

Supplementary Materials

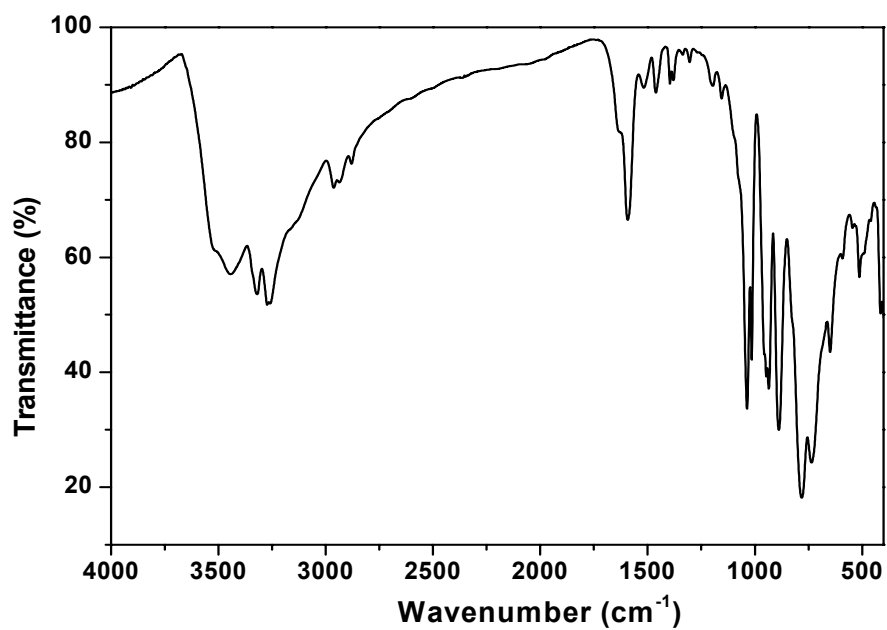


Fig.S1 FT-IR spectrum of compound 1.

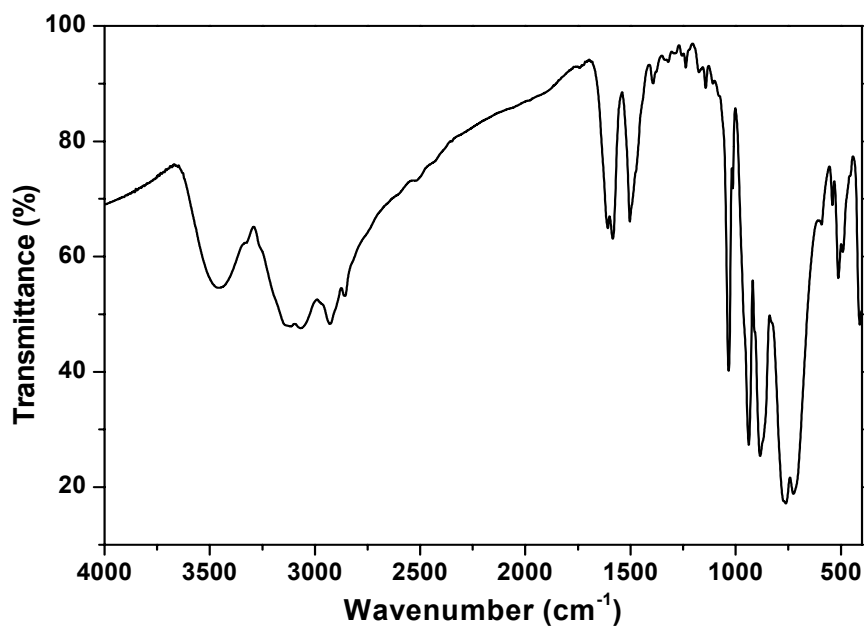


Fig.S2 FT-IR spectrum of compound 2.

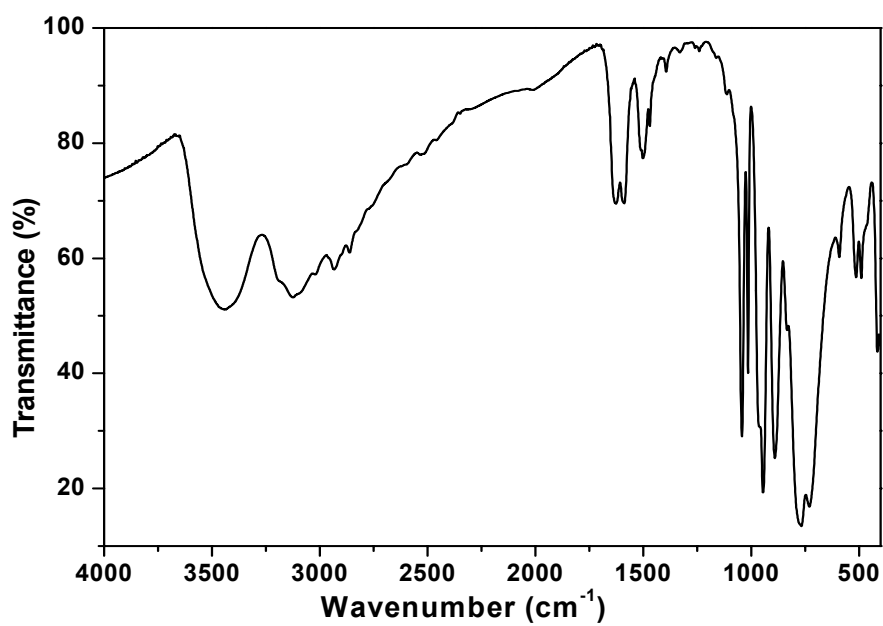


Fig.S3 FT-IR spectrum of compound 3.

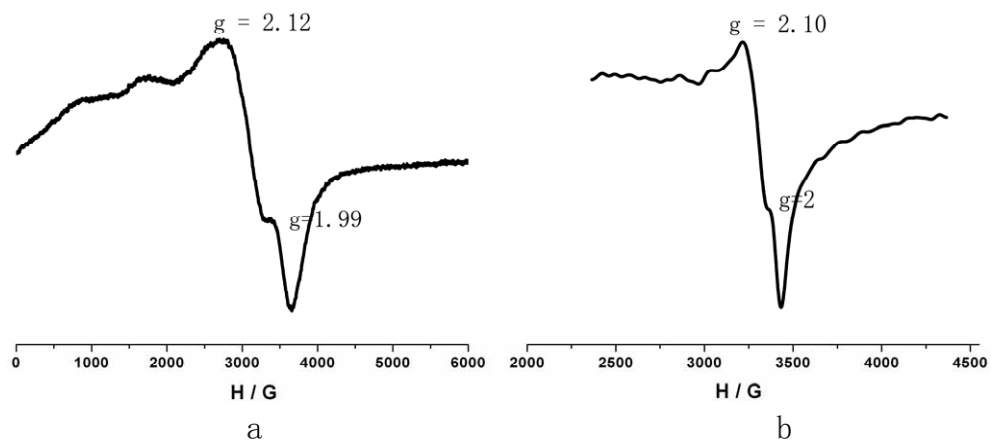


Fig. S4. The EPR spectra for **1** (a) and **2** (b) measured at room temperature.

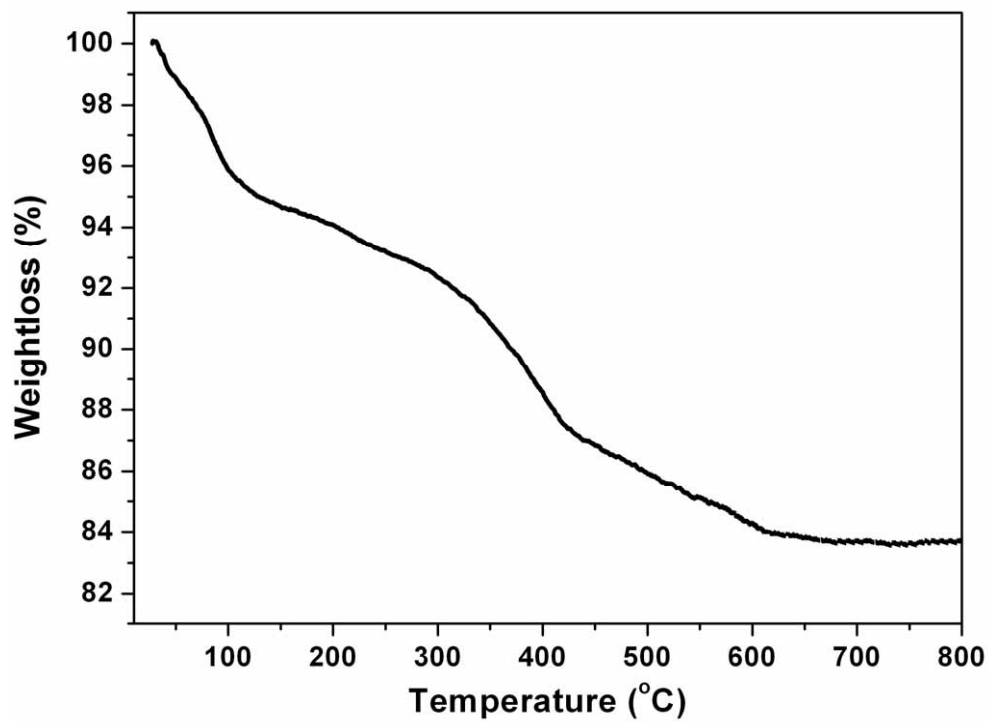


Fig. S5. TG curve for compound 1.

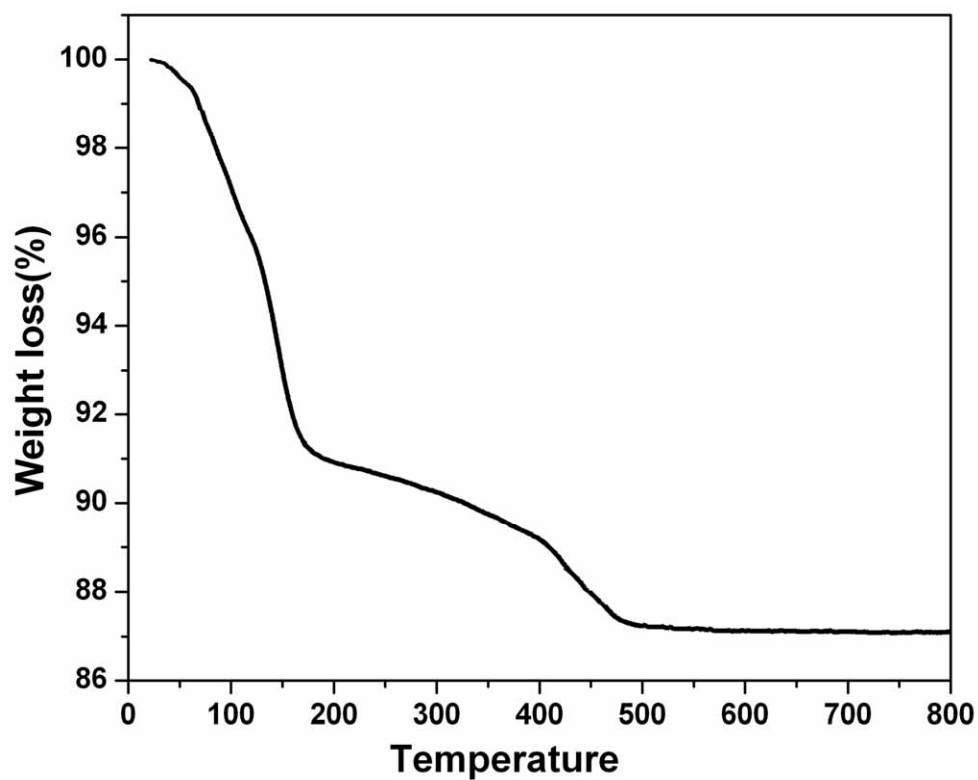


Fig. S6. TG curve for compound 2.

Table S1. Selected bond lengths [\AA] and angles [$^\circ$] for **1** and **2**.

Compound 1			
W(1)-O(18)	1.743(9)	W(2)-O(8)	1.762(9)
W(1)-O(28)	1.769(9)	W(2)-O(24)	1.775(10)
W(1)-O(20)#1	1.885(9)	W(2)-O(10)	1.912(9)
W(1)-O(4)	2.000(10)	W(2)-O(12)#1	1.987(10)
W(1)-O(6)	2.003(10)	W(2)-O(27)	2.048(10)
W(1)-O(29)	2.411(9)	W(2)-O(26)	2.434(10)
W(3)-O(17)	1.734(9)	W(4)-O(13)	1.711(10)
W(3)-O(19)	1.820(10)	W(4)-O(1)	1.775(9)
W(3)-O(2)	1.863(11)	W(4)-O(20)	1.930(10)
W(3)-O(11)#1	1.935(10)	W(4)-O(15)	1.938(10)
W(3)-O(16)#1	1.944(10)	W(4)-O(19)	2.043(10)
W(3)-O(32)	2.520(9)	W(4)-O(32)	2.487(9)
W(5)-O(33)	1.756(9)	W(6)-O(22)	1.701(10)
W(5)-O(9)	1.839(9)	W(6)-O(4)	1.882(10)
W(5)-O(12)	1.900(10)	W(6)-O(11)	1.892(10)
W(5)-O(30)	1.934(11)	W(6)-O(21)	1.897(10)
W(5)-O(5)	1.991(10)	W(6)-O(7)	1.907(10)
W(5)-O(26)#1	2.417(9)	W(6)-O(29)	2.498(9)
W(7)-O(31)	1.752(9)	W(8)-O(14)	1.733(10)
W(7)-O(27)#1	1.855(10)	W(8)-O(25)	1.774(9)
W(7)-O(5)	1.894(10)	W(8)-O(15)	1.923(9)
W(7)-O(16)	1.901(9)	W(8)-O(10)	1.930(9)
W(7)-O(7)	1.932(10)	W(8)-O(2)	2.001(9)
W(7)-O(26)#1	2.491(9)	W(8)-O(32)	2.393(10)
W(9)-O(34)	1.760(10)	W(9)-O(29)	2.416(9)
W(9)-O(3)	1.810(10)	P(1)-O(32)#1	1.531(10)
W(9)-O(6)	1.850(10)	P(1)-O(26)#1	1.539(10)
W(9)-O(30)	1.929(10)	P(1)-O(23)#1	1.542(10)
W(9)-O(21)	1.983(10)	P(1)-O(29)	1.555(10)
Ni(1)-O(24)	1.976(10)	Ni(2)-O(25)	2.002(9)
Ni(1)-O(28)	1.986(9)	Ni(2)-O(1)	2.010(10)
Ni(1)-O(9)#1	2.045(10)	Ni(2)-O(9)	2.057(9)
Ni(1)-O(3)	2.052(11)	Ni(2)-O(3)	2.097(9)
Ni(1)-O(23)	2.158(9)	Ni(2)-N(1)	2.108(14)
Ni(1)-O(23)#1	2.168(9)	Ni(2)-O(23)	2.217(10)
Ni(3)-N(3)	2.073(11)	Ni(4)-N(2)#3	2.064(13)
Ni(3)-N(3)#2	2.073(11)	Ni(4)-N(2)	2.064(13)
Ni(3)-N(5)#2	2.105(14)	Ni(4)-O(14)	2.087(10)
Ni(3)-N(5)	2.105(14)	Ni(4)-O(14)#3	2.087(10)
Ni(3)-O(18)#2	2.162(10)	Ni(4)-N(6)	2.099(13)

Ni(3)-O(18)	2.162(10)	Ni(4)-N(6)#3	2.099(13)
Ni(5)-N(11)	1.99(2)	Ni(5)-N(10)	2.08(2)
Ni(5)-N(7)	2.053(17)	Ni(5)-O(35)	2.16(2)
Ni(5)-N(4)	2.079(13)	Ni(5)-O(17)	2.175(10)
O(24)-Ni(1)-O(28)	93.7(4)	O(25)-Ni(2)-O(1)	93.9(4)
O(24)-Ni(1)-O(9)#1	96.4(4)	O(25)-Ni(2)-O(9)	169.2(4)
O(28)-Ni(1)-O(9)#1	91.1(4)	O(1)-Ni(2)-O(9)	90.6(4)
O(24)-Ni(1)-O(3)	91.3(4)	O(25)-Ni(2)-O(3)	89.2(4)
O(28)-Ni(1)-O(3)	95.1(4)	O(1)-Ni(2)-O(3)	171.8(4)
O(9)#1-Ni(1)-O(3)	169.8(4)	O(9)-Ni(2)-O(3)	85.1(4)
O(24)-Ni(1)-O(23)	91.5(3)	O(25)-Ni(2)-N(1)	90.9(5)
O(28)-Ni(1)-O(23)	174.8(4)	O(1)-Ni(2)-N(1)	89.1(5)
O(9)#1-Ni(1)-O(23)	88.7(4)	O(9)-Ni(2)-N(1)	99.1(5)
O(3)-Ni(1)-O(23)	84.4(4)	O(3)-Ni(2)-N(1)	98.5(5)
O(24)-Ni(1)-O(23)#1	177.1(3)	O(25)-Ni(2)-O(23)	87.6(4)
O(28)-Ni(1)-O(23)#1	89.2(4)	O(1)-Ni(2)-O(23)	90.7(4)
O(9)#1-Ni(1)-O(23)#1	84.0(4)	O(9)-Ni(2)-O(23)	82.4(4)
O(3)-Ni(1)-O(23)#1	88.0(4)	O(3)-Ni(2)-O(23)	81.9(4)
O(23)-Ni(1)-O(23)#1	85.6(3)	N(1)-Ni(2)-O(23)	178.5(4)
N(3)-Ni(3)-N(3)#2	180.000(2)	N(2)#3-Ni(4)-N(2)	180.000(2)
N(3)-Ni(3)-N(5)#2	97.5(5)	N(2)#3-Ni(4)-O(14)	89.4(4)
N(3)#2-Ni(3)-N(5)#2	82.5(5)	N(2)-Ni(4)-O(14)	90.6(4)
N(3)-Ni(3)-N(5)	82.5(5)	N(2)#3-Ni(4)-O(14)#3	90.6(4)
N(3)#2-Ni(3)-N(5)	97.5(5)	N(2)-Ni(4)-O(14)#3	89.4(4)
N(5)#2-Ni(3)-N(5)	180.000(2)	O(14)-Ni(4)-O(14)#3	180.0(4)
N(3)-Ni(3)-O(18)#2	89.4(4)	N(2)#3-Ni(4)-N(6)	98.6(5)
N(3)#2-Ni(3)-O(18)#2	90.6(4)	N(2)-Ni(4)-N(6)	81.4(5)
N(5)#2-Ni(3)-O(18)#2	89.5(5)	O(14)-Ni(4)-N(6)	90.4(5)
N(5)-Ni(3)-O(18)#2	90.5(5)	O(14)#3-Ni(4)-N(6)	89.6(5)
N(3)-Ni(3)-O(18)	90.6(4)	N(2)#3-Ni(4)-N(6)#3	81.4(5)
N(3)#2-Ni(3)-O(18)	89.4(4)	N(2)-Ni(4)-N(6)#3	98.6(5)
N(5)#2-Ni(3)-O(18)	90.5(5)	O(14)-Ni(4)-N(6)#3	89.6(5)
N(5)-Ni(3)-O(18)	89.5(5)	O(14)#3-Ni(4)-N(6)#3	90.4(5)
O(18)#2-Ni(3)-O(18)	180.000(2)	N(6)-Ni(4)-N(6)#3	180.0(6)
N(11)-Ni(5)-N(7)	96.9(9)	N(4)-Ni(5)-O(35)	93.2(7)
N(11)-Ni(5)-N(4)	92.8(8)	N(10)-Ni(5)-O(35)	89.8(8)
N(7)-Ni(5)-N(4)	81.7(6)	N(11)-Ni(5)-O(17)	174.5(8)
N(11)-Ni(5)-N(10)	88.4(9)	N(7)-Ni(5)-O(17)	87.7(6)
N(7)-Ni(5)-N(10)	95.1(8)	N(4)-Ni(5)-O(17)	90.9(4)
N(4)-Ni(5)-N(10)	176.7(8)	N(10)-Ni(5)-O(17)	88.2(7)
N(11)-Ni(5)-O(35)	90.7(9)	O(35)-Ni(5)-O(17)	85.0(7)
N(7)-Ni(5)-O(35)	171.1(7)		
Compound 2			

W(1)-O(31)	1.714(15)	W(2)-O(26)	1.691(18)
W(1)-O(18)	1.793(13)	W(2)-O(10)	1.814(14)
W(1)-O(20)	1.886(15)	W(2)-O(4)	1.900(14)
W(1)-O(5)	1.965(17)	W(2)-O(7)	1.927(13)
W(1)-O(8)	2.020(14)	W(2)-O(15)	2.015(15)
W(1)-O(24)	2.392(13)	W(2)-O(17)	2.381(16)
W(3)-O(25)	1.742(16)	W(4)-O(33)	1.669(15)
W(3)-O(6)	1.781(13)	W(4)-O(21)	1.839(17)
W(3)-O(9)	1.886(17)	W(4)-O(22)	1.863(16)
W(3)-O(4)	1.958(16)	W(4)-O(2)	1.918(15)
W(3)-O(13)	1.999(14)	W(4)-O(1)	1.949(17)
W(3)-O(17)	2.355(13)	W(4)-O(12)#1	2.487(13)
W(5)-O(14)	1.702(17)	W(6)-O(34)	1.696(16)
W(5)-O(30)#1	1.757(13)	W(6)-O(32)	1.859(19)
W(5)-O(16)	1.906(16)	W(6)-O(8)	1.862(15)
W(5)-O(20)	1.953(15)	W(6)-O(3)	1.894(15)
W(5)-O(21)	2.052(15)	W(6)-O(2)	1.916(16)
W(5)-O(12)#1	2.376(15)	W(6)-O(24)	2.519(11)
W(7)-O(28)	1.788(13)	W(8)-O(23)	1.692(16)
W(7)-O(19)	1.819(12)	W(8)-O(13)	1.857(14)
W(7)-O(7)	1.924(14)	W(8)-O(1)	1.879(17)
W(7)-O(5)	1.928(17)	W(8)-O(15)	1.880(17)
W(7)-O(32)	2.036(15)	W(8)-O(3)	1.960(14)
W(7)-O(24)	2.342(14)	W(8)-O(17)	2.529(14)
W(9)-O(27)	1.758(14)	W(9)-O(12)#1	2.451(14)
W(9)-O(29)	1.760(14)	P(1)-O(12)	1.534(16)
W(9)-O(9)	1.931(18)	P(1)-O(17)#1	1.581(16)
W(9)-O(16)	1.955(17)	P(1)-O(11)	1.582(12)
W(9)-O(22)	1.998(14)	P(1)-O(24)#1	1.590(13)
Ni(1)-O(6)	2.006(13)	Ni(2)-O(27)#1	2.023(14)
Ni(1)-O(18)#1	2.010(14)	Ni(2)-O(30)	2.056(14)
Ni(1)-O(10)	2.058(16)	Ni(2)-N(1)	2.08(2)
Ni(1)-O(19)#1	2.069(15)	Ni(2)-O(19)	2.085(13)
Ni(1)-O(11)#1	2.138(12)	Ni(2)-O(10)	2.123(15)
Ni(1)-O(11)	2.143(14)	Ni(2)-O(11)	2.153(14)
O(6)-Ni(1)-O(18)#1	90.1(6)	O(27)#1-Ni(2)-O(30)	94.5(5)
O(6)-Ni(1)-O(10)	93.6(6)	O(27)#1-Ni(2)-N(1)	88.3(7)
O(18)#1-Ni(1)-O(10)	91.3(6)	O(30)-Ni(2)-N(1)	90.8(7)
O(6)-Ni(1)-O(19)#1	92.7(6)	O(27)#1-Ni(2)-O(19)	91.4(5)
O(18)#1-Ni(1)-O(19)#1	95.1(6)	O(30)-Ni(2)-O(19)	171.1(6)
O(10)-Ni(1)-O(19)#1	171.1(6)	N(1)-Ni(2)-O(19)	96.1(7)
O(6)-Ni(1)-O(11)#1	92.2(5)	O(27)#1-Ni(2)-O(10)	172.1(6)
O(18)#1-Ni(1)-O(11)#1	177.2(6)	O(30)-Ni(2)-O(10)	89.1(5)

O(10)-Ni(1)-O(11)#1	90.1(5)	N(1)-Ni(2)-O(10)	98.6(7)
O(19)#1-Ni(1)-O(11)#1	83.4(5)	O(19)-Ni(2)-O(10)	84.2(5)
O(6)-Ni(1)-O(11)	176.9(5)	O(27)#1-Ni(2)-O(11)	90.5(6)
O(18)#1-Ni(1)-O(11)	92.2(5)	O(30)-Ni(2)-O(11)	90.6(5)
O(10)-Ni(1)-O(11)	84.2(6)	N(1)-Ni(2)-O(11)	178.2(7)
O(19)#1-Ni(1)-O(11)	89.2(5)	O(19)-Ni(2)-O(11)	82.6(5)
O(11)#1-Ni(1)-O(11)	85.5(5)	O(10)-Ni(2)-O(11)	82.4(6)

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