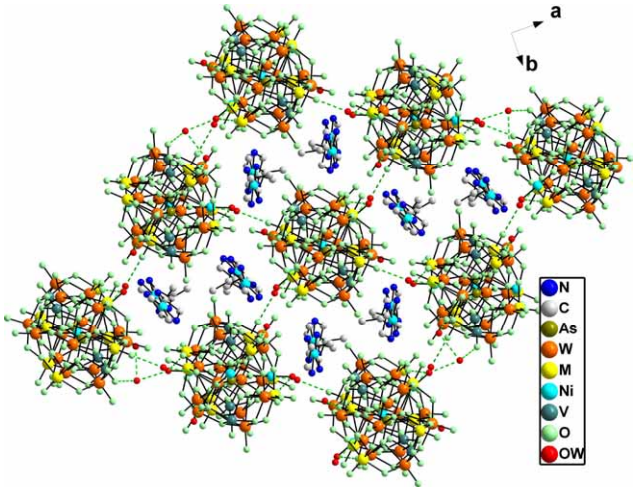
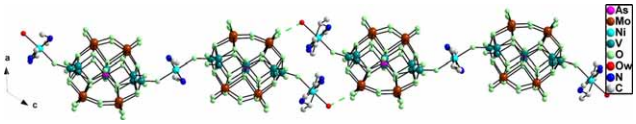
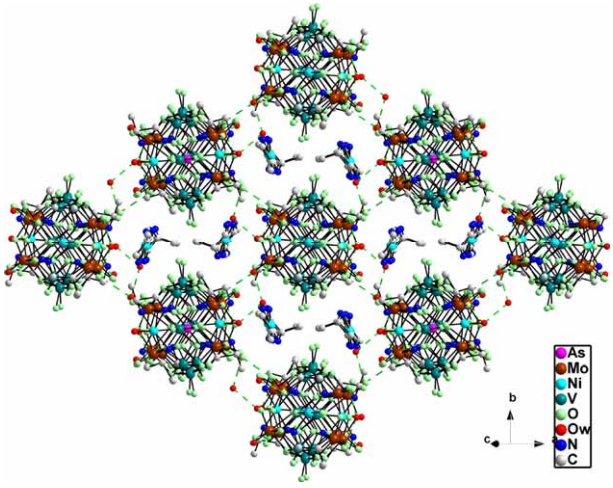
Supplementary materials



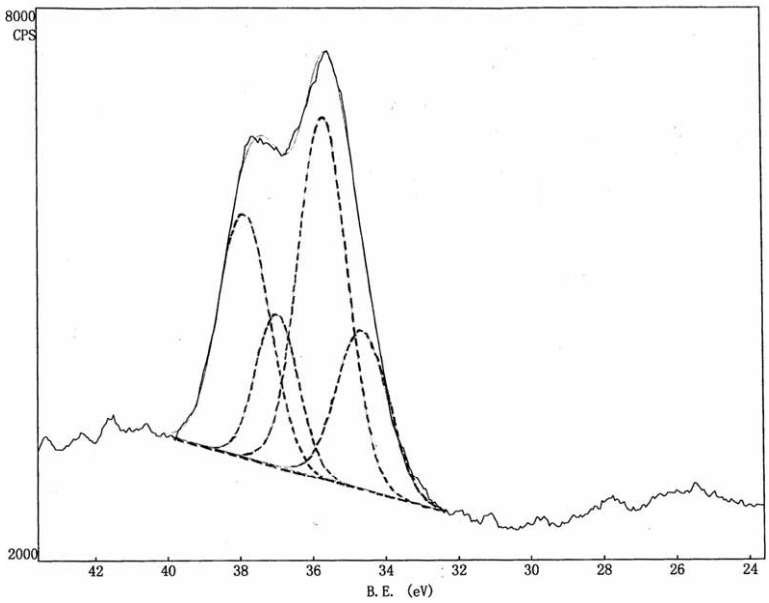
S-Fig. 1 Showing the charge–compensating components $\{[Ni(2)(enMe)_2]^{2+}$ and $[Ni(4)(enMe)_2]^{2+}\}$ filled in the 1-D channel for **2.**



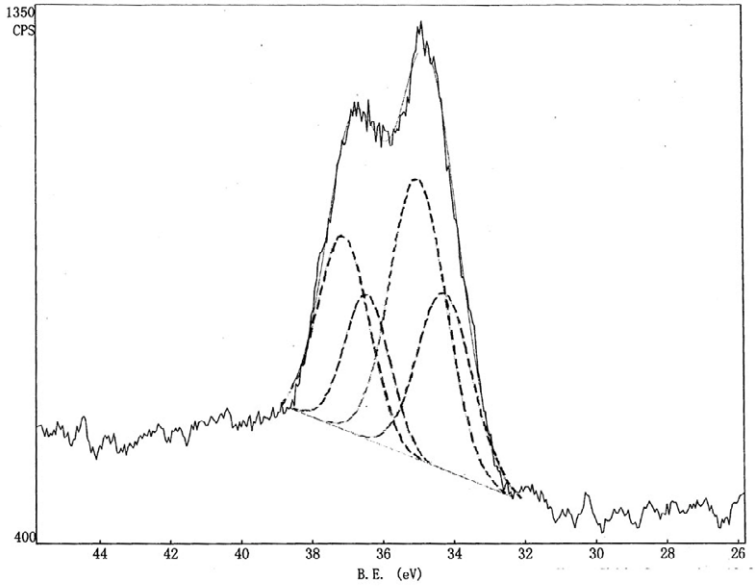
S-Fig.2 1-D supramolecular chain consists of the discrete dimer in **3**.



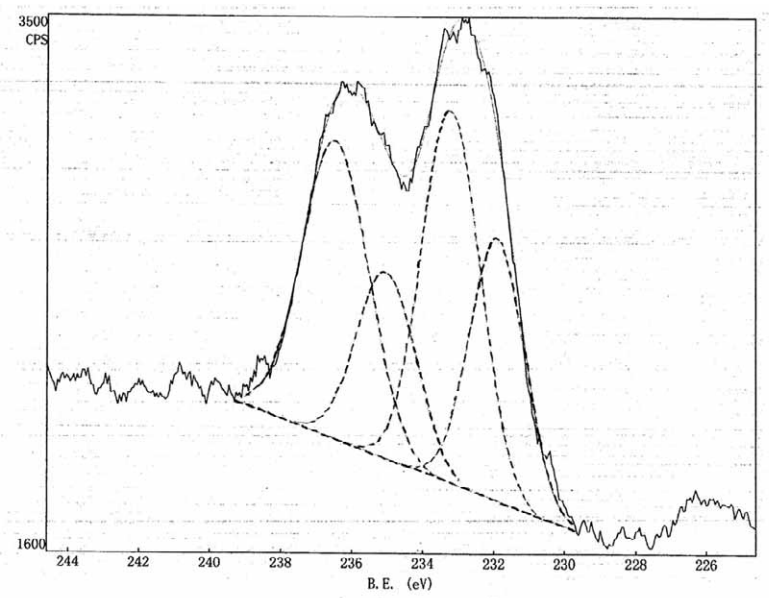
S-Fig. 3 Showing the charge–compensating components $\{[Ni(3)(enMe)_2]^{2+}$ and $[Ni(4)(enMe)_2]^{2+}\}$ filled in the 1-D channel for **3**



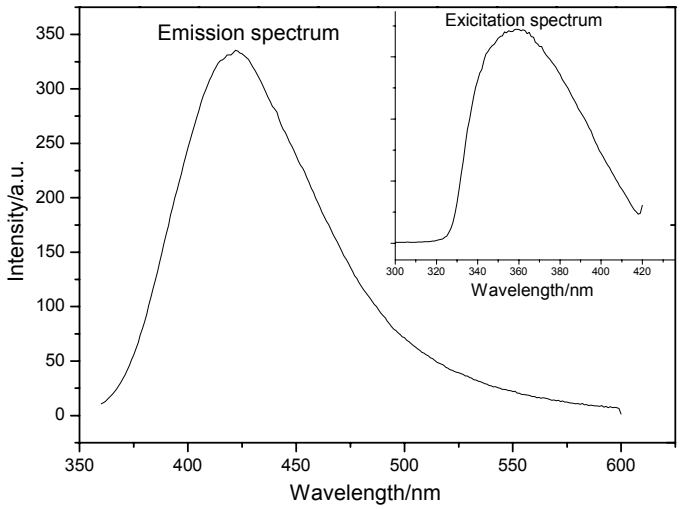
S-Fig . 4 xps for compound **1**



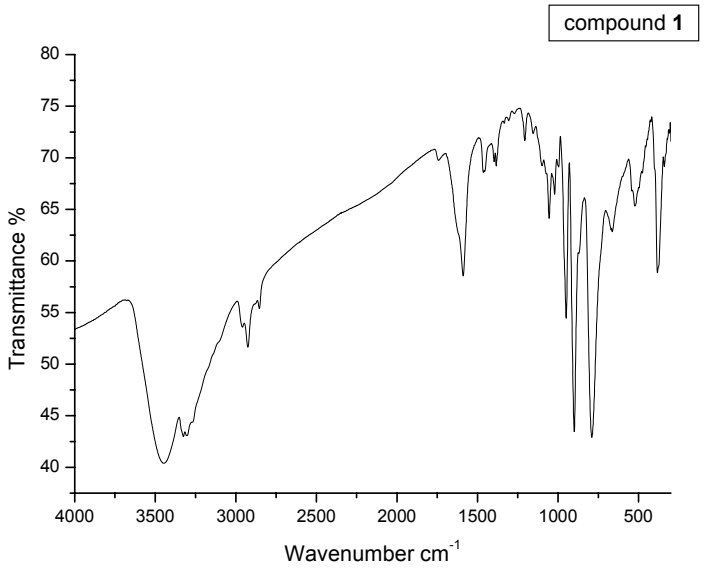
S-Fig. 5 Xps for compound **2**



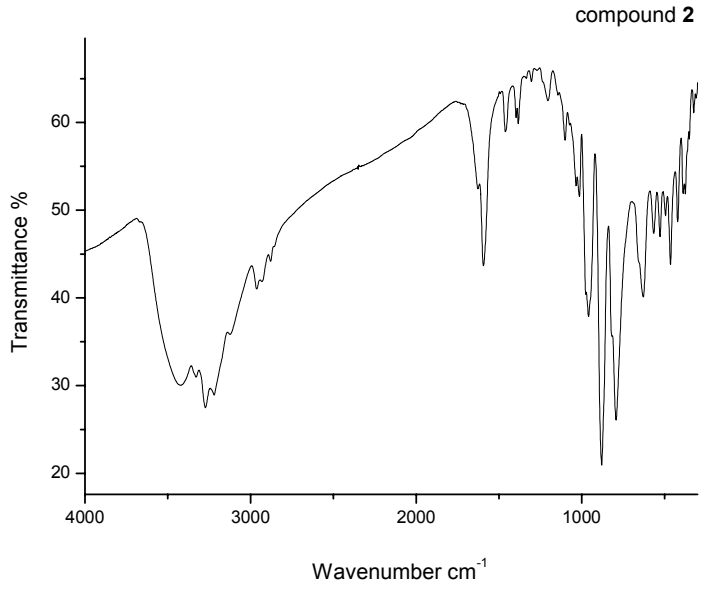
S-Fig.6 Xps for compound **3**



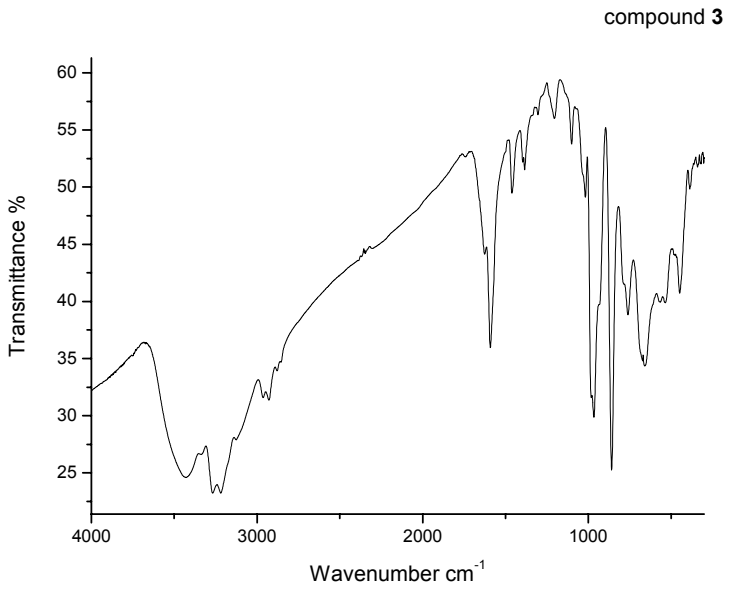
S-Fig.7 Emission spectra of enMe



S-Fig. 8 IR for compound **1**



S-Fig. 9 IR for compound **2**



S-Fig. 10 IR for compound **3**

S-Table 1 Selected bond lengths (Å) and bond angle (°) for **1**-**3**.

Compound **1**			
N(2)-C(3)	1.44(2)	P(1)-O(1)#1	1.555(7)
N(2)-Ni(2)	2.040(14)	Ni(1)-N(6)	1.945(13)
N(2)-H(2C)	0.8967	Ni(1)-N(6)#2	1.945(13)
N(2)-H(2D)	0.8976	Ni(1)-N(5)	1.960(13)
W(1)-O(15)	1.716(9)	Ni(1)-N(5)#2	1.961(13)
W(1)-O(6)	1.901(9)	Ni(1)-O(13)	2.627(12)
W(1)-O(4)#1	1.919(9)	Ni(2)-N(3)	2.066(12)
W(1)-O(2)	1.931(9)	Ni(2)-N(1)	2.081(12)
W(1)-O(14)#1	1.950(9)	Ni(2)-N(4)	2.117(11)
W(1)-O(1)	2.397(8)	Ni(2)-O(1W)	2.146(11)
W(2)-O(17)	1.714(10)	Ni(2)-O(2W)	2.186(11)
W(2)-O(2)	1.888(9)	O(1)-W(4)#1	2.387(8)
W(2)-O(14)	1.904(9)	O(1)-W(2)#1	2.394(9)
W(2)-O(12)	1.920(9)	O(4)-W(1)#1	1.919(9)
W(2)-O(5)	1.951(8)	O(7)-W(6)#1	1.916(9)
W(2)-O(1)#1	2.394(9)	O(9)-W(6)#1	2.397(8)
W(3)-O(19)	1.713(11)	O(10)-W(3)#1	1.923(9)
W(3)-O(12)	1.889(9)	O(14)-W(1)#1	1.950(9)
W(3)-O(16)	1.912(9)	C(1)-C(3)	1.49(3)
W(3)-O(6)	1.922(9)	C(1)-H(1A)	0.9600
W(3)-O(10)#1	1.923(9)	C(1)-H(1B)	0.9600

W(3)-O(9)	2.398(8)	C(1)-H(1C)	0.9600
W(4)-O(11)	1.714(9)	C(2)-C(3)	1.31(2)
W(4)-O(3)	1.902(9)	C(2)-N(1)	1.45(2)
W(4)-O(8)	1.911(9)	C(2)-H(2A)	0.9700
W(4)-O(5)	1.921(9)	C(2)-H(2B)	0.9700
W(4)-O(4)	1.961(9)	C(3)-H(3)	0.9800
W(4)-O(1)#1	2.387(8)	C(4)-N(4)	1.47(2)
W(5)-O(13)	1.709(10)	C(4)-C(5)	1.48(2)
W(5)-O(18)	1.887(10)	C(4)-C(6)	1.52(2)
W(5)-O(8)	1.909(9)	C(4)-H(4)	0.9800
W(5)-O(7)	1.927(9)	C(5)-N(3)	1.46(2)
W(5)-O(16)	1.951(9)	C(5)-H(5A)	0.9700
W(5)-O(9)	2.414(8)	C(5)-H(5B)	0.9700
W(6)-O(20)	1.705(9)	C(6)-H(6A)	0.9600
W(6)-O(7)#1	1.916(9)	C(6)-H(6B)	0.9600
W(6)-O(3)	1.922(9)	C(6)-H(6C)	0.9600
W(6)-O(18)	1.926(10)	C(7)-C(8)	1.44(2)
W(6)-O(10)	1.925(10)	C(7)-N(5)	1.49(2)
W(6)-O(9)#1	2.397(8)	C(7)-C(9)	1.50(2)
P(1)-O(9)	1.519(8)	C(7)-H(7)	0.9800
P(1)-O(9)#1	1.519(8)	C(8)-N(6)	1.44(2)
P(1)-O(1)	1.555(7)	C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700	N(3)-H(3B)	0.9000
C(9)-H(9A)	0.9600	N(4)-H(4A)	0.9000
C(9)-H(9B)	0.9600	N(4)-H(4B)	0.9000
C(9)-H(9C)	0.9600	N(5)-H(5C)	0.9000
N(1)-H(1D)	0.9000	N(5)-H(5D)	0.9000
N(1)-H(1E)	0.9000	N(6)-H(6D)	0.9000
N(3)-H(3A)	0.9000	N(6)-H(6E)	0.9000
C(3)-N(2)-Ni(2)	108.7(11)	O(4)#1-W(1)-O(1)	75.3(3)
C(3)-N(2)-H(2C)	109.7	O(2)-W(1)-O(1)	83.1(3)
Ni(2)-N(2)-H(2C)	110.0	O(14)#1-W(1)-O(1)	74.3(3)
C(3)-N(2)-H(2D)	109.6	O(17)-W(2)-O(2)	102.6(4)
Ni(2)-N(2)-H(2D)	110.0	O(17)-W(2)-O(14)	100.3(4)
H(2C)-N(2)-H(2D)	108.8	O(2)-W(2)-O(14)	91.0(4)
O(15)-W(1)-O(6)	102.5(4)	O(17)-W(2)-O(12)	101.6(5)
O(15)-W(1)-O(4)#1	99.0(4)	O(2)-W(2)-O(12)	86.5(4)
O(6)-W(1)-O(4)#1	90.7(4)	O(14)-W(2)-O(12)	158.0(4)
O(15)-W(1)-O(2)	102.6(4)	O(17)-W(2)-O(5)	98.1(4)
O(6)-W(1)-O(2)	86.4(4)	O(2)-W(2)-O(5)	159.1(4)
O(4)#1-W(1)-O(2)	158.4(4)	O(14)-W(2)-O(5)	88.2(4)
O(15)-W(1)-O(14)#1	100.4(4)	O(12)-W(2)-O(5)	86.4(4)

O(6)-W(1)-O(14)#1	157.0(4)	O(17)-W(2)-O(1)#1	171.0(4)
O(4)#1-W(1)-O(14)#1	88.4(4)	O(2)-W(2)-O(1)#1	85.5(3)
O(2)-W(1)-O(14)#1	86.1(4)	O(14)-W(2)-O(1)#1	75.2(3)
O(15)-W(1)-O(1)	172.1(4)	O(12)-W(2)-O(1)#1	82.8(3)
O(6)-W(1)-O(1)	83.2(3)	O(8)-W(5)-O(9)	83.5(3)
O(5)-W(2)-O(1)#1	74.2(3)	O(7)-W(5)-O(9)	74.8(3)
O(19)-W(3)-O(12)	100.3(4)	O(16)-W(5)-O(9)	74.7(3)
O(19)-W(3)-O(16)	99.3(4)	O(20)-W(6)-O(7)#1	100.3(4)
O(12)-W(3)-O(16)	90.8(4)	O(20)-W(6)-O(3)	101.0(4)
O(19)-W(3)-O(6)	101.7(4)	O(7)#1-W(6)-O(3)	158.6(4)
O(12)-W(3)-O(6)	85.8(4)	O(20)-W(6)-O(18)	102.3(5)
O(16)-W(3)-O(6)	159.0(4)	O(7)#1-W(6)-O(18)	88.4(4)
O(19)-W(3)-O(10)#1	100.9(4)	O(3)-W(6)-O(18)	85.2(4)
O(12)-W(3)-O(10)#1	158.5(4)	O(20)-W(6)-O(10)	98.5(5)
O(16)-W(3)-O(10)#1	88.9(4)	O(7)#1-W(6)-O(10)	89.1(4)
O(6)-W(3)-O(10)#1	86.9(4)	O(3)-W(6)-O(10)	89.7(4)
O(19)-W(3)-O(9)	173.9(4)	O(18)-W(6)-O(10)	159.2(4)
O(12)-W(3)-O(9)	83.5(4)	O(20)-W(6)-O(9)#1	172.5(5)
O(16)-W(3)-O(9)	75.7(3)	O(7)#1-W(6)-O(9)#1	75.4(3)
O(6)-W(3)-O(9)	83.3(3)	O(3)-W(6)-O(9)#1	83.6(3)
O(10)#1-W(3)-O(9)	75.6(3)	O(18)-W(6)-O(9)#1	83.8(3)
O(11)-W(4)-O(3)	101.9(4)	O(10)-W(6)-O(9)#1	75.6(3)
O(11)-W(4)-O(8)	102.9(4)	O(9)-P(1)-O(9)#1	109.3(7)
O(3)-W(4)-O(8)	87.3(4)	O(9)-P(1)-O(1)	109.6(4)
O(11)-W(4)-O(5)	100.2(4)	O(9)#1-P(1)-O(1)	109.7(5)
O(3)-W(4)-O(5)	157.7(4)	O(9)-P(1)-O(1)#1	109.7(5)
O(8)-W(4)-O(5)	90.6(4)	O(9)#1-P(1)-O(1)#1	109.6(4)
O(11)-W(4)-O(4)	96.3(4)	O(1)-P(1)-O(1)#1	108.8(6)
O(3)-W(4)-O(4)	87.2(4)	N(6)-Ni(1)-N(6)#2	93.0(8)
O(8)-W(4)-O(4)	160.7(4)	N(6)-Ni(1)-N(5)	85.1(5)
O(5)-W(4)-O(4)	87.5(4)	N(6)#2-Ni(1)-N(5)	177.2(6)
O(11)-W(4)-O(1)#1	169.9(4)	N(6)-Ni(1)-N(5)#2	177.2(6)
O(3)-W(4)-O(1)#1	82.9(3)	N(6)#2-Ni(1)-N(5)#2	85.1(5)
O(8)-W(4)-O(1)#1	86.1(3)	N(5)-Ni(1)-N(5)#2	96.8(7)
O(5)-W(4)-O(1)#1	74.8(3)	N(6)-Ni(1)-O(13)	86.0(5)
O(4)-W(4)-O(1)#1	74.8(3)	N(6)#2-Ni(1)-O(13)	88.8(5)
O(13)-W(5)-O(18)	103.3(5)	N(5)-Ni(1)-O(13)	93.2(5)
O(13)-W(5)-O(8)	100.0(4)	N(5)#2-Ni(1)-O(13)	91.8(5)
O(18)-W(5)-O(8)	86.3(4)	N(2)-Ni(2)-N(3)	95.0(5)
O(13)-W(5)-O(7)	101.6(4)	N(2)-Ni(2)-N(1)	83.0(5)
O(18)-W(5)-O(7)	90.6(4)	N(3)-Ni(2)-N(1)	177.7(5)
O(8)-W(5)-O(7)	158.3(4)	N(2)-Ni(2)-N(4)	93.8(5)
O(13)-W(5)-O(16)	98.3(5)	N(3)-Ni(2)-N(4)	82.5(5)

O(18)-W(5)-O(16)	158.1(4)	N(1)-Ni(2)-N(4)	96.3(5)
O(8)-W(5)-O(16)	86.6(4)	N(2)-Ni(2)-O(1W)	173.5(5)
O(7)-W(5)-O(16)	88.3(4)	N(3)-Ni(2)-O(1W)	90.7(5)
O(13)-W(5)-O(9)	172.1(4)	N(1)-Ni(2)-O(1W)	91.4(5)
O(18)-W(5)-O(9)	83.9(3)	C(2)-C(3)-N(2)	117.5(19)
N(4)-Ni(2)-O(1W)	89.9(5)	C(2)-C(3)-C(1)	122(2)
N(2)-Ni(2)-O(2W)	92.5(5)	N(2)-C(3)-C(1)	115.8(17)
N(3)-Ni(2)-O(2W)	90.1(5)	C(2)-C(3)-H(3)	97.3
N(1)-Ni(2)-O(2W)	91.2(5)	N(2)-C(3)-H(3)	97.3
N(4)-Ni(2)-O(2W)	170.7(5)	C(1)-C(3)-H(3)	97.3
O(1W)-Ni(2)-O(2W)	84.4(4)	N(4)-C(4)-C(5)	110.2(16)
P(1)-O(1)-W(4)#1	125.0(4)	N(4)-C(4)-C(6)	112.7(14)
P(1)-O(1)-W(2)#1	125.1(4)	C(5)-C(4)-C(6)	114.5(16)
W(4)#1-O(1)-W(2)#1	89.8(3)	N(4)-C(4)-H(4)	106.3
P(1)-O(1)-W(1)	126.8(5)	C(5)-C(4)-H(4)	106.3
W(4)#1-O(1)-W(1)	89.5(2)	C(6)-C(4)-H(4)	106.3
W(2)#1-O(1)-W(1)	89.1(3)	N(3)-C(5)-C(4)	112.7(15)
W(2)-O(2)-W(1)	150.1(5)	N(3)-C(5)-H(5A)	109.1
W(4)-O(3)-W(6)	150.6(5)	C(4)-C(5)-H(5A)	109.1
W(1)#1-O(4)-W(4)	120.4(4)	N(3)-C(5)-H(5B)	109.1
W(4)-O(5)-W(2)	121.2(5)	C(4)-C(5)-H(5B)	109.1
W(1)-O(6)-W(3)	151.3(5)	H(5A)-C(5)-H(5B)	107.8
W(6)#1-O(7)-W(5)	121.4(4)	C(4)-C(6)-H(6A)	109.5
W(5)-O(8)-W(4)	149.1(6)	C(4)-C(6)-H(6B)	109.5
P(1)-O(9)-W(6)#1	126.2(5)	H(6A)-C(6)-H(6B)	109.5
P(1)-O(9)-W(3)	126.1(5)	C(4)-C(6)-H(6C)	109.5
W(6)#1-O(9)-W(3)	88.3(3)	H(6A)-C(6)-H(6C)	109.5
P(1)-O(9)-W(5)	126.9(4)	H(6B)-C(6)-H(6C)	109.5
W(6)#1-O(9)-W(5)	88.3(3)	C(8)-C(7)-N(5)	106.3(15)
W(3)-O(9)-W(5)	88.6(3)	C(8)-C(7)-C(9)	113.0(16)
W(3)#1-O(10)-W(6)	120.4(5)	N(5)-C(7)-C(9)	112.5(14)
W(3)-O(12)-W(2)	151.7(5)	C(8)-C(7)-H(7)	108.3
W(5)-O(13)-Ni(1)	131.7(6)	N(5)-C(7)-H(7)	108.3
W(2)-O(14)-W(1)#1	121.4(4)	C(9)-C(7)-H(7)	108.3
W(3)-O(16)-W(5)	120.9(5)	N(6)-C(8)-C(7)	111.9(14)
W(5)-O(18)-W(6)	151.7(5)	N(6)-C(8)-H(8A)	109.2
C(3)-C(1)-H(1A)	109.5	C(7)-C(8)-H(8A)	109.2
C(3)-C(1)-H(1B)	109.5	N(6)-C(8)-H(8B)	109.2
H(1A)-C(1)-H(1B)	109.5	C(7)-C(8)-H(8B)	109.2
C(3)-C(1)-H(1C)	109.5	H(8A)-C(8)-H(8B)	107.9
H(1A)-C(1)-H(1C)	109.5	C(7)-C(9)-H(9A)	109.5
H(1B)-C(1)-H(1C)	109.5	C(7)-C(9)-H(9B)	109.5
C(3)-C(2)-N(1)	118.4(18)	H(9A)-C(9)-H(9B)	109.5

C(3)-C(2)-H(2A)	107.7	C(7)-C(9)-H(9C)	109.5
N(1)-C(2)-H(2A)	107.7	H(9A)-C(9)-H(9C)	109.5
C(3)-C(2)-H(2B)	107.7	H(9B)-C(9)-H(9C)	109.5
N(1)-C(2)-H(2B)	107.7	C(2)-N(1)-Ni(2)	107.3(10)
H(2A)-C(2)-H(2B)	107.1	C(7)-N(5)-Ni(1)	110.0(9)
C(2)-N(1)-H(1D)	110.2	C(7)-N(5)-H(5C)	109.7
Ni(2)-N(1)-H(1D)	110.2	Ni(1)-N(5)-H(5C)	109.7
C(2)-N(1)-H(1E)	110.2	C(7)-N(5)-H(5D)	109.7
Ni(2)-N(1)-H(1E)	110.2	Ni(1)-N(5)-H(5D)	109.7
H(1D)-N(1)-H(1E)	108.5	H(5C)-N(5)-H(5D)	108.2
C(5)-N(3)-Ni(2)	110.4(10)	C(8)-N(6)-Ni(1)	108.8(10)
C(5)-N(3)-H(3A)	109.6	C(8)-N(6)-H(6D)	109.9
Ni(2)-N(3)-H(3A)	109.6	Ni(1)-N(6)-H(6D)	109.9
C(5)-N(3)-H(3B)	109.6	C(8)-N(6)-H(6E)	109.9
Ni(2)-N(3)-H(3B)	109.6	Ni(1)-N(6)-H(6E)	109.9
H(3A)-N(3)-H(3B)	108.1	H(6D)-N(6)-H(6E)	108.3
C(4)-N(4)-Ni(2)	108.1(9)	Ni(2)-N(4)-H(4B)	110.1
C(4)-N(4)-H(4A)	110.1	H(4A)-N(4)-H(4B)	108.4
Ni(2)-N(4)-H(4A)	110.1	C(4)-N(4)-H(4B)	110.1
Symmetry code: (#1) -x+1,y,-z+1/2; (#2) -x+2,y,-z+1/2.			
Compound **2**			
As(1)-O(13)	1.649(18)	V(1)-O(27)	1.93(2)
As(1)-O(25)	1.654(19)	V(1)-O(40)	2.034(19)
As(1)-O(10)	1.672(18)	V(1)-O(11)	2.046(19)
As(1)-O(20)	1.676(18)	V(2)-O(42)	1.62(2)
W(1)-O(29)	1.710(19)	V(2)-O(26)	1.924(19)
W(1)-O(4)	1.791(18)	V(2)-O(16)	1.931(19)
W(1)-O(17)	1.836(19)	V(2)-O(5)	1.996(19)
W(1)-O(3)	2.024(18)	V(2)-O(7)	2.02(2)
W(1)-O(11)	2.056(19)	Ni(1)-N(2)	2.08(3)
W(1)-O(10)	2.409(18)	Ni(1)-N(2)#1	2.08(3)
W(1)-V(1)	3.149(5)	Ni(1)-O(12)#1	2.10(2)
W(2)-O(22)	1.727(19)	Ni(1)-O(12)	2.10(2)
W(2)-O(15)	1.806(18)	Ni(1)-N(1)	2.11(3)
W(2)-O(2)	1.814(18)	Ni(1)-N(1)#1	2.11(3)
W(2)-O(5)	2.032(18)	Ni(2)-N(10)	1.88(3)
W(2)-O(16)	2.068(19)	Ni(2)-N(7)	1.90(3)
W(2)-O(20)	2.358(18)	Ni(2)-N(8)	1.91(2)
W(2)-V(2)	3.129(5)	Ni(2)-N(9)	1.93(3)
W(3)-O(12)	1.75(2)	Ni(3)-N(5)	2.07(3)
W(3)-O(24)	1.821(19)	Ni(3)-O(9)	2.086(19)
W(3)-O(23)	1.823(19)	Ni(3)-N(3)	2.10(4)
W(3)-O(27)	2.049(19)	Ni(3)-O(1W)	2.09(4)

W(3)-O(11)	2.057(19)	Ni(3)-N(4)	2.07(4)
W(3)-O(10)	2.331(18)	Ni(3)-N(6)	2.15(4)
W(3)-V(1)	3.108(5)	Ni(4)-N(13)	1.88(3)
W(4)-O(33)	1.709(18)	Ni(4)-N(11)	1.89(3)
W(4)-O(19)	1.781(19)	Ni(4)-N(12)	1.91(3)
W(4)-O(21)	1.832(18)	Ni(4)-N(14)	1.91(3)
W(4)-O(40)	2.049(19)	C(1)-N(2)	1.42(2)
W(4)-O(27)	2.063(18)	C(1)-C(2)	1.42(2)
W(4)-O(13)	2.402(18)	C(1)-H(1A)	0.9700
W(4)-V(1)	3.115(5)	C(1)-H(1B)	0.9700
W(5)-O(38)	1.72(2)	C(2)-C(3)	1.55(7)
W(5)-O(32)	1.801(18)	C(2)-N(1)	1.60(6)
W(5)-O(1)	1.829(18)	C(2)-H(2)	0.9800
W(5)-O(40)	2.037(19)	C(3)-H(3A)	0.9600
W(5)-O(3)	2.104(18)	C(3)-H(3B)	0.9600
W(5)-O(13)	2.389(19)	C(3)-H(3C)	0.9600
W(5)-V(1)	3.114(5)	C(4)-C(5)	1.36(9)
W(6)-O(9)	1.727(19)	C(4)-N(3)	1.46(8)
W(6)-O(28)	1.817(19)	C(4)-H(4A)	0.9700
W(6)-O(31)	1.839(19)	C(4)-H(4B)	0.9700
W(6)-O(26)	2.061(19)	C(5)-C(6)	1.50(3)
W(6)-O(5)	2.079(18)	C(5)-N(4)	1.52(3)
W(6)-O(20)	2.341(18)	C(5)-H(5)	0.9800
W(6)-V(2)	3.106(5)	C(6)-H(6A)	0.9600
W(7)-O(36)	1.75(2)	C(6)-H(6B)	0.9600
W(7)-O(6)	1.800(19)	C(6)-H(6C)	0.9600
W(7)-O(34)	1.857(19)	C(7)-N(5)	1.51(7)
W(7)-O(26)	2.030(19)	C(7)-C(8)	1.54(9)
W(7)-O(7)	2.095(19)	C(7)-H(7A)	0.9700
W(7)-O(25)	2.384(18)	C(7)-H(7B)	0.9700
W(7)-V(2)	3.118(5)	C(8)-N(6)	1.45(8)
W(8)-O(41)	1.71(2)	C(8)-C(9)	1.53(3)
W(8)-O(30)	1.823(19)	C(8)-H(8)	0.9800
W(8)-O(18)	1.868(19)	C(9)-H(9A)	0.9600
W(8)-O(16)	2.039(19)	C(9)-H(9B)	0.9600
W(8)-O(7)	2.049(19)	C(9)-H(9C)	0.9600
W(8)-O(25)	2.399(19)	C(10)-C(11)	1.41(6)
W(8)-V(2)	3.113(5)	C(10)-N(9)	1.44(5)
W(9)-O(35)	1.627(19)	C(10)-H(10A)	0.9700
W(9)-O(1)	1.939(18)	C(10)-H(10B)	0.9700
W(9)-O(31)	1.953(19)	C(11)-N(10)	1.39(5)
W(9)-O(4)	1.983(18)	C(11)-C(12)	1.44(6)
W(9)-O(2)	2.008(18)	C(11)-H(11)	0.9800

W(9)-O(20)	2.451(19)	C(12)-H(12A)	0.9600
W(10)-O(8)	1.638(18)	C(12)-H(12B)	0.9600
W(10)-O(28)	1.934(19)	C(12)-H(12C)	0.9600
W(10)-O(6)	1.974(19)	C(13)-N(7)	1.43(5)
W(10)-O(32)	1.975(19)	C(13)-C(14)	1.46(6)
W(10)-O(21)	1.981(19)	C(13)-C(15)	1.50(2)
W(10)-O(13)	2.380(18)	C(13)-H(13)	0.9800
W(11)-O(37)	1.62(2)	C(14)-N(8)	1.46(5)
W(11)-O(18)	1.955(19)	C(14)-H(14A)	0.9700
W(11)-O(24)	1.966(19)	C(14)-H(14B)	0.9700
W(11)-O(19)	1.992(19)	C(15)-H(15A)	0.9600
W(11)-O(34)	1.998(19)	C(15)-H(15B)	0.9600
W(11)-O(25)	2.401(19)	C(15)-H(15C)	0.9600
W(12)-O(14)	1.627(18)	C(16)-N(12)	1.43(2)
W(12)-O(30)	1.94(2)	C(16)-C(17)	1.45(7)
W(12)-O(15)	1.968(18)	C(16)-H(16A)	0.9700
W(12)-O(23)	1.980(19)	C(16)-H(16B)	0.9700
W(12)-O(17)	1.983(19)	C(17)-C(18)	1.37(7)
W(12)-O(10)	2.398(18)	C(17)-N(11)	1.42(6)
V(1)-O(39)	1.62(2)	C(17)-H(17)	0.9800
V(1)-O(3)	1.919(19)	C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600	N(6)-H(6E)	0.9000
C(18)-H(18C)	0.9600	N(7)-H(7C)	0.9000
C(19)-C(20)	1.51(2)	N(7)-H(7D)	0.9000
C(19)-N(14)	1.52(2)	N(8)-H(8A)	0.9000
C(19)-H(19A)	0.9700	N(8)-H(8B)	0.9000
C(19)-H(19B)	0.9700	N(9)-H(9D)	0.9000
C(20)-N(13)	1.50(2)	N(9)-H(9E)	0.9000
C(20)-C(21)	1.504(18)	N(10)-H(10C)	0.9000
C(20)-H(20)	0.9800	N(10)-H(10D)	0.9000
C(21)-H(21A)	0.9602	N(11)-H(11A)	0.9000
C(21)-H(21B)	0.9602	N(11)-H(11B)	0.9000
C(21)-H(21C)	0.9602	N(12)-H(12D)	0.9000
N(1)-H(1C)	0.9000	N(12)-H(12E)	0.9000
N(1)-H(1D)	0.9000	N(13)-H(13A)	0.9000
N(2)-H(2A)	0.9000	N(13)-H(13B)	0.9000
N(2)-H(2B)	0.9000	N(14)-H(14C)	0.9000
N(3)-H(3D)	0.9000	N(14)-H(14D)	0.9000
N(3)-H(3E)	0.9000	N(5)-H(5A)	0.9000
N(4)-H(4C)	0.9000	N(5)-H(5B)	0.9000
N(4)-H(4D)	0.9000	N(6)-H(6D)	0.9000
O(4)-W(1)-O(3)	86.8(8)	O(13)-As(1)-O(25)	109.7(9)

O(17)-W(1)-O(3)	157.3(8)	O(13)-As(1)-O(10)	110.3(9)
O(29)-W(1)-O(11)	99.8(8)	O(25)-As(1)-O(10)	109.1(9)
O(4)-W(1)-O(11)	151.8(7)	O(13)-As(1)-O(20)	109.2(9)
O(17)-W(1)-O(11)	89.9(8)	O(25)-As(1)-O(20)	108.9(9)
O(3)-W(1)-O(11)	75.6(7)	O(10)-As(1)-O(20)	109.6(9)
O(29)-W(1)-O(10)	167.2(8)	O(29)-W(1)-O(4)	104.6(9)
O(4)-W(1)-O(10)	88.0(7)	O(29)-W(1)-O(17)	101.2(8)
O(17)-W(1)-O(10)	74.7(7)	O(4)-W(1)-O(17)	99.0(8)
O(3)-W(1)-O(10)	83.6(7)	O(29)-W(1)-O(3)	98.5(8)
O(11)-W(1)-O(10)	68.5(7)	O(29)-W(1)-V(1)	100.6(6)
O(4)-W(1)-V(1)	120.2(6)	N(7)-Ni(2)-N(8)	84.5(12)
O(17)-W(1)-V(1)	127.8(6)	N(10)-Ni(2)-N(9)	86.1(12)
O(3)-W(1)-V(1)	35.9(5)	N(7)-Ni(2)-N(9)	96.1(11)
O(11)-W(1)-V(1)	39.7(5)	N(8)-Ni(2)-N(9)	177.4(13)
O(10)-W(1)-V(1)	73.8(4)	N(5)-Ni(3)-O(9)	88.4(10)
O(22)-W(2)-O(15)	104.5(8)	N(5)-Ni(3)-N(3)	179.3(14)
O(22)-W(2)-O(2)	101.7(9)	O(9)-Ni(3)-N(3)	91.1(10)
O(15)-W(2)-O(2)	98.4(8)	N(5)-Ni(3)-O(1W)	88.1(13)
O(22)-W(2)-O(5)	98.5(8)	O(9)-Ni(3)-O(1W)	176.5(12)
O(15)-W(2)-O(5)	152.5(8)	N(3)-Ni(3)-O(1W)	92.3(13)
O(2)-W(2)-O(5)	91.4(8)	N(5)-Ni(3)-N(4)	96.3(13)
O(22)-W(2)-O(16)	99.2(8)	O(9)-Ni(3)-N(4)	86.8(11)
O(15)-W(2)-O(16)	86.0(8)	N(3)-Ni(3)-N(4)	84.3(16)
O(2)-W(2)-O(16)	156.8(8)	O(1W)-Ni(3)-N(4)	94.0(14)
O(5)-W(2)-O(16)	75.5(7)	N(5)-Ni(3)-N(6)	80.5(15)
O(22)-W(2)-O(20)	167.4(7)	O(9)-Ni(3)-N(6)	86.6(13)
O(15)-W(2)-O(20)	88.0(7)	N(3)-Ni(3)-N(6)	98.9(17)
O(2)-W(2)-O(20)	74.8(7)	O(1W)-Ni(3)-N(6)	92.4(15)
O(5)-W(2)-O(20)	69.7(7)	N(4)-Ni(3)-N(6)	172.8(15)
O(16)-W(2)-O(20)	82.6(7)	N(13)-Ni(4)-N(11)	95.0(15)
O(22)-W(2)-V(2)	99.7(6)	N(13)-Ni(4)-N(12)	178.4(13)
O(15)-W(2)-V(2)	120.9(6)	N(11)-Ni(4)-N(12)	85.4(14)
O(2)-W(2)-V(2)	128.0(6)	N(13)-Ni(4)-N(14)	84.9(15)
O(5)-W(2)-V(2)	38.6(5)	N(11)-Ni(4)-N(14)	179.3(14)
O(16)-W(2)-V(2)	37.0(5)	N(12)-Ni(4)-N(14)	94.8(15)
O(20)-W(2)-V(2)	74.2(5)	W(5)-O(1)-W(9)	153.7(11)
O(12)-W(3)-O(24)	103.3(9)	W(2)-O(2)-W(9)	125.3(10)
O(12)-W(3)-O(23)	101.9(9)	V(1)-O(3)-W(1)	105.9(9)
O(24)-W(3)-O(23)	95.4(9)	V(1)-O(3)-W(5)	101.3(8)
O(12)-W(3)-O(27)	97.0(8)	W(1)-O(3)-W(5)	142.6(10)
O(24)-W(3)-O(27)	87.1(8)	W(1)-O(4)-W(9)	155.7(10)
O(23)-W(3)-O(27)	159.8(8)	V(2)-O(5)-W(2)	102.0(8)
O(12)-W(3)-O(11)	100.1(8)	V(2)-O(5)-W(6)	99.3(8)

O(24)-W(3)-O(11)	153.5(8)	W(2)-O(5)-W(6)	118.9(9)
O(23)-W(3)-O(11)	91.8(8)	W(7)-O(6)-W(10)	154.0(11)
O(27)-W(3)-O(11)	77.8(7)	V(2)-O(7)-W(8)	99.9(8)
O(12)-W(3)-O(10)	169.7(8)	V(2)-O(7)-W(7)	98.6(8)
O(24)-W(3)-O(10)	86.9(8)	W(8)-O(7)-W(7)	120.5(9)
O(23)-W(3)-O(10)	76.2(7)	W(6)-O(9)-Ni(3)	148.9(11)
O(27)-W(3)-O(10)	83.9(7)	As(1)-O(10)-W(3)	124.9(10)
O(11)-W(3)-O(10)	70.0(7)	As(1)-O(10)-W(12)	123.9(10)
O(12)-W(3)-V(1)	99.0(7)	W(3)-O(10)-W(12)	89.4(6)
O(24)-W(3)-V(1)	122.1(6)	As(1)-O(10)-W(1)	122.5(9)
O(23)-W(3)-V(1)	130.9(6)	W(3)-O(10)-W(1)	97.8(7)
O(27)-W(3)-V(1)	37.2(5)	W(12)-O(10)-W(1)	88.7(6)
O(11)-W(3)-V(1)	40.6(5)	V(1)-O(11)-W(1)	100.3(8)
O(10)-W(3)-V(1)	75.6(5)	V(1)-O(11)-W(3)	98.5(8)
O(33)-W(4)-O(19)	104.2(9)	W(1)-O(11)-W(3)	120.5(9)
O(33)-W(4)-O(21)	101.6(9)	W(3)-O(12)-Ni(1)	139.2(11)
O(19)-W(4)-O(21)	97.1(8)	As(1)-O(13)-W(10)	125.1(10)
O(33)-W(4)-O(40)	101.2(9)	As(1)-O(13)-W(5)	124.9(9)
O(19)-W(4)-O(40)	150.9(8)	W(10)-O(13)-W(5)	89.0(6)
O(21)-W(4)-O(40)	91.4(8)	As(1)-O(13)-W(4)	122.6(10)
O(33)-W(4)-O(27)	99.0(8)	W(10)-O(13)-W(4)	89.0(6)
O(19)-W(4)-O(27)	85.1(8)	W(5)-O(13)-W(4)	96.4(7)
O(21)-W(4)-O(27)	158.1(8)	W(2)-O(15)-W(12)	153.3(10)
O(40)-W(4)-O(27)	77.1(7)	V(2)-O(16)-W(8)	103.2(8)
O(33)-W(4)-O(13)	169.3(8)	V(2)-O(16)-W(2)	102.9(8)
O(19)-W(4)-O(13)	86.3(8)	W(8)-O(16)-W(2)	144.5(10)
O(21)-W(4)-O(13)	74.9(7)	W(1)-O(17)-W(12)	123.3(9)
O(40)-W(4)-O(13)	69.1(7)	W(8)-O(18)-W(11)	121.8(10)
O(27)-W(4)-O(13)	83.5(7)	W(4)-O(19)-W(11)	156.7(11)
O(33)-W(4)-V(1)	100.6(7)	As(1)-O(20)-W(6)	123.2(9)
O(19)-W(4)-V(1)	120.0(6)	As(1)-O(20)-W(2)	125.1(9)
O(21)-W(4)-V(1)	129.8(6)	W(6)-O(20)-W(2)	97.8(7)
O(40)-W(4)-V(1)	40.1(5)	As(1)-O(20)-W(9)	123.1(9)
O(27)-W(4)-V(1)	37.2(5)	W(6)-O(20)-W(9)	87.9(6)
O(13)-W(4)-V(1)	75.1(4)	W(2)-O(20)-W(9)	89.8(6)
O(38)-W(5)-O(32)	102.0(9)	W(4)-O(21)-W(10)	122.9(10)
O(38)-W(5)-O(1)	103.9(9)	W(3)-O(23)-W(12)	122.1(10)
O(32)-W(5)-O(1)	98.1(8)	W(3)-O(24)-W(11)	153.0(11)
O(38)-W(5)-O(40)	98.6(9)	As(1)-O(25)-W(7)	124.2(10)
O(32)-W(5)-O(40)	90.5(8)	As(1)-O(25)-W(11)	124.5(10)
O(1)-W(5)-O(40)	153.6(8)	W(7)-O(25)-W(11)	89.3(6)
O(38)-W(5)-O(3)	98.4(8)	As(1)-O(25)-W(8)	123.3(10)
O(32)-W(5)-O(3)	157.5(8)	W(7)-O(25)-W(8)	97.6(7)

O(1)-W(5)-O(3)	85.9(8)	W(11)-O(25)-W(8)	88.2(6)
O(40)-W(5)-O(3)	77.1(7)	V(2)-O(26)-W(7)	104.1(9)
O(38)-W(5)-O(13)	167.3(8)	V(2)-O(26)-W(6)	102.4(8)
O(32)-W(5)-O(13)	74.3(7)	W(7)-O(26)-W(6)	144.2(10)
O(1)-W(5)-O(13)	88.8(7)	V(1)-O(27)-W(3)	102.8(8)
O(40)-W(5)-O(13)	69.5(7)	V(1)-O(27)-W(4)	102.6(9)
O(3)-W(5)-O(13)	83.7(7)	W(3)-O(27)-W(4)	144.6(10)
O(38)-W(5)-V(1)	98.8(7)	W(6)-O(28)-W(10)	153.2(11)
O(32)-W(5)-V(1)	128.8(6)	W(8)-O(30)-W(12)	152.4(11)
O(1)-W(5)-V(1)	121.3(6)	W(6)-O(31)-W(9)	122.7(10)
O(40)-W(5)-V(1)	40.1(5)	W(5)-O(32)-W(10)	124.6(10)
O(3)-W(5)-V(1)	37.2(5)	W(7)-O(34)-W(11)	121.4(10)
O(13)-W(5)-V(1)	75.2(4)	V(1)-O(40)-W(5)	99.8(8)
O(9)-W(6)-O(28)	104.9(9)	V(1)-O(40)-W(4)	99.5(8)
O(9)-W(6)-O(31)	100.1(9)	W(5)-O(40)-W(4)	121.8(9)
O(28)-W(6)-O(31)	96.7(8)	N(2)-C(1)-C(2)	113(4)
O(9)-W(6)-O(26)	98.0(8)	N(2)-C(1)-H(1A)	109.0
O(28)-W(6)-O(26)	86.6(8)	C(2)-C(1)-H(1A)	109.0
O(31)-W(6)-O(26)	160.1(8)	N(2)-C(1)-H(1B)	109.0
O(9)-W(6)-O(5)	97.3(8)	C(2)-C(1)-H(1B)	109.0
O(28)-W(6)-O(5)	153.8(8)	H(1A)-C(1)-H(1B)	107.8
O(31)-W(6)-O(5)	93.0(8)	C(1)-C(2)-C(3)	112(4)
O(26)-W(6)-O(5)	76.5(7)	C(1)-C(2)-N(1)	111(4)
O(9)-W(6)-O(20)	165.9(8)	C(3)-C(2)-N(1)	109(4)
O(28)-W(6)-O(20)	89.2(7)	C(1)-C(2)-H(2)	108.1
O(31)-W(6)-O(20)	76.7(7)	C(3)-C(2)-H(2)	108.1
O(26)-W(6)-O(20)	83.8(7)	N(1)-C(2)-H(2)	108.1
O(5)-W(6)-O(20)	69.4(7)	C(2)-C(3)-H(3A)	109.5
O(9)-W(6)-V(2)	98.0(7)	C(2)-C(3)-H(3B)	109.5
O(28)-W(6)-V(2)	122.0(6)	H(3A)-C(3)-H(3B)	109.5
O(31)-W(6)-V(2)	130.8(6)	C(2)-C(3)-H(3C)	109.5
O(26)-W(6)-V(2)	37.2(5)	H(3A)-C(3)-H(3C)	109.5
O(5)-W(6)-V(2)	39.4(5)	H(3B)-C(3)-H(3C)	109.5
O(20)-W(6)-V(2)	74.9(5)	C(5)-C(4)-N(3)	114(7)
O(36)-W(7)-O(6)	105.1(9)	C(5)-C(4)-H(4A)	109.0
O(36)-W(7)-O(34)	101.7(9)	N(3)-C(4)-H(4A)	108.8
O(6)-W(7)-O(34)	98.0(8)	C(5)-C(4)-H(4B)	108.5
O(36)-W(7)-O(26)	98.0(9)	N(3)-C(4)-H(4B)	108.7
O(6)-W(7)-O(26)	86.4(8)	H(4A)-C(4)-H(4B)	107.6
O(34)-W(7)-O(26)	157.8(8)	C(4)-C(5)-C(6)	113(5)
O(36)-W(7)-O(7)	99.1(8)	C(4)-C(5)-N(4)	124(7)
O(6)-W(7)-O(7)	152.0(8)	C(6)-C(5)-N(4)	122(6)
O(34)-W(7)-O(7)	90.5(8)	C(4)-C(5)-H(5)	94.3

O(26)-W(7)-O(7)	76.4(8)	C(6)-C(5)-H(5)	94.3
O(36)-W(7)-O(25)	167.8(8)	N(4)-C(5)-H(5)	94.3
O(6)-W(7)-O(25)	87.1(7)	C(5)-C(6)-H(6A)	109.6
O(34)-W(7)-O(25)	75.9(7)	C(5)-C(6)-H(6B)	109.6
O(26)-W(7)-O(25)	82.7(7)	H(6A)-C(6)-H(6B)	109.5
O(7)-W(7)-O(25)	69.1(7)	C(5)-C(6)-H(6C)	109.2
O(36)-W(7)-V(2)	98.7(7)	H(6A)-C(6)-H(6C)	109.5
O(6)-W(7)-V(2)	121.1(6)	H(6B)-C(6)-H(6C)	109.5
O(34)-W(7)-V(2)	128.7(6)	N(5)-C(7)-C(8)	108(5)
O(26)-W(7)-V(2)	36.8(5)	N(5)-C(7)-H(7A)	110.1
O(7)-W(7)-V(2)	39.7(5)	C(8)-C(7)-H(7A)	110.1
O(25)-W(7)-V(2)	74.5(5)	N(5)-C(7)-H(7B)	110.1
O(41)-W(8)-O(30)	103.9(9)	C(8)-C(7)-H(7B)	110.1
O(41)-W(8)-O(18)	102.1(9)	H(7A)-C(7)-H(7B)	108.4
O(30)-W(8)-O(18)	96.4(8)	N(6)-C(8)-C(9)	123(6)
O(41)-W(8)-O(16)	97.7(9)	N(6)-C(8)-C(7)	112(6)
O(30)-W(8)-O(16)	86.9(8)	C(9)-C(8)-C(7)	110(6)
O(18)-W(8)-O(16)	158.5(8)	N(6)-C(8)-H(8)	102.5
O(41)-W(8)-O(7)	98.5(9)	C(9)-C(8)-H(8)	102.5
O(30)-W(8)-O(7)	153.8(8)	C(7)-C(8)-H(8)	102.5
O(18)-W(8)-O(7)	91.9(8)	C(8)-C(9)-H(9A)	109.5
O(16)-W(8)-O(7)	76.7(7)	C(8)-C(9)-H(9B)	109.5
O(41)-W(8)-O(25)	167.5(8)	H(9A)-C(9)-H(9B)	109.5
O(30)-W(8)-O(25)	88.6(8)	C(8)-C(9)-H(9C)	109.5
O(18)-W(8)-O(25)	75.6(7)	H(9A)-C(9)-H(9C)	109.5
O(16)-W(8)-O(25)	83.2(7)	H(9B)-C(9)-H(9C)	109.5
O(7)-W(8)-O(25)	69.5(7)	C(11)-C(10)-N(9)	116(4)
O(41)-W(8)-V(2)	98.7(7)	C(11)-C(10)-H(10A)	108.2
O(30)-W(8)-V(2)	122.1(6)	N(9)-C(10)-H(10A)	108.2
O(18)-W(8)-V(2)	129.7(6)	C(11)-C(10)-H(10B)	108.2
O(16)-W(8)-V(2)	37.1(5)	N(9)-C(10)-H(10B)	108.2
O(7)-W(8)-V(2)	39.7(6)	H(10A)-C(10)-H(10B)	107.3
O(25)-W(8)-V(2)	74.5(5)	N(10)-C(11)-C(10)	112(4)
O(35)-W(9)-O(1)	102.6(9)	N(10)-C(11)-C(12)	124(4)
O(35)-W(9)-O(31)	101.8(9)	C(10)-C(11)-C(12)	120(4)
O(1)-W(9)-O(31)	92.7(8)	N(10)-C(11)-H(11)	96.5
O(35)-W(9)-O(4)	103.4(9)	C(10)-C(11)-H(11)	96.5
O(1)-W(9)-O(4)	84.9(7)	C(12)-C(11)-H(11)	96.5
O(31)-W(9)-O(4)	154.7(8)	C(11)-C(12)-H(12A)	109.5
O(35)-W(9)-O(2)	101.1(9)	C(11)-C(12)-H(12B)	109.5
O(1)-W(9)-O(2)	156.3(8)	H(12A)-C(12)-H(12B)	109.5
O(31)-W(9)-O(2)	82.9(7)	C(11)-C(12)-H(12C)	109.5
O(4)-W(9)-O(2)	89.3(7)	H(12A)-C(12)-H(12C)	109.5

O(35)-W(9)-O(20)	169.1(8)	H(12B)-C(12)-H(12C)	109.5
O(1)-W(9)-O(20)	86.8(7)	N(7)-C(13)-C(14)	111(4)
O(31)-W(9)-O(20)	72.1(7)	N(7)-C(13)-C(15)	128(4)
O(4)-W(9)-O(20)	82.6(7)	C(14)-C(13)-C(15)	99(3)
O(2)-W(9)-O(20)	69.6(7)	N(7)-C(13)-H(13)	105.6
O(8)-W(10)-O(28)	101.2(9)	C(14)-C(13)-H(13)	105.6
O(8)-W(10)-O(6)	102.6(9)	C(15)-C(13)-H(13)	105.7
O(28)-W(10)-O(6)	86.5(8)	N(8)-C(14)-C(13)	108(3)
O(8)-W(10)-O(32)	101.3(9)	N(8)-C(14)-H(14A)	110.0
O(28)-W(10)-O(32)	91.0(8)	C(13)-C(14)-H(14A)	110.0
O(6)-W(10)-O(32)	155.9(8)	N(8)-C(14)-H(14B)	110.0
O(8)-W(10)-O(21)	101.7(9)	C(13)-C(14)-H(14B)	110.0
O(28)-W(10)-O(21)	157.1(8)	H(14A)-C(14)-H(14B)	108.4
O(6)-W(10)-O(21)	88.7(8)	C(13)-C(15)-H(15A)	114.7
O(32)-W(10)-O(21)	84.3(8)	C(13)-C(15)-H(15B)	106.7
O(8)-W(10)-O(13)	171.4(8)	H(15A)-C(15)-H(15B)	109.5
O(28)-W(10)-O(13)	84.3(7)	C(13)-C(15)-H(15C)	106.9
O(6)-W(10)-O(13)	84.2(7)	H(15A)-C(15)-H(15C)	109.5
O(32)-W(10)-O(13)	71.7(7)	H(15B)-C(15)-H(15C)	109.5
O(21)-W(10)-O(13)	73.0(7)	N(12)-C(16)-C(17)	110(4)
O(37)-W(11)-O(18)	100.1(9)	N(12)-C(16)-H(16A)	109.6
O(37)-W(11)-O(24)	100.4(9)	C(17)-C(16)-H(16A)	109.6
O(18)-W(11)-O(24)	88.5(8)	N(12)-C(16)-H(16B)	109.6
O(37)-W(11)-O(19)	103.9(9)	C(17)-C(16)-H(16B)	109.6
O(18)-W(11)-O(19)	156.0(8)	H(16A)-C(16)-H(16B)	108.1
O(24)-W(11)-O(19)	86.1(8)	C(18)-C(17)-N(11)	124(5)
O(37)-W(11)-O(34)	102.8(9)	C(18)-C(17)-C(16)	111(5)
O(18)-W(11)-O(34)	85.8(8)	N(11)-C(17)-C(16)	103(4)
O(24)-W(11)-O(34)	156.7(8)	C(18)-C(17)-H(17)	105.6
O(19)-W(11)-O(34)	90.0(8)	N(11)-C(17)-H(17)	105.6
O(37)-W(11)-O(25)	173.0(9)	C(16)-C(17)-H(17)	105.6
O(18)-W(11)-O(25)	74.1(7)	C(17)-C(18)-H(18A)	109.5
O(24)-W(11)-O(25)	83.6(7)	C(17)-C(18)-H(18B)	109.5
O(19)-W(11)-O(25)	82.0(7)	H(18A)-C(18)-H(18B)	109.5
O(34)-W(11)-O(25)	73.1(7)	C(17)-C(18)-H(18C)	109.5
O(14)-W(12)-O(30)	102.9(9)	H(18A)-C(18)-H(18C)	109.5
O(14)-W(12)-O(15)	100.0(8)	H(18B)-C(18)-H(18C)	109.5
O(30)-W(12)-O(15)	87.4(8)	C(20)-C(19)-N(14)	112(4)
O(14)-W(12)-O(23)	102.7(9)	C(20)-C(19)-H(19A)	109.3
O(30)-W(12)-O(23)	89.8(8)	N(14)-C(19)-H(19A)	109.3
O(15)-W(12)-O(23)	157.2(8)	C(20)-C(19)-H(19B)	109.3
O(14)-W(12)-O(17)	99.4(9)	N(14)-C(19)-H(19B)	109.3
O(30)-W(12)-O(17)	157.7(8)	H(19A)-C(19)-H(19B)	108.0

O(15)-W(12)-O(17)	90.0(8)	N(13)-C(20)-C(21)	111(4)
O(23)-W(12)-O(17)	84.1(8)	N(13)-C(20)-C(19)	102(4)
O(14)-W(12)-O(10)	170.5(8)	C(21)-C(20)-C(19)	119(5)
O(30)-W(12)-O(10)	85.1(7)	N(13)-C(20)-H(20)	108.2
O(15)-W(12)-O(10)	85.3(7)	C(21)-C(20)-H(20)	108.2
O(23)-W(12)-O(10)	72.0(7)	C(19)-C(20)-H(20)	108.2
O(17)-W(12)-O(10)	72.6(7)	C(20)-C(21)-H(21A)	109.5
O(39)-V(1)-O(3)	125.1(10)	C(20)-C(21)-H(21B)	109.5
O(39)-V(1)-O(27)	119.4(10)	H(21A)-C(21)-H(21B)	109.5
O(3)-V(1)-O(27)	115.3(8)	C(20)-C(21)-H(21C)	109.5
O(39)-V(1)-O(40)	110.3(10)	H(21A)-C(21)-H(21C)	109.4
O(3)-V(1)-O(40)	81.5(8)	H(21B)-C(21)-H(21C)	109.4
O(27)-V(1)-O(40)	80.6(8)	C(2)-N(1)-Ni(1)	106(2)
O(39)-V(1)-O(11)	106.6(9)	C(2)-N(1)-H(1C)	110.6
O(3)-V(1)-O(11)	78.1(8)	Ni(1)-N(1)-H(1C)	110.6
O(27)-V(1)-O(11)	80.8(8)	C(2)-N(1)-H(1D)	110.6
O(40)-V(1)-O(11)	143.1(8)	Ni(1)-N(1)-H(1D)	110.6
O(39)-V(1)-W(3)	118.7(8)	H(1C)-N(1)-H(1D)	108.7
O(3)-V(1)-W(3)	100.4(6)	C(1)-N(2)-Ni(1)	113(3)
O(27)-V(1)-W(3)	40.0(6)	C(1)-N(2)-H(2A)	109.1
O(40)-V(1)-W(3)	115.5(6)	Ni(1)-N(2)-H(2A)	109.1
O(11)-V(1)-W(3)	40.9(5)	C(1)-N(2)-H(2B)	109.1
O(39)-V(1)-W(5)	125.2(8)	Ni(1)-N(2)-H(2B)	109.1
O(3)-V(1)-W(5)	41.5(5)	H(2A)-N(2)-H(2B)	107.8
O(27)-V(1)-W(5)	101.7(6)	C(4)-N(3)-Ni(3)	112(4)
O(40)-V(1)-W(5)	40.1(5)	C(4)-N(3)-H(3D)	109.2
O(11)-V(1)-W(5)	114.9(5)	Ni(3)-N(3)-H(3D)	109.2
W(3)-V(1)-W(5)	116.14(16)	C(4)-N(3)-H(3E)	109.3
O(39)-V(1)-W(4)	120.9(8)	Ni(3)-N(3)-H(3E)	109.2
O(3)-V(1)-W(4)	102.8(6)	H(3D)-N(3)-H(3E)	107.9
O(27)-V(1)-W(4)	40.3(6)	C(5)-N(4)-Ni(3)	106(4)
O(40)-V(1)-W(4)	40.4(6)	C(5)-N(4)-H(4C)	110.4
O(11)-V(1)-W(4)	116.1(6)	Ni(3)-N(4)-H(4C)	110.6
W(3)-V(1)-W(4)	78.00(12)	C(5)-N(4)-H(4D)	110.7
W(5)-V(1)-W(4)	69.95(11)	Ni(3)-N(4)-H(4D)	110.6
O(39)-V(1)-W(1)	122.9(8)	H(4C)-N(4)-H(4D)	108.7
O(3)-V(1)-W(1)	38.2(5)	C(7)-N(5)-Ni(3)	114(3)
O(27)-V(1)-W(1)	101.3(6)	C(7)-N(5)-H(5A)	108.7
O(40)-V(1)-W(1)	114.7(6)	Ni(3)-N(5)-H(5A)	108.7
O(11)-V(1)-W(1)	40.0(5)	C(7)-N(5)-H(5B)	108.7
W(3)-V(1)-W(1)	69.60(11)	Ni(3)-N(5)-H(5B)	108.7
W(5)-V(1)-W(1)	77.27(12)	H(5A)-N(5)-H(5B)	107.6
W(4)-V(1)-W(1)	116.09(16)	C(8)-N(6)-Ni(3)	112(3)

O(42)-V(2)-O(26)	123.2(10)	C(8)-N(6)-H(6D)	109.2
O(42)-V(2)-O(16)	122.4(11)	Ni(3)-N(6)-H(6D)	109.1
O(26)-V(2)-O(16)	114.4(8)	C(8)-N(6)-H(6E)	109.1
O(42)-V(2)-O(5)	106.8(10)	Ni(3)-N(6)-H(6E)	109.1
O(26)-V(2)-O(5)	81.7(8)	H(6D)-N(6)-H(6E)	107.9
O(16)-V(2)-O(5)	79.5(8)	C(13)-N(7)-Ni(2)	113(2)
O(42)-V(2)-O(7)	108.9(10)	C(13)-N(7)-H(7C)	109.0
O(26)-V(2)-O(7)	80.7(8)	Ni(2)-N(7)-H(7C)	109.0
O(16)-V(2)-O(7)	80.0(8)	C(13)-N(7)-H(7D)	109.0
O(5)-V(2)-O(7)	144.3(8)	Ni(2)-N(7)-H(7D)	109.0
O(42)-V(2)-W(6)	121.8(9)	H(7C)-N(7)-H(7D)	107.8
O(26)-V(2)-W(6)	40.4(6)	C(14)-N(8)-Ni(2)	113(2)
O(16)-V(2)-W(6)	100.7(6)	C(14)-N(8)-H(8A)	108.9
O(5)-V(2)-W(6)	41.3(5)	Ni(2)-N(8)-H(8A)	108.9
O(7)-V(2)-W(6)	116.1(6)	C(14)-N(8)-H(8B)	108.9
O(42)-V(2)-W(8)	122.5(9)	Ni(2)-N(8)-H(8B)	108.9
O(26)-V(2)-W(8)	101.1(6)	H(8A)-N(8)-H(8B)	107.7
O(16)-V(2)-W(8)	39.6(6)	C(10)-N(9)-Ni(2)	108(2)
O(5)-V(2)-W(8)	114.8(6)	C(10)-N(9)-H(9D)	110.1
O(7)-V(2)-W(8)	40.4(5)	Ni(2)-N(9)-H(9D)	110.1
W(6)-V(2)-W(8)	115.70(16)	C(10)-N(9)-H(9E)	110.2
O(42)-V(2)-W(7)	122.8(9)	Ni(2)-N(9)-H(9E)	110.2
O(26)-V(2)-W(7)	39.1(6)	H(9D)-N(9)-H(9E)	108.5
O(16)-V(2)-W(7)	101.7(6)	C(11)-N(10)-Ni(2)	114(3)
O(5)-V(2)-W(7)	116.2(6)	C(11)-N(10)-H(10C)	108.7
O(7)-V(2)-W(7)	41.6(6)	Ni(2)-N(10)-H(10C)	108.7
W(6)-V(2)-W(7)	77.40(12)	C(11)-N(10)-H(10D)	108.7
W(8)-V(2)-W(7)	70.56(12)	Ni(2)-N(10)-H(10D)	108.7
O(42)-V(2)-W(2)	120.7(9)	H(10C)-N(10)-H(10D)	107.6
O(26)-V(2)-W(2)	101.4(6)	C(17)-N(11)-Ni(4)	111(3)
O(16)-V(2)-W(2)	40.1(6)	C(17)-N(11)-H(11A)	109.4
O(5)-V(2)-W(2)	39.4(5)	Ni(4)-N(11)-H(11A)	109.5
O(7)-V(2)-W(2)	115.6(6)	C(17)-N(11)-H(11B)	109.5
W(6)-V(2)-W(2)	69.20(11)	Ni(4)-N(11)-H(11B)	109.5
W(8)-V(2)-W(2)	77.61(12)	H(11A)-N(11)-H(11B)	108.0
W(7)-V(2)-W(2)	116.45(16)	C(16)-N(12)-Ni(4)	106(3)
N(2)-Ni(1)-N(2)#1	179.997(10)	C(16)-N(12)-H(12D)	110.4
N(2)-Ni(1)-O(12)#1	91.9(9)	Ni(4)-N(12)-H(12D)	110.4
N(2)#1-Ni(1)-O(12)#1	88.1(9)	C(16)-N(12)-H(12E)	110.4
N(2)-Ni(1)-O(12)	88.1(9)	Ni(4)-N(12)-H(12E)	110.4
N(2)#1-Ni(1)-O(12)	91.9(9)	H(12D)-N(12)-H(12E)	108.6
O(12)#1-Ni(1)-O(12)	180.0(6)	C(20)-N(13)-Ni(4)	115(3)
N(2)-Ni(1)-N(1)	82.3(12)	C(20)-N(13)-H(13A)	108.4

N(2)#1-Ni(1)-N(1)	97.7(12)	Ni(4)-N(13)-H(13A)	108.4
O(12)#1-Ni(1)-N(1)	88.9(9)	C(20)-N(13)-H(13B)	108.4
O(12)-Ni(1)-N(1)	91.1(9)	Ni(4)-N(13)-H(13B)	108.4
N(2)-Ni(1)-N(1)#1	97.7(12)	H(13A)-N(13)-H(13B)	107.5
N(2)#1-Ni(1)-N(1)#1	82.3(12)	C(19)-N(14)-Ni(4)	111(3)
O(12)#1-Ni(1)-N(1)#1	91.2(9)	C(19)-N(14)-H(14C)	109.4
O(12)-Ni(1)-N(1)#1	88.9(9)	Ni(4)-N(14)-H(14C)	109.4
N(1)-Ni(1)-N(1)#1	180.0(7)	C(19)-N(14)-H(14D)	109.4
N(10)-Ni(2)-N(7)	175.4(14)	Ni(4)-N(14)-H(14D)	109.4
N(10)-Ni(2)-N(8)	93.4(13)	H(14C)-N(14)-H(14D)	108.0
Symmetry code: (#1) -x+2,-y,-z+2			
Compound **3**			
As(1)-O(19)	1.658(6)	V(1)-V(5)	2.901(3)
As(1)-O(31)	1.667(7)	V(1)-V(4)	2.986(3)
As(1)-O(14)	1.667(7)	V(2)-O(38)	1.645(7)
As(1)-O(30)	1.680(7)	V(2)-O(11)	1.888(7)
Mo(1)-O(40)	1.647(7)	V(2)-O(2)	1.931(7)
Mo(1)-O(20)	1.831(7)	V(2)-O(15)	2.005(7)
Mo(1)-O(9)	1.832(7)	V(2)-O(10)	2.011(7)
Mo(1)-O(6)	2.074(7)	V(2)-O(30)	2.424(7)
Mo(1)-O(1)	2.078(7)	V(2)-V(7)	2.800(3)
Mo(1)-O(19)	2.418(7)	V(2)-V(4)	2.949(2)
Mo(1)-V(6)	3.119(2)	V(3)-O(25)	1.616(7)
Mo(2)-O(24)	1.689(8)	V(3)-O(3)	1.934(7)
Mo(2)-O(29)	1.815(7)	V(3)-O(8)	1.937(7)
Mo(2)-O(18)	1.880(7)	V(3)-O(1)	1.975(7)
Mo(2)-O(4)	2.039(7)	V(3)-O(5)	1.994(7)
Mo(2)-O(15)	2.068(7)	V(3)-O(14)	2.400(7)
Mo(2)-O(31)	2.409(7)	V(3)-V(5)	2.868(3)
Mo(2)-V(4)	3.075(2)	V(3)-V(6)	2.922(2)
Mo(3)-O(23)	1.657(7)	V(4)-O(36)	1.612(8)
Mo(3)-O(28)	1.816(7)	V(4)-O(15)	1.862(7)
Mo(3)-O(32)	1.867(7)	V(4)-O(22)	1.875(7)
Mo(3)-O(5)	2.026(7)	V(4)-O(10)	1.945(7)
Mo(3)-O(16)	2.047(7)	V(4)-O(4)	1.973(7)
Mo(3)-O(14)	2.396(7)	V(5)-O(39)	1.593(9)
Mo(3)-V(6)	3.050(2)	V(5)-O(3)	1.843(7)
Mo(4)-O(37)	1.630(8)	V(5)-O(17)	1.870(7)
Mo(4)-O(33)	1.865(8)	V(5)-O(8)	1.983(7)
Mo(4)-O(32)	1.921(7)	V(5)-O(7)	2.005(8)
Mo(4)-O(17)	2.024(7)	V(6)-O(43)	1.620(8)
Mo(4)-O(8)	2.045(7)	V(6)-O(1)	1.888(7)
Mo(4)-O(14)	2.414(7)	V(6)-O(16)	1.892(7)

Mo(4)-V(5)	3.024(2)	V(6)-O(5)	1.973(7)
Mo(5)-O(27)	1.626(7)	V(6)-O(6)	2.018(8)
Mo(5)-O(29)	1.886(7)	V(6)-V(8)	3.001(2)
Mo(5)-O(9)	1.930(7)	V(7)-O(44)	1.577(10)
Mo(5)-O(11)	2.013(7)	V(7)-O(26)	1.870(8)
Mo(5)-O(13)	2.046(8)	V(7)-O(11)	1.900(7)
Mo(5)-O(19)	2.387(7)	V(7)-O(2)	1.940(7)
Mo(5)-V(7)	3.092(3)	V(7)-O(13)	2.119(9)
Mo(6)-O(34)	1.644(7)	V(7)-V(8)	2.994(3)
Mo(6)-O(20)	1.876(7)	V(8)-O(12)	1.637(7)
Mo(6)-O(18)	1.920(7)	V(8)-O(26)	1.933(7)
Mo(6)-O(7)	2.001(7)	V(8)-O(16)	1.971(7)
Mo(6)-O(3)	2.067(7)	V(8)-O(13)	1.981(8)
Mo(6)-O(31)	2.429(7)	V(8)-O(6)	2.014(7)
Mo(6)-V(5)	3.001(2)	V(8)-O(19)	2.361(7)
Mo(7)-O(42)	1.624(8)	C(1)-N(1)	1.446(17)
Mo(7)-O(33)	1.836(8)	C(1)-C(2)	1.524(18)
Mo(7)-O(35)	1.880(7)	C(1)-H(1A)	0.9700
Mo(7)-O(10)	2.062(7)	C(1)-H(1B)	0.9700
Mo(7)-O(22)	2.075(7)	C(2)-N(2)	1.45(3)
Mo(7)-O(30)	2.369(7)	C(2)-C(3)	1.555(18)
Mo(7)-V(4)	3.073(2)	C(2)-H(2)	0.9800
Mo(8)-O(41)	1.606(8)	C(3)-H(3A)	0.9600
Mo(8)-O(35)	1.897(7)	C(3)-H(3B)	0.9600
Mo(8)-O(28)	1.899(7)	C(3)-H(3C)	0.9600
Mo(8)-O(26)	2.034(7)	C(4)-N(3)	1.46(3)
Mo(8)-O(2)	2.042(7)	C(4)-C(5)	1.512(18)
Mo(8)-O(30)	2.389(7)	C(4)-H(4A)	0.9700
Mo(8)-V(7)	2.975(3)	C(4)-H(4B)	0.9700
Ni(1)-N(5)#1	2.033(13)	C(5)-N(4)	1.422(17)
Ni(1)-N(5)	2.033(13)	C(5)-C(6)	1.471(17)
Ni(1)-N(6)#1	2.056(13)	C(5)-H(5)	0.9800
Ni(1)-N(6)	2.056(13)	C(6)-H(6A)	0.9600
Ni(1)-O(12)	2.132(7)	C(6)-H(6B)	0.9600
Ni(1)-O(12)#1	2.132(7)	C(6)-H(6C)	0.9600
Ni(2)-N(4)	1.982(16)	C(7)-N(6)	1.440(15)
Ni(2)-O(21)	2.064(8)	C(7)-C(8)#1	1.53(3)
Ni(2)-N(3)	2.088(18)	C(7)-H(7A)	0.9700
Ni(2)-N(2)	2.128(17)	C(7)-H(7B)	0.9700
Ni(2)-N(1)	2.130(18)	C(8)-C(9)	1.40(3)
Ni(2)-O(5W)	2.190(16)	C(8)-N(5)	1.48(2)
Ni(3)-N(9)	1.881(11)	C(8)-C(7)#1	1.53(3)
Ni(3)-N(8)	1.893(11)	C(8)-H(8)	0.9800

Ni(3)-N(10)	1.900(12)	C(9)-H(9A)	0.9600
Ni(3)-N(7)	1.910(11)	C(9)-H(9B)	0.9600
Ni(4)-N(12)	1.899(10)	C(9)-H(9C)	0.9600
Ni(4)-N(13)	1.904(9)	C(10)-C(11)	1.49(2)
Ni(4)-N(11)	1.929(10)	C(10)-N(7)	1.555(15)
Ni(4)-N(14)	1.937(11)	C(10)-H(10A)	0.9700
V(1)-O(21)	1.633(7)	C(10)-H(10B)	0.9700
V(1)-O(17)	1.928(7)	C(11)-N(8)	1.43(2)
V(1)-O(7)	1.949(7)	C(11)-C(12)	1.48(3)
V(1)-O(22)	1.962(7)	C(11)-H(11)	0.9800
V(1)-O(4)	2.020(7)	C(12)-H(12A)	0.9600
V(1)-O(31)	2.372(7)	C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600	N(1)-H(1C)	0.9000
C(13)-C(14)	1.51(2)	N(1)-H(1D)	0.9000
C(13)-N(9)	1.512(19)	N(2)-H(2A)	0.9000
C(13)-H(13A)	0.9700	N(2)-H(2B)	0.9000
C(13)-H(13B)	0.9700	N(3)-H(3D)	0.9000
C(14)-C(15)	1.42(3)	N(3)-H(3E)	0.9000
C(14)-N(10)	1.45(2)	N(4)-H(4C)	0.9000
C(14)-H(14)	0.9800	N(4)-H(4D)	0.9000
C(15)-H(15A)	0.9600	N(5)-H(5A)	0.9000
C(15)-H(15B)	0.9600	N(5)-H(5B)	0.9000
C(15)-H(15C)	0.9600	N(6)-H(6D)	0.9000
C(16)-C(17)	1.47(3)	N(6)-H(6E)	0.9000
C(16)-N(11)	1.49(2)	N(7)-H(7C)	0.9000
C(16)-H(16A)	0.9700	N(7)-H(7D)	0.9000
C(16)-H(16B)	0.9700	N(8)-H(8A)	0.9000
C(17)-N(12)	1.41(2)	N(8)-H(8B)	0.9000
C(17)-C(18)	1.59(4)	N(9)-H(9D)	0.9000
C(17)-H(17)	0.9800	N(9)-H(9E)	0.9000
C(18)-H(18A)	0.9600	N(10)-H(10C)	0.9000
C(18)-H(18B)	0.9600	N(10)-H(10D)	0.9000
C(18)-H(18C)	0.9600	N(11)-H(11A)	0.9000
C(19)-N(13)	1.411(19)	N(11)-H(11B)	0.9000
C(19)-C(20)	1.52(2)	N(12)-H(12D)	0.9000
C(19)-H(19A)	0.9700	N(12)-H(12E)	0.9000
C(19)-H(19B)	0.9700	N(13)-H(13C)	0.9000
C(20)-N(14)	1.357(19)	N(13)-H(13D)	0.9000
C(20)-C(21)	1.42(2)	N(14)-H(14A)	0.9000
C(20)-H(20)	0.9800	N(14)-H(14B)	0.9000
C(21)-H(21A)	0.9600	C(21)-H(21C)	0.9600
C(21)-H(21B)	0.9600		

O(19)-As(1)-O(31)	109.9(3)	O(26)-V(7)-V(8)	38.8(2)
O(19)-As(1)-O(14)	108.7(3)	O(11)-V(7)-V(8)	103.1(2)
O(31)-As(1)-O(14)	109.6(3)	O(2)-V(7)-V(8)	119.7(2)
O(19)-As(1)-O(30)	109.6(3)	O(13)-V(7)-V(8)	41.3(2)
O(31)-As(1)-O(30)	109.5(3)	V(2)-V(7)-V(8)	120.41(9)
O(14)-As(1)-O(30)	109.5(3)	Mo(8)-V(7)-V(8)	78.78(7)
O(40)-Mo(1)-O(20)	104.8(3)	O(44)-V(7)-Mo(5)	121.4(4)
O(40)-Mo(1)-O(9)	101.2(3)	O(26)-V(7)-Mo(5)	101.9(2)
O(20)-Mo(1)-O(9)	97.0(3)	O(11)-V(7)-Mo(5)	39.1(2)
O(40)-Mo(1)-O(6)	99.0(3)	O(2)-V(7)-Mo(5)	119.5(2)
O(20)-Mo(1)-O(6)	152.6(3)	O(13)-V(7)-Mo(5)	41.2(2)
O(9)-Mo(1)-O(6)	91.6(3)	V(2)-V(7)-Mo(5)	78.53(6)
O(40)-Mo(1)-O(1)	97.2(3)	Mo(8)-V(7)-Mo(5)	118.90(8)
O(20)-Mo(1)-O(1)	87.8(3)	V(8)-V(7)-Mo(5)	69.68(6)
O(9)-Mo(1)-O(1)	159.1(3)	O(12)-V(8)-O(26)	102.3(3)
O(6)-Mo(1)-O(1)	75.7(3)	O(12)-V(8)-O(16)	100.8(3)
O(40)-Mo(1)-O(19)	167.2(3)	O(26)-V(8)-O(16)	89.7(3)
O(20)-Mo(1)-O(19)	87.8(3)	O(12)-V(8)-O(13)	100.1(4)
O(9)-Mo(1)-O(19)	74.5(3)	O(26)-V(8)-O(13)	82.2(3)
O(6)-Mo(1)-O(19)	69.4(3)	O(16)-V(8)-O(13)	158.9(3)
O(1)-Mo(1)-O(19)	85.4(3)	O(12)-V(8)-O(6)	100.4(3)
O(40)-Mo(1)-V(6)	101.7(3)	O(26)-V(8)-O(6)	156.5(3)
O(20)-Mo(1)-V(6)	120.2(2)	O(16)-V(8)-O(6)	80.0(3)
O(9)-Mo(1)-V(6)	128.7(2)	O(13)-V(8)-O(6)	99.8(3)
O(6)-Mo(1)-V(6)	39.7(2)	O(12)-V(8)-O(19)	168.0(3)
O(1)-Mo(1)-V(6)	36.03(18)	O(26)-V(8)-O(19)	86.9(3)
O(19)-Mo(1)-V(6)	73.16(17)	O(16)-V(8)-O(19)	86.8(3)
O(24)-Mo(2)-O(29)	106.0(3)	O(13)-V(8)-O(19)	73.3(3)
O(24)-Mo(2)-O(18)	99.3(4)	O(6)-V(8)-O(19)	71.6(2)
O(29)-Mo(2)-O(18)	99.1(3)	O(12)-V(8)-V(7)	105.7(3)
O(24)-Mo(2)-O(4)	99.7(3)	O(26)-V(8)-V(7)	37.3(2)
O(29)-Mo(2)-O(4)	150.6(3)	O(16)-V(8)-V(7)	124.3(2)
O(18)-Mo(2)-O(4)	90.3(3)	O(13)-V(8)-V(7)	44.9(2)
O(24)-Mo(2)-O(15)	99.0(3)	O(6)-V(8)-V(7)	138.9(2)
O(29)-Mo(2)-O(15)	86.8(3)	O(19)-V(8)-V(7)	76.92(17)
O(18)-Mo(2)-O(15)	158.4(3)	O(12)-V(8)-V(6)	104.1(3)
O(4)-Mo(2)-O(15)	75.3(3)	O(26)-V(8)-V(6)	124.8(2)
O(24)-Mo(2)-O(31)	167.9(3)	O(16)-V(8)-V(6)	38.1(2)
O(29)-Mo(2)-O(31)	85.4(3)	O(13)-V(8)-V(6)	137.6(2)
O(18)-Mo(2)-O(31)	74.7(3)	O(6)-V(8)-V(6)	42.0(2)
O(4)-Mo(2)-O(31)	70.3(3)	O(19)-V(8)-V(6)	76.21(17)
O(15)-Mo(2)-O(31)	85.1(3)	V(7)-V(8)-V(6)	148.46(8)
O(24)-Mo(2)-V(4)	103.1(3)	V(6)-O(1)-V(3)	98.3(3)

O(29)-Mo(2)-V(4)	119.0(2)	V(6)-O(1)-Mo(1)	103.6(3)
O(18)-Mo(2)-V(4)	127.2(2)	V(3)-O(1)-Mo(1)	143.3(4)
O(4)-Mo(2)-V(4)	39.2(2)	V(2)-O(2)-V(7)	92.7(3)
O(15)-Mo(2)-V(4)	36.19(19)	V(2)-O(2)-Mo(8)	123.4(4)
O(31)-Mo(2)-V(4)	73.53(17)	V(7)-O(2)-Mo(8)	96.7(3)
O(23)-Mo(3)-O(28)	104.9(4)	V(5)-O(3)-V(3)	98.8(3)
O(23)-Mo(3)-O(32)	101.8(4)	V(5)-O(3)-Mo(6)	100.1(3)
O(28)-Mo(3)-O(32)	96.3(3)	V(3)-O(3)-Mo(6)	144.2(4)
O(23)-Mo(3)-O(5)	100.7(3)	V(4)-O(4)-V(1)	96.8(3)
O(28)-Mo(3)-O(5)	151.9(3)	V(4)-O(4)-Mo(2)	100.1(3)
O(32)-Mo(3)-O(5)	89.6(3)	V(1)-O(4)-Mo(2)	120.3(3)
O(23)-Mo(3)-O(16)	98.2(3)	V(6)-O(5)-V(3)	94.9(3)
O(28)-Mo(3)-O(16)	87.8(3)	V(6)-O(5)-Mo(3)	99.4(3)
O(32)-Mo(3)-O(16)	157.8(3)	V(3)-O(5)-Mo(3)	123.7(3)
O(5)-Mo(3)-O(16)	77.1(3)	V(8)-O(6)-V(6)	96.2(3)
O(23)-Mo(3)-O(14)	169.0(3)	V(8)-O(6)-Mo(1)	120.4(3)
O(28)-Mo(3)-O(14)	85.9(3)	V(6)-O(6)-Mo(1)	99.3(3)
O(32)-Mo(3)-O(14)	74.4(3)	V(1)-O(7)-Mo(6)	122.7(4)
O(5)-Mo(3)-O(14)	69.2(3)	V(1)-O(7)-V(5)	94.4(3)
O(16)-Mo(3)-O(14)	84.2(2)	Mo(6)-O(7)-V(5)	97.0(3)
O(23)-Mo(3)-V(6)	102.2(3)	V(3)-O(8)-V(5)	94.0(3)
O(28)-Mo(3)-V(6)	121.7(2)	V(3)-O(8)-Mo(4)	123.0(4)
O(32)-Mo(3)-V(6)	127.0(2)	V(5)-O(8)-Mo(4)	97.3(3)
O(5)-Mo(3)-V(6)	39.7(2)	Mo(1)-O(9)-Mo(5)	123.5(4)
O(16)-Mo(3)-V(6)	37.5(2)	V(4)-O(10)-V(2)	96.4(3)
O(14)-Mo(3)-V(6)	73.19(16)	V(4)-O(10)-Mo(7)	100.1(3)
O(37)-Mo(4)-O(33)	105.3(4)	V(2)-O(10)-Mo(7)	122.2(3)
O(37)-Mo(4)-O(32)	100.4(3)	V(2)-O(11)-V(7)	95.3(3)
O(33)-Mo(4)-O(32)	94.3(3)	V(2)-O(11)-Mo(5)	146.6(4)
O(37)-Mo(4)-O(17)	98.8(3)	V(7)-O(11)-Mo(5)	104.4(3)
O(33)-Mo(4)-O(17)	89.7(3)	V(8)-O(12)-Ni(1)	146.9(5)
O(32)-Mo(4)-O(17)	158.6(3)	V(8)-O(13)-Mo(5)	119.5(4)
O(37)-Mo(4)-O(8)	99.3(3)	V(8)-O(13)-V(7)	93.8(3)
O(33)-Mo(4)-O(8)	153.9(3)	Mo(5)-O(13)-V(7)	95.9(3)
O(32)-Mo(4)-O(8)	89.8(3)	As(1)-O(14)-Mo(3)	123.6(4)
O(17)-Mo(4)-O(8)	77.8(3)	As(1)-O(14)-V(3)	124.8(3)
O(37)-Mo(4)-O(14)	167.3(3)	Mo(3)-O(14)-V(3)	95.3(2)
O(33)-Mo(4)-O(14)	86.4(3)	As(1)-O(14)-Mo(4)	122.5(3)
O(32)-Mo(4)-O(14)	73.1(3)	Mo(3)-O(14)-Mo(4)	87.8(2)
O(17)-Mo(4)-O(14)	86.2(3)	V(3)-O(14)-Mo(4)	93.3(2)
O(8)-Mo(4)-O(14)	70.1(2)	V(4)-O(15)-V(2)	99.3(3)
O(37)-Mo(4)-V(5)	103.0(3)	V(4)-O(15)-Mo(2)	102.8(3)
O(33)-Mo(4)-V(5)	122.9(2)	V(2)-O(15)-Mo(2)	143.0(4)

O(32)-Mo(4)-V(5)	127.6(2)	V(6)-O(16)-V(8)	102.0(3)
O(17)-Mo(4)-V(5)	37.2(2)	V(6)-O(16)-Mo(3)	101.4(3)
O(8)-Mo(4)-V(5)	40.6(2)	V(8)-O(16)-Mo(3)	143.9(4)
O(14)-Mo(4)-V(5)	73.87(17)	V(5)-O(17)-V(1)	99.6(3)
O(27)-Mo(5)-O(29)	102.9(3)	V(5)-O(17)-Mo(4)	101.8(3)
O(27)-Mo(5)-O(9)	99.4(3)	V(1)-O(17)-Mo(4)	143.4(4)
O(29)-Mo(5)-O(9)	94.1(3)	Mo(2)-O(18)-Mo(6)	122.9(4)
O(27)-Mo(5)-O(11)	99.9(3)	As(1)-O(19)-V(8)	124.7(4)
O(29)-Mo(5)-O(11)	87.7(3)	As(1)-O(19)-Mo(5)	122.9(3)
O(9)-Mo(5)-O(11)	159.7(3)	V(8)-O(19)-Mo(5)	94.2(2)
O(27)-Mo(5)-O(13)	99.8(3)	As(1)-O(19)-Mo(1)	122.7(3)
O(29)-Mo(5)-O(13)	155.5(3)	V(8)-O(19)-Mo(1)	95.8(2)
O(9)-Mo(5)-O(13)	91.2(3)	Mo(5)-O(19)-Mo(1)	87.2(2)
O(11)-Mo(5)-O(13)	79.4(3)	Mo(1)-O(20)-Mo(6)	155.7(4)
O(27)-Mo(5)-O(19)	168.4(3)	V(1)-O(21)-Ni(2)	151.4(5)
O(29)-Mo(5)-O(19)	87.0(3)	V(4)-O(22)-V(1)	102.1(3)
O(9)-Mo(5)-O(19)	73.6(3)	V(4)-O(22)-Mo(7)	102.0(3)
O(11)-Mo(5)-O(19)	86.3(3)	V(1)-O(22)-Mo(7)	142.7(4)
O(13)-Mo(5)-O(19)	71.6(3)	V(7)-O(26)-V(8)	103.9(3)
O(27)-Mo(5)-V(7)	104.7(3)	V(7)-O(26)-Mo(8)	99.2(3)
O(29)-Mo(5)-V(7)	120.7(2)	V(8)-O(26)-Mo(8)	145.5(4)
O(9)-Mo(5)-V(7)	130.7(2)	Mo(3)-O(28)-Mo(8)	157.0(4)
O(11)-Mo(5)-V(7)	36.5(2)	Mo(2)-O(29)-Mo(5)	156.1(4)
O(13)-Mo(5)-V(7)	43.0(2)	As(1)-O(30)-Mo(7)	124.2(3)
O(19)-Mo(5)-V(7)	74.60(17)	As(1)-O(30)-Mo(8)	124.0(3)
O(34)-Mo(6)-O(20)	105.7(3)	Mo(7)-O(30)-Mo(8)	88.3(2)
O(34)-Mo(6)-O(18)	98.8(3)	As(1)-O(30)-V(2)	122.0(3)
O(20)-Mo(6)-O(18)	96.1(3)	Mo(7)-O(30)-V(2)	96.2(2)
O(34)-Mo(6)-O(7)	100.3(3)	Mo(8)-O(30)-V(2)	93.2(2)
O(20)-Mo(6)-O(7)	152.4(3)	As(1)-O(31)-V(1)	123.4(4)
O(18)-Mo(6)-O(7)	89.0(3)	As(1)-O(31)-Mo(2)	124.8(3)
O(34)-Mo(6)-O(3)	99.6(3)	V(1)-O(31)-Mo(2)	94.9(2)
O(20)-Mo(6)-O(3)	87.8(3)	As(1)-O(31)-Mo(6)	124.3(3)
O(18)-Mo(6)-O(3)	159.4(3)	V(1)-O(31)-Mo(6)	92.4(2)
O(7)-Mo(6)-O(3)	78.7(3)	Mo(2)-O(31)-Mo(6)	87.2(2)
O(34)-Mo(6)-O(31)	167.9(3)	Mo(3)-O(32)-Mo(4)	123.4(4)
O(20)-Mo(6)-O(31)	84.8(3)	Mo(7)-O(33)-Mo(4)	154.5(4)
O(18)-Mo(6)-O(31)	73.6(3)	Mo(7)-O(35)-Mo(8)	122.7(4)
O(7)-Mo(6)-O(31)	70.6(3)	N(1)-C(1)-C(2)	102(2)
O(3)-Mo(6)-O(31)	86.7(3)	N(1)-C(1)-H(1A)	111.3
O(34)-Mo(6)-V(5)	104.3(3)	C(2)-C(1)-H(1A)	111.4
O(20)-Mo(6)-V(5)	120.6(2)	N(1)-C(1)-H(1B)	111.3
O(18)-Mo(6)-V(5)	127.9(2)	C(2)-C(1)-H(1B)	111.3

O(7)-Mo(6)-V(5)	41.5(2)	H(1A)-C(1)-H(1B)	109.2
O(3)-Mo(6)-V(5)	37.20(19)	N(2)-C(2)-C(3)	110(2)
O(31)-Mo(6)-V(5)	74.50(17)	N(2)-C(2)-C(1)	140(2)
O(42)-Mo(7)-O(33)	106.1(4)	C(3)-C(2)-C(1)	110(2)
O(42)-Mo(7)-O(35)	99.8(4)	N(2)-C(2)-H(2)	92.0
O(33)-Mo(7)-O(35)	97.1(3)	C(3)-C(2)-H(2)	92.0
O(42)-Mo(7)-O(10)	98.8(4)	C(1)-C(2)-H(2)	92.0
O(33)-Mo(7)-O(10)	152.1(3)	C(2)-C(3)-H(3A)	109.5
O(35)-Mo(7)-O(10)	90.7(3)	C(2)-C(3)-H(3B)	109.5
O(42)-Mo(7)-O(22)	99.1(3)	H(3A)-C(3)-H(3B)	109.5
O(33)-Mo(7)-O(22)	88.5(3)	C(2)-C(3)-H(3C)	109.5
O(35)-Mo(7)-O(22)	157.9(3)	H(3A)-C(3)-H(3C)	109.5
O(10)-Mo(7)-O(22)	75.2(3)	H(3B)-C(3)-H(3C)	109.5
O(42)-Mo(7)-O(30)	166.6(4)	N(3)-C(4)-C(5)	119(2)
O(33)-Mo(7)-O(30)	86.7(3)	N(3)-C(4)-H(4A)	107.5
O(35)-Mo(7)-O(30)	74.3(3)	C(5)-C(4)-H(4A)	107.5
O(10)-Mo(7)-O(30)	69.7(2)	N(3)-C(4)-H(4B)	107.5
O(22)-Mo(7)-O(30)	84.8(3)	C(5)-C(4)-H(4B)	107.5
O(42)-Mo(7)-V(4)	101.7(3)	H(4A)-C(4)-H(4B)	107.0
O(33)-Mo(7)-V(4)	121.8(2)	N(4)-C(5)-C(6)	116.4(17)
O(35)-Mo(7)-V(4)	127.1(2)	N(4)-C(5)-C(4)	105(2)
O(10)-Mo(7)-V(4)	38.55(19)	C(6)-C(5)-C(4)	113.7(18)
O(22)-Mo(7)-V(4)	36.6(2)	N(4)-C(5)-H(5)	107.1
O(30)-Mo(7)-V(4)	73.73(17)	C(6)-C(5)-H(5)	107.1
O(41)-Mo(8)-O(35)	101.3(4)	C(4)-C(5)-H(5)	107.1
O(41)-Mo(8)-O(28)	103.9(4)	C(5)-C(6)-H(6A)	109.5
O(35)-Mo(8)-O(28)	95.2(3)	C(5)-C(6)-H(6B)	109.5
O(41)-Mo(8)-O(26)	99.5(3)	H(6A)-C(6)-H(6B)	109.5
O(35)-Mo(8)-O(26)	157.6(3)	C(5)-C(6)-H(6C)	109.5
O(28)-Mo(8)-O(26)	87.5(3)	H(6A)-C(6)-H(6C)	109.5
O(41)-Mo(8)-O(2)	101.8(4)	H(6B)-C(6)-H(6C)	109.5
O(35)-Mo(8)-O(2)	89.1(3)	N(6)-C(7)-C(8)#1	109.8(18)
O(28)-Mo(8)-O(2)	152.5(3)	N(6)-C(7)-H(7A)	109.7
O(26)-Mo(8)-O(2)	78.7(3)	C(8)#1-C(7)-H(7A)	109.7
O(41)-Mo(8)-O(30)	170.7(3)	N(6)-C(7)-H(7B)	109.7
O(35)-Mo(8)-O(30)	73.5(3)	C(8)#1-C(7)-H(7B)	109.7
O(28)-Mo(8)-O(30)	84.4(3)	H(7A)-C(7)-H(7B)	108.2
O(26)-Mo(8)-O(30)	84.7(3)	C(9)-C(8)-N(5)	121(2)
O(2)-Mo(8)-O(30)	70.8(3)	C(9)-C(8)-C(7)#1	111(2)
O(41)-Mo(8)-V(7)	103.2(3)	N(5)-C(8)-C(7)#1	104.5(17)
O(35)-Mo(8)-V(7)	127.2(2)	C(9)-C(8)-H(8)	106.4
O(28)-Mo(8)-V(7)	122.5(2)	N(5)-C(8)-H(8)	106.4
O(26)-Mo(8)-V(7)	38.3(2)	C(7)#1-C(8)-H(8)	106.4

O(2)-Mo(8)-V(7)	40.4(2)	C(8)-C(9)-H(9A)	109.5
O(30)-Mo(8)-V(7)	74.94(17)	C(8)-C(9)-H(9B)	109.6
N(5)#1-Ni(1)-N(5)	179.998(4)	H(9A)-C(9)-H(9B)	109.5
N(5)#1-Ni(1)-N(6)#1	100.0(6)	C(8)-C(9)-H(9C)	109.3
N(5)-Ni(1)-N(6)#1	80.0(6)	H(9A)-C(9)-H(9C)	109.5
N(5)#1-Ni(1)-N(6)	80.0(6)	H(9B)-C(9)-H(9C)	109.5
N(5)-Ni(1)-N(6)	100.0(6)	C(11)-C(10)-N(7)	104.6(14)
N(6)#1-Ni(1)-N(6)	179.997(2)	C(11)-C(10)-H(10A)	110.8
N(5)#1-Ni(1)-O(12)	90.1(4)	N(7)-C(10)-H(10A)	110.8
N(5)-Ni(1)-O(12)	89.9(4)	C(11)-C(10)-H(10B)	110.8
N(6)#1-Ni(1)-O(12)	89.9(4)	N(7)-C(10)-H(10B)	110.8
N(6)-Ni(1)-O(12)	90.1(4)	H(10A)-C(10)-H(10B)	108.9
N(5)#1-Ni(1)-O(12)#1	89.9(4)	N(8)-C(11)-C(10)	106.4(14)
N(5)-Ni(1)-O(12)#1	90.1(4)	N(8)-C(11)-C(12)	123.4(18)
N(6)#1-Ni(1)-O(12)#1	90.1(4)	C(10)-C(11)-C(12)	109.6(17)
N(6)-Ni(1)-O(12)#1	89.9(4)	N(8)-C(11)-H(11)	105.4
O(12)-Ni(1)-O(12)#1	179.998(2)	C(10)-C(11)-H(11)	105.4
N(4)-Ni(2)-O(21)	87.4(6)	C(12)-C(11)-H(11)	105.4
N(4)-Ni(2)-N(3)	87.7(8)	C(11)-C(12)-H(12A)	109.5
O(21)-Ni(2)-N(3)	87.3(5)	C(11)-C(12)-H(12B)	109.5
N(4)-Ni(2)-N(2)	172.7(6)	H(12A)-C(12)-H(12B)	109.5
O(21)-Ni(2)-N(2)	85.7(5)	C(11)-C(12)-H(12C)	109.5
N(3)-Ni(2)-N(2)	94.5(7)	H(12A)-C(12)-H(12C)	109.5
N(4)-Ni(2)-N(1)	89.1(8)	H(12B)-C(12)-H(12C)	109.5
O(21)-Ni(2)-N(1)	91.0(5)	C(14)-C(13)-N(9)	107.6(13)
N(3)-Ni(2)-N(1)	176.4(7)	C(14)-C(13)-H(13A)	110.2
N(2)-Ni(2)-N(1)	88.5(7)	N(9)-C(13)-H(13A)	110.2
N(4)-Ni(2)-O(5W)	93.8(8)	C(14)-C(13)-H(13B)	110.2
O(21)-Ni(2)-O(5W)	176.5(5)	N(9)-C(13)-H(13B)	110.2
N(3)-Ni(2)-O(5W)	89.4(7)	H(13A)-C(13)-H(13B)	108.5
N(2)-Ni(2)-O(5W)	93.3(7)	C(15)-C(14)-N(10)	128.4(17)
N(1)-Ni(2)-O(5W)	92.4(7)	C(15)-C(14)-C(13)	112.6(17)
N(9)-Ni(3)-N(8)	177.3(5)	N(10)-C(14)-C(13)	108.3(15)
N(9)-Ni(3)-N(10)	87.0(5)	C(15)-C(14)-H(14)	100.9
N(8)-Ni(3)-N(10)	95.6(5)	N(10)-C(14)-H(14)	100.9
N(9)-Ni(3)-N(7)	92.2(5)	C(13)-C(14)-H(14)	100.9
N(8)-Ni(3)-N(7)	85.1(5)	C(14)-C(15)-H(15A)	109.5
N(10)-Ni(3)-N(7)	178.6(5)	C(14)-C(15)-H(15B)	109.5
N(12)-Ni(4)-N(13)	178.5(5)	H(15A)-C(15)-H(15B)	109.5
N(12)-Ni(4)-N(11)	86.2(5)	C(14)-C(15)-H(15C)	109.5
N(13)-Ni(4)-N(11)	93.5(4)	H(15A)-C(15)-H(15C)	109.5
N(12)-Ni(4)-N(14)	93.9(5)	H(15B)-C(15)-H(15C)	109.5
N(13)-Ni(4)-N(14)	86.5(5)	C(17)-C(16)-N(11)	102.8(16)

N(11)-Ni(4)-N(14)	178.2(5)	C(17)-C(16)-H(16A)	111.2
O(21)-V(1)-O(17)	102.6(4)	N(11)-C(16)-H(16A)	111.2
O(21)-V(1)-O(7)	100.3(3)	C(17)-C(16)-H(16B)	111.2
O(17)-V(1)-O(7)	83.0(3)	N(11)-C(16)-H(16B)	111.2
O(21)-V(1)-O(22)	100.8(3)	H(16A)-C(16)-H(16B)	109.1
O(17)-V(1)-O(22)	90.5(3)	N(12)-C(17)-C(16)	113.8(15)
O(7)-V(1)-O(22)	158.8(3)	N(12)-C(17)-C(18)	123(2)
O(21)-V(1)-O(4)	98.1(3)	C(16)-C(17)-C(18)	108(2)
O(17)-V(1)-O(4)	158.2(3)	N(12)-C(17)-H(17)	103.5
O(7)-V(1)-O(4)	100.1(3)	C(16)-C(17)-H(17)	103.5
O(22)-V(1)-O(4)	78.9(3)	C(18)-C(17)-H(17)	103.5
O(21)-V(1)-O(31)	165.5(3)	C(17)-C(18)-H(18A)	109.5
O(17)-V(1)-O(31)	89.3(3)	C(17)-C(18)-H(18B)	109.5
O(7)-V(1)-O(31)	72.7(3)	H(18A)-C(18)-H(18B)	109.5
O(22)-V(1)-O(31)	87.1(3)	C(17)-C(18)-H(18C)	109.5
O(4)-V(1)-O(31)	71.4(3)	H(18A)-C(18)-H(18C)	109.5
O(21)-V(1)-V(5)	106.7(3)	H(18B)-C(18)-H(18C)	109.5
O(17)-V(1)-V(5)	39.5(2)	N(13)-C(19)-C(20)	114.8(13)
O(7)-V(1)-V(5)	43.6(2)	N(13)-C(19)-H(19A)	108.6
O(22)-V(1)-V(5)	126.5(2)	C(20)-C(19)-H(19A)	108.6
O(4)-V(1)-V(5)	138.4(2)	N(13)-C(19)-H(19B)	108.6
O(31)-V(1)-V(5)	77.28(17)	C(20)-C(19)-H(19B)	108.6
O(21)-V(1)-V(4)	103.0(3)	H(19A)-C(19)-H(19B)	107.5
O(17)-V(1)-V(4)	125.6(2)	N(14)-C(20)-C(21)	130.7(18)
O(7)-V(1)-V(4)	136.7(2)	N(14)-C(20)-C(19)	110.2(14)
O(22)-V(1)-V(4)	37.9(2)	C(21)-C(20)-C(19)	113.2(16)
O(4)-V(1)-V(4)	41.0(2)	N(14)-C(20)-H(20)	97.9
O(31)-V(1)-V(4)	75.77(17)	C(21)-C(20)-H(20)	97.9
V(5)-V(1)-V(4)	149.28(8)	C(19)-C(20)-H(20)	97.9
O(38)-V(2)-O(11)	103.4(4)	C(20)-C(21)-H(21A)	109.5
O(38)-V(2)-O(2)	101.3(4)	C(20)-C(21)-H(21B)	109.5
O(11)-V(2)-O(2)	86.2(3)	H(21A)-C(21)-H(21B)	109.5
O(38)-V(2)-O(15)	100.0(3)	C(20)-C(21)-H(21C)	109.5
O(11)-V(2)-O(15)	88.3(3)	H(21A)-C(21)-H(21C)	109.5
O(2)-V(2)-O(15)	158.7(3)	H(21B)-C(21)-H(21C)	109.5
O(38)-V(2)-O(10)	100.2(4)	C(1)-N(1)-Ni(2)	113.9(15)
O(11)-V(2)-O(10)	155.0(3)	C(1)-N(1)-H(1C)	108.8
O(2)-V(2)-O(10)	97.2(3)	Ni(2)-N(1)-H(1C)	108.8
O(15)-V(2)-O(10)	79.5(3)	C(1)-N(1)-H(1D)	108.8
O(38)-V(2)-O(30)	165.9(3)	Ni(2)-N(1)-H(1D)	108.8
O(11)-V(2)-O(30)	88.6(3)	H(1C)-N(1)-H(1D)	107.7
O(2)-V(2)-O(30)	71.7(3)	C(2)-N(2)-Ni(2)	95.2(14)
O(15)-V(2)-O(30)	87.6(3)	C(2)-N(2)-H(2A)	112.7

O(10)-V(2)-O(30)	69.3(3)	Ni(2)-N(2)-H(2A)	112.7
O(38)-V(2)-V(7)	105.9(3)	C(2)-N(2)-H(2B)	112.7
O(11)-V(2)-V(7)	42.5(2)	Ni(2)-N(2)-H(2B)	112.7
O(2)-V(2)-V(7)	43.8(2)	H(2A)-N(2)-H(2B)	110.2
O(15)-V(2)-V(7)	128.1(2)	C(4)-N(3)-Ni(2)	99.8(14)
O(10)-V(2)-V(7)	136.2(2)	C(4)-N(3)-H(3D)	111.8
O(30)-V(2)-V(7)	77.87(17)	Ni(2)-N(3)-H(3D)	111.8
O(38)-V(2)-V(4)	103.1(3)	C(4)-N(3)-H(3E)	111.8
O(11)-V(2)-V(4)	123.7(2)	Ni(2)-N(3)-H(3E)	111.8
O(2)-V(2)-V(4)	134.6(2)	H(3D)-N(3)-H(3E)	109.5
O(15)-V(2)-V(4)	38.6(2)	C(5)-N(4)-Ni(2)	106.0(12)
O(10)-V(2)-V(4)	41.0(2)	C(5)-N(4)-H(4C)	110.5
O(30)-V(2)-V(4)	75.45(16)	Ni(2)-N(4)-H(4C)	110.5
V(7)-V(2)-V(4)	150.32(8)	C(5)-N(4)-H(4D)	110.5
O(25)-V(3)-O(3)	102.0(4)	Ni(2)-N(4)-H(4D)	110.5
O(25)-V(3)-O(8)	100.1(3)	H(4C)-N(4)-H(4D)	108.7
O(3)-V(3)-O(8)	83.0(3)	C(8)-N(5)-Ni(1)	113.9(12)
O(25)-V(3)-O(1)	102.2(3)	C(8)-N(5)-H(5A)	108.8
O(3)-V(3)-O(1)	88.5(3)	Ni(1)-N(5)-H(5A)	108.8
O(8)-V(3)-O(1)	157.3(3)	C(8)-N(5)-H(5B)	108.8
O(25)-V(3)-O(5)	100.2(3)	Ni(1)-N(5)-H(5B)	108.8
O(3)-V(3)-O(5)	157.2(3)	H(5A)-N(5)-H(5B)	107.7
O(8)-V(3)-O(5)	97.9(3)	C(7)-N(6)-Ni(1)	113.0(11)
O(1)-V(3)-O(5)	82.0(3)	C(7)-N(6)-H(6D)	109.0
O(25)-V(3)-O(14)	165.5(3)	Ni(1)-N(6)-H(6D)	109.0
O(3)-V(3)-O(14)	89.3(3)	C(7)-N(6)-H(6E)	109.0
O(8)-V(3)-O(14)	72.1(3)	Ni(1)-N(6)-H(6E)	109.0
O(1)-V(3)-O(14)	86.8(3)	H(6D)-N(6)-H(6E)	107.8
O(5)-V(3)-O(14)	69.6(3)	C(10)-N(7)-Ni(3)	108.8(9)
O(25)-V(3)-V(5)	106.0(3)	C(10)-N(7)-H(7C)	109.9
O(3)-V(3)-V(5)	39.4(2)	Ni(3)-N(7)-H(7C)	109.9
O(8)-V(3)-V(5)	43.6(2)	C(10)-N(7)-H(7D)	109.9
O(1)-V(3)-V(5)	124.4(2)	Ni(3)-N(7)-H(7D)	109.9
O(5)-V(3)-V(5)	136.2(2)	H(7C)-N(7)-H(7D)	108.3
O(14)-V(3)-V(5)	77.12(16)	C(11)-N(8)-Ni(3)	113.9(10)
O(25)-V(3)-V(6)	104.1(3)	C(11)-N(8)-H(8A)	108.8
O(3)-V(3)-V(6)	125.6(2)	Ni(3)-N(8)-H(8A)	108.8
O(8)-V(3)-V(6)	136.2(2)	C(11)-N(8)-H(8B)	108.8
O(1)-V(3)-V(6)	39.74(19)	Ni(3)-N(8)-H(8B)	108.8
O(5)-V(3)-V(6)	42.3(2)	H(8A)-N(8)-H(8B)	107.7
O(14)-V(3)-V(6)	75.63(16)	C(13)-N(9)-Ni(3)	112.0(9)
V(5)-V(3)-V(6)	148.98(8)	C(13)-N(9)-H(9D)	109.2
O(36)-V(4)-O(15)	118.4(4)	Ni(3)-N(9)-H(9D)	109.2

O(36)-V(4)-O(22)	117.7(4)	C(13)-N(9)-H(9E)	109.2
O(15)-V(4)-O(22)	123.8(3)	Ni(3)-N(9)-H(9E)	109.2
O(36)-V(4)-O(10)	106.3(4)	H(9D)-N(9)-H(9E)	107.9
O(15)-V(4)-O(10)	84.8(3)	C(14)-N(10)-Ni(3)	110.9(11)
O(22)-V(4)-O(10)	82.7(3)	C(14)-N(10)-H(10C)	109.5
O(36)-V(4)-O(4)	104.4(4)	Ni(3)-N(10)-H(10C)	109.5
O(15)-V(4)-O(4)	81.7(3)	C(14)-N(10)-H(10D)	109.5
O(22)-V(4)-O(4)	82.2(3)	Ni(3)-N(10)-H(10D)	109.5
O(10)-V(4)-O(4)	149.3(3)	H(10C)-N(10)-H(10D)	108.0
O(36)-V(4)-V(2)	120.8(3)	C(16)-N(11)-Ni(4)	110.7(10)
O(15)-V(4)-V(2)	42.2(2)	C(16)-N(11)-H(11A)	109.5
O(22)-V(4)-V(2)	107.0(2)	Ni(4)-N(11)-H(11A)	109.5
O(10)-V(4)-V(2)	42.7(2)	C(16)-N(11)-H(11B)	109.5
O(4)-V(4)-V(2)	118.8(2)	Ni(4)-N(11)-H(11B)	109.5
O(36)-V(4)-V(1)	119.2(3)	H(11A)-N(11)-H(11B)	108.1
O(15)-V(4)-V(1)	105.8(2)	C(17)-N(12)-Ni(4)	107.8(11)
O(22)-V(4)-V(1)	40.0(2)	C(17)-N(12)-H(12D)	110.1
O(10)-V(4)-V(1)	117.7(2)	Ni(4)-N(12)-H(12D)	110.1
O(4)-V(4)-V(1)	42.2(2)	C(17)-N(12)-H(12E)	110.1
V(2)-V(4)-V(1)	119.99(7)	Ni(4)-N(12)-H(12E)	110.1
O(36)-V(4)-Mo(7)	120.3(3)	H(12D)-N(12)-H(12E)	108.5
O(15)-V(4)-Mo(7)	107.7(2)	C(19)-N(13)-Ni(4)	110.4(9)
O(22)-V(4)-Mo(7)	41.3(2)	C(19)-N(13)-H(13C)	109.6
O(10)-V(4)-Mo(7)	41.3(2)	Ni(4)-N(13)-H(13C)	109.6
O(4)-V(4)-Mo(7)	118.6(2)	C(19)-N(13)-H(13D)	109.6
V(2)-V(4)-Mo(7)	72.60(5)	Ni(4)-N(13)-H(13D)	109.6
V(1)-V(4)-Mo(7)	78.29(6)	H(13C)-N(13)-H(13D)	108.1
O(36)-V(4)-Mo(2)	120.0(3)	C(20)-N(14)-Ni(4)	113.2(11)
O(15)-V(4)-Mo(2)	41.0(2)	C(20)-N(14)-H(14A)	108.9
O(22)-V(4)-Mo(2)	104.8(2)	Ni(4)-N(14)-H(14A)	108.9
O(10)-V(4)-Mo(2)	119.8(2)	C(20)-N(14)-H(14B)	108.9
O(4)-V(4)-Mo(2)	40.8(2)	Ni(4)-N(14)-H(14B)	108.9
V(2)-V(4)-Mo(2)	79.73(6)	H(14A)-N(14)-H(14B)	107.8
V(1)-V(4)-Mo(2)	71.02(5)	O(43)-V(6)-O(6)	104.4(4)
Mo(7)-V(4)-Mo(2)	119.62(6)	O(1)-V(6)-O(6)	81.3(3)
O(39)-V(5)-O(3)	115.8(4)	O(16)-V(6)-O(6)	81.8(3)
O(39)-V(5)-O(17)	117.6(4)	O(5)-V(6)-O(6)	148.4(3)
O(3)-V(5)-O(17)	126.5(3)	O(43)-V(6)-V(3)	120.6(3)
O(39)-V(5)-O(8)	106.1(4)	O(1)-V(6)-V(3)	42.0(2)
O(3)-V(5)-O(8)	84.1(3)	O(16)-V(6)-V(3)	106.8(2)
O(17)-V(5)-O(8)	83.0(3)	O(5)-V(6)-V(3)	42.8(2)
O(39)-V(5)-O(7)	102.9(4)	O(6)-V(6)-V(3)	118.4(2)
O(3)-V(5)-O(7)	84.1(3)	O(43)-V(6)-V(8)	119.3(3)

O(17)-V(5)-O(7)	83.0(3)	O(1)-V(6)-V(8)	105.3(2)
O(8)-V(5)-O(7)	151.0(3)	O(16)-V(6)-V(8)	40.0(2)
O(39)-V(5)-V(3)	119.8(3)	O(5)-V(6)-V(8)	117.3(2)
O(3)-V(5)-V(3)	41.8(2)	O(6)-V(6)-V(8)	41.8(2)
O(17)-V(5)-V(3)	107.8(2)	V(3)-V(6)-V(8)	120.10(7)
O(8)-V(5)-V(3)	42.34(19)	O(43)-V(6)-Mo(3)	121.2(3)
O(7)-V(5)-V(3)	120.4(2)	O(1)-V(6)-Mo(3)	107.2(2)
O(39)-V(5)-V(1)	118.7(3)	O(16)-V(6)-Mo(3)	41.1(2)
O(3)-V(5)-V(1)	108.4(2)	O(5)-V(6)-Mo(3)	40.9(2)
O(17)-V(5)-V(1)	40.9(2)	O(6)-V(6)-Mo(3)	118.1(2)
O(8)-V(5)-V(1)	119.0(2)	V(3)-V(6)-Mo(3)	72.78(6)
O(7)-V(5)-V(1)	42.1(2)	V(8)-V(6)-Mo(3)	78.27(6)
V(3)-V(5)-V(1)	121.48(8)	O(43)-V(6)-Mo(1)	120.1(3)
O(39)-V(5)-Mo(6)	117.7(4)	O(1)-V(6)-Mo(1)	40.4(2)
O(3)-V(5)-Mo(6)	42.7(2)	O(16)-V(6)-Mo(1)	104.0(2)
O(17)-V(5)-Mo(6)	106.9(2)	O(5)-V(6)-Mo(1)	118.9(2)
O(8)-V(5)-Mo(6)	121.0(2)	O(6)-V(6)-Mo(1)	41.0(2)
O(7)-V(5)-Mo(6)	41.4(2)	V(3)-V(6)-Mo(1)	79.04(6)
V(3)-V(5)-Mo(6)	80.84(6)	V(8)-V(6)-Mo(1)	70.83(5)
V(1)-V(5)-Mo(6)	71.91(6)	Mo(3)-V(6)-Mo(1)	118.69(6)
O(39)-V(5)-Mo(4)	121.3(4)	O(44)-V(7)-O(26)	117.4(5)
O(3)-V(5)-Mo(4)	108.2(2)	O(44)-V(7)-O(11)	121.2(5)
O(17)-V(5)-Mo(4)	40.9(2)	O(26)-V(7)-O(11)	120.9(3)
O(8)-V(5)-Mo(4)	42.1(2)	O(44)-V(7)-O(2)	106.0(5)
O(7)-V(5)-Mo(4)	118.8(2)	O(26)-V(7)-O(2)	85.4(3)
V(3)-V(5)-Mo(4)	72.81(6)	O(11)-V(7)-O(2)	85.7(3)
V(1)-V(5)-Mo(4)	78.55(7)	O(44)-V(7)-O(13)	103.4(5)
Mo(6)-V(5)-Mo(4)	120.90(7)	O(26)-V(7)-O(13)	80.1(3)
O(43)-V(6)-O(1)	118.3(4)	O(11)-V(7)-O(13)	80.2(3)
O(43)-V(6)-O(16)	118.9(4)	O(2)-V(7)-O(13)	150.6(3)
O(1)-V(6)-O(16)	122.7(3)	O(44)-V(7)-V(2)	121.8(4)
O(43)-V(6)-O(5)	107.2(4)	O(26)-V(7)-V(2)	108.5(2)
O(1)-V(6)-O(5)	84.8(3)	O(11)-V(7)-V(2)	42.2(2)
O(16)-V(6)-O(5)	82.1(3)	O(2)-V(7)-V(2)	43.5(2)
O(2)-V(7)-Mo(8)	43.0(2)	O(13)-V(7)-V(2)	118.5(2)
O(13)-V(7)-Mo(8)	118.5(2)	O(44)-V(7)-Mo(8)	119.4(4)
V(2)-V(7)-Mo(8)	74.49(6)	O(26)-V(7)-Mo(8)	42.5(2)
O(44)-V(7)-V(8)	117.8(4)	O(11)-V(7)-Mo(8)	108.0(2)
Symmetry code: (#1) -x+2,-y+1,-z+1			

S-Table 2 Bond valence sum of **1-3**

Compound **1**						
W(1)	W(2)	W(3)	W(4)	W(5)	W(6)	P(1)
5.68	5.78	5.83	5.68	5.76	5.74	5.15
Compound **2**						
W(1)	W(2)	W(3)	W(4)	W(5)	W(6)	W(7)
5.85	5.98	5.48	5.96	5.52	5.50	5.28
W(8)	W(9)	W(10)	W(11)	W(12)	As(1)	V(1)
5.54	5.67	5.60	5.46	5.66	5.14	3.82
V(2)	V(9)	V(10)	V(11)	V(12)		
3.89	4.05	4.00	3.91	4.04		
Compound **3**						
Mo(1)	Mo(2)	Mo(3)	Mo(4)	Mo(5)	Mo(6)	Mo(7)
5.84	5.69	5.84	5.74	5.65	5.54	5.85
Mo(8)	As(1)	V(1)	V(2)	V(3)	V(4)	V(5)
5.87	5.13	4.05	3.99	4.12	4.30	4.36
V(6)	V(7)	V(8)				
4.06	4.21	3.99				