.17(4)	N(2)-C(26)-C(25)	122.82(15)
S(1)-Zn(1)-S(3)	116.448(17)	C(38)-C(25)-C(26)	120.15(15)
N(3)-Zn(2)-S(2)	107.45(4)	C(21)-C(24)-C(18)	117.95(19)
N(3)-Zn(2)-S(4)	99.03(4)	C(21)-C(24)-S(4)	123.69(14)
S(2)-Zn(2)-S(4)	124.041(19)	C(18)-C(24)-S(4)	118.35(17)
N(3)-Zn(2)-S(3)	108.41(4)	C(7)-C(23)-C(30)	120.58(19)
S(2)-Zn(2)-S(3)	98.357(16)	C(20)-C(22)-C(40)	119.70(17)
S(4)-Zn(2)-S(3)	118.784(16)	C(24)-C(21)-C(2)	120.9(2)
C(24)-S(4)-Zn(2)	107.27(6)	N(1)-C(20)-C(22)	123.23(16)
C(41)-S(3)-Zn(1)	104.03(5)	C(10)-C(19)-C(32)	120.8(2)
C(41)-S(3)-Zn(2)	114.61(5)	C(24)-C(18)-C(8)	120.0(3)
Zn(1)-S(3)-Zn(2)	120.522(17)	C(12)-C(17)-C(16)	120.88(19)
C(32)-S(2)-Zn(2)	107.67(6)	C(41)-C(16)-C(17)	120.40(17)
C(30)-S(1)-Zn(1)	96.26(5)	C(13)-C(15)-C(30)	121.09(19)
C(39)-C(42)-C(34)	117.06(13)	C(13)-C(14)-C(7)	119.8(2)
C(39)-C(42)-C(35)	123.74(14)	C(14)-C(13)-C(15)	120.0(2)
C(34)-C(42)-C(35)	119.13(14)	C(5)-C(12)-C(17)	119.27(18)
C(11)-C(41)-C(16)	118.16(15)	C(41)-C(11)-C(5)	120.33(18)
C(11)-C(41)-S(3)	121.67(13)	C(4)-C(10)-C(19)	121.3(3)
C(16)-C(41)-S(3)	119.99(12)	C(32)-C(9)-C(6)	119.9(2)
C(27)-C(40)-C(22)	116.76(15)	C(3)-C(8)-C(18)	121.2(2)
C(27)-C(40)-C(1)	123.11(15)	C(23)-C(7)-C(14)	120.5(2)
C(22)-C(40)-C(1)	120.13(16)	C(4)-C(6)-C(9)	121.0(2)
C(36)-C(39)-C(42)	119.62(14)	C(12)-C(5)-C(11)	121.0(2)
C(25)-C(38)-C(29)	116.68(14)	C(6)-C(4)-C(10)	119.2(2)
C(25)-C(38)-C(37)	119.88(14)	C(2)-C(3)-C(8)	119.2(2)
C(29)-C(38)-C(37)	123.40(14)	C(3)-C(2)-C(21)	120.7(3)
C(35)-C(37)-C(38)	124.75(15)	C(1)#2-C(1)-C(40)	124.5(2)
N(3)-C(36)-C(39)	123.02(14)	C(33)-N(3)-C(36)	117.65(12)
C(37)-C(35)-C(42)	124.95(15)	C(33)-N(3)-Zn(2)	119.59(10)
C(33)-C(34)-C(42)	119.75(14)	C(36)-N(3)-Zn(2)	122.37(10)
N(3)-C(33)-C(34)	122.74(14)	C(31)-N(2)-C(26)	117.27(13)
C(9)-C(32)-C(19)	117.73(18)	C(31)-N(2)-Zn(1)#3	120.08(11)
C(9)-C(32)-S(2)	118.71(17)	C(26)-N(2)-Zn(1)#3	122.46(11)
C(19)-C(32)-S(2)	123.56(13)	C(20)-N(1)-C(28)	117.06(14)
N(2)-C(31)-C(29)	123.19(15)	C(20)-N(1)-Zn(1)	123.95(11)
C(23)-C(30)-C(15)	117.96(17)	C(28)-N(1)-Zn(1)	118.94(12)
C(23)-C(30)-S(1)	120.76(14)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y-1/2,-z+1/2; #2 -x+1,-y+1,-z; #3 -x+1/2,y+1/2,-z+1/2

Table S3. Selected bond lengths (Å) and angles (deg) for NTU-3.

Bond lengths	(Å)	Bond lengths	(Å)
Zn(1)-N(1)	2.058(2)	C(15)-C(18)	1.463(4)
Zn(1)-N(3)#1	2.093(2)	C(16)-C(17)	1.376(4)
Zn(1)-S(1)	2.2753(9)	C(17)-C(18)	1.367(4)

Zn(1)-S(2)	2.3483(9)	C(18)-C(19)	1.343(4)
Zn(2)-N(2)#2	2.095(2)	C(19)-C(20)	1.363(4)
Zn(2)-S(3)	2.2736(9)	C(21)-C(22)	1.297(4)
Zn(2)-S(4)	2.2846(9)	C(22)-C(25)	1.480(4)
Zn(2)-S(2)	2.4271(9)	C(23)-C(24)	1.384(4)
S(1)-C(28)	1.753(4)	C(24)-C(25)	1.358(4)
S(2)-C(34)	1.780(3)	C(25)-C(26)	1.383(4)
S(3)-C(40)	1.771(4)	C(26)-C(27)	1.384(4)
S(4)-C(46)	1.757(3)	C(28)-C(33)	1.379(4)
N(1)-C(1)	1.314(4)	C(28)-C(29)	1.393(5)
N(1)-C(5)	1.325(4)	C(29)-C(30)	1.366(6)
N(2)-C(27)	1.322(4)	C(30)-C(31)	1.378(6)
N(2)-C(23)	1.326(4)	C(31)-C(32)	1.355(6)
N(2)-Zn(2)#3	2.095(2)	C(32)-C(33)	1.386(5)
N(3)-C(16)	1.310(4)	C(34)-C(35)	1.372(5)
N(3)-C(20)	1.323(4)	C(34)-C(39)	1.386(5)
N(3)-Zn(1)#4	2.093(2)	C(35)-C(36)	1.381(5)
C(1)-C(2)	1.377(4)	C(36)-C(37)	1.357(7)
C(2)-C(3)	1.356(4)	C(37)-C(38)	1.330(7)
C(3)-C(4)	1.366(4)	C(38)-C(39)	1.371(5)
C(3)-C(6)	1.465(4)	C(40)-C(41)	1.374(5)
C(4)-C(5)	1.371(4)	C(40)-C(45)	1.389(4)
C(6)-C(7)	1.327(4)	C(41)-C(42)	1.383(5)
C(7)-C(8)	1.471(4)	C(42)-C(43)	1.399(6)
C(8)-C(13)	1.387(4)	C(43)-C(44)	1.361(6)
C(8)-C(9)	1.402(4)	C(44)-C(45)	1.377(5)
C(9)-C(10)	1.399(4)	C(46)-C(51)	1.367(5)
C(10)-C(11)	1.392(4)	C(46)-C(47)	1.374(4)
C(10)-C(14)	1.464(4)	C(47)-C(48)	1.374(5)
C(11)-C(12)	1.391(4)	C(48)-C(49)	1.340(6)
C(12)-C(13)	1.392(4)	C(49)-C(50)	1.369(6)
C(12)-C(21)	1.469(4)	C(50)-C(51)	1.368(5)
C(14)-C(15)	1.321(4)		
Bond angles	(deg)	Bond angles	(deg)
N(1)-Zn(1)-N(3)#1	108.33(9)	C(14)-C(15)-C(18)	126.2(3)
N(1)-Zn(1)-S(1)	109.50(7)	N(3)-C(16)-C(17)	124.3(3)
N(3)#1-Zn(1)-S(1)	102.95(7)	C(18)-C(17)-C(16)	121.0(3)
N(1)-Zn(1)-S(2)	111.06(7)	C(19)-C(18)-C(17)	114.1(3)
N(3)#1-Zn(1)-S(2)	101.24(7)	C(19)-C(18)-C(15)	123.4(3)
S(1)-Zn(1)-S(2)	122.32(3)	C(17)-C(18)-C(15)	122.4(3)
N(2)#2-Zn(2)-S(3)	106.28(7)	C(18)-C(19)-C(20)	122.3(3)
N(2)#2-Zn(2)-S(4)	109.32(7)	N(3)-C(20)-C(19)	123.9(3)
S(3)-Zn(2)-S(4)	127.31(4)	C(22)-C(21)-C(12)	128.1(3)
N(2)#2-Zn(2)-S(2)	110.04(7)	C(21)-C(22)-C(25)	126.4(3)
S(3)-Zn(2)-S(2)	104.22(3)	N(2)-C(23)-C(24)	123.7(3)
S(4)-Zn(2)-S(2)	98.59(3)	C(25)-C(24)-C(23)	120.3(3)
C(28)-S(1)-Zn(1)	108.17(13)	C(24)-C(25)-C(26)	116.5(3)
C(34)-S(2)-Zn(1)	108.69(12)	C(24)-C(25)-C(22)	120.7(3)
C(34)-S(2)-Zn(2)	101.64(11)	C(26)-C(25)-C(22)	122.7(3)
Zn(1)-S(2)-Zn(2)	137.64(4)	C(25)-C(26)-C(27)	119.5(3)
C(40)-S(3)-Zn(2)	106.67(11)	N(2)-C(27)-C(26)	124.0(3)
C(46)-S(4)-Zn(2)	109.25(11)	C(33)-C(28)-C(29)	116.1(3)
C(1)-N(1)-C(5)	115.4(3)	C(33)-C(28)-S(1)	119.5(3)

C(1)-N(1)-Zn(1)	121.7(2)	C(29)-C(28)-S(1)	124.3(3)
C(5)-N(1)-Zn(1)	121.9(2)	C(30)-C(29)-C(28)	121.8(4)
C(27)-N(2)-C(23)	115.9(3)	C(29)-C(30)-C(31)	120.9(5)
C(27)-N(2)-Zn(2)#3	119.4(2)	C(32)-C(31)-C(30)	118.4(4)
C(23)-N(2)-Zn(2)#3	124.3(2)	C(31)-C(32)-C(33)	120.9(4)
C(16)-N(3)-C(20)	114.4(3)	C(28)-C(33)-C(32)	121.8(4)
C(16)-N(3)-Zn(1)#4	131.4(2)	C(35)-C(34)-C(39)	118.0(3)
C(20)-N(3)-Zn(1)#4	113.7(2)	C(35)-C(34)-S(2)	122.5(3)
N(1)-C(1)-C(2)	123.7(3)	C(39)-C(34)-S(2)	119.4(3)
C(3)-C(2)-C(1)	121.1(3)	C(34)-C(35)-C(36)	120.8(4)
C(2)-C(3)-C(4)	115.4(3)	C(37)-C(36)-C(35)	119.4(5)
C(2)-C(3)-C(6)	125.6(3)	C(38)-C(37)-C(36)	120.8(4)
C(4)-C(3)-C(6)	119.0(3)	C(37)-C(38)-C(39)	120.8(4)
C(3)-C(4)-C(5)	120.6(3)	C(38)-C(39)-C(34)	120.1(4)
N(1)-C(5)-C(4)	123.8(3)	C(41)-C(40)-C(45)	117.9(3)
C(7)-C(6)-C(3)	128.0(3)	C(41)-C(40)-S(3)	122.9(3)
C(6)-C(7)-C(8)	125.4(3)	C(45)-C(40)-S(3)	119.2(3)
C(13)-C(8)-C(9)	118.2(2)	C(40)-C(41)-C(42)	122.0(4)
C(13)-C(8)-C(7)	122.1(2)	C(41)-C(42)-C(43)	118.7(4)
C(9)-C(8)-C(7)	119.7(2)	C(44)-C(43)-C(42)	119.9(4)
C(10)-C(9)-C(8)	121.7(2)	C(43)-C(44)-C(45)	120.4(4)
C(11)-C(10)-C(9)	117.8(2)	C(44)-C(45)-C(40)	121.0(4)
C(11)-C(10)-C(14)	122.0(2)	C(51)-C(46)-C(47)	116.6(3)
C(9)-C(10)-C(14)	120.2(2)	C(51)-C(46)-S(4)	124.9(3)
C(12)-C(11)-C(10)	122.0(2)	C(47)-C(46)-S(4)	118.5(3)
C(11)-C(12)-C(13)	118.5(2)	C(48)-C(47)-C(46)	121.4(4)
C(11)-C(12)-C(21)	118.3(2)	C(49)-C(48)-C(47)	121.4(4)
C(13)-C(12)-C(21)	123.1(2)	C(48)-C(49)-C(50)	118.1(4)
C(8)-C(13)-C(12)	121.7(2)	C(51)-C(50)-C(49)	120.8(4)
C(15)-C(14)-C(10)	126.6(3)	C(50)-C(51)-C(46)	121.6(4)

Symmetry transformations used to generate equivalent atoms: #1 x,y,z+1; #2 x+1,-y+1/2,z+1/2; #3 x-1,-y+1/2,z-1/2; #4 x,y,z-1

Table S4. Selected bond lengths (Å) and angles (deg) for NTU-4.

Bond lengths	(Å)	Bond lengths	(Å)
Zn(1)-N(2)#1	2.0606(15)	C(45)-C(30)	1.383(3)
Zn(1)-N(3)	2.0715(15)	C(44)-C(37)	1.365(3)
Zn(1)-S(4)	2.2951(6)	C(43)-C(38)	1.377(3)
Zn(1)-S(3)	2.2970(5)	C(42)-C(32)	1.371(3)
Zn(2)-N(1)#2	2.0719(17)	C(41)-C(36)	1.366(3)
Zn(2)-N(4)	2.0879(16)	C(39)-C(30)	1.369(3)
Zn(2)-S(1)	2.2677(8)	C(35)-C(15)	1.406(4)
Zn(2)-S(2)	2.2794(8)	C(34)-C(29)	1.386(3)
S(2)-C(22)	1.728(3)	C(33)-C(16)	1.376(3)
S(3)-C(47)	1.768(2)	C(31)-C(18)	1.410(4)
S(4)-C(46)	1.775(2)	C(28)-C(23)	1.266(6)
O(3)-C(49)	1.342(2)	C(28)-C(27)#5	1.396(6)
O(3)-C(55)	1.443(2)	C(27)-C(23)	1.361(7)
O(1)-C(45)	1.343(2)	C(27)-C(28)#5	1.396(6)
O(1)-C(53)	1.421(2)	C(27)-C(10)	1.498(9)

O(4)-C(51)	1.339(2)	C(26)-C(25)	1.357(5)
O(4)-C(48)	1.440(2)	C(26)-C(20)	1.385(5)
O(2)-C(54)	1.364(2)	C(25)-C(18)	1.381(4)
O(2)-C(50)	1.426(2)	C(24)-C(11)	1.335(6)
N(4)-C(37)	1.326(3)	C(24)-C(22)	1.370(4)
N(4)-C(34)	1.340(3)	C(22)-C(12)	1.351(6)
N(3)-C(40)	1.329(2)	C(21)-C(19)	1.364(5)
N(3)-C(42)	1.352(3)	C(21)-C(17)	1.384(4)
N(2)-C(43)	1.318(2)	C(19)-C(15)	1.389(4)
N(2)-C(41)	1.337(3)	C(14)-C(13)	1.328(10)
N(2)-Zn(1)#3	2.0606(15)	C(14)-C(12)	1.486(8)
N(1)-C(16)	1.316(3)	C(13)-C(11)	1.367(9)
N(1)-C(39)	1.319(3)	S(1)-C(6)	1.688(4)
N(1)-Zn(2)#4	2.0719(17)	S(1)-C(6B)	1.759(9)
C(56)-C(48)	1.521(2)	C(1)-C(6)	1.367(7)
C(56)-C(55)	1.528(2)	C(1)-C(2)	1.431(9)
C(56)-C(50)	1.530(2)	C(2)-C(3)	1.243(11)
C(56)-C(53)	1.534(2)	C(3)-C(4)	1.360(11)
C(54)-C(38)	1.370(3)	C(4)-C(5)	1.365(8)
C(54)-C(36)	1.375(3)	C(5)-C(6)	1.329(7)
C(52)-C(40)	1.380(2)	C(1B)-C(6B)	1.316(13)
C(52)-C(49)	1.386(2)	C(1B)-C(2B)	1.442(16)
C(51)-C(29)	1.381(3)	C(2B)-C(3B)	1.421(17)
C(51)-C(44)	1.388(3)	C(3B)-C(4B)	1.298(18)
C(49)-C(32)	1.394(3)	C(4B)-C(5B)	1.430(17)
C(47)-C(31)	1.370(3)	C(5B)-C(6B)	1.449(14)
C(47)-C(20)	1.401(4)	C(80)-C(81)#6	1.369(8)
C(46)-C(17)	1.378(3)	C(80)-C(82)	1.827(12)
C(46)-C(35)	1.384(3)	C(81)-C(80)#6	1.369(8)
C(45)-C(33)45	1.357(3)	C(81)-C(82)	1.488(8)
Bond angles	(deg)	Bond angles	(deg)
N(2)#1-Zn(1)-N(3)	99.07(6)	C(37)-C(44)-C(51)	118.37(19)
N(2)#1-Zn(1)-S(4)	106.39(5)	N(2)-C(43)-C(38)	123.21(18)
N(3)-Zn(1)-S(4)	107.65(4)	N(3)-C(42)-C(32)	123.21(19)
N(2)#1-Zn(1)-S(3)	108.33(4)	N(2)-C(41)-C(36)	123.97(19)
N(3)-Zn(1)-S(3)	105.22(5)	N(3)-C(40)-C(52)	124.87(17)
S(4)-Zn(1)-S(3)	126.79(2)	N(1)-C(39)-C(30)	123.6(2)
N(1)#2-Zn(2)-N(4)	100.79(6)	C(54)-C(38)-C(43)	119.11(17)
N(1)#2-Zn(2)-S(1)	109.33(5)	N(4)-C(37)-C(44)	124.94(19)
N(4)-Zn(2)-S(1)	111.79(5)	C(41)-C(36)-C(54)	118.25(19)
N(1)#2-Zn(2)-S(2)	113.52(5)	C(46)-C(35)-C(15)	121.0(2)
N(4)-Zn(2)-S(2)	109.95(5)	N(4)-C(34)-C(29)	123.9(2)
S(1)-Zn(2)-S(2)	111.07(3)	C(45)-C(33)-C(16)	118.5(2)
C(22)-S(2)-Zn(2)	104.98(10)	C(42)-C(32)-C(49)	118.71(19)
C(47)-S(3)-Zn(1)	104.94(7)	C(47)-C(31)-C(18)	121.0(2)
C(46)-S(4)-Zn(1)	106.42(7)	C(39)-C(30)-C(45)	119.4(2)
C(49)-O(3)-C(55)	118.89(13)	C(51)-C(29)-C(34)	118.21(19)
C(45)-O(1)-C(53)	119.77(14)	C(23)-C(28)-C(27)#5	115.6(5)
C(51)-O(4)-C(48)	118.46(13)	C(23)-C(27)-C(28)#5	123.1(4)
C(54)-O(2)-C(50)	116.59(13)	C(23)-C(27)-C(10)	123.2(5)
C(37)-N(4)-C(34)	116.07(17)	C(28)#5-C(27)-C(10)	113.4(5)
C(37)-N(4)-Zn(2)	122.49(13)	C(25)-C(26)-C(20)	122.6(3)
C(34)-N(4)-Zn(2)	121.14(14)	C(26)-C(25)-C(18)	119.4(3)

C(40)-N(3)-C(42)	116.62(16)	C(11)-C(24)-C(22)	124.9(4)
C(40)-N(3)-Zn(1)	122.69(12)	C(28)-C(23)-C(27)	121.3(4)
C(42)-N(3)-Zn(1)	120.68(13)	C(12)-C(22)-C(24)	119.3(4)
C(43)-N(2)-C(41)	116.90(16)	C(12)-C(22)-S(2)	117.2(3)
C(43)-N(2)-Zn(1)#3	123.27(13)	C(24)-C(22)-S(2)	123.4(3)
C(41)-N(2)-Zn(1)#3	119.82(13)	C(19)-C(21)-C(17)	120.4(3)
C(16)-N(1)-C(39)	115.96(19)	C(26)-C(20)-C(47)	118.7(3)
C(16)-N(1)-Zn(2)#4	119.22(14)	C(21)-C(19)-C(15)	120.6(3)
C(39)-N(1)-Zn(2)#4	124.81(15)	C(25)-C(18)-C(31)	119.2(3)
C(48)-C(56)-C(55)	111.35(13)	C(46)-C(17)-C(21)	120.9(3)
C(48)-C(56)-C(50)	107.58(13)	N(1)-C(16)-C(33)	125.0(2)
C(55)-C(56)-C(50)	110.01(13)	C(19)-C(15)-C(35)	118.4(3)
C(48)-C(56)-C(53)	108.81(13)	C(13)-C(14)-C(12)	118.5(6)
C(55)-C(56)-C(53)	108.58(13)	C(14)-C(13)-C(11)	123.5(6)
C(50)-C(56)-C(53)	110.52(13)	C(22)-C(12)-C(14)	116.9(5)
O(3)-C(55)-C(56)	105.82(13)	C(24)-C(11)-C(13)	116.6(5)
O(2)-C(54)-C(38)	116.35(15)	C(6)-S(1)-C(6B)	141.9(3)
O(2)-C(54)-C(36)	125.09(16)	C(6)-S(1)-Zn(2)	107.05(12)
C(38)-C(54)-C(36)	118.56(16)	C(6B)-S(1)-Zn(2)	108.1(3)
O(1)-C(53)-C(56)	107.04(13)	C(6)-C(1)-C(2)	118.3(6)
C(40)-C(52)-C(49)	117.51(16)	C(3)-C(2)-C(1)	122.8(7)
O(4)-C(51)-C(29)	116.18(16)	C(2)-C(3)-C(4)	120.8(6)
O(4)-C(51)-C(44)	125.36(17)	C(3)-C(4)-C(5)	116.7(7)
C(29)-C(51)-C(44)	118.46(18)	C(6)-C(5)-C(4)	125.8(6)
O(2)-C(50)-C(56)	108.56(13)	C(5)-C(6)-C(1)	115.4(5)
O(3)-C(49)-C(52)	126.00(16)	C(5)-C(6)-S(1)	121.4(4)
O(3)-C(49)-C(32)	114.99(16)	C(1)-C(6)-S(1)	123.1(4)
C(52)-C(49)-C(32)	119.01(17)	C(6B)-C(1B)-C(2B)	124.0(9)
O(4)-C(48)-C(56)	107.51(13)	C(3B)-C(2B)-C(1B)	115.1(10)
C(31)-C(47)-C(20)	119.2(2)	C(4B)-C(3B)-C(2B)	121.6(10)
C(31)-C(47)-S(3)	124.04(17)	C(3B)-C(4B)-C(5B)	120.7(11)
C(20)-C(47)-S(3)	116.75(19)	C(4B)-C(5B)-C(6B)	118.8(10)
C(17)-C(46)-C(35)	118.7(2)	C(1B)-C(6B)-C(5B)	117.0(9)
C(17)-C(46)-S(4)	117.56(17)	C(1B)-C(6B)-S(1)	124.3(7)
C(35)-C(46)-S(4)	123.70(16)	C(5B)-C(6B)-S(1)	118.4(7)
O(1)-C(45)-C(33)	126.10(18)	C(81)#6-C(80)-C(82)	82.1(6)
O(1)-C(45)-C(30)	116.36(17)	C(80)#6-C(81)-C(82)	145.9(6)
C(33)-C(45)-C(30)	117.51(19)	C(81)-C(82)-C(80)	132.0(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y+1/2,-z+1/2;
#2 -x,y+1/2,-z+1/2; #3 -x+1,y-1/2,-z+1/2; #4 -x,y-1/2,-z+1/2; #5 -x+1,-y+1,-z+2 ; #6 -x+1,-y+2,-z