SUPPLEMENTARY MATERIALS

Table 1. Crystal data and structure refinement for **1-Fe**.

Identification code	**1-Fe**	
Empirical formula	C40 H52 Fe N6 O4 S2	
Formula weight	800.84	
Temperature	100(2) K	
Wavelength	0.9699 E	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 17.231(3) Å	α= 90°.
	b = 23.699(5) Å	β= 118.93(3)°.
	c = 11.442(2) Å	γ = 90°.
Volume	4089.7(17) Å ^{3}	
Z	4	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	1.200 mm^{-1}	
F(000)	1696	
Crystal size	0.200 x 0.150 x 0.020 mm^3	
Theta range for data collection	2.184 to 38.406°.	
Index ranges	-20<=h<=20, -28<=k<=28, -14<=l<=14	
Reflections collected	24323	
Independent reflections	4333 [R(int) = 0.0774]	
Completeness to theta = 35.587°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.80	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4333 / 11 / 240	
Goodness-of-fit on F^2	1.171	
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1433	
R indices (all data)	R1 = 0.0764, wR2 = 0.1568	
Extinction coefficient	0.0013(3)	
Largest diff. peak and hole	0.613 and -0.802 e. Å $^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1-Fe**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5000	2717(1)	2500	19(1)
S(1)	4654(1)	3416(1)	4289(1)	19(1)
O(1)	4219(1)	3517(1)	2849(2)	22(1)
O(2)	4079(1)	3335(1)	4868(2)	22(1)
N(1)	5289(1)	2893(1)	4441(2)	20(1)
N(2)	6121(1)	2191(1)	3341(2)	20(1)
N(3)	6164(2)	1086(2)	946(3)	24(1)
N(3A)	6025(5)	1347(3)	496(6)	24(1)
C(1)	5862(2)	2643(1)	5679(2)	18(1)
C(2)	5842(2)	2762(1)	6867(3)	22(1)
C(3)	6413(2)	2496(1)	8059(2)	23(1)
C(4)	7028(2)	2112(1)	8103(3)	26(1)
C(5)	7075(2)	1985(1)	6959(3)	23(1)
C(6)	6494(2)	2239(1)	5721(2)	20(1)
C(7)	6615(2)	2073(1)	4595(2)	20(1)
C(8)	5358(2)	3992(1)	5138(2)	21(1)
C(9)	6034(2)	4143(1)	4861(2)	22(1)
C(10)	6590(2)	4592(1)	5543(3)	24(1)
C(11)	6480(2)	4902(1)	6497(2)	21(1)
C(12)	5783(2)	4752(1)	6732(3)	23(1)
C(13)	5222(2)	4304(1)	6062(2)	22(1)
C(14)	7095(2)	5386(1)	7239(3)	29(1)
C(15)	6400(2)	1949(1)	2410(2)	23(1)
C(16)	6092(3)	1337(1)	2070(4)	33(1)
C(17)	7051(2)	1190(2)	1095(4)	33(1)
C(18)	7300(3)	806(2)	278(5)	33(1)
C(19)	5428(3)	1258(2)	-344(4)	33(1)
C(20)	4605(3)	899(2)	-772(5)	33(1)
C(16A)	5740(4)	1524(3)	1465(7)	33(1)
C(17A)	6677(5)	886(3)	1035(7)	33(1)
C(18A)	7066(6)	731(5)	140(10)	33(1)
C(19A)	5308(6)	1237(4)	-803(8)	33(1)
C(20A)	4704(6)	742(3)	-990(9)	33(1)

Table 3. Bond lengths [Å] and angles [°] for **1-Fe**.

Fe(1)-N(1)#1	2.070(2)	C(12)-H(12)	0.9500
Fe(1)-N(1)	2.070(2)	C(13)-H(13)	0.9500
Fe(1)-N(2)#1	2.102(2)	C(14)-H(14A)	0.9800
Fe(1)-N(2)	2.102(2)	C(14)-H(14B)	0.9800
S(1)-O(2)	1.4467(18)	C(14)-H(14C)	0.9800
S(1)-O(1)	1.4625(18)	C(15)-C(16A)	1.512(3)
S(1)-N(1)	1.605(2)	C(15)-C(16)	1.528(3)
S(1)-C(8)	1.772(3)	C(15)-H(15A)	0.9900
N(1)-C(1)	1.407(3)	C(15)-H(15B)	0.9900
N(2)-C(7)	1.296(3)	C(15)-H(15C)	0.9900
N(2)-C(15)	1.479(3)	C(15)-H(15D)	0.9900
N(3)-C(19)	1.464(6)	C(16)-H(16A)	0.9900
N(3)-C(17)	1.474(3)	C(16)-H(16B)	0.9900
N(3)-C(16)	1.476(3)	C(17)-C(18)	1.509(3)
N(3A)-C(19A)	1.423(10)	C(17)-H(17A)	0.9900
N(3A)-C(17A)	1.472(3)	C(17)-H(17B)	0.9900
N(3A)-C(16A)	1.475(3)	C(18)-H(18A)	0.9800
C(1)-C(2)	1.405(3)	C(18)-H(18B)	0.9800
C(1)-C(6)	1.433(4)	C(18)-H(18C)	0.9800
C(2)-C(3)	1.388(4)	C(19)-C(20)	1.519(3)
C(2)-H(2)	0.9500	C(19)-H(19A)	0.9900
C(3)-C(4)	1.379(4)	C(19)-H(19B)	0.9900
C(3)-H(3)	0.9500	C(20)-H(20A)	0.9800
C(4)-C(5)	1.382(4)	C(20)-H(20B)	0.9800
C(4)-H(4)	0.9500	C(20)-H(20C)	0.9800
C(5)-C(6)	1.414(3)	C(16A)-H(16C)	0.9900
C(5)-H(5)	0.9500	C(16A)-H(16D)	0.9900
C(6)-C(7)	1.456(3)	C(17A)-C(18A)	1.515(3)
C(7)-H(7)	0.9500	C(17A)-H(17C)	0.9900
C(8)-C(9)	1.394(4)	C(17A)-H(17D)	0.9900
C(8)-C(13)	1.400(3)	C(18A)-H(18D)	0.9800
C(9)-C(10)	1.391(4)	C(18A)-H(18E)	0.9800
C(9)-H(9)	0.9500	C(18A)-H(18F)	0.9800
C(10)-C(11)	1.403(3)	C(19A)-C(20A)	1.514(3)
C(10)-H(10)	0.9500	C(19A)-H(19C)	0.9900
C(11)-C(12)	1.398(4)	C(19A)-H(19D)	0.9900
C(11)-C(14)	1.512(4)	C(20A)-H(20D)	0.9800
C(12)-C(13)	1.390(4)	C(20A)-H(20E)	0.9800

C(20A)-H(20F)	0.9800

N(1)#1-Fe(1)-N(1)	156.79(12)	C(6)-C(5)-H(5)	119.4
N(1)#1-Fe(1)-N(2)#1	86.41(8)	C(5)-C(6)-C(1)	118.5(2)
N(1)-Fe(1)-N(2)#1	107.55(8)	C(5)-C(6)-C(7)	115.9(2)
N(1)#1-Fe(1)-N(2)	107.55(8)	C(1)-C(6)-C(7)	125.6(2)
N(1)-Fe(1)-N(2)	86.41(8)	N(2)-C(7)-C(6)	128.6(2)
N(2)#1-Fe(1)-N(2)	107.16(11)	N(2)-C(7)-H(7)	115.7
O(2)-S(1)-O(1)	116.46(11)	C(6)-C(7)-H(7)	115.7
O(2)-S(1)-N(1)	115.49(11)	C(9)-C(8)-C(13)	120.0(2)
O(1)-S(1)-N(1)	101.56(10)	C(9)-C(8)-S(1)	119.90(19)
O(2)-S(1)-C(8)	106.83(11)	C(13)-C(8)-S(1)	120.1(2)
O(1)-S(1)-C(8)	109.41(11)	C(10)-C(9)-C(8)	119.5(2)
N(1)-S(1)-C(8)	106.63(12)	C(10)-C(9)-H(9)	120.2
C(1)-N(1)-S(1)	122.96(17)	C(8)-C(9)-H(9)	120.2
C(1)-N(1)-Fe(1)	133.05(17)	C(9)-C(10)-C(11)	121.5(2)
S(1)-N(1)-Fe(1)	103.97(10)	C(9)-C(10)-H(10)	119.3
C(7)-N(2)-C(15)	116.5(2)	C(11)-C(10)-H(10)	119.3
C(7)-N(2)-Fe(1)	126.95(18)	C(12)-C(11)-C(10)	117.9(2)
C(15)-N(2)-Fe(1)	116.53(15)	C(12)-C(11)-C(14)	121.2(2)
C(19)-N(3)-C(17)	114.4(3)	C(10)-C(11)-C(14)	120.9(2)
C(19)-N(3)-C(16)	111.6(3)	C(13)-C(12)-C(11)	121.4(2)
C(17)-N(3)-C(16)	110.5(3)	C(13)-C(12)-H(12)	119.3
C(19A)-N(3A)-C(17A)	113.8(7)	C(11)-C(12)-H(12)	119.3
C(19A)-N(3A)-C(16A)	113.6(6)	C(12)-C(13)-C(8)	119.6(2)
C(17A)-N(3A)-C(16A)	111.2(6)	C(12)-C(13)-H(13)	120.2
C(2)-C(1)-N(1)	123.8(2)	C(8)-C(13)-H(13)	120.2
C(2)-C(1)-C(6)	118.3(2)	C(11)-C(14)-H(14A)	109.5
N(1)-C(1)-C(6)	117.9(2)	C(11)-C(14)-H(14B)	109.5
C(3)-C(2)-C(1)	121.5(2)	H(14A)-C(14)-H(14B)	109.5
C(3)-C(2)-H(2)	119.2	C(11)-C(14)-H(14C)	109.5
C(1)-C(2)-H(2)	119.2	H(14A)-C(14)-H(14C)	109.5
C(4)-C(3)-C(2)	120.1(2)	H(14B)-C(14)-H(14C)	109.5
C(4)-C(3)-H(3)	119.9	N(2)-C(15)-C(16A)	112.3(3)
C(2)-C(3)-H(3)	119.9	N(2)-C(15)-C(16)	110.9(2)
C(3)-C(4)-C(5)	120.3(2)	N(2)-C(15)-H(15A)	109.5
C(3)-C(4)-H(4)	119.9	C(16)-C(15)-H(15A)	109.5
C(5)-C(4)-H(4)	119.9	N(2)-C(15)-H(15B)	109.5
C(4)-C(5)-C(6)	121.2(2)	C(16)-C(15)-H(15B)	109.5
C(4)-C(5)-H(5)	119.4	H(15A)-C(15)-H(15B)	108.0

N(2)-C(15)-H(15C)	109.2	H(20A)-C(20)-H(20C)	109.5
C(16A)-C(15)-H(15C)	109.2	H(20B)-C(20)-H(20C)	109.5
N(2)-C(15)-H(15D)	109.2	N(3A)-C(16A)-C(15)	108.6(4)
C(16A)-C(15)-H(15D)	109.2	N(3A)-C(16A)-H(16C)	110.0
H(15C)-C(15)-H(15D)	107.9	C(15)-C(16A)-H(16C)	110.0
N(3)-C(16)-C(15)	116.1(3)	N(3A)-C(16A)-H(16D)	110.0
N(3)-C(16)-H(16A)	108.3	C(15)-C(16A)-H(16D)	110.0
C(15)-C(16)-H(16A)	108.3	H(16C)-C(16A)-H(16D)	108.4
N(3)-C(16)-H(16B)	108.3	N(3A)-C(17A)-C(18A)	113.2(6)
C(15)-C(16)-H(16B)	108.3	N(3A)-C(17A)-H(17C)	108.9
H(16A)-C(16)-H(16B)	107.4	C(18A)-C(17A)-H(17C)	108.9
N(3)-C(17)-C(18)	114.7(3)	N(3A)-C(17A)-H(17D)	108.9
N(3)-C(17)-H(17A)	108.6	C(18A)-C(17A)-H(17D)	108.9
C(18)-C(17)-H(17A)	108.6	H(17C)-C(17A)-H(17D)	107.7
N(3)-C(17)-H(17B)	108.6	C(17A)-C(18A)-H(18D)	109.5
C(18)-C(17)-H(17B)	108.6	C(17A)-C(18A)-H(18E)	109.5
H(17A)-C(17)-H(17B)	107.6	H(18D)-C(18A)-H(18E)	109.5
C(17)-C(18)-H(18A)	109.5	C(17A)-C(18A)-H(18F)	109.5
C(17)-C(18)-H(18B)	109.5	H(18D)-C(18A)-H(18F)	109.5
H(18A)-C(18)-H(18B)	109.5	H(18E)-C(18A)-H(18F)	109.5
C(17)-C(18)-H(18C)	109.5	N(3A)-C(19A)-C(20A)	118.6(7)
H(18A)-C(18)-H(18C)	109.5	N(3A)-C(19A)-H(19C)	107.7
H(18B)-C(18)-H(18C)	109.5	C(20A)-C(19A)-H(19C)	107.7
N(3)-C(19)-C(20)	112.8(4)	N(3A)-C(19A)-H(19D)	107.7
N(3)-C(19)-H(19A)	109.0	C(20A)-C(19A)-H(19D)	107.7
C(20)-C(19)-H(19A)	109.0	H(19C)-C(19A)-H(19D)	107.1
N(3)-C(19)-H(19B)	109.0	C(19A)-C(20A)-H(20D)	109.5
C(20)-C(19)-H(19B)	109.0	C(19A)-C(20A)-H(20E)	109.5
H(19A)-C(19)-H(19B)	107.8	H(20D)-C(20A)-H(20E)	109.5
C(19)-C(20)-H(20A)	109.5	C(19A)-C(20A)-H(20F)	109.5
C(19)-C(20)-H(20B)	109.5	H(20D)-C(20A)-H(20F)	109.5
H(20A)-C(20)-H(20B)	109.5	H(20E)-C(20A)-H(20F)	109.5
C(19)-C(20)-H(20C)	109.5		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1-Fe**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	20(1)	23(1)	12(1)	0	7(1)	0
S(1)	19(1)	23(1)	14(1)	1(1)	8(1)	1(1)
O(1)	22(1)	29(1)	13(1)	3(1)	8(1)	3(1)
O(2)	20(1)	29(1)	20(1)	1(1)	12(1)	-1(1)
N(1)	21(1)	22(1)	14(1)	1(1)	7(1)	2(1)
N(2)	20(1)	22(1)	17(1)	0(1)	9(1)	-1(1)
N(3)	29(2)	25(2)	17(2)	-1(1)	10(2)	4(2)
N(3A)	29(2)	25(2)	17(2)	-1(1)	10(2)	4(2)
C(1)	18(1)	21(1)	14(1)	1(1)	6(1)	-3(1)
C(2)	23(1)	24(1)	18(1)	-2(1)	10(1)	1(1)
C(3)	26(2)	30(1)	15(1)	-1(1)	11(1)	-2(1)
C(4)	24(2)	32(2)	16(1)	3(1)	6(1)	1(1)
C(5)	20(1)	24(1)	21(1)	2(1)	8(1)	1(1)
C(6)	17(1)	22(1)	18(1)	-1(1)	7(1)	-2(1)
C(7)	18(1)	19(1)	23(1)	-1(1)	11(1)	0(1)
C(8)	24(1)	21(1)	17(1)	5(1)	10(1)	5(1)
C(9)	26(2)	23(1)	20(1)	-1(1)	13(1)	1(1)
C(10)	24(2)	26(1)	25(1)	2(1)	15(1)	0(1)
C(11)	23(1)	20(1)	18(1)	1(1)	7(1)	2(1)
C(12)	27(2)	24(1)	20(1)	-2(1)	12(1)	3(1)
C(13)	21(1)	29(2)	19(1)	2(1)	11(1)	2(1)
C(14)	33(2)	27(2)	29(2)	-5(1)	16(1)	-6(1)
C(15)	24(1)	28(1)	18(1)	1(1)	12(1)	5(1)
C(16)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(17)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(18)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(19)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(20)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(16A)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(17A)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(18A)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(19A)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)
C(20A)	32(1)	38(1)	26(1)	-4(1)	12(1)	6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1-Fe**.

	x	y	z	U(iso)
H(2)	5430	3031	6854	26
H(3)	6379	2578	8845	28
H(4)	7422	1934	8923	31
H(5)	7506	1723	7006	27
H(7)	7124	1849	4807	24
H(9)	6114	3941	4211	26
H(10)	7054	4690	5359	28
H(12)	5692	4960	7364	28
H(13)	4749	4211	6230	27
H(14A)	7007	5693	6613	43
H(14B)	7711	5256	7652	43
H(14C)	6964	5523	7934	43
H(15A)	7054	1965	2822	27
H(15B)	6145	2176	1580	27
H(15C)	6983	1764	2931	27
H(15D)	6469	2258	1885	27
H(16A)	6443	1104	2874	39
H(16B)	5465	1316	1863	39
H(17A)	7497	1148	2049	39
H(17B)	7077	1586	838	39
H(18A)	6920	887	-674	49
H(18B)	7222	412	459	49
H(18C)	7922	871	517	49
H(19A)	5618	1233	-1032	39
H(19B)	5279	1657	-288	39
H(20A)	4167	992	-1694	49
H(20B)	4352	973	-182	49
H(20C)	4764	499	-717	49
H(16C)	5712	1193	1972	39
H(16D)	5142	1696	991	39
H(17C)	6389	549	1164	39
H(17D)	7164	999	1920	39
H(18D)	6614	542	-663	49
H(18E)	7572	477	621	49
H(18F)	7265	1074	-116	49
H(19C)	5560	1182	-1410	39

H(19D)	4936	1581	-1105	39
H(20D)	4176	765	-1872	49
H(20E)	4525	750	-297	49
H(20F)	5020	389	-922	49

Table 6. Torsion angles [°] for **1-Fe**.

O(2)-S(1)-N(1)-C(1)	-53.8(2)	C(13)-C(8)-C(9)-C(10)	2.3(4)
O(1)-S(1)-N(1)-C(1)	179.25(19)	S(1)-C(8)-C(9)-C(10)	-179.22(19)
C(8)-S(1)-N(1)-C(1)	64.7(2)	C(8)-C(9)-C(10)-C(11)	-0.8(4)
O(2)-S(1)-N(1)-Fe(1)	124.67(11)	C(9)-C(10)-C(11)-C(12)	-0.8(4)
O(1)-S(1)-N(1)-Fe(1)	-2.30(13)	C(9)-C(10)-C(11)-C(14)	179.5(2)
C(8)-S(1)-N(1)-Fe(1)	-116.83(11)	C(10)-C(11)-C(12)-C(13)	0.9(4)
S(1)-N(1)-C(1)-C(2)	10.2(4)	C(14)-C(11)-C(12)-C(13)	-179.4(2)
Fe(1)-N(1)-C(1)-C(2)	-167.71(19)	C(11)-C(12)-C(13)-C(8)	0.5(4)
S(1)-N(1)-C(1)-C(6)	-170.45(18)	C(9)-C(8)-C(13)-C(12)	-2.2(4)
Fe(1)-N(1)-C(1)-C(6)	11.6(3)	S(1)-C(8)-C(13)-C(12)	179.32(19)
N(1)-C(1)-C(2)-C(3)	178.8(2)	C(7)-N(2)-C(15)-C(16A)	114.5(4)
C(6)-C(1)-C(2)-C(3)	-0.5(4)	Fe(1)-N(2)-C(15)-C(16A)	-68.2(4)
C(1)-C(2)-C(3)-C(4)	1.3(4)	C(7)-N(2)-C(15)-C(16)	81.7(3)
C(2)-C(3)-C(4)-C(5)	-0.7(4)	Fe(1)-N(2)-C(15)-C(16)	-100.9(3)
C(3)-C(4)-C(5)-C(6)	-0.5(4)	C(19)-N(3)-C(16)-C(15)	-80.0(4)
C(4)-C(5)-C(6)-C(1)	1.3(4)	C(17)-N(3)-C(16)-C(15)	48.6(5)
C(4)-C(5)-C(6)-C(7)	179.6(2)	N(2)-C(15)-C(16)-N(3)	167.8(3)
C(2)-C(1)-C(6)-C(5)	-0.7(4)	C(16A)-C(15)-C(16)-N(3)	69.2(6)
N(1)-C(1)-C(6)-C(5)	179.9(2)	C(19)-N(3)-C(17)-C(18)	-71.6(5)
C(2)-C(1)-C(6)-C(7)	-178.9(2)	C(16)-N(3)-C(17)-C(18)	161.4(4)
N(1)-C(1)-C(6)-C(7)	1.7(4)	C(17)-N(3)-C(19)-C(20)	149.8(4)
C(15)-N(2)-C(7)-C(6)	-178.4(2)	C(16)-N(3)-C(19)-C(20)	-83.7(4)
Fe(1)-N(2)-C(7)-C(6)	4.6(4)	C(19A)-N(3A)-C(16A)-C(15)	-145.2(7)
C(5)-C(6)-C(7)-N(2)	171.7(2)	C(17A)-N(3A)-C(16A)-C(15)	84.9(8)
C(1)-C(6)-C(7)-N(2)	-10.1(4)	N(2)-C(15)-C(16A)-N(3A)	174.7(5)
O(2)-S(1)-C(8)-C(9)	175.21(19)	C(16)-C(15)-C(16A)-N(3A)	-91.6(7)
O(1)-S(1)-C(8)-C(9)	-57.9(2)	C(19A)-N(3A)-C(17A)-C(18A)	56.4(10)
N(1)-S(1)-C(8)-C(9)	51.2(2)	C(16A)-N(3A)-C(17A)-C(18A)	-173.7(7)
O(2)-S(1)-C(8)-C(13)	-6.3(2)	C(17A)-N(3A)-C(19A)-C(20A)	62.1(10)
O(1)-S(1)-C(8)-C(13)	120.6(2)	C(16A)-N(3A)-C(19A)-C(20A)	-66.5(10)
N(1)-S(1)-C(8)-C(13)	-130.3(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table 1. Crystal data and structure refinement for **2-Zn**.

Identification code	**2-Zn**	
Empirical formula	C35.50 H41.50 N4.50 O8.50 S2 Zn	
Formula weight	796.72	
Temperature	100(2) K	
Wavelength	0.96990 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4379(17) Å	α = 78.68(3)°.
	b = 11.489(2) Å	β = 86.99(3)°.
	c = 20.085(4) Å	γ = 75.58(3)°.
Volume	1849.1(7) Å^3	
Z	2	
Density (calculated)	1.431 Mg/m^3	
Absorption coefficient	1.920 mm^{-1}	
F(000)	832	
Crystal size	0.20 x 0.15 x 0.05 mm^3	
Theta range for data collection	3.135 to 38.443°.	
Index ranges	-10<=h<=8, -12<=k<=14, -25<=l<=25	
Reflections collected	17994	
Independent reflections	7593 [R(int) = 0.1167]	
Completeness to theta = 35.587°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.900 and 0.700	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7593 / 22 / 387	
Goodness-of-fit on F^2	1.046	
Final R indices [for 4327 rflns with I>2σ(I)]	R1 = 0.1175, wR2 = 0.2425	
R indices (all data)	R1 = 0.1655, wR2 = 0.2822	
Extinction coefficient	0.0171(16)	
Largest diff. peak and hole	1.530 and -1.319 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2-Zn**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Zn(1)	8126(1)	6147(1)	7600(1)	38(1)
S(1)	6374(2)	4635(2)	6991(1)	36(1)
S(2)	7619(2)	8535(2)	6637(1)	37(1)
O(1)	5446(6)	5859(4)	7033(3)	38(1)
O(2)	5655(6)	3654(5)	7328(3)	39(1)
O(3)	11975(12)	6113(7)	8843(4)	100(2)
O(4)	11645(12)	8576(7)	8979(4)	100(2)
O(5)	8666(6)	9380(5)	6540(3)	40(1)
O(6)	8209(6)	7426(4)	6357(3)	38(1)
O(7)	4750(30)	5231(14)	9270(8)	108(3)
O(8)	6270(30)	2944(15)	9961(7)	108(3)
O(7A)	8570(30)	4348(15)	9736(7)	108(3)
O(8A)	6840(30)	2387(16)	9795(9)	108(3)
N(1)	8121(7)	4566(5)	7288(3)	31(1)
N(2)	10619(7)	5727(6)	7618(3)	37(2)
N(3)	7312(12)	7995(7)	7424(4)	66(1)
N(4)	7062(12)	5985(7)	8548(4)	66(1)
C(1)	9456(9)	3536(7)	7302(4)	33(2)
C(2)	9277(10)	2394(6)	7191(4)	36(2)
C(3)	10557(10)	1413(7)	7189(4)	42(2)
C(4)	12149(11)	1474(8)	7311(5)	48(2)
C(5)	12389(10)	2545(7)	7437(5)	45(2)
C(6)	11044(9)	3617(7)	7441(4)	34(2)
C(7)	11547(11)	4683(8)	7548(4)	45(2)
C(8)	6708(9)	4492(7)	6134(4)	35(2)
C(9)	6201(10)	3577(8)	5879(4)	43(2)
C(10)	6552(9)	3453(7)	5212(4)	38(2)
C(11)	7366(9)	4215(7)	4782(4)	36(2)
C(12)	7819(10)	5130(7)	5037(4)	41(2)
C(13)	7503(10)	5267(7)	5704(4)	41(2)
C(14)	7798(11)	4056(8)	4058(4)	50(2)
C(15)	11470(20)	6692(11)	7666(6)	100(2)
C(16)	11220(20)	7063(11)	8344(6)	100(2)
C(17)	11860(20)	8201(11)	8342(6)	100(2)
C(18)	6832(15)	8735(9)	7912(5)	66(1)

C(19)	6698(14)	10016(9)	7775(5)	66(1)
C(20)	6267(14)	10729(9)	8272(5)	66(1)
C(21)	5921(14)	10217(8)	8913(5)	66(1)
C(22)	5963(14)	8979(9)	9048(5)	66(1)
C(23)	6471(14)	8208(9)	8572(5)	66(1)
C(24)	6421(14)	6914(8)	8836(5)	66(1)
C(25)	5693(9)	9332(7)	6278(4)	34(2)
C(26)	4367(9)	8784(7)	6362(4)	36(2)
C(27)	2848(10)	9411(8)	6069(4)	42(2)
C(28)	2620(10)	10597(7)	5678(4)	37(2)
C(29)	3944(10)	11117(7)	5588(4)	41(2)
C(30)	5483(11)	10504(7)	5882(4)	43(2)
C(31)	988(10)	11270(8)	5374(4)	45(2)
C(32)	7440(30)	4761(13)	8988(12)	108(3)
C(33)	5840(30)	4456(15)	8886(11)	108(3)
C(34)	6070(40)	3138(17)	9248(8)	108(3)
C(32A)	6610(30)	4834(15)	8856(14)	108(3)
C(33A)	8180(30)	3957(16)	9150(9)	108(3)
C(34A)	8100(30)	2628(17)	9333(12)	108(3)
O(9)	800(30)	3389(15)	10265(9)	122(5)
N(5)	1750(20)	2201(14)	9478(7)	122(5)
C(35)	810(20)	2478(15)	10018(8)	122(5)
C(36)	1680(40)	1102(18)	9219(12)	122(5)
C(37)	2750(30)	3070(20)	9208(13)	122(5)

Table 3. Bond lengths [Å] and angles [°] for **2-Zn**.

Zn(1)-N(3)	2.027(8)	C(5)-C(6)	1.453(10)
Zn(1)-N(1)	2.035(5)	C(5)-H(5)	0.9500
Zn(1)-N(2)	2.039(6)	C(6)-C(7)	1.449(10)
Zn(1)-N(4)	2.057(7)	C(7)-H(7)	0.9500
S(1)-O(1)	1.445(5)	C(8)-C(13)	1.387(11)
S(1)-O(2)	1.448(5)	C(8)-C(9)	1.417(10)
S(1)-N(1)	1.597(6)	C(9)-C(10)	1.383(11)
S(1)-C(8)	1.762(8)	C(9)-H(9)	0.9500
S(2)-O(5)	1.448(5)	C(10)-C(11)	1.387(11)
S(2)-O(6)	1.458(5)	C(10)-H(10)	0.9500
S(2)-N(3)	1.614(8)	C(11)-C(12)	1.395(10)
S(2)-C(25)	1.768(8)	C(11)-C(14)	1.515(11)
O(3)-C(16)	1.375(14)	C(12)-C(13)	1.384(11)
O(3)-H(3A)	0.9002	C(12)-H(12)	0.9500
O(4)-C(17)	1.418(13)	C(13)-H(13)	0.9500
O(4)-H(4A)	0.9000	C(14)-H(14A)	0.9800
O(7)-C(33)	1.420(3)	C(14)-H(14B)	0.9800
O(7)-H(7A)	0.9000	C(14)-H(14C)	0.9800
O(8)-C(34)	1.420(3)	C(15)-C(16)	1.496(16)
O(8)-H(8A)	0.9000	C(15)-H(15A)	0.9900
O(7A)-C(33A)	1.420(3)	C(15)-H(15B)	0.9900
O(7A)-H(7B)	0.9000	C(16)-C(17)	1.533(16)
O(8A)-C(34A)	1.419(3)	C(16)-H(16)	1.0000
O(8A)-H(8B)	0.9000	C(17)-H(17A)	0.9900
N(1)-C(1)	1.413(9)	C(17)-H(17B)	0.9900
N(2)-C(7)	1.288(10)	C(18)-C(23)	1.397(13)
N(2)-C(15)	1.483(13)	C(18)-C(19)	1.420(13)
N(3)-C(18)	1.401(10)	C(19)-C(20)	1.389(11)
N(4)-C(24)	1.299(10)	C(19)-H(19)	0.9500
N(4)-C(32A)	1.476(3)	C(20)-C(21)	1.356(13)
N(4)-C(32)	1.476(3)	C(20)-H(20)	0.9500
C(1)-C(6)	1.412(10)	C(21)-C(22)	1.386(12)
C(1)-C(2)	1.417(9)	C(21)-H(21)	0.9500
C(2)-C(3)	1.354(11)	C(22)-C(23)	1.408(11)
C(2)-H(2)	0.9500	C(22)-H(22)	0.9500
C(3)-C(4)	1.400(12)	C(23)-C(24)	1.488(13)
C(3)-H(3)	0.9500	C(24)-H(24)	0.9500
C(4)-C(5)	1.367(11)	C(25)-C(30)	1.397(11)
C(4)-H(4)	0.9500	C(25)-C(26)	1.402(10)

C(26)-C(27)	1.401(11)	C(32A)-C(33A)	1.515(3)
C(26)-H(26)	0.9500	C(32A)-H(32C)	0.9900
C(27)-C(28)	1.405(11)	C(32A)-H(32D)	0.9900
C(27)-H(27)	0.9500	C(33A)-C(34A)	1.515(3)
C(28)-C(29)	1.382(11)	C(33A)-H(33B)	1.0000
C(28)-C(31)	1.496(11)	C(34A)-H(34C)	0.9900
C(29)-C(30)	1.412(12)	C(34A)-H(34D)	0.9900
C(29)-H(29)	0.9500	O(9)-C(35)	1.241(3)
C(30)-H(30)	0.9500	N(5)-C(35)	1.350(3)
C(31)-H(31A)	0.9800	N(5)-C(36)	1.470(3)
C(31)-H(31B)	0.9800	N(5)-C(37)	1.471(3)
C(31)-H(31C)	0.9800	C(35)-H(35)	0.9500
C(32)-C(33)	1.514(3)	C(36)-H(36A)	0.9800
C(32)-H(32A)	0.9900	C(36)-H(36B)	0.9800
C(32)-H(32B)	0.9900	C(36)-H(36C)	0.9800
C(33)-C(34)	1.515(3)	C(37)-H(37A)	0.9800
C(33)-H(33A)	1.0000	C(37)-H(37B)	0.9800
C(34)-H(34A)	0.9900	C(37)-H(37C)	0.9800
C(34)-H(34B)	0.9900		

N(3)-Zn(1)-N(1)	146.4(3)	C(34)-O(8)-H(8A)	110.1
N(3)-Zn(1)-N(2)	108.0(3)	C(33A)-O(7A)-H(7B)	107.3
N(1)-Zn(1)-N(2)	91.8(2)	C(34A)-O(8A)-H(8B)	108.3
N(3)-Zn(1)-N(4)	91.9(3)	C(1)-N(1)-S(1)	122.5(5)
N(1)-Zn(1)-N(4)	104.9(3)	C(1)-N(1)-Zn(1)	126.7(5)
N(2)-Zn(1)-N(4)	113.8(3)	S(1)-N(1)-Zn(1)	110.8(3)
O(1)-S(1)-O(2)	115.7(3)	C(7)-N(2)-C(15)	115.9(9)
O(1)-S(1)-N(1)	103.5(3)	C(7)-N(2)-Zn(1)	124.6(6)
O(2)-S(1)-N(1)	113.2(3)	C(15)-N(2)-Zn(1)	119.4(7)
O(1)-S(1)-C(8)	110.0(4)	C(18)-N(3)-S(2)	123.0(7)
O(2)-S(1)-C(8)	107.8(3)	C(18)-N(3)-Zn(1)	126.8(7)
N(1)-S(1)-C(8)	106.1(3)	S(2)-N(3)-Zn(1)	109.3(4)
O(5)-S(2)-O(6)	116.4(3)	C(24)-N(4)-C(32A)	115.4(14)
O(5)-S(2)-N(3)	113.7(4)	C(24)-N(4)-C(32)	117.3(14)
O(6)-S(2)-N(3)	102.3(3)	C(24)-N(4)-Zn(1)	123.4(7)
O(5)-S(2)-C(25)	107.9(3)	C(32A)-N(4)-Zn(1)	119.4(12)
O(6)-S(2)-C(25)	108.8(3)	C(32)-N(4)-Zn(1)	117.2(13)
N(3)-S(2)-C(25)	107.3(4)	C(6)-C(1)-N(1)	119.8(6)
C(16)-O(3)-H(3A)	103.1	C(6)-C(1)-C(2)	117.4(7)
C(17)-O(4)-H(4A)	108.7	N(1)-C(1)-C(2)	122.8(7)
C(33)-O(7)-H(7A)	107.9	C(3)-C(2)-C(1)	123.0(7)

C(3)-C(2)-H(2)	118.5	N(2)-C(15)-C(16)	111.9(11)
C(1)-C(2)-H(2)	118.5	N(2)-C(15)-H(15A)	109.2
C(2)-C(3)-C(4)	120.9(7)	C(16)-C(15)-H(15A)	109.2
C(2)-C(3)-H(3)	119.6	N(2)-C(15)-H(15B)	109.2
C(4)-C(3)-H(3)	119.6	C(16)-C(15)-H(15B)	109.2
C(5)-C(4)-C(3)	118.7(8)	H(15A)-C(15)-H(15B)	107.9
C(5)-C(4)-H(4)	120.7	O(3)-C(16)-C(15)	110.4(11)
C(3)-C(4)-H(4)	120.7	O(3)-C(16)-C(17)	110.7(11)
C(4)-C(5)-C(6)	121.9(8)	C(15)-C(16)-C(17)	110.8(12)
C(4)-C(5)-H(5)	119.0	O(3)-C(16)-H(16)	108.3
C(6)-C(5)-H(5)	119.0	C(15)-C(16)-H(16)	108.3
C(1)-C(6)-C(7)	127.8(7)	C(17)-C(16)-H(16)	108.3
C(1)-C(6)-C(5)	118.2(6)	O(4)-C(17)-C(16)	112.1(11)
C(7)-C(6)-C(5)	113.9(7)	O(4)-C(17)-H(17A)	109.2
N(2)-C(7)-C(6)	127.4(8)	C(16)-C(17)-H(17A)	109.2
N(2)-C(7)-H(7)	116.3	O(4)-C(17)-H(17B)	109.2
C(6)-C(7)-H(7)	116.3	C(16)-C(17)-H(17B)	109.2
C(13)-C(8)-C(9)	119.3(7)	H(17A)-C(17)-H(17B)	107.9
C(13)-C(8)-S(1)	119.8(6)	C(23)-C(18)-N(3)	119.5(8)
C(9)-C(8)-S(1)	120.9(6)	C(23)-C(18)-C(19)	117.1(8)
C(10)-C(9)-C(8)	119.3(7)	N(3)-C(18)-C(19)	123.4(9)
C(10)-C(9)-H(9)	120.3	C(20)-C(19)-C(18)	122.5(9)
C(8)-C(9)-H(9)	120.3	C(20)-C(19)-H(19)	118.8
C(9)-C(10)-C(11)	121.7(7)	C(18)-C(19)-H(19)	118.8
C(9)-C(10)-H(10)	119.2	C(21)-C(20)-C(19)	120.4(9)
C(11)-C(10)-H(10)	119.2	C(21)-C(20)-H(20)	119.8
C(10)-C(11)-C(12)	118.2(7)	C(19)-C(20)-H(20)	119.8
C(10)-C(11)-C(14)	121.8(7)	C(20)-C(21)-C(22)	117.9(8)
C(12)-C(11)-C(14)	120.0(7)	C(20)-C(21)-H(21)	121.0
C(13)-C(12)-C(11)	121.4(7)	C(22)-C(21)-H(21)	121.0
C(13)-C(12)-H(12)	119.3	C(21)-C(22)-C(23)	123.6(9)
C(11)-C(12)-H(12)	119.3	C(21)-C(22)-H(22)	118.2
C(12)-C(13)-C(8)	120.1(7)	C(23)-C(22)-H(22)	118.2
C(12)-C(13)-H(13)	120.0	C(18)-C(23)-C(22)	118.3(9)
C(8)-C(13)-H(13)	120.0	C(18)-C(23)-C(24)	127.8(8)
C(11)-C(14)-H(14A)	109.5	C(22)-C(23)-C(24)	113.7(9)
C(11)-C(14)-H(14B)	109.5	N(4)-C(24)-C(23)	126.2(9)
H(14A)-C(14)-H(14B)	109.5	N(4)-C(24)-H(24)	116.9
C(11)-C(14)-H(14C)	109.5	C(23)-C(24)-H(24)	116.9
H(14A)-C(14)-H(14C)	109.5	C(30)-C(25)-C(26)	118.8(7)
H(14B)-C(14)-H(14C)	109.5	C(30)-C(25)-S(2)	120.4(6)

C(26)-C(25)-S(2)	120.7(6)	N(4)-C(32A)-H(32C)	110.5
C(27)-C(26)-C(25)	120.6(7)	C(33A)-C(32A)-H(32C)	110.5
C(27)-C(26)-H(26)	119.7	N(4)-C(32A)-H(32D)	110.5
C(25)-C(26)-H(26)	119.7	C(33A)-C(32A)-H(32D)	110.5
C(26)-C(27)-C(28)	121.0(7)	H(32C)-C(32A)-H(32D)	108.7
C(26)-C(27)-H(27)	119.5	O(7A)-C(33A)-C(34A)	109.7(16)
C(28)-C(27)-H(27)	119.5	O(7A)-C(33A)-C(32A)	108(2)
C(29)-C(28)-C(27)	117.8(8)	C(34A)-C(33A)-C(32A)	114.8(18)
C(29)-C(28)-C(31)	121.4(7)	O(7A)-C(33A)-H(33B)	108.2
C(27)-C(28)-C(31)	120.7(7)	C(34A)-C(33A)-H(33B)	108.2
C(28)-C(29)-C(30)	122.1(7)	C(32A)-C(33A)-H(33B)	108.2
C(28)-C(29)-H(29)	118.9	O(8A)-C(34A)-C(33A)	115.3(18)
C(30)-C(29)-H(29)	118.9	O(8A)-C(34A)-H(34C)	108.5
C(25)-C(30)-C(29)	119.6(7)	C(33A)-C(34A)-H(34C)	108.5
C(25)-C(30)-H(30)	120.2	O(8A)-C(34A)-H(34D)	108.5
C(29)-C(30)-H(30)	120.2	C(33A)-C(34A)-H(34D)	108.5
C(28)-C(31)-H(31A)	109.5	H(34C)-C(34A)-H(34D)	107.5
C(28)-C(31)-H(31B)	109.5	C(35)-N(5)-C(36)	119.0(17)
H(31A)-C(31)-H(31B)	109.5	C(35)-N(5)-C(37)	114.3(17)
C(28)-C(31)-H(31C)	109.5	C(36)-N(5)-C(37)	126.7(18)
H(31A)-C(31)-H(31C)	109.5	O(9)-C(35)-N(5)	122.7(18)
H(31B)-C(31)-H(31C)	109.5	O(9)-C(35)-H(35)	118.7
N(4)-C(32)-C(33)	96.4(12)	N(5)-C(35)-H(35)	118.7
N(4)-C(32)-H(32A)	112.5	N(5)-C(36)-H(36A)	109.5
C(33)-C(32)-H(32A)	112.5	N(5)-C(36)-H(36B)	109.5
N(4)-C(32)-H(32B)	112.5	H(36A)-C(36)-H(36B)	109.5
C(33)-C(32)-H(32B)	112.5	N(5)-C(36)-H(36C)	109.5
H(32A)-C(32)-H(32B)	110.0	H(36A)-C(36)-H(36C)	109.5
O(7)-C(33)-C(32)	101(2)	H(36B)-C(36)-H(36C)	109.5
O(7)-C(33)-C(34)	109.1(18)	N(5)-C(37)-H(37A)	109.5
C(32)-C(33)-C(34)	104.5(18)	N(5)-C(37)-H(37B)	109.5
O(7)-C(33)-H(33A)	113.7	H(37A)-C(37)-H(37B)	109.5
C(32)-C(33)-H(33A)	113.7	N(5)-C(37)-H(37C)	109.5
C(34)-C(33)-H(33A)	113.7	H(37A)-C(37)-H(37C)	109.5
O(8)-C(34)-C(33)	114.7(17)	H(37B)-C(37)-H(37C)	109.5
O(8)-C(34)-H(34A)	108.6		
C(33)-C(34)-H(34A)	108.6		
O(8)-C(34)-H(34B)	108.6		
C(33)-C(34)-H(34B)	108.6		
H(34A)-C(34)-H(34B)	107.6		
N(4)-C(32A)-C(33A)	106.0(13)		

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

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	39(1)	33(1)	48(1)	-18(1)	6(1)	-14(1)
S(1)	31(1)	33(1)	50(1)	-16(1)	5(1)	-13(1)
S(2)	32(1)	32(1)	53(1)	-18(1)	7(1)	-13(1)
O(1)	30(3)	22(3)	62(4)	-15(2)	4(3)	-1(2)
O(2)	37(3)	36(3)	52(3)	-15(3)	8(2)	-21(2)
O(3)	168(5)	61(3)	83(3)	-24(2)	-29(3)	-34(3)
O(4)	168(5)	61(3)	83(3)	-24(2)	-29(3)	-34(3)
O(5)	33(3)	35(3)	59(4)	-16(3)	8(3)	-17(2)
O(6)	35(3)	27(3)	56(4)	-20(2)	10(3)	-10(2)
O(7)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
O(8)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
O(7A)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
O(8A)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
N(1)	24(3)	24(3)	50(4)	-16(3)	0(3)	-6(2)
N(2)	24(4)	38(4)	50(4)	-17(3)	0(3)	-3(3)
N(3)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
N(4)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(1)	34(5)	30(4)	39(4)	-14(3)	6(3)	-10(3)
C(2)	30(4)	24(4)	56(5)	-14(3)	5(4)	-8(3)
C(3)	42(5)	36(5)	54(5)	-14(4)	3(4)	-19(4)
C(4)	43(6)	32(5)	70(6)	-18(4)	11(4)	-5(4)
C(5)	28(5)	35(5)	75(6)	-22(4)	4(4)	-7(4)
C(6)	32(4)	28(4)	48(5)	-21(3)	10(3)	-12(3)
C(7)	46(6)	38(5)	60(6)	-23(4)	6(4)	-16(4)
C(8)	28(4)	26(4)	57(5)	-14(4)	2(4)	-12(3)
C(9)	39(5)	47(5)	53(5)	-18(4)	2(4)	-23(4)
C(10)	32(5)	35(4)	52(5)	-19(4)	-2(4)	-10(3)
C(11)	28(4)	33(4)	48(5)	-12(4)	4(4)	-5(3)
C(12)	44(5)	37(5)	46(5)	-9(4)	4(4)	-17(4)
C(13)	37(5)	38(5)	52(5)	-15(4)	-6(4)	-11(4)
C(14)	48(6)	50(5)	59(6)	-21(4)	6(4)	-16(4)
C(15)	168(5)	61(3)	83(3)	-24(2)	-29(3)	-34(3)
C(16)	168(5)	61(3)	83(3)	-24(2)	-29(3)	-34(3)
C(17)	168(5)	61(3)	83(3)	-24(2)	-29(3)	-34(3)
C(18)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)

C(19)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(20)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(21)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(22)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(23)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(24)	103(3)	40(2)	60(2)	-24(2)	25(2)	-20(2)
C(25)	31(4)	28(4)	47(5)	-18(3)	8(3)	-9(3)
C(26)	33(5)	24(4)	55(5)	-10(3)	7(4)	-15(3)
C(27)	39(5)	42(5)	54(5)	-12(4)	4(4)	-21(4)
C(28)	33(5)	36(4)	47(5)	-15(4)	6(4)	-11(3)
C(29)	40(5)	24(4)	53(5)	-6(4)	4(4)	0(3)
C(30)	46(6)	38(5)	53(5)	-13(4)	9(4)	-23(4)
C(31)	32(5)	45(5)	53(5)	-9(4)	-3(4)	0(4)
C(32)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
C(33)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
C(34)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
C(32A)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
C(33A)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
C(34A)	197(9)	67(5)	77(5)	-27(3)	17(5)	-59(5)
O(9)	201(14)	80(8)	100(9)	-48(6)	45(8)	-48(8)
N(5)	201(14)	80(8)	100(9)	-48(6)	45(8)	-48(8)
C(35)	201(14)	80(8)	100(9)	-48(6)	45(8)	-48(8)
C(36)	201(14)	80(8)	100(9)	-48(6)	45(8)	-48(8)
C(37)	201(14)	80(8)	100(9)	-48(6)	45(8)	-48(8)

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

Atom	x	y	z	U(iso)
H(3A)	11520	6340	9227	150
H(4A)	12359	8037	9276	150
H(7A)	3778	5482	9059	161
H(8A)	7022	3323	10058	161
H(7B)	9524	3847	9897	161
H(8B)	6013	3062	9747	161
H(2)	8211	2314	7116	43
H(3)	10372	674	7103	50
H(4)	13046	786	7307	58
H(5)	13465	2590	7525	54
H(7)	12692	4603	7569	54
H(9)	5626	3054	6163	52
H(10)	6227	2830	5045	45
H(12)	8357	5671	4747	49
H(13)	7831	5892	5868	49
H(14A)	8828	3433	4054	75
H(14B)	7920	4835	3785	75
H(14C)	6925	3797	3868	75
H(15A)	11052	7417	7307	120
H(15B)	12655	6387	7585	120
H(16)	10023	7269	8444	120
H(17A)	13044	8021	8224	120
H(17B)	11284	8879	7988	120
H(19)	6910	10400	7328	79
H(20)	6214	11580	8161	79
H(21)	5659	10692	9259	79
H(22)	5630	8632	9486	79
H(24)	5867	6751	9255	79
H(26)	4500	7980	6622	43
H(27)	1960	9029	6135	51
H(29)	3815	11914	5321	49
H(30)	6371	10886	5812	52
H(31A)	573	12012	5564	67
H(31B)	220	10744	5479	67
H(31C)	1102	11495	4881	67
H(32A)	7618	4795	9467	129

H(32B)	8395	4192	8821	129
H(33A)	5522	4599	8398	129
H(34A)	5102	2850	9157	129
H(34B)	7036	2631	9053	129
H(32C)	6163	4503	8508	129
H(32D)	5783	4973	9217	129
H(33B)	9074	4021	8809	129
H(34C)	7959	2345	8910	129
H(34D)	9169	2137	9531	129
H(35)	133	1953	10217	146
H(36A)	1428	1327	8733	183
H(36B)	836	738	9463	183
H(36C)	2747	508	9287	183
H(37A)	3450	3124	9570	183
H(37B)	2032	3879	9042	183
H(37C)	3433	2787	8834	183

Table 6. Torsion angles [°] for **2-Zn**.

O(1)-S(1)-N(1)-C(1)	-176.0(6)	S(1)-C(8)-C(9)-C(10)	-176.9(6)
O(2)-S(1)-N(1)-C(1)	57.9(7)	C(8)-C(9)-C(10)-C(11)	-1.1(13)
C(8)-S(1)-N(1)-C(1)	-60.1(7)	C(9)-C(10)-C(11)-C(12)	-0.5(12)
O(1)-S(1)-N(1)-Zn(1)	2.3(4)	C(9)-C(10)-C(11)-C(14)	178.1(8)
O(2)-S(1)-N(1)-Zn(1)	-123.7(3)	C(10)-C(11)-C(12)-C(13)	1.3(12)
C(8)-S(1)-N(1)-Zn(1)	118.2(4)	C(14)-C(11)-C(12)-C(13)	-177.3(8)
O(5)-S(2)-N(3)-C(18)	49.4(10)	C(11)-C(12)-C(13)-C(8)	-0.5(13)
O(6)-S(2)-N(3)-C(18)	175.7(9)	C(9)-C(8)-C(13)-C(12)	-1.1(12)
C(25)-S(2)-N(3)-C(18)	-69.9(10)	S(1)-C(8)-C(13)-C(12)	177.7(6)
O(5)-S(2)-N(3)-Zn(1)	-120.3(4)	C(7)-N(2)-C(15)-C(16)	-115.1(12)
O(6)-S(2)-N(3)-Zn(1)	6.1(5)	Zn(1)-N(2)-C(15)-C(16)	69.1(12)
C(25)-S(2)-N(3)-Zn(1)	120.5(4)	N(2)-C(15)-C(16)-O(3)	66.5(16)
S(1)-N(1)-C(1)-C(6)	167.3(6)	N(2)-C(15)-C(16)-C(17)	-170.5(11)
Zn(1)-N(1)-C(1)-C(6)	-10.8(10)	O(3)-C(16)-C(17)-O(4)	-57.3(17)
S(1)-N(1)-C(1)-C(2)	-13.7(10)	C(15)-C(16)-C(17)-O(4)	179.9(12)
Zn(1)-N(1)-C(1)-C(2)	168.2(6)	S(2)-N(3)-C(18)-C(23)	175.2(9)
C(6)-C(1)-C(2)-C(3)	-2.6(12)	Zn(1)-N(3)-C(18)-C(23)	-17.1(16)
N(1)-C(1)-C(2)-C(3)	178.4(8)	S(2)-N(3)-C(18)-C(19)	-5.2(17)
C(1)-C(2)-C(3)-C(4)	1.3(13)	Zn(1)-N(3)-C(18)-C(19)	162.5(9)
C(2)-C(3)-C(4)-C(5)	0.3(13)	C(23)-C(18)-C(19)-C(20)	1.6(18)
C(3)-C(4)-C(5)-C(6)	-0.6(13)	N(3)-C(18)-C(19)-C(20)	-178.0(11)
N(1)-C(1)-C(6)-C(7)	-3.2(12)	C(18)-C(19)-C(20)-C(21)	-1.4(19)
C(2)-C(1)-C(6)-C(7)	177.8(8)	C(19)-C(20)-C(21)-C(22)	-2.0(18)
N(1)-C(1)-C(6)-C(5)	-178.8(7)	C(20)-C(21)-C(22)-C(23)	5.4(18)
C(2)-C(1)-C(6)-C(5)	2.2(11)	N(3)-C(18)-C(23)-C(22)	-178.8(11)
C(4)-C(5)-C(6)-C(1)	-0.7(13)	C(19)-C(18)-C(23)-C(22)	1.6(17)
C(4)-C(5)-C(6)-C(7)	-176.9(8)	N(3)-C(18)-C(23)-C(24)	-4.3(19)
C(15)-N(2)-C(7)-C(6)	-175.1(9)	C(19)-C(18)-C(23)-C(24)	176.1(12)
Zn(1)-N(2)-C(7)-C(6)	0.4(13)	C(21)-C(22)-C(23)-C(18)	-5.2(19)
C(1)-C(6)-C(7)-N(2)	9.0(14)	C(21)-C(22)-C(23)-C(24)	179.6(11)
C(5)-C(6)-C(7)-N(2)	-175.2(8)	C(32A)-N(4)-C(24)-C(23)	-170.5(15)
O(1)-S(1)-C(8)-C(13)	57.7(7)	C(32)-N(4)-C(24)-C(23)	157.0(14)
O(2)-S(1)-C(8)-C(13)	-175.2(6)	Zn(1)-N(4)-C(24)-C(23)	-5.9(17)
N(1)-S(1)-C(8)-C(13)	-53.6(7)	C(18)-C(23)-C(24)-N(4)	17(2)
O(1)-S(1)-C(8)-C(9)	-123.4(7)	C(22)-C(23)-C(24)-N(4)	-168.2(11)
O(2)-S(1)-C(8)-C(9)	3.6(8)	O(5)-S(2)-C(25)-C(30)	9.6(7)
N(1)-S(1)-C(8)-C(9)	125.2(7)	O(6)-S(2)-C(25)-C(30)	-117.5(6)
C(13)-C(8)-C(9)-C(10)	1.9(12)	N(3)-S(2)-C(25)-C(30)	132.5(6)

O(5)-S(2)-C(25)-C(26)	-172.8(6)	C(24)-N(4)-C(32)-C(33)	93.0(17)
O(6)-S(2)-C(25)-C(26)	60.1(7)	Zn(1)-N(4)-C(32)-C(33)	-103.1(16)
N(3)-S(2)-C(25)-C(26)	-49.9(7)	N(4)-C(32)-C(33)-O(7)	-72.7(19)
C(30)-C(25)-C(26)-C(27)	-1.4(11)	N(4)-C(32)-C(33)-C(34)	174.0(16)
S(2)-C(25)-C(26)-C(27)	-179.1(6)	O(7)-C(33)-C(34)-O(8)	-43(3)
C(25)-C(26)-C(27)-C(28)	0.6(12)	C(32)-C(33)-C(34)-O(8)	65(3)
C(26)-C(27)-C(28)-C(29)	0.5(12)	C(24)-N(4)-C(32A)-C(33A)	-114.1(17)
C(26)-C(27)-C(28)-C(31)	-179.0(7)	Zn(1)-N(4)-C(32A)-C(33A)	81(2)
C(27)-C(28)-C(29)-C(30)	-0.8(12)	N(4)-C(32A)-C(33A)-O(7A)	72(2)
C(31)-C(28)-C(29)-C(30)	178.7(7)	N(4)-C(32A)-C(33A)-C(34A)	-165.2(17)
C(26)-C(25)-C(30)-C(29)	1.1(11)	O(7A)-C(33A)-C(34A)-O(8A)	65(3)
S(2)-C(25)-C(30)-C(29)	178.8(6)	C(32A)-C(33A)-C(34A)-O(8A)	-57(3)
C(28)-C(29)-C(30)-C(25)	0.0(12)		

Table 7. Hydrogen bonds for **2-Zn** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...O(7A)#1	0.90	2.08	2.834(17)	140.3
O(4)-H(4A)...O(8)#1	0.90	1.95	2.84(2)	169.6
O(4)-H(4A)...O(8A)#1	0.90	1.94	2.73(2)	145.4
O(7)-H(7A)...O(3)#2	0.90	1.56	2.44(2)	165.1
C(13)-H(13)...O(6)	0.95	2.27	3.212(9)	170.3
C(19)-H(19)...O(5)	0.95	2.39	3.021(11)	124.0
C(24)-H(24)...O(8)#3	0.95	2.34	3.23(2)	156.0
C(26)-H(26)...O(1)	0.95	2.36	3.281(9)	163.3

Symmetry transformations used to generate equivalent atoms:

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

Table 1. Crystal data and structure refinement for **3-Cu**.

Identification code	**3-Cu**	
Empirical formula	C38 H44 Cu2 N4 O8 S2	
Formula weight	875.97	
Temperature	100(2) K	
Wavelength	0.96990 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.1000(18) Å	α = 90°.
	b = 13.647(3) Å	β = 103.10(3)°.
	c = 15.877(3) Å	γ = 90°.
Volume	1920.3(7) $Å^3$	
Z	2	
Density (calculated)	1.515 Mg/m^3	
Absorption coefficient	2.945 mm^{-1}	
F(000)	908	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	3.596 to 38.203°.	
Index ranges	-9<=h<=10, -17<=k<=11, -19<=l<=19	
Reflections collected	12853	
Independent reflections	3777 [R(int) = 0.0804]	
Completeness to theta = 35.587°	96.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.750 and 0.550	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3777 / 38 / 233	
Goodness-of-fit on F^2	1.057	
Final R indices [for 2436 rflns with I>2σ(I)]	R1 = 0.0768, wR2 = 0.1762	
R indices (all data)	R1 = 0.1124, wR2 = 0.1980	
Extinction coefficient	0.0040(6)	
Largest diff. peak and hole	0.800 and -0.920 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3-Cu**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Cu(1)	8727(1)	633(1)	5083(1)	24(1)
S(1)	8670(1)	2000(1)	6570(1)	28(1)
O(1)	9884(3)	317(2)	4249(2)	26(1)
O(2)	7519(4)	2978(2)	3260(2)	63(1)
O(3)	8546(3)	1868(2)	7447(2)	38(1)
O(4)	10194(3)	1932(2)	6428(2)	42(1)
N(1)	7232(4)	1098(2)	4079(2)	27(1)
N(2)	7692(3)	1255(2)	5890(2)	27(1)
C(1)	9070(4)	366(2)	3385(2)	28(1)
C(2)	7851(5)	1156(2)	3291(2)	32(1)
C(3)	5858(5)	1306(2)	4091(3)	32(1)
C(4)	5243(5)	1307(2)	4873(2)	29(1)
C(5)	6122(4)	1299(2)	5724(2)	25(1)
C(6)	5338(5)	1359(2)	6407(3)	34(1)
C(7)	3782(5)	1445(3)	6232(3)	40(1)
C(8)	2922(5)	1434(2)	5393(3)	35(1)
C(9)	3645(5)	1360(3)	4715(3)	35(1)
C(10)	8611(5)	2181(2)	3301(3)	44(1)
C(11)	6625(5)	982(3)	2462(3)	48(1)
C(12)	7217(6)	994(5)	1674(3)	82(2)
C(13)	8051(1)	3206(1)	6281(1)	49(1)
C(14)	7354(1)	3781(1)	6803(1)	49(1)
C(15)	6884(1)	4730(1)	6547(1)	49(1)
C(16)	7111(1)	5104(1)	5768(1)	49(1)
C(17)	7809(1)	4526(1)	5246(1)	49(1)
C(18)	8279(1)	3578(1)	5503(1)	49(1)
C(19)	6607(1)	6126(1)	5489(1)	49(1)
C(13A)	7820(1)	3141(1)	6216(1)	49(1)
C(14A)	7359(1)	3717(1)	6835(1)	49(1)
C(15A)	6680(1)	4625(1)	6604(1)	49(1)
C(16A)	6460(1)	4958(1)	5754(1)	49(1)
C(17A)	6921(1)	4381(1)	5134(1)	49(1)
C(18A)	7600(1)	3474(1)	5365(1)	49(1)
C(19A)	5727(1)	5936(1)	5520(7)	49(1)

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

Cu(1)-O(1)	1.918(3)	C(10)-H(10B)	0.9900
Cu(1)-N(2)	1.949(3)	C(11)-C(12)	1.470(7)
Cu(1)-O(1)#1	1.948(2)	C(11)-H(11A)	0.9900
Cu(1)-N(1)	1.952(3)	C(11)-H(11B)	0.9900
Cu(1)-O(4)	2.862(3)	C(12)-H(12A)	0.9800
Cu(1)-Cu(1)#1	2.9484(10)	C(12)-H(12B)	0.9800
S(1)-O(3)	1.433(3)	C(12)-H(12C)	0.9800
S(1)-O(4)	1.457(3)	C(13)-C(18)	1.3939(13)
S(1)-N(2)	1.600(3)	C(13)-C(14)	1.3942(8)
S(1)-C(13)	1.7655(5)	C(14)-C(15)	1.3957(13)
S(1)-C(13A)	1.7723(6)	C(14)-H(14A)	0.9500
O(1)-C(1)	1.404(4)	C(15)-C(16)	1.3950(16)
O(1)-Cu(1)#1	1.948(2)	C(15)-H(15A)	0.9500
O(2)-C(10)	1.465(5)	C(16)-C(17)	1.3966(14)
O(2)-H(2O)	0.9090	C(16)-C(19)	1.5034(15)
N(1)-C(3)	1.286(5)	C(17)-C(18)	1.3949(14)
N(1)-C(2)	1.487(5)	C(17)-H(17A)	0.9500
N(2)-C(5)	1.394(5)	C(18)-H(18A)	0.9500
C(1)-C(2)	1.530(5)	C(19)-H(19A)	0.9800
C(1)-H(1A)	0.9900	C(19)-H(19B)	0.9800
C(1)-H(1B)	0.9900	C(19)-H(19C)	0.9800
C(2)-C(11)	1.538(5)	C(13A)-C(14A)	1.3953(16)
C(2)-C(10)	1.559(5)	C(13A)-C(18A)	1.3960(19)
C(3)-C(4)	1.473(6)	C(14A)-C(15A)	1.3950(11)
C(3)-H(3)	0.9500	C(14A)-H(14B)	0.9500
C(4)-C(5)	1.406(5)	C(15A)-C(16A)	1.395(2)
C(4)-C(9)	1.420(6)	C(15A)-H(15B)	0.9500
C(5)-C(6)	1.429(6)	C(16A)-C(17A)	1.3961(18)
C(6)-C(7)	1.385(6)	C(16A)-C(19A)	1.5012(19)
C(6)-H(6)	0.9500	C(17A)-C(18A)	1.3949(12)
C(7)-C(8)	1.384(6)	C(17A)-H(17B)	0.9500
C(7)-H(7)	0.9500	C(18A)-H(18B)	0.9500
C(8)-C(9)	1.387(6)	C(19A)-H(19D)	0.9800
C(8)-H(8)	0.9500	C(19A)-H(19E)	0.9800
C(9)-H(9)	0.9500	C(19A)-H(19F)	0.9800
C(10)-H(10A)	0.9900		

O(1)-Cu(1)-N(2)	167.06(11)	O(1)-Cu(1)-O(1)#1	80.62(11)

N(2)-Cu(1)-O(1)#1	106.38(11)	N(1)-C(3)-C(4)	124.7(3)
O(1)-Cu(1)-N(1)	84.22(12)	N(1)-C(3)-H(3)	117.6
N(2)-Cu(1)-N(1)	92.52(13)	C(4)-C(3)-H(3)	117.6
O(1)#1-Cu(1)-N(1)	155.09(11)	C(5)-C(4)-C(9)	120.5(4)
O(1)-Cu(1)-O(4)	114.73(10)	C(5)-C(4)-C(3)	124.6(4)
N(2)-Cu(1)-O(4)	56.82(10)	C(9)-C(4)-C(3)	114.8(3)
O(1)#1-Cu(1)-O(4)	82.56(9)	N(2)-C(5)-C(4)	121.2(4)
N(1)-Cu(1)-O(4)	121.92(10)	N(2)-C(5)-C(6)	121.8(3)
O(3)-S(1)-O(4)	115.47(16)	C(4)-C(5)-C(6)	117.1(4)
O(3)-S(1)-N(2)	114.90(15)	C(7)-C(6)-C(5)	121.1(4)
O(4)-S(1)-N(2)	104.93(16)	C(7)-C(6)-H(6)	119.4
O(3)-S(1)-C(13)	106.20(10)	C(5)-C(6)-H(6)	119.4
O(4)-S(1)-C(13)	106.17(10)	C(8)-C(7)-C(6)	121.4(4)
N(2)-S(1)-C(13)	108.74(10)	C(8)-C(7)-H(7)	119.3
O(3)-S(1)-C(13A)	107.08(11)	C(6)-C(7)-H(7)	119.3
O(4)-S(1)-C(13A)	111.71(10)	C(7)-C(8)-C(9)	118.9(4)
N(2)-S(1)-C(13A)	102.01(10)	C(7)-C(8)-H(8)	120.5
C(1)-O(1)-Cu(1)	114.4(2)	C(9)-C(8)-H(8)	120.5
C(1)-O(1)-Cu(1)#1	134.2(2)	C(8)-C(9)-C(4)	120.9(4)
Cu(1)-O(1)-Cu(1)#1	99.37(11)	C(8)-C(9)-H(9)	119.6
C(10)-O(2)-H(2O)	108.0	C(4)-C(9)-H(9)	119.6
S(1)-O(4)-Cu(1)	81.77(11)	O(2)-C(10)-C(2)	111.7(4)
C(3)-N(1)-C(2)	123.8(3)	O(2)-C(10)-H(10A)	109.3
C(3)-N(1)-Cu(1)	124.0(3)	C(2)-C(10)-H(10A)	109.3
C(2)-N(1)-Cu(1)	112.2(2)	O(2)-C(10)-H(10B)	109.3
C(5)-N(2)-S(1)	119.3(2)	C(2)-C(10)-H(10B)	109.3
C(5)-N(2)-Cu(1)	121.5(2)	H(10A)-C(10)-H(10B)	107.9
S(1)-N(2)-Cu(1)	116.29(17)	C(12)-C(11)-C(2)	113.1(4)
O(1)-C(1)-C(2)	109.8(3)	C(12)-C(11)-H(11A)	109.0
O(1)-C(1)-H(1A)	109.7	C(2)-C(11)-H(11A)	109.0
C(2)-C(1)-H(1A)	109.7	C(12)-C(11)-H(11B)	109.0
O(1)-C(1)-H(1B)	109.7	C(2)-C(11)-H(11B)	109.0
C(2)-C(1)-H(1B)	109.7	H(11A)-C(11)-H(11B)	107.8
H(1A)-C(1)-H(1B)	108.2	C(11)-C(12)-H(12A)	109.5
N(1)-C(2)-C(1)	106.5(3)	C(11)-C(12)-H(12B)	109.5
N(1)-C(2)-C(11)	111.9(4)	H(12A)-C(12)-H(12B)	109.5
C(1)-C(2)-C(11)	110.2(3)	C(11)-C(12)-H(12C)	109.5
N(1)-C(2)-C(10)	106.9(3)	H(12A)-C(12)-H(12C)	109.5
C(1)-C(2)-C(10)	108.7(3)	H(12B)-C(12)-H(12C)	109.5
C(11)-C(2)-C(10)	112.4(3)	C(18)-C(13)-C(14)	120.09(6)

C(18)-C(13)-S(1)	117.84(5)	C(14A)-C(13A)-S(1)	116.79(10)
C(14)-C(13)-S(1)	122.07(4)	C(18A)-C(13A)-S(1)	123.35(8)
C(13)-C(14)-C(15)	119.96(8)	C(15A)-C(14A)-C(13A)	120.09(13)
C(13)-C(14)-H(14A)	120.0	C(15A)-C(14A)-H(14B)	120.0
C(15)-C(14)-H(14A)	120.0	C(13A)-C(14A)-H(14B)	120.0
C(16)-C(15)-C(14)	120.07(9)	C(14A)-C(15A)-C(16A)	120.07(13)
C(16)-C(15)-H(15A)	120.0	C(14A)-C(15A)-H(15B)	120.0
C(14)-C(15)-H(15A)	120.0	C(16A)-C(15A)-H(15B)	120.0
C(15)-C(16)-C(17)	119.84(9)	C(15A)-C(16A)-C(17A)	119.85(9)
C(15)-C(16)-C(19)	120.29(10)	C(15A)-C(16A)-C(19A)	119.2(4)
C(17)-C(16)-C(19)	119.87(11)	C(17A)-C(16A)-C(19A)	121.0(4)
C(18)-C(17)-C(16)	120.09(11)	C(18A)-C(17A)-C(16A)	120.07(14)
C(18)-C(17)-H(17A)	120.0	C(18A)-C(17A)-H(17B)	120.0
C(16)-C(17)-H(17A)	120.0	C(16A)-C(17A)-H(17B)	120.0
C(13)-C(18)-C(17)	119.95(9)	C(17A)-C(18A)-C(13A)	120.06(12)
C(13)-C(18)-H(18A)	120.0	C(17A)-C(18A)-H(18B)	120.0
C(17)-C(18)-H(18A)	120.0	C(13A)-C(18A)-H(18B)	120.0
C(16)-C(19)-H(19A)	109.5	C(16A)-C(19A)-H(19D)	109.5
C(16)-C(19)-H(19B)	109.5	C(16A)-C(19A)-H(19E)	109.5
H(19A)-C(19)-H(19B)	109.5	H(19D)-C(19A)-H(19E)	109.5
C(16)-C(19)-H(19C)	109.5	C(16A)-C(19A)-H(19F)	109.5
H(19A)-C(19)-H(19C)	109.5	H(19D)-C(19A)-H(19F)	109.5
H(19B)-C(19)-H(19C)	109.5	H(19E)-C(19A)-H(19F)	109.5
C(14A)-C(13A)-C(18A)	119.86(6)		

Symmetry transformations used to generate equivalent atoms:

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

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

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	21(1)	20(1)	30(1)	1(1)	1(1)	4(1)
S(1)	23(1)	22(1)	36(1)	-6(1)	-2(1)	2(1)
O(1)	18(2)	27(1)	32(1)	-1(1)	4(1)	5(1)
O(2)	82(3)	49(2)	61(2)	15(1)	24(2)	31(2)
O(3)	44(2)	32(1)	29(2)	-3(1)	-9(1)	1(1)
O(4)	18(2)	33(1)	71(2)	-15(1)	3(1)	1(1)
N(1)	23(2)	24(1)	32(2)	-2(1)	0(2)	6(1)
N(2)	15(2)	23(1)	39(2)	0(1)	0(1)	2(1)
C(1)	25(2)	30(2)	27(2)	1(2)	-2(2)	9(2)
C(2)	38(3)	28(2)	29(2)	6(2)	5(2)	11(2)
C(3)	32(2)	22(2)	39(2)	2(2)	-2(2)	5(2)
C(4)	30(2)	20(1)	33(2)	1(1)	0(2)	3(2)
C(5)	23(2)	14(1)	37(2)	-3(1)	2(2)	1(1)
C(6)	25(2)	33(2)	42(2)	-8(2)	3(2)	-2(2)
C(7)	35(3)	37(2)	49(3)	-10(2)	10(2)	-7(2)
C(8)	17(2)	25(2)	66(3)	-9(2)	14(2)	-4(2)
C(9)	19(2)	30(2)	50(3)	-2(2)	-6(2)	4(2)
C(10)	64(3)	29(2)	46(2)	5(2)	29(2)	9(2)
C(11)	48(3)	62(2)	32(2)	7(2)	2(2)	33(2)
C(12)	73(4)	145(5)	29(3)	25(3)	12(3)	53(3)
C(13)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(14)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(15)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(16)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(17)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(18)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(19)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(13A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(14A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(15A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(16A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(17A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(18A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)
C(19A)	66(2)	28(1)	51(1)	-2(1)	14(1)	3(1)

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

Atom	x	y	z	U(iso)
H(2O)	6890	2968	2726	94
H(1A)	8596	-277	3207	34
H(1B)	9764	522	3005	34
H(3)	5193	1471	3558	39
H(6)	5893	1340	6990	41
H(7)	3294	1512	6699	48
H(8)	1853	1478	5283	42
H(9)	3064	1343	4137	42
H(10A)	9412	2247	3836	52
H(10B)	9091	2232	2802	52
H(11A)	6139	341	2506	58
H(11B)	5842	1495	2415	58
H(12A)	6435	764	1183	123
H(12B)	8098	562	1751	123
H(12C)	7511	1664	1561	123
H(14A)	7199	3527	7333	58
H(15A)	6409	5122	6902	58
H(17A)	7965	4780	4716	58
H(18A)	8754	3185	5147	58
H(19A)	5981	6384	5866	73
H(19B)	6018	6114	4890	73
H(19C)	7492	6547	5528	73
H(14B)	7508	3492	7414	58
H(15B)	6367	5016	7027	58
H(17B)	6772	4607	4555	58
H(18B)	7913	3083	4943	58
H(19D)	6507	6434	5530	73
H(19E)	5126	6111	5938	73
H(19F)	5070	5903	4939	73

Table 6. Torsion angles [°] for **3-Cu**.

O(3)-S(1)-O(4)-Cu(1)	130.66(11)	Cu(1)-N(2)-C(5)-C(6)	153.4(2)
N(2)-S(1)-O(4)-Cu(1)	3.09(12)	C(9)-C(4)-C(5)-N(2)	-179.5(3)
C(13)-S(1)-O(4)-Cu(1)	-111.96(4)	C(3)-C(4)-C(5)-N(2)	-2.3(5)
C(13A)-S(1)-O(4)-Cu(1)	-106.66(7)	C(9)-C(4)-C(5)-C(6)	-0.9(4)
O(3)-S(1)-N(2)-C(5)	66.1(3)	C(3)-C(4)-C(5)-C(6)	176.4(3)
O(4)-S(1)-N(2)-C(5)	-166.0(3)	N(2)-C(5)-C(6)-C(7)	177.2(3)
C(13)-S(1)-N(2)-C(5)	-52.7(3)	C(4)-C(5)-C(6)-C(7)	-1.5(5)
C(13A)-S(1)-N(2)-C(5)	-49.4(3)	C(5)-C(6)-C(7)-C(8)	2.7(5)
O(3)-S(1)-N(2)-Cu(1)	-132.94(17)	C(6)-C(7)-C(8)-C(9)	-1.5(5)
O(4)-S(1)-N(2)-Cu(1)	-5.0(2)	C(7)-C(8)-C(9)-C(4)	-0.8(5)
C(13)-S(1)-N(2)-Cu(1)	108.24(13)	C(5)-C(4)-C(9)-C(8)	2.0(5)
C(13A)-S(1)-N(2)-Cu(1)	111.61(14)	C(3)-C(4)-C(9)-C(8)	-175.5(3)
Cu(1)-O(1)-C(1)-C(2)	31.6(4)	N(1)-C(2)-C(10)-O(2)	-62.3(4)
Cu(1)#1-O(1)-C(1)-C(2)	165.2(2)	C(1)-C(2)-C(10)-O(2)	-176.9(3)
C(3)-N(1)-C(2)-C(1)	-148.8(3)	C(11)-C(2)-C(10)-O(2)	60.9(4)
Cu(1)-N(1)-C(2)-C(1)	29.5(3)	N(1)-C(2)-C(11)-C(12)	-177.5(4)
C(3)-N(1)-C(2)-C(11)	-28.5(4)	C(1)-C(2)-C(11)-C(12)	-59.3(5)
Cu(1)-N(1)-C(2)-C(11)	149.9(2)	C(10)-C(2)-C(11)-C(12)	62.1(5)
C(3)-N(1)-C(2)-C(10)	95.1(4)	O(3)-S(1)-C(13)-C(18)	170.15(11)
Cu(1)-N(1)-C(2)-C(10)	-86.6(3)	O(4)-S(1)-C(13)-C(18)	46.74(12)
O(1)-C(1)-C(2)-N(1)	-38.6(4)	N(2)-S(1)-C(13)-C(18)	-65.70(13)
O(1)-C(1)-C(2)-C(11)	-160.1(3)	O(3)-S(1)-C(13)-C(14)	-9.86(11)
O(1)-C(1)-C(2)-C(10)	76.3(4)	O(4)-S(1)-C(13)-C(14)	-133.26(12)
C(2)-N(1)-C(3)-C(4)	-176.4(3)	N(2)-S(1)-C(13)-C(14)	114.30(13)
Cu(1)-N(1)-C(3)-C(4)	5.4(5)	O(3)-S(1)-C(13A)-C(14A)	6.34(11)
N(1)-C(3)-C(4)-C(5)	15.0(5)	O(4)-S(1)-C(13A)-C(14A)	-121.01(12)
N(1)-C(3)-C(4)-C(9)	-167.6(3)	N(2)-S(1)-C(13A)-C(14A)	127.38(12)
S(1)-N(2)-C(5)-C(4)	132.0(3)	O(3)-S(1)-C(13A)-C(18A)	-173.66(11)
Cu(1)-N(2)-C(5)-C(4)	-28.0(4)	O(4)-S(1)-C(13A)-C(18A)	58.99(12)
S(1)-N(2)-C(5)-C(6)	-46.7(4)	N(2)-S(1)-C(13A)-C(18A)	-52.62(12)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for **3-Cu** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(4)#2	0.91	2.28	3.189(4)	174.5

Symmetry transformations used to generate equivalent atoms:

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

Table 1. Crystal data and structure refinement for **3-Ni**.

Identification code	**3-Ni**	
Empirical formula	C718 H931 K4 N73 Ni48 O220 S36	
Formula weight	18232.06	
Temperature	100(2) K	
Wavelength	0.96990 Å	
Crystal system	Trigonal	
Space group	R-3c	
Unit cell dimensions	a = 23.754(3) Å	$\alpha = 90°$.
	b = 23.754(3) Å	$\beta = 90°$.
	c = 139.71(3) Å	$\gamma = 120°$.
Volume	68270(26) $Å^3$	
Z	3	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	2.651 mm^{-1}	
F(000)	28518	
Crystal size	0.12 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.087 to 38.544°.	
Index ranges	-25<=h<=30, -29<=k<=25, -176<=l<=176	
Reflections collected	223428	
Independent reflections	16597 [R(int) = 0.1040]	
Completeness to theta = 35.587°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.940 and 0.740	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16597 / 31 / 714	
Goodness-of-fit on F^2	1.084	
Final R indices [I>2sigma(I)]	R1 = 0.0983, wR2 = 0.1662	
R indices (all data)	R1 = 0.1870, wR2 = 0.1967	
Extinction coefficient	0.000060(3)	
Largest diff. peak and hole	1.206 and -0.880 e. $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3-Ni**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Ni(1)	4212(1)	7136(1)	2943(1)	65(1)
Ni(2)	3333	6667	3124(1)	66(1)
Ni(3)	3167(1)	5837(1)	2240(1)	56(1)
Ni(4)	3333	6667	2060(1)	83(1)
S(1)	4784(1)	6798(1)	2757(1)	71(1)
S(2)	3751(1)	5597(1)	2433(1)	66(1)
K(1)	3333	6667	2598(1)	69(1)
O(1)	3333	6667	2873(1)	65(2)
O(2)	3713(3)	7428(3)	3030(1)	66(1)
O(3)	4132(3)	7134(3)	3212(1)	74(2)
O(4)	4427(3)	7103(3)	2720(1)	76(2)
O(5)	4514(3)	6129(3)	2727(1)	84(2)
O(6)	4593(3)	8010(2)	2856(1)	72(2)
O(7)	3333	6667	2308(1)	48(2)
O(8)	2624(2)	6077(2)	2152(1)	65(1)
O(9)	3187(4)	5898(4)	1971(1)	109(2)
O(10)	3300(3)	5818(3)	2461(1)	68(1)
O(11)	4419(3)	6021(3)	2465(1)	77(2)
O(12)	2325(2)	5233(2)	2328(1)	66(1)
N(1)	4910(3)	7626(3)	3042(1)	64(2)
N(2)	4839(3)	6904(3)	2870(1)	69(2)
N(3)	2914(3)	5124(3)	2143(1)	73(2)
N(4)	3668(3)	5479(3)	2321(1)	61(2)
C(1)	5344(4)	7485(4)	3064(1)	65(2)
C(2)	5494(4)	7035(4)	3014(1)	62(2)
C(3)	5889(4)	6867(5)	3065(1)	79(3)
C(4)	6074(5)	6437(5)	3032(1)	94(3)
C(5)	5838(5)	6151(5)	2944(1)	96(3)
C(6)	5428(5)	6297(4)	2889(1)	78(2)
C(7)	5250(4)	6736(4)	2923(1)	69(2)
C(8)	4778(4)	8050(4)	3106(1)	72(2)
C(9)	4169(4)	8053(4)	3066(1)	71(2)
C(10)	4660(4)	7780(5)	3209(1)	77(2)
C(11)	5358(5)	8736(4)	3111(1)	116(3)
C(12)	5689(5)	9059(5)	3018(1)	116(3)

C(13)	5580(5)	7234(6)	2711(1)	99(1)
C(14)	6058(5)	7789(6)	2759(1)	99(1)
C(15)	6696(5)	8155(6)	2721(1)	99(1)
C(16)	6844(5)	7963(6)	2637(1)	99(1)
C(17)	6361(5)	7397(6)	2590(1)	99(1)
C(18)	5726(5)	7035(6)	2626(1)	99(1)
C(19)	7532(5)	8345(5)	2594(1)	99(1)
C(20)	3241(4)	4844(4)	2127(1)	88(1)
C(21)	3779(4)	4893(4)	2183(1)	88(1)
C(22)	4112(4)	4599(4)	2138(1)	88(1)
C(23)	4635(4)	4615(4)	2180(1)	88(1)
C(24)	4829(4)	4882(4)	2268(1)	88(1)
C(25)	4537(4)	5176(4)	2318(1)	88(1)
C(26)	3997(4)	5197(4)	2273(1)	88(1)
C(27)	2368(4)	5041(4)	2076(1)	115(2)
C(28)	2111(4)	5471(4)	2113(1)	77(2)
C(29)	2641(6)	5243(6)	1975(1)	109(4)
C(30)	1855(4)	4323(4)	2082(1)	115(2)
C(31)	1279(5)	4114(5)	2016(1)	115(2)
C(32)	3465(5)	4837(5)	2489(1)	117(2)
C(33)	2957(5)	4283(5)	2455(1)	117(2)
C(34)	2711(5)	3709(5)	2507(1)	117(2)
C(35)	2964(5)	3672(5)	2592(1)	117(2)
C(36)	3417(5)	4240(5)	2633(1)	117(2)
C(37)	3697(5)	4838(5)	2581(1)	117(2)
C(38)	2716(5)	3050(5)	2650(1)	117(2)
Ni(5)	3481(1)	5997(1)	3731(1)	47(1)
Ni(6)	3333	6667	3550(1)	51(1)
S(3)	4240(1)	5911(1)	3919(1)	56(1)
O(13)	3333	6667	3804(1)	45(2)
O(14)	2760(2)	5947(2)	3643(1)	48(1)
O(15)	3442(2)	6011(2)	3465(1)	62(1)
O(16)	4826(2)	6375(2)	3968(1)	66(1)
O(17)	3644(2)	5875(2)	3955(1)	59(1)
O(18)	2726(2)	5247(2)	3820(1)	53(1)
N(5)	3459(3)	5352(3)	3637(1)	54(2)
N(6)	4254(3)	6022(3)	3807(1)	53(2)
C(39)	3938(4)	5252(4)	3621(1)	64(2)
C(40)	4576(4)	5585(4)	3667(1)	59(2)
C(41)	5074(4)	5544(4)	3618(1)	70(2)

C(42)	5715(4)	5884(5)	3647(1)	79(3)
C(43)	5873(4)	6263(5)	3729(1)	80(3)
C(44)	5397(4)	6307(4)	3781(1)	67(2)
C(45)	4740(4)	5967(4)	3752(1)	56(2)
C(46)	2874(4)	5065(3)	3573(1)	56(2)
C(47)	2414(4)	5302(3)	3609(1)	58(2)
C(48)	3098(4)	5312(4)	3470(1)	66(2)
C(49)	2511(4)	4303(4)	3572(1)	73(2)
C(50)	2354(6)	3989(4)	3672(1)	119(4)
C(51)	4171(3)	5137(4)	3934(1)	55(2)
C(52)	4615(4)	5060(4)	3989(1)	68(2)
C(53)	4536(4)	4454(4)	4003(1)	72(2)
C(54)	4016(4)	3903(4)	3963(1)	73(2)
C(55)	3593(4)	3993(4)	3905(1)	71(2)
C(56)	3676(4)	4597(4)	3889(1)	64(2)
C(57)	3929(4)	3235(4)	3979(1)	99(3)
O(19)	4354(3)	6454(3)	3338(1)	102(2)
O(20)	5389(3)	7047(5)	3293(1)	102(2)
C(58)	4919(3)	6541(4)	3338(1)	102(2)
C(59)	5107(6)	6104(7)	3385(1)	102(2)
O(20')	4600(6)	5697(4)	3379(1)	102(2)
C(58')	4733(3)	6233(4)	3333(1)	102(2)
C(59')	5336(5)	6534(8)	3276(1)	102(2)
O(21)	4124(11)	5795(10)	1881(2)	84(7)
O(22)	3709(10)	4723(10)	1889(2)	84(7)
C(60)	4206(8)	5315(10)	1877(1)	84(7)
C(61)	4838(9)	5362(15)	1858(2)	84(7)
N(7)	3333	6667	4134(1)	57(4)
C(62)	3922(1)	6667	4167	57(4)
C(63)	4524(2)	7222(8)	4122(2)	57(4)

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

Ni(1)-N(1)	2.018(7)	O(1)-Ni(1)#2	2.060(4)
Ni(1)-O(2)	2.041(5)	O(1)-Ni(1)#1	2.060(4)
Ni(1)-O(1)	2.060(4)	O(2)-C(9)	1.424(9)
Ni(1)-N(2)	2.093(6)	O(2)-Ni(1)#2	2.130(5)
Ni(1)-O(2)#1	2.131(5)	O(3)-C(10)	1.416(10)
Ni(1)-O(6)	2.178(5)	O(3)-H(3O)	0.9237
Ni(2)-O(2)#2	2.043(5)	O(6)-H(6A)	0.9062
Ni(2)-O(2)#1	2.043(5)	O(6)-H(6B)	0.9150
Ni(2)-O(2)	2.044(5)	O(7)-Ni(3)#1	2.044(4)
Ni(2)-O(3)#2	2.059(5)	O(7)-Ni(3)#2	2.044(4)
Ni(2)-O(3)	2.059(5)	O(8)-C(28)	1.449(9)
Ni(2)-O(3)#1	2.059(5)	O(8)-Ni(3)#1	2.131(5)
Ni(3)-N(3)	2.012(6)	O(9)-C(29)	1.446(11)
Ni(3)-O(7)	2.044(4)	O(9)-H(9O)	0.9089
Ni(3)-O(8)	2.055(5)	O(12)-H(12D)	0.8900
Ni(3)-N(4)	2.101(6)	O(12)-H(12E)	0.9182
Ni(3)-O(8)#2	2.131(5)	N(1)-C(1)	1.271(10)
Ni(3)-O(12)	2.170(5)	N(1)-C(8)	1.494(10)
Ni(4)-O(8)#1	2.028(5)	N(2)-C(7)	1.433(10)
Ni(4)-O(8)	2.028(6)	N(3)-C(20)	1.269(10)
Ni(4)-O(8)#2	2.028(5)	N(3)-C(27)	1.531(11)
Ni(4)-O(9)#1	2.089(7)	N(4)-C(26)	1.421(10)
Ni(4)-O(9)#2	2.089(7)	C(1)-C(2)	1.465(11)
Ni(4)-O(9)	2.089(7)	C(1)-H(1)	0.9500
S(1)-O(5)	1.446(6)	C(2)-C(3)	1.382(11)
S(1)-O(4)	1.459(6)	C(2)-C(7)	1.427(10)
S(1)-N(2)	1.597(6)	C(3)-C(4)	1.374(12)
S(1)-C(13)	1.763(11)	C(3)-H(3)	0.9500
S(2)-O(11)	1.459(5)	C(4)-C(5)	1.379(12)
S(2)-O(10)	1.462(5)	C(4)-H(4)	0.9500
S(2)-N(4)	1.594(7)	C(5)-C(6)	1.411(12)
S(2)-C(32)	1.760(10)	C(5)-H(5)	0.9500
K(1)-O(10)#1	2.747(6)	C(6)-C(7)	1.392(11)
K(1)-O(10)#2	2.747(6)	C(6)-H(6)	0.9500
K(1)-O(10)	2.747(6)	C(8)-C(11)	1.520(3)
K(1)-O(4)#2	2.839(6)	C(8)-C(10)	1.539(11)
K(1)-O(4)#1	2.839(6)	C(8)-C(9)	1.556(11)
K(1)-O(4)	2.839(6)	C(9)-H(9A)	0.9900

C(9)-H(9B)	0.9900	C(29)-H(29A)	0.9900
C(10)-H(10A)	0.9900	C(29)-H(29B)	0.9900
C(10)-H(10B)	0.9900	C(30)-C(31)	1.519(3)
C(11)-C(12)	1.515(3)	C(30)-H(30A)	0.9900
C(11)-H(11A)	0.9900	C(30)-H(30B)	0.9900
C(11)-H(11B)	0.9900	C(31)-H(31A)	0.9800
C(12)-H(12A)	0.9800	C(31)-H(31B)	0.9800
C(12)-H(12B)	0.9800	C(31)-H(31C)	0.9800
C(12)-H(12C)	0.9800	C(32)-C(33)	1.349(13)
C(13)-C(18)	1.378(13)	C(32)-C(37)	1.399(13)
C(13)-C(14)	1.407(14)	C(33)-C(34)	1.390(12)
C(14)-C(15)	1.419(13)	C(33)-H(33)	0.9500
C(14)-H(14)	0.9500	C(34)-C(35)	1.354(13)
C(15)-C(16)	1.367(13)	C(34)-H(34)	0.9500
C(15)-H(15)	0.9500	C(35)-C(36)	1.357(14)
C(16)-C(17)	1.416(14)	C(35)-C(38)	1.518(13)
C(16)-C(19)	1.540(13)	C(36)-C(37)	1.427(12)
C(17)-C(18)	1.404(13)	C(36)-H(36)	0.9500
C(17)-H(17)	0.9500	C(37)-H(37)	0.9500
C(18)-H(18)	0.9500	C(38)-H(38A)	0.9800
C(19)-H(19A)	0.9800	C(38)-H(38B)	0.9800
C(19)-H(19B)	0.9800	C(38)-H(38C)	0.9800
C(19)-H(19C)	0.9800	Ni(5)-N(5)	2.005(6)
C(20)-C(21)	1.449(13)	Ni(5)-O(13)	2.058(4)
C(20)-H(20)	0.9500	Ni(5)-O(14)	2.064(4)
C(21)-C(26)	1.424(13)	Ni(5)-N(6)	2.089(5)
C(21)-C(22)	1.431(11)	Ni(5)-O(14)#2	2.118(4)
C(22)-C(23)	1.356(12)	Ni(5)-O(18)	2.175(4)
C(22)-H(22)	0.9500	Ni(6)-O(14)#1	2.035(5)
C(23)-C(24)	1.361(13)	Ni(6)-O(14)#2	2.035(5)
C(23)-H(23)	0.9500	Ni(6)-O(14)	2.036(5)
C(24)-C(25)	1.389(11)	Ni(6)-O(15)#1	2.076(5)
C(24)-H(24)	0.9500	Ni(6)-O(15)#2	2.076(5)
C(25)-C(26)	1.446(13)	Ni(6)-O(15)	2.076(5)
C(25)-H(25)	0.9500	S(3)-O(16)	1.445(5)
C(27)-C(29)	1.522(3)	S(3)-O(17)	1.466(5)
C(27)-C(28)	1.523(3)	S(3)-N(6)	1.587(6)
C(27)-C(30)	1.525(3)	S(3)-C(51)	1.774(8)
C(28)-H(28A)	0.9900	O(13)-Ni(5)#1	2.057(4)
C(28)-H(28B)	0.9900	O(13)-Ni(5)#2	2.057(4)

O(14)-C(47)	1.412(8)	C(54)-C(55)	1.386(11)
O(14)-Ni(5)#1	2.118(4)	C(54)-C(57)	1.514(11)
O(15)-C(48)	1.442(8)	C(55)-C(56)	1.365(10)
O(15)-H(15O)	0.9227	C(55)-H(55)	0.9500
O(18)-H(18A)	0.9178	C(56)-H(56)	0.9500
O(18)-H(18B)	0.9184	C(57)-H(57A)	0.9800
N(5)-C(39)	1.293(9)	C(57)-H(57B)	0.9800
N(5)-C(46)	1.501(9)	C(57)-H(57C)	0.9800
N(6)-C(45)	1.442(9)	O(19)-C(58')	1.252(3)
C(39)-C(40)	1.462(11)	O(19)-C(58)	1.252(3)
C(39)-H(39)	0.9500	O(20)-C(58)	1.318(3)
C(40)-C(41)	1.412(10)	O(20)-H(20A)	0.8502
C(40)-C(45)	1.421(10)	C(58)-C(59)	1.473(3)
C(41)-C(42)	1.381(11)	C(59)-H(59A)	0.9800
C(41)-H(41)	0.9500	C(59)-H(59B)	0.9800
C(42)-C(43)	1.387(12)	C(59)-H(59C)	0.9800
C(42)-H(42)	0.9500	O(20')-C(58')	1.321(3)
C(43)-C(44)	1.393(11)	O(20')-H(20B)	0.8500
C(43)-H(43)	0.9500	C(58')-C(59')	1.470(3)
C(44)-C(45)	1.412(10)	C(59')-H(59D)	0.9800
C(44)-H(44)	0.9500	C(59')-H(59E)	0.9800
C(46)-C(48)	1.539(10)	C(59')-H(59F)	0.9800
C(46)-C(47)	1.544(10)	O(21)-C(60)	1.252(3)
C(46)-C(49)	1.567(10)	O(22)-C(60)	1.321(3)
C(47)-H(47A)	0.9900	O(22)-H(22O)	0.8498
C(47)-H(47B)	0.9900	C(60)-C(61)	1.471(3)
C(48)-H(48A)	0.9900	C(61)-H(61A)	0.9800
C(48)-H(48B)	0.9900	C(61)-H(61B)	0.9800
C(49)-C(50)	1.529(13)	C(61)-H(61C)	0.9800
C(49)-H(49A)	0.9900	N(7)-C(62)	1.472(2)
C(49)-H(49B)	0.9900	N(7)-H(7N)	0.9100
C(50)-H(50A)	0.9800	C(62)-N(7)#3	1.472(2)
C(50)-H(50B)	0.9800	C(62)-C(63)#4	1.512(3)
C(50)-H(50C)	0.9800	C(62)-C(63)	1.512(3)
C(51)-C(56)	1.382(10)	C(62)-H(62A)	0.9598
C(51)-C(52)	1.388(10)	C(62)-H(62B)	0.9599
C(52)-C(53)	1.371(11)	C(63)-H(63D)	0.9600
C(52)-H(52)	0.9500	C(63)-H(63A)	0.9581
C(53)-C(54)	1.394(11)	C(63)-H(63B)	0.9610
C(53)-H(53)	0.9500		

N(1)-Ni(1)-O(2)	81.3(2)	N(4)-Ni(3)-O(8)#2	101.8(2)
N(1)-Ni(1)-O(1)	163.0(3)	N(3)-Ni(3)-O(12)	92.1(2)
O(2)-Ni(1)-O(1)	82.1(2)	O(7)-Ni(3)-O(12)	92.38(18)
N(1)-Ni(1)-N(2)	90.0(3)	O(8)-Ni(3)-O(12)	91.2(2)
O(2)-Ni(1)-N(2)	171.2(2)	N(4)-Ni(3)-O(12)	87.2(2)
O(1)-Ni(1)-N(2)	106.6(2)	O(8)#2-Ni(3)-O(12)	169.4(2)
N(1)-Ni(1)-O(2)#1	93.7(2)	O(8)#1-Ni(4)-O(8)	83.7(2)
O(2)-Ni(1)-O(2)#1	81.0(3)	O(8)#1-Ni(4)-O(8)#2	83.7(2)
O(1)-Ni(1)-O(2)#1	80.0(2)	O(8)-Ni(4)-O(8)#2	83.7(2)
N(2)-Ni(1)-O(2)#1	99.1(2)	O(8)#1-Ni(4)-O(9)#1	93.3(2)
N(1)-Ni(1)-O(6)	90.2(2)	O(8)-Ni(4)-O(9)#1	94.7(2)
O(2)-Ni(1)-O(6)	92.5(2)	O(8)#2-Ni(4)-O(9)#1	176.8(3)
O(1)-Ni(1)-O(6)	94.20(19)	O(8)#1-Ni(4)-O(9)#2	94.7(2)
N(2)-Ni(1)-O(6)	88.0(2)	O(8)-Ni(4)-O(9)#2	176.7(3)
O(2)#1-Ni(1)-O(6)	171.8(2)	O(8)#2-Ni(4)-O(9)#2	93.3(2)
O(2)#2-Ni(2)-O(2)#1	83.1(2)	O(9)#1-Ni(4)-O(9)#2	88.2(3)
O(2)#2-Ni(2)-O(2)	83.1(2)	O(8)#1-Ni(4)-O(9)	176.8(3)
O(2)#1-Ni(2)-O(2)	83.1(2)	O(8)-Ni(4)-O(9)	93.3(2)
O(2)#2-Ni(2)-O(3)#2	91.5(2)	O(8)#2-Ni(4)-O(9)	94.7(2)
O(2)#1-Ni(2)-O(3)#2	174.5(2)	O(9)#1-Ni(4)-O(9)	88.2(3)
O(2)-Ni(2)-O(3)#2	97.4(2)	O(9)#2-Ni(4)-O(9)	88.2(3)
O(2)#2-Ni(2)-O(3)	174.5(2)	O(5)-S(1)-O(4)	113.4(4)
O(2)#1-Ni(2)-O(3)	97.4(2)	O(5)-S(1)-N(2)	114.5(4)
O(2)-Ni(2)-O(3)	91.6(2)	O(4)-S(1)-N(2)	106.9(3)
O(3)#2-Ni(2)-O(3)	88.0(2)	O(5)-S(1)-C(13)	107.3(5)
O(2)#2-Ni(2)-O(3)#1	97.4(2)	O(4)-S(1)-C(13)	107.4(4)
O(2)#1-Ni(2)-O(3)#1	91.5(2)	N(2)-S(1)-C(13)	107.0(4)
O(2)-Ni(2)-O(3)#1	174.5(2)	O(11)-S(2)-O(10)	114.3(3)
O(3)#2-Ni(2)-O(3)#1	88.0(2)	O(11)-S(2)-N(4)	114.6(3)
O(3)-Ni(2)-O(3)#1	88.0(2)	O(10)-S(2)-N(4)	106.1(3)
N(3)-Ni(3)-O(7)	163.5(3)	O(11)-S(2)-C(32)	107.7(4)
N(3)-Ni(3)-O(8)	82.3(2)	O(10)-S(2)-C(32)	105.9(5)
O(7)-Ni(3)-O(8)	81.74(19)	N(4)-S(2)-C(32)	107.8(5)
N(3)-Ni(3)-N(4)	90.7(3)	O(10)#1-K(1)-O(10)#2	77.12(17)
O(7)-Ni(3)-N(4)	105.3(2)	O(10)#1-K(1)-O(10)	77.12(17)
O(8)-Ni(3)-N(4)	172.8(2)	O(10)#2-K(1)-O(10)	77.12(17)
N(3)-Ni(3)-O(8)#2	93.3(2)	O(10)#1-K(1)-O(4)#2	86.93(15)
O(7)-Ni(3)-O(8)#2	79.9(2)	O(10)#2-K(1)-O(4)#2	111.86(16)
O(8)-Ni(3)-O(8)#2	80.5(3)	O(10)-K(1)-O(4)#2	159.64(17)

O(10)#1-K(1)-O(4)#1	111.86(16)	H(12D)-O(12)-H(12E)	103.7
O(10)#2-K(1)-O(4)#1	159.64(17)	C(1)-N(1)-C(8)	120.3(7)
O(10)-K(1)-O(4)#1	86.93(15)	C(1)-N(1)-Ni(1)	123.6(6)
O(4)#2-K(1)-O(4)#1	87.37(16)	C(8)-N(1)-Ni(1)	114.3(5)
O(10)#1-K(1)-O(4)	159.64(17)	C(7)-N(2)-S(1)	118.8(5)
O(10)#2-K(1)-O(4)	86.93(15)	C(7)-N(2)-Ni(1)	119.6(5)
O(10)-K(1)-O(4)	111.86(15)	S(1)-N(2)-Ni(1)	120.9(4)
O(4)#2-K(1)-O(4)	87.37(16)	C(20)-N(3)-C(27)	121.7(7)
O(4)#1-K(1)-O(4)	87.37(16)	C(20)-N(3)-Ni(3)	123.6(7)
Ni(1)#2-O(1)-Ni(1)	99.1(2)	C(27)-N(3)-Ni(3)	113.6(5)
Ni(1)#2-O(1)-Ni(1)#1	99.1(2)	C(26)-N(4)-S(2)	119.5(6)
Ni(1)-O(1)-Ni(1)#1	99.1(2)	C(26)-N(4)-Ni(3)	119.9(6)
C(9)-O(2)-Ni(1)	107.2(4)	S(2)-N(4)-Ni(3)	120.2(3)
C(9)-O(2)-Ni(2)	117.7(4)	N(1)-C(1)-C(2)	127.1(8)
Ni(1)-O(2)-Ni(2)	98.9(2)	N(1)-C(1)-H(1)	116.4
C(9)-O(2)-Ni(1)#2	133.4(5)	C(2)-C(1)-H(1)	116.4
Ni(1)-O(2)-Ni(1)#2	97.4(2)	C(3)-C(2)-C(7)	118.6(8)
Ni(2)-O(2)-Ni(1)#2	96.1(2)	C(3)-C(2)-C(1)	114.5(8)
C(10)-O(3)-Ni(2)	130.1(5)	C(7)-C(2)-C(1)	126.8(8)
C(10)-O(3)-H(3O)	107.0	C(4)-C(3)-C(2)	123.9(8)
Ni(2)-O(3)-H(3O)	120.1	C(4)-C(3)-H(3)	118.0
S(1)-O(4)-K(1)	133.2(3)	C(2)-C(3)-H(3)	118.0
Ni(1)-O(6)-H(6A)	103.5	C(3)-C(4)-C(5)	117.4(9)
Ni(1)-O(6)-H(6B)	115.2	C(3)-C(4)-H(4)	121.3
H(6A)-O(6)-H(6B)	104.3	C(5)-C(4)-H(4)	121.3
Ni(3)-O(7)-Ni(3)#1	99.9(2)	C(4)-C(5)-C(6)	121.5(9)
Ni(3)-O(7)-Ni(3)#2	99.9(2)	C(4)-C(5)-H(5)	119.2
Ni(3)#1-O(7)-Ni(3)#2	99.9(2)	C(6)-C(5)-H(5)	119.2
C(28)-O(8)-Ni(4)	116.2(5)	C(7)-C(6)-C(5)	120.2(9)
C(28)-O(8)-Ni(3)	106.4(4)	C(7)-C(6)-H(6)	119.9
Ni(4)-O(8)-Ni(3)	98.7(2)	C(5)-C(6)-H(6)	119.9
C(28)-O(8)-Ni(3)#1	135.7(4)	C(6)-C(7)-C(2)	118.4(8)
Ni(4)-O(8)-Ni(3)#1	96.3(2)	C(6)-C(7)-N(2)	122.5(8)
Ni(3)-O(8)-Ni(3)#1	96.7(2)	C(2)-C(7)-N(2)	119.1(7)
C(29)-O(9)-Ni(4)	125.8(5)	N(1)-C(8)-C(11)	111.3(7)
C(29)-O(9)-H(9O)	98.8	N(1)-C(8)-C(10)	109.5(7)
Ni(4)-O(9)-H(9O)	129.7	C(11)-C(8)-C(10)	106.7(7)
S(2)-O(10)-K(1)	133.6(3)	N(1)-C(8)-C(9)	107.2(6)
Ni(3)-O(12)-H(12D)	104.0	C(11)-C(8)-C(9)	110.9(8)
Ni(3)-O(12)-H(12E)	115.4	C(10)-C(8)-C(9)	111.3(7)

O(2)-C(9)-C(8)	110.3(6)	C(13)-C(18)-H(18)	120.8
O(2)-C(9)-H(9A)	109.6	C(17)-C(18)-H(18)	120.8
C(8)-C(9)-H(9A)	109.6	C(16)-C(19)-H(19A)	109.5
O(2)-C(9)-H(9B)	109.6	C(16)-C(19)-H(19B)	109.5
C(8)-C(9)-H(9B)	109.6	H(19A)-C(19)-H(19B)	109.5
H(9A)-C(9)-H(9B)	108.1	C(16)-C(19)-H(19C)	109.5
O(3)-C(10)-C(8)	111.0(6)	H(19A)-C(19)-H(19C)	109.5
O(3)-C(10)-H(10A)	109.4	H(19B)-C(19)-H(19C)	109.5
C(8)-C(10)-H(10A)	109.4	N(3)-C(20)-C(21)	127.9(9)
O(3)-C(10)-H(10B)	109.4	N(3)-C(20)-H(20)	116.1
C(8)-C(10)-H(10B)	109.4	C(21)-C(20)-H(20)	116.1
H(10A)-C(10)-H(10B)	108.0	C(26)-C(21)-C(22)	119.1(9)
C(12)-C(11)-C(8)	118.1(8)	C(26)-C(21)-C(20)	126.7(8)
C(12)-C(11)-H(11A)	107.8	C(22)-C(21)-C(20)	114.2(9)
C(8)-C(11)-H(11A)	107.8	C(23)-C(22)-C(21)	121.4(10)
C(12)-C(11)-H(11B)	107.8	C(23)-C(22)-H(22)	119.3
C(8)-C(11)-H(11B)	107.8	C(21)-C(22)-H(22)	119.3
H(11A)-C(11)-H(11B)	107.1	C(22)-C(23)-C(24)	119.8(9)
C(11)-C(12)-H(12A)	109.5	C(22)-C(23)-H(23)	120.1
C(11)-C(12)-H(12B)	109.5	C(24)-C(23)-H(23)	120.1
H(12A)-C(12)-H(12B)	109.5	C(23)-C(24)-C(25)	123.1(10)
C(11)-C(12)-H(12C)	109.5	C(23)-C(24)-H(24)	118.4
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-H(24)	118.4
H(12B)-C(12)-H(12C)	109.5	C(24)-C(25)-C(26)	118.7(10)
C(18)-C(13)-C(14)	120.4(10)	C(24)-C(25)-H(25)	120.6
C(18)-C(13)-S(1)	119.5(9)	C(26)-C(25)-H(25)	120.6
C(14)-C(13)-S(1)	120.2(8)	N(4)-C(26)-C(21)	120.5(9)
C(13)-C(14)-C(15)	120.7(10)	N(4)-C(26)-C(25)	121.7(9)
C(13)-C(14)-H(14)	119.6	C(21)-C(26)-C(25)	117.8(8)
C(15)-C(14)-H(14)	119.6	C(29)-C(27)-C(28)	110.9(8)
C(16)-C(15)-C(14)	119.3(11)	C(29)-C(27)-C(30)	112.7(8)
C(16)-C(15)-H(15)	120.4	C(28)-C(27)-C(30)	111.4(7)
C(14)-C(15)-H(15)	120.4	C(29)-C(27)-N(3)	109.2(7)
C(15)-C(16)-C(17)	119.3(10)	C(28)-C(27)-N(3)	107.4(6)
C(15)-C(16)-C(19)	120.8(11)	C(30)-C(27)-N(3)	105.0(6)
C(17)-C(16)-C(19)	119.9(9)	O(8)-C(28)-C(27)	112.1(6)
C(18)-C(17)-C(16)	121.9(10)	O(8)-C(28)-H(28A)	109.2
C(18)-C(17)-H(17)	119.0	C(27)-C(28)-H(28A)	109.2
C(16)-C(17)-H(17)	119.0	O(8)-C(28)-H(28B)	109.2
C(13)-C(18)-C(17)	118.3(11)	C(27)-C(28)-H(28B)	109.2

H(28A)-C(28)-H(28B)	107.9	C(35)-C(38)-H(38C)	109.5
O(9)-C(29)-C(27)	112.8(7)	H(38A)-C(38)-H(38C)	109.5
O(9)-C(29)-H(29A)	109.0	H(38B)-C(38)-H(38C)	109.5
C(27)-C(29)-H(29A)	109.0	N(5)-Ni(5)-O(13)	165.0(2)
O(9)-C(29)-H(29B)	109.0	N(5)-Ni(5)-O(14)	81.9(2)
C(27)-C(29)-H(29B)	109.0	O(13)-Ni(5)-O(14)	83.19(18)
H(29A)-C(29)-H(29B)	107.8	N(5)-Ni(5)-N(6)	92.2(2)
C(31)-C(30)-C(27)	114.4(8)	O(13)-Ni(5)-N(6)	102.6(2)
C(31)-C(30)-H(30A)	108.7	O(14)-Ni(5)-N(6)	173.3(2)
C(27)-C(30)-H(30A)	108.7	N(5)-Ni(5)-O(14)#2	94.3(2)
C(31)-C(30)-H(30B)	108.7	O(13)-Ni(5)-O(14)#2	81.88(18)
C(27)-C(30)-H(30B)	108.7	O(14)-Ni(5)-O(14)#2	80.8(2)
H(30A)-C(30)-H(30B)	107.6	N(6)-Ni(5)-O(14)#2	96.5(2)
C(30)-C(31)-H(31A)	109.5	N(5)-Ni(5)-O(18)	93.1(2)
C(30)-C(31)-H(31B)	109.5	O(13)-Ni(5)-O(18)	87.92(17)
H(31A)-C(31)-H(31B)	109.5	O(14)-Ni(5)-O(18)	88.39(17)
C(30)-C(31)-H(31C)	109.5	N(6)-Ni(5)-O(18)	95.2(2)
H(31A)-C(31)-H(31C)	109.5	O(14)#2-Ni(5)-O(18)	165.88(17)
H(31B)-C(31)-H(31C)	109.5	O(14)#1-Ni(6)-O(14)#2	83.46(18)
C(33)-C(32)-C(37)	118.7(10)	O(14)#1-Ni(6)-O(14)	83.45(18)
C(33)-C(32)-S(2)	123.1(8)	O(14)#2-Ni(6)-O(14)	83.45(18)
C(37)-C(32)-S(2)	117.0(8)	O(14)#1-Ni(6)-O(15)#1	91.11(18)
C(32)-C(33)-C(34)	120.5(10)	O(14)#2-Ni(6)-O(15)#1	174.47(19)
C(32)-C(33)-H(33)	119.7	O(14)-Ni(6)-O(15)#1	94.94(18)
C(34)-C(33)-H(33)	119.7	O(14)#1-Ni(6)-O(15)#2	94.94(18)
C(35)-C(34)-C(33)	122.7(11)	O(14)#2-Ni(6)-O(15)#2	91.11(19)
C(35)-C(34)-H(34)	118.7	O(14)-Ni(6)-O(15)#2	174.46(19)
C(33)-C(34)-H(34)	118.7	O(15)#1-Ni(6)-O(15)#2	90.4(2)
C(34)-C(35)-C(36)	117.2(10)	O(14)#1-Ni(6)-O(15)	174.47(19)
C(34)-C(35)-C(38)	123.8(10)	O(14)#2-Ni(6)-O(15)	94.94(18)
C(36)-C(35)-C(38)	118.6(10)	O(14)-Ni(6)-O(15)	91.12(19)
C(35)-C(36)-C(37)	121.5(10)	O(15)#1-Ni(6)-O(15)	90.4(2)
C(35)-C(36)-H(36)	119.3	O(15)#2-Ni(6)-O(15)	90.4(2)
C(37)-C(36)-H(36)	119.3	O(16)-S(3)-O(17)	114.5(3)
C(32)-C(37)-C(36)	118.5(10)	O(16)-S(3)-N(6)	114.2(3)
C(32)-C(37)-H(37)	120.7	O(17)-S(3)-N(6)	106.7(3)
C(36)-C(37)-H(37)	120.7	O(16)-S(3)-C(51)	106.8(3)
C(35)-C(38)-H(38A)	109.5	O(17)-S(3)-C(51)	108.2(3)
C(35)-C(38)-H(38B)	109.5	N(6)-S(3)-C(51)	106.1(3)
H(38A)-C(38)-H(38B)	109.5	Ni(5)#1-O(13)-Ni(5)#2	97.9(2)

Ni(5)#1-O(13)-Ni(5)	97.9(2)	C(40)-C(45)-N(6)	121.3(7)
Ni(5)#2-O(13)-Ni(5)	97.9(2)	N(5)-C(46)-C(48)	108.4(6)
C(47)-O(14)-Ni(6)	118.4(4)	N(5)-C(46)-C(47)	107.6(6)
C(47)-O(14)-Ni(5)	106.4(4)	C(48)-C(46)-C(47)	109.9(6)
Ni(6)-O(14)-Ni(5)	98.41(18)	N(5)-C(46)-C(49)	112.1(6)
C(47)-O(14)-Ni(5)#1	134.1(4)	C(48)-C(46)-C(49)	108.9(6)
Ni(6)-O(14)-Ni(5)#1	96.70(18)	C(47)-C(46)-C(49)	110.0(6)
Ni(5)-O(14)-Ni(5)#1	95.77(18)	O(14)-C(47)-C(46)	111.9(6)
C(48)-O(15)-Ni(6)	128.6(4)	O(14)-C(47)-H(47A)	109.2
C(48)-O(15)-H(15O)	110.5	C(46)-C(47)-H(47A)	109.2
Ni(6)-O(15)-H(15O)	119.0	O(14)-C(47)-H(47B)	109.2
Ni(5)-O(18)-H(18A)	104.5	C(46)-C(47)-H(47B)	109.2
Ni(5)-O(18)-H(18B)	115.3	H(47A)-C(47)-H(47B)	107.9
H(18A)-O(18)-H(18B)	104.1	O(15)-C(48)-C(46)	112.1(6)
C(39)-N(5)-C(46)	121.1(6)	O(15)-C(48)-H(48A)	109.2
C(39)-N(5)-Ni(5)	124.3(5)	C(46)-C(48)-H(48A)	109.2
C(46)-N(5)-Ni(5)	113.9(4)	O(15)-C(48)-H(48B)	109.2
C(45)-N(6)-S(3)	117.1(4)	C(46)-C(48)-H(48B)	109.2
C(45)-N(6)-Ni(5)	117.7(4)	H(48A)-C(48)-H(48B)	107.9
S(3)-N(6)-Ni(5)	123.2(3)	C(50)-C(49)-C(46)	114.9(7)
N(5)-C(39)-C(40)	126.4(7)	C(50)-C(49)-H(49A)	108.5
N(5)-C(39)-H(39)	116.8	C(46)-C(49)-H(49A)	108.5
C(40)-C(39)-H(39)	116.8	C(50)-C(49)-H(49B)	108.5
C(41)-C(40)-C(45)	118.4(7)	C(46)-C(49)-H(49B)	108.5
C(41)-C(40)-C(39)	115.1(7)	H(49A)-C(49)-H(49B)	107.5
C(45)-C(40)-C(39)	126.4(7)	C(49)-C(50)-H(50A)	109.5
C(42)-C(41)-C(40)	122.5(8)	C(49)-C(50)-H(50B)	109.5
C(42)-C(41)-H(41)	118.8	H(50A)-C(50)-H(50B)	109.5
C(40)-C(41)-H(41)	118.8	C(49)-C(50)-H(50C)	109.5
C(41)-C(42)-C(43)	118.7(8)	H(50A)-C(50)-H(50C)	109.5
C(41)-C(42)-H(42)	120.6	H(50B)-C(50)-H(50C)	109.5
C(43)-C(42)-H(42)	120.6	C(56)-C(51)-C(52)	118.6(7)
C(42)-C(43)-C(44)	120.9(8)	C(56)-C(51)-S(3)	120.1(6)
C(42)-C(43)-H(43)	119.5	C(52)-C(51)-S(3)	121.3(6)
C(44)-C(43)-H(43)	119.5	C(53)-C(52)-C(51)	120.3(8)
C(43)-C(44)-C(45)	120.9(8)	C(53)-C(52)-H(52)	119.9
C(43)-C(44)-H(44)	119.6	C(51)-C(52)-H(52)	119.9
C(45)-C(44)-H(44)	119.6	C(52)-C(53)-C(54)	121.2(8)
C(44)-C(45)-C(40)	118.5(7)	C(52)-C(53)-H(53)	119.4
C(44)-C(45)-N(6)	120.1(7)	C(54)-C(53)-H(53)	119.4

C(55)-C(54)-C(53)	117.6(8)	C(58')-C(59')-H(59F)	109.5
C(55)-C(54)-C(57)	121.3(8)	H(59D)-C(59')-H(59F)	109.5
C(53)-C(54)-C(57)	121.0(8)	H(59E)-C(59')-H(59F)	109.5
C(56)-C(55)-C(54)	121.3(8)	C(60)-O(22)-H(22O)	119.4
C(56)-C(55)-H(55)	119.3	O(21)-C(60)-O(22)	120.0(3)
C(54)-C(55)-H(55)	119.3	O(21)-C(60)-C(61)	124.0(3)
C(55)-C(56)-C(51)	120.8(7)	O(22)-C(60)-C(61)	116.0(3)
C(55)-C(56)-H(56)	119.6	C(60)-C(61)-H(61A)	109.5
C(51)-C(56)-H(56)	119.6	C(60)-C(61)-H(61B)	109.5
C(54)-C(57)-H(57A)	109.5	H(61A)-C(61)-H(61B)	109.5
C(54)-C(57)-H(57B)	109.5	C(60)-C(61)-H(61C)	109.5
H(57A)-C(57)-H(57B)	109.5	H(61A)-C(61)-H(61C)	109.5
C(54)-C(57)-H(57C)	109.5	H(61B)-C(61)-H(61C)	109.5
H(57A)-C(57)-H(57C)	109.5	C(62)#2-N(7)-C(62)#1	110.7(3)
H(57B)-C(57)-H(57C)	109.5	C(62)#2-N(7)-C(62)	110.7(3)
C(58)-O(20)-H(20A)	119.4	C(62)#1-N(7)-C(62)	110.7(3)
O(19)-C(58)-O(20)	120.1(3)	C(62)#2-N(7)-H(7N)	108.2
O(19)-C(58)-C(59)	123.9(3)	C(62)#1-N(7)-H(7N)	108.2
O(20)-C(58)-C(59)	115.9(3)	C(62)-N(7)-H(7N)	108.2
C(58)-C(59)-H(59A)	109.5	N(7)#3-C(62)-C(63)#4	110.8(3)
C(58)-C(59)-H(59B)	109.5	N(7)-C(62)-C(63)	110.8(3)
H(59A)-C(59)-H(59B)	109.5	N(7)-C(62)-H(62A)	109.4
C(58)-C(59)-H(59C)	109.5	C(63)-C(62)-H(62A)	106.9
H(59A)-C(59)-H(59C)	109.5	N(7)-C(62)-H(62B)	109.9
H(59B)-C(59)-H(59C)	109.5	C(63)-C(62)-H(62B)	111.6
C(58')-O(20')-H(20B)	119.3	H(62A)-C(62)-H(62B)	108.1
O(19)-C(58')-O(20')	120.0(3)	C(62)-C(63)-H(63D)	110.1
O(19)-C(58')-C(59')	123.9(3)	C(62)-C(63)-H(63A)	111.5
O(20')-C(58')-C(59')	116.1(3)	H(63D)-C(63)-H(63A)	109.4
C(58')-C(59')-H(59D)	109.5	C(62)-C(63)-H(63B)	106.7
C(58')-C(59')-H(59E)	109.5	H(63D)-C(63)-H(63B)	109.4
H(59D)-C(59')-H(59E)	109.5	H(63A)-C(63)-H(63B)	109.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,-x+1,z #2 -y+1,x-y+1,z #3 y-1/3,x+1/3,-z+5/6 #4 x-y+2/3,-y+4/3,-z+5/6

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

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	70(1)	74(1)	49(1)	-3(1)	1(1)	35(1)
Ni(2)	76(1)	76(1)	46(1)	0	0	38(1)
Ni(3)	56(1)	53(1)	56(1)	-6(1)	3(1)	26(1)
Ni(4)	101(1)	101(1)	46(1)	0	0	50(1)
S(1)	80(2)	91(2)	50(1)	-4(1)	-1(1)	47(1)
S(2)	69(1)	58(1)	72(1)	10(1)	5(1)	32(1)
K(1)	80(1)	80(1)	46(2)	0	0	40(1)
O(1)	72(4)	72(4)	51(5)	0	0	36(2)
O(2)	72(4)	64(3)	55(3)	-5(3)	-2(3)	30(3)
O(3)	84(4)	79(4)	49(3)	-5(3)	-7(3)	33(4)
O(4)	84(4)	115(5)	47(3)	-4(3)	-2(3)	62(4)
O(5)	110(5)	78(4)	59(3)	-10(3)	0(3)	43(4)
O(6)	79(4)	71(4)	58(3)	6(3)	3(3)	32(3)
O(7)	43(3)	43(3)	56(5)	0	0	22(1)
O(8)	68(3)	65(3)	64(3)	-25(3)	-11(3)	34(3)
O(9)	122(6)	129(6)	76(4)	-32(4)	10(4)	62(5)
O(10)	76(4)	73(4)	65(3)	12(3)	11(3)	46(3)
O(11)	59(4)	58(3)	95(4)	4(3)	-9(3)	16(3)
O(12)	56(3)	57(3)	80(4)	-8(3)	9(3)	25(3)
N(1)	58(4)	68(4)	60(4)	-2(3)	2(3)	27(4)
N(2)	69(4)	85(5)	54(4)	-4(3)	-2(3)	41(4)
N(3)	52(4)	65(4)	88(5)	-27(4)	-3(4)	19(4)
N(4)	59(4)	51(4)	83(5)	5(3)	10(3)	35(3)
C(1)	75(6)	57(5)	54(5)	2(4)	9(4)	25(5)
C(2)	63(5)	62(5)	57(5)	2(4)	-8(4)	28(4)
C(3)	90(7)	80(6)	63(5)	-7(5)	-13(5)	39(6)
C(4)	125(9)	100(8)	73(6)	2(6)	-20(6)	67(7)
C(5)	128(9)	103(8)	77(7)	3(6)	-3(6)	74(7)
C(6)	106(7)	81(6)	58(5)	2(5)	0(5)	54(6)
C(7)	83(6)	69(6)	52(5)	9(4)	7(4)	36(5)
C(8)	77(6)	72(6)	65(5)	-11(4)	2(4)	35(5)
C(9)	75(6)	86(6)	60(5)	-1(4)	4(4)	45(5)
C(10)	79(6)	97(7)	48(5)	-14(4)	0(4)	38(6)
C(11)	125(7)	98(6)	108(6)	0(5)	-1(5)	42(5)
C(12)	125(7)	98(6)	108(6)	0(5)	-1(5)	42(5)

C(13)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(14)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(15)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(16)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(17)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(18)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(19)	99(3)	153(4)	68(2)	22(2)	7(2)	80(3)
C(20)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(21)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(22)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(23)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(24)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(25)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(26)	62(2)	63(2)	134(3)	-9(2)	21(2)	29(2)
C(27)	106(5)	115(5)	133(5)	-71(5)	-34(4)	61(4)
C(28)	81(6)	81(6)	74(5)	-33(5)	-18(5)	45(5)
C(29)	109(9)	125(10)	80(7)	-48(6)	-8(6)	50(8)
C(30)	106(5)	115(5)	133(5)	-71(5)	-34(4)	61(4)
C(31)	106(5)	115(5)	133(5)	-71(5)	-34(4)	61(4)
C(32)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(33)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(34)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(35)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(36)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(37)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
C(38)	102(3)	81(3)	128(4)	37(3)	-26(3)	17(2)
Ni(5)	47(1)	46(1)	50(1)	-2(1)	-3(1)	25(1)
Ni(6)	53(1)	53(1)	47(1)	0	0	26(1)
S(3)	54(1)	60(1)	55(1)	-7(1)	-9(1)	29(1)
O(13)	41(3)	41(3)	54(4)	0	0	21(1)
O(14)	44(3)	45(3)	54(3)	-8(2)	-8(2)	22(2)
O(15)	74(4)	58(3)	56(3)	-8(2)	-1(3)	33(3)
O(16)	59(3)	69(4)	66(3)	-18(3)	-17(3)	28(3)
O(17)	59(3)	67(3)	57(3)	-1(2)	-1(2)	37(3)
O(18)	43(3)	52(3)	64(3)	8(2)	1(2)	23(2)
N(5)	62(4)	48(4)	56(4)	1(3)	-5(3)	30(3)
N(6)	48(4)	63(4)	58(3)	-3(3)	-3(3)	37(3)
C(39)	86(6)	58(5)	61(5)	-3(4)	5(4)	46(5)
C(40)	69(5)	68(5)	56(4)	-1(4)	-2(4)	47(5)
C(41)	82(6)	83(6)	64(5)	9(4)	13(5)	54(5)

C(42)	61(6)	110(8)	83(6)	15(6)	7(5)	56(6)
C(43)	64(6)	112(8)	84(6)	7(6)	-6(5)	58(6)
C(44)	56(5)	81(6)	77(5)	-5(4)	-13(4)	43(5)
C(45)	60(5)	63(5)	60(5)	8(4)	-4(4)	41(4)
C(46)	61(5)	43(4)	61(5)	-4(3)	-5(4)	25(4)
C(47)	70(5)	46(4)	56(4)	-1(3)	-2(4)	28(4)
C(48)	76(6)	55(5)	68(5)	-17(4)	-10(4)	33(4)
C(49)	80(6)	61(5)	83(6)	-17(5)	-8(5)	37(5)
C(50)	154(11)	50(6)	131(10)	-2(6)	6(8)	36(7)
C(51)	49(4)	60(5)	54(4)	-2(4)	-8(4)	25(4)
C(52)	55(5)	79(6)	61(5)	-3(4)	-16(4)	28(5)
C(53)	68(6)	70(6)	85(6)	13(5)	-15(5)	40(5)
C(54)	58(5)	69(6)	90(6)	12(5)	-7(5)	30(5)
C(55)	61(5)	59(5)	98(6)	-5(5)	-22(5)	34(4)
C(56)	57(5)	62(5)	76(5)	-8(4)	-19(4)	33(4)
C(57)	68(6)	65(6)	159(10)	25(6)	-8(6)	30(5)
O(19)	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
O(20)	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
C(58)	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
C(59)	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
O(20')	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
C(58')	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
C(59')	105(4)	138(5)	88(3)	-16(3)	-15(3)	80(4)
O(21)	48(11)	113(18)	65(11)	-55(12)	11(9)	20(11)
O(22)	48(11)	113(18)	65(11)	-55(12)	11(9)	20(11)
C(60)	48(11)	113(18)	65(11)	-55(12)	11(9)	20(11)
C(61)	48(11)	113(18)	65(11)	-55(12)	11(9)	20(11)
N(7)	45(5)	45(5)	82(12)	0	0	22(3)
C(62)	45(5)	45(5)	82(12)	0	0	22(3)
C(63)	45(5)	45(5)	82(12)	0	0	22(3)

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

Atom	x	y	z	U(iso)
H(3O)	4265	6895	3248	111
H(6A)	4594	7864	2796	108
H(6B)	4331	8189	2851	108
H(9O)	3483	5812	1943	164
H(12D)	2479	5325	2388	99
H(12E)	2004	5342	2327	99
H(1)	5599	7696	3119	78
H(3)	6041	7060	3126	95
H(4)	6353	6342	3069	113
H(5)	5954	5849	2920	115
H(6)	5274	6094	2829	93
H(9A)	3964	8176	3117	85
H(9B)	4302	8379	3014	85
H(10A)	5057	7790	3233	93
H(10B)	4566	8057	3251	93
H(11A)	5214	9016	3142	140
H(11B)	5689	8727	3153	140
H(12A)	5390	9132	2978	175
H(12B)	5812	8778	2983	175
H(12C)	6080	9477	3031	175
H(14)	5953	7920	2817	119
H(15)	7017	8530	2753	119
H(17)	6470	7258	2533	119
H(18)	5406	6661	2593	119
H(19A)	7516	8546	2533	149
H(19B)	7698	8047	2582	149
H(19C)	7820	8683	2639	149
H(20)	3118	4570	2073	105
H(22)	3963	4389	2078	105
H(23)	4865	4441	2147	105
H(24)	5182	4867	2298	105
H(25)	4689	5359	2379	105
H(28A)	1894	5568	2060	92
H(28B)	1783	5234	2164	92
H(29A)	2779	4938	1951	130
H(29B)	2293	5209	1932	130

H(30A)	2063	4061	2068	139
H(30B)	1694	4224	2149	139
H(31A)	1407	4084	1950	173
H(31B)	1134	4435	2018	173
H(31C)	923	3689	2036	173
H(33)	2766	4285	2396	140
H(34)	2352	3327	2482	140
H(36)	3550	4240	2697	140
H(37)	4033	5227	2608	140
H(38A)	2536	3093	2711	175
H(38B)	3075	2968	2662	175
H(38C)	2376	2686	2613	175
H(15O)	3814	6159	3429	93
H(18A)	2898	5332	3881	80
H(18B)	2352	5270	3826	80
H(39)	3870	4929	3575	77
H(41)	4963	5273	3564	84
H(42)	6043	5858	3612	95
H(43)	6312	6495	3750	96
H(44)	5515	6569	3837	81
H(47A)	2124	5277	3556	69
H(47B)	2138	5012	3661	69
H(48A)	3385	5149	3447	79
H(48B)	2714	5135	3427	79
H(49A)	2100	4140	3536	88
H(49B)	2783	4162	3538	88
H(50A)	2083	3517	3665	178
H(50B)	2119	4156	3709	178
H(50C)	2759	4093	3705	178
H(52)	4975	5430	4017	81
H(53)	4841	4408	4042	87
H(55)	3239	3627	3875	85
H(56)	3390	4648	3847	76
H(57A)	3489	2941	4003	148
H(57B)	4247	3263	4026	148
H(57C)	3996	3067	3918	148
H(20A)	5771	7100	3293	153
H(59A)	5566	6351	3403	153
H(59B)	5038	5755	3340	153
H(59C)	4840	5915	3442	153

H(20B)	4860	5550	3375	153
H(59D)	5582	6313	3290	153
H(59E)	5599	6994	3293	153
H(59F)	5229	6495	3208	153
H(22O)	3769	4399	1886	126
H(61A)	4767	4956	1829	126
H(61B)	5074	5435	1919	126
H(61C)	5093	5725	1815	126
H(7N)	3333	6667	4069	86
H(62A)	3905	6273	4146	69
H(62B)	3943	6683	4235	69
H(63D)	4904	7216	4144	86
H(63A)	4505	7202	4054	86
H(63B)	4543	7616	4143	86

Table 6. Torsion angles [°] for **3-Ni**.

O(5)-S(1)-O(4)-K(1)	-2.2(5)	Ni(1)-N(1)-C(8)-C(11)	-129.4(7)
N(2)-S(1)-O(4)-K(1)	-129.4(4)	C(1)-N(1)-C(8)-C(10)	-52.1(9)
C(13)-S(1)-O(4)-K(1)	116.1(5)	Ni(1)-N(1)-C(8)-C(10)	112.8(6)
O(11)-S(2)-O(10)-K(1)	-19.1(5)	C(1)-N(1)-C(8)-C(9)	-172.9(7)
N(4)-S(2)-O(10)-K(1)	-146.4(4)	Ni(1)-N(1)-C(8)-C(9)	-8.0(7)
C(32)-S(2)-O(10)-K(1)	99.2(5)	Ni(1)-O(2)-C(9)-C(8)	-48.8(7)
O(5)-S(1)-N(2)-C(7)	62.6(7)	Ni(2)-O(2)-C(9)-C(8)	61.4(7)
O(4)-S(1)-N(2)-C(7)	-170.9(6)	Ni(1)#2-O(2)-C(9)-C(8)	-167.4(5)
C(13)-S(1)-N(2)-C(7)	-56.1(7)	N(1)-C(8)-C(9)-O(2)	37.3(8)
O(5)-S(1)-N(2)-Ni(1)	-107.4(5)	C(11)-C(8)-C(9)-O(2)	159.0(7)
O(4)-S(1)-N(2)-Ni(1)	19.1(5)	C(10)-C(8)-C(9)-O(2)	-82.4(8)
C(13)-S(1)-N(2)-Ni(1)	133.9(5)	Ni(2)-O(3)-C(10)-C(8)	-27.2(10)
O(11)-S(2)-N(4)-C(26)	59.3(7)	N(1)-C(8)-C(10)-O(3)	-58.3(9)
O(10)-S(2)-N(4)-C(26)	-173.6(6)	C(11)-C(8)-C(10)-O(3)	-178.9(8)
C(32)-S(2)-N(4)-C(26)	-60.5(7)	C(9)-C(8)-C(10)-O(3)	60.0(9)
O(11)-S(2)-N(4)-Ni(3)	-113.5(4)	N(1)-C(8)-C(11)-C(12)	45.6(13)
O(10)-S(2)-N(4)-Ni(3)	13.5(5)	C(10)-C(8)-C(11)-C(12)	165.0(10)
C(32)-S(2)-N(4)-Ni(3)	126.6(5)	C(9)-C(8)-C(11)-C(12)	-73.6(12)
C(8)-N(1)-C(1)-C(2)	174.3(7)	O(5)-S(1)-C(13)-C(18)	30.0(9)
Ni(1)-N(1)-C(1)-C(2)	10.8(11)	O(4)-S(1)-C(13)-C(18)	-92.2(9)
N(1)-C(1)-C(2)-C(3)	-166.5(8)	N(2)-S(1)-C(13)-C(18)	153.3(8)
N(1)-C(1)-C(2)-C(7)	9.8(13)	O(5)-S(1)-C(13)-C(14)	-151.3(8)
C(7)-C(2)-C(3)-C(4)	1.5(14)	O(4)-S(1)-C(13)-C(14)	86.5(8)
C(1)-C(2)-C(3)-C(4)	178.2(9)	N(2)-S(1)-C(13)-C(14)	-28.0(9)
C(2)-C(3)-C(4)-C(5)	-1.3(16)	C(18)-C(13)-C(14)-C(15)	0.5(15)
C(3)-C(4)-C(5)-C(6)	0.7(16)	S(1)-C(13)-C(14)-C(15)	-178.2(7)
C(4)-C(5)-C(6)-C(7)	-0.3(15)	C(13)-C(14)-C(15)-C(16)	0.0(14)
C(5)-C(6)-C(7)-C(2)	0.4(13)	C(14)-C(15)-C(16)-C(17)	-1.1(14)
C(5)-C(6)-C(7)-N(2)	179.6(8)	C(14)-C(15)-C(16)-C(19)	-179.4(8)
C(3)-C(2)-C(7)-C(6)	-1.0(12)	C(15)-C(16)-C(17)-C(18)	1.9(15)
C(1)-C(2)-C(7)-C(6)	-177.2(8)	C(19)-C(16)-C(17)-C(18)	-179.8(8)
C(3)-C(2)-C(7)-N(2)	179.8(7)	C(14)-C(13)-C(18)-C(17)	0.2(14)
C(1)-C(2)-C(7)-N(2)	3.6(12)	S(1)-C(13)-C(18)-C(17)	178.9(7)
S(1)-N(2)-C(7)-C(6)	-22.1(11)	C(16)-C(17)-C(18)-C(13)	-1.4(14)
Ni(1)-N(2)-C(7)-C(6)	148.0(7)	C(27)-N(3)-C(20)-C(21)	178.0(8)
S(1)-N(2)-C(7)-C(2)	157.1(6)	Ni(3)-N(3)-C(20)-C(21)	10.5(14)
Ni(1)-N(2)-C(7)-C(2)	-32.8(10)	N(3)-C(20)-C(21)-C(26)	9.2(17)
C(1)-N(1)-C(8)-C(11)	65.6(10)	N(3)-C(20)-C(21)-C(22)	-170.6(9)

C(26)-C(21)-C(22)-C(23)	-1.1(14)
C(20)-C(21)-C(22)-C(23)	178.6(9)
C(21)-C(22)-C(23)-C(24)	3.8(14)
C(22)-C(23)-C(24)-C(25)	-3.4(14)
C(23)-C(24)-C(25)-C(26)	0.4(14)
S(2)-N(4)-C(26)-C(21)	159.3(7)
Ni(3)-N(4)-C(26)-C(21)	-27.8(11)
S(2)-N(4)-C(26)-C(25)	-17.3(11)
Ni(3)-N(4)-C(26)-C(25)	155.6(7)
C(22)-C(21)-C(26)-N(4)	-178.5(8)
C(20)-C(21)-C(26)-N(4)	1.7(15)
C(22)-C(21)-C(26)-C(25)	-1.8(13)
C(20)-C(21)-C(26)-C(25)	178.4(9)
C(24)-C(25)-C(26)-N(4)	178.9(8)
C(24)-C(25)-C(26)-C(21)	2.2(13)
C(20)-N(3)-C(27)-C(29)	-56.6(10)
Ni(3)-N(3)-C(27)-C(29)	112.0(7)
C(20)-N(3)-C(27)-C(28)	-176.9(8)
Ni(3)-N(3)-C(27)-C(28)	-8.3(8)
C(20)-N(3)-C(27)-C(30)	64.4(10)
Ni(3)-N(3)-C(27)-C(30)	-127.0(6)
Ni(4)-O(8)-C(28)-C(27)	61.6(8)
Ni(3)-O(8)-C(28)-C(27)	-47.1(8)
Ni(3)#1-O(8)-C(28)-C(27)	-165.6(5)
C(29)-C(27)-C(28)-O(8)	-82.5(10)
C(30)-C(27)-C(28)-O(8)	151.1(8)
N(3)-C(27)-C(28)-O(8)	36.6(9)
Ni(4)-O(9)-C(29)-C(27)	-30.8(12)
C(28)-C(27)-C(29)-O(9)	62.2(11)
C(30)-C(27)-C(29)-O(9)	-172.2(8)
N(3)-C(27)-C(29)-O(9)	-55.9(10)
C(29)-C(27)-C(30)-C(31)	-57.6(11)
C(28)-C(27)-C(30)-C(31)	67.8(11)
N(3)-C(27)-C(30)-C(31)	-176.3(8)
O(11)-S(2)-C(32)-C(33)	-159.2(11)
O(10)-S(2)-C(32)-C(33)	78.1(13)
N(4)-S(2)-C(32)-C(33)	-35.1(13)
O(11)-S(2)-C(32)-C(37)	33.3(12)
O(10)-S(2)-C(32)-C(37)	-89.4(11)
N(4)-S(2)-C(32)-C(37)	157.4(10)
C(37)-C(32)-C(33)-C(34)	-6(2)
S(2)-C(32)-C(33)-C(34)	-173.5(10)
C(32)-C(33)-C(34)-C(35)	0(2)
C(33)-C(34)-C(35)-C(36)	9(2)
C(33)-C(34)-C(35)-C(38)	-178.7(12)
C(34)-C(35)-C(36)-C(37)	-10(2)
C(38)-C(35)-C(36)-C(37)	176.6(11)
C(33)-C(32)-C(37)-C(36)	4(2)
S(2)-C(32)-C(37)-C(36)	172.5(9)
C(35)-C(36)-C(37)-C(32)	4(2)
O(16)-S(3)-N(6)-C(45)	62.4(6)
O(17)-S(3)-N(6)-C(45)	-170.1(5)
C(51)-S(3)-N(6)-C(45)	-55.0(6)
O(16)-S(3)-N(6)-Ni(5)	-134.1(4)
O(17)-S(3)-N(6)-Ni(5)	-6.7(5)
C(51)-S(3)-N(6)-Ni(5)	108.5(4)
C(46)-N(5)-C(39)-C(40)	169.1(7)
Ni(5)-N(5)-C(39)-C(40)	-0.8(11)
N(5)-C(39)-C(40)-C(41)	-160.7(8)
N(5)-C(39)-C(40)-C(45)	15.5(13)
C(45)-C(40)-C(41)-C(42)	-3.0(12)
C(39)-C(40)-C(41)-C(42)	173.5(8)
C(40)-C(41)-C(42)-C(43)	2.1(13)
C(41)-C(42)-C(43)-C(44)	-0.6(13)
C(42)-C(43)-C(44)-C(45)	0.0(13)
C(43)-C(44)-C(45)-C(40)	-0.9(11)
C(43)-C(44)-C(45)-N(6)	-179.6(7)
C(41)-C(40)-C(45)-C(44)	2.3(11)
C(39)-C(40)-C(45)-C(44)	-173.8(7)
C(41)-C(40)-C(45)-N(6)	-179.0(6)
C(39)-C(40)-C(45)-N(6)	4.9(11)
S(3)-N(6)-C(45)-C(44)	-50.0(9)
Ni(5)-N(6)-C(45)-C(44)	145.7(6)
S(3)-N(6)-C(45)-C(40)	131.3(6)
Ni(5)-N(6)-C(45)-C(40)	-33.0(8)
C(39)-N(5)-C(46)-C(48)	-59.0(8)
Ni(5)-N(5)-C(46)-C(48)	111.9(5)
C(39)-N(5)-C(46)-C(47)	-177.7(6)
Ni(5)-N(5)-C(46)-C(47)	-6.9(7)
C(39)-N(5)-C(46)-C(49)	61.2(9)

Ni(5)-N(5)-C(46)-C(49)	-127.9(5)	O(16)-S(3)-C(51)-C(56)	-175.7(6)
Ni(6)-O(14)-C(47)-C(46)	62.3(6)	O(17)-S(3)-C(51)-C(56)	60.6(7)
Ni(5)-O(14)-C(47)-C(46)	-47.1(6)	N(6)-S(3)-C(51)-C(56)	-53.5(7)
Ni(5)#1-O(14)-C(47)-C(46)	-162.5(4)	O(16)-S(3)-C(51)-C(52)	2.8(7)
N(5)-C(46)-C(47)-O(14)	36.2(8)	O(17)-S(3)-C(51)-C(52)	-120.9(6)
C(48)-C(46)-C(47)-O(14)	-81.6(7)	N(6)-S(3)-C(51)-C(52)	125.0(6)
C(49)-C(46)-C(47)-O(14)	158.6(6)	C(56)-C(51)-C(52)-C(53)	-4.3(12)
Ni(6)-O(15)-C(48)-C(46)	-29.2(9)	S(3)-C(51)-C(52)-C(53)	177.2(6)
N(5)-C(46)-C(48)-O(15)	-57.3(8)	C(51)-C(52)-C(53)-C(54)	0.7(13)
C(47)-C(46)-C(48)-O(15)	60.0(8)	C(52)-C(53)-C(54)-C(55)	2.0(13)
C(49)-C(46)-C(48)-O(15)	-179.5(6)	C(53)-C(54)-C(55)-C(56)	-1.1(13)
N(5)-C(46)-C(49)-C(50)	50.7(10)	C(54)-C(55)-C(56)-C(51)	-2.6(13)
C(48)-C(46)-C(49)-C(50)	170.7(8)	C(52)-C(51)-C(56)-C(55)	5.2(12)
C(47)-C(46)-C(49)-C(50)	-68.9(10)	S(3)-C(51)-C(56)-C(55)	-176.2(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,-x+1,z #2 -y+1,x-y+1,z #3 y-1/3,x+1/3,-z+5/6 #4 x-y+2/3,-y+4/3,-z+5/6

Table 7. Hydrogen bonds for **3-Ni** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3O)...O(19)	0.92	1.72	2.616(8)	163.6
O(6)-H(6A)...O(4)	0.91	1.96	2.745(7)	144.6
O(6)-H(6B)...O(5)#2	0.91	2.22	2.916(8)	132.2
O(9)-H(9O)...O(21)	0.91	1.77	2.67(2)	169.2
O(12)-H(12D)...O(10)	0.90	1.98	2.743(7)	141.6
O(12)-H(12E)...O(11)#1	0.92	2.34	2.950(7)	123.8
O(15)-H(15O)...O(19)	0.92	1.69	2.580(8)	163.1
O(18)-H(18A)...O(17)	0.92	1.90	2.697(7)	144.7
O(18)-H(18B)...N(6)#1	0.92	2.20	3.051(7)	153.4

Symmetry transformations used to generate equivalent atoms:

#1 -x+y, -x+1, z #2 -y+1, x-y+1, z #3 y-1/3, x+1/3, -z+5/6 #4 x-y+2/3, -y+4/3, -z+5/6