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Table S3. Bond Lengths (Å) and Angles (°) for Complexes **1**, **2** and **3**.For **1**

Bond lengths		Bond lengths	
V1–O1	1.596(5)	O3–C2	1.432(10)
V1–O4	1.983(5)	O4–C4	1.284(9)
V1–O5	1.994(5)	O5–C6	1.264(9)
V1–O2	2.021(6)	O6–C6	1.258(9)
V1–O3	2.070(5)	O7–C4	1.221(9)
V1–N1	2.307(6)	C1–C2	1.517(12)
N1–C5	1.449(9)	C3–C4	1.549(10)
N1–C3	1.460(9)	C5–C6	1.506(10)
N1–C1	1.477(10)		

Bond angles		Bond angles	
O1–V1–O4	104.4(3)	C3–N1–C1	112.8(6)
O1–V1–O5	104.9(3)	C5–N1–V1	104.5(4)
O4–V1–O5	150.5(2)	C3–N1–V1	107.2(4)
O1–V1–O2	103.2(3)	C1–N1–V1	106.9(5)
O4–V1–O2	86.2(2)	C2–O3–V1	118.1(5)
O5–V1–O2	84.5(2)	C4–O4–V1	123.7(5)
O1–V1–O3	92.9(3)	C6–O5–V1	120.3(5)
O4–V1–O3	89.5(2)	N1–C1–C2	109.9(7)
O5–V1–O3	91.8(2)	O3–C2–C1	104.2(7)
O2–V1–O3	163.9(2)	N1–C3–C4	112.0(6)
O1–V1–N1	168.5(3)	O7–C4–O4	124.4(7)
O4–V1–N1	77.1(2)	O7–C4–C3	119.5(6)
O5–V1–N1	74.7(2)	O4–C4–C3	116.0(6)
O2–V1–N1	88.2(2)	N1–C5–C6	110.0(6)

O3-V1-N1	75.7(2)	O6-C6-O5	123.0(7)
C5-N1-C3	116.1(6)	O6-C6-C5	119.5(7)
C5-N1-C1	108.6(6)	O5-C6-C5	117.5(6)

For 2

Bond lengths		Bond lengths	
V1-O2	1.624(3)	V1-O1	1.663(3)
V1-O4	1.969(3)	V1-O5	1.988(3)
V1-N1	2.251(3)	V1-O3	2.287(3)
N1-C3	1.474(5)	N1-C5	1.477(5)
N1-C1	1.482(5)	C1-C2	1.500(5)
C2-O3	1.448(5)	C3-C4	1.531(5)
C4-O7	1.239(5)	C4-O4	1.293(5)
C5-C6	1.524(5)	C6-O6	1.225(5)
C6-O5	1.302(5)	O6-Na1	2.309(4)
O7-Na1 ¹	2.382(3)	Na1-W8	2.369(5)
Na1-O7 ²	2.382(3)	Na1-W10	2.368(3)
Na1-W10 ³	2.452(3)	Na1-W9	2.479(4)
Na1-Na1 ³	3.623(3)	W10-Na1 ³	2.452(3)

Bond angles		Bond angles	
O2-V1-O1	105.7(2)	O2-V1-O4	96.54(14)
O1-V1-O4	100.25(13)	O2-V1-O5	95.7(2)
O1-V1-O5	102.33(13)	O4-V1-O5	150.30(12)
O2-V1-N1	93.96(13)	O1-V1-N1	160.35(14)
O4-V1-N1	77.05(12)	O5-V1-N1	75.18(12)
O2-V1-O3	167.83(13)	O1-V1-O3	86.35(13)
O4-V1-O3	79.24(12)	O5-V1-O3	83.20(12)

N1-V1-O3	74.01(11)	C3-N1-C5	115.7(3)
C3-N1-C1	112.2(3)	C5-N1-C1	109.0(3)
C3-N1-V1	104.6(2)	C5-N1-V1	102.4(2)
C1-N1-V1	112.5(2)	N1-C1-C2	111.1(3)
O3-C2-C1	106.4(3)	N1-C3-C4	109.1(3)
O7-C4-O4	122.8(4)	O7-C4-C3	121.5(3)
O4-C4-C3	115.6(3)	N1-C5-C6	107.5(3)
O6-C6-O5	122.3(4)	O6-C6-C5	121.7(4)
O5-C6-C5	115.9(3)	C2-O3-V1	113.5(2)
C4-O4-V1	121.0(2)	C6-O5-V1	117.4(3)
C6-O6-Na1	149.2(3)	C4-O7-Na1 ¹	144.3(3)
O6-Na1-W8	85.5(2)	O6-Na1-O7 ²	90.66(13)
W8-Na1-O7 ²	103.5(2)	O6-Na1-W10	177.82(13)
W8-Na1-W10	94.4(2)	O7 ² -Na1-W10	87.25(12)
O6-Na1-W10 ³	99.15(12)	W8-Na1-W10 ³	96.8(2)
O7 ² -Na1-W10 ³	158.02(14)	W10-Na1-W10 ³	83.03(12)
O6-Na1-W9	80.3(2)	W8-Na1-W9	165.1(2)
O7 ² -Na1-W9	81.26(13)	W10-Na1-W9	100.0(2)
W10 ³ -Na1-W9	81.08(13)	O6-Na1-Na1 ³	139.98(12)
W8-Na1-Na1 ³	97.5(2)	O7 ² -Na1-Na1 ³	126.58(11)
W10-Na1-Na1 ³	42.20(8)	W10 ³ -Na1-Na1 ³	40.83(8)
W9-Na1-Na1 ³	90.52(12)	Na1-W10-Na1 ³	96.97(12)

For 3

Bond lengths		Bond lengths	
V-O1	1.6071(15)	O6-C6	1.233(2)
V-O2	1.8033(4)	O7-C4	1.239(2)
V-O5	1.9807(15)	N1-C5	1.473(2)

V-O4	1.9851(15)	N1-C3	1.478(2)
V-O3	2.1109(15)	N1-C1	1.483(2)
V-N1	2.277(2)	C1-C2	1.512(3)
O3-C	-1.446(2)	C3-C4	1.521(3)
O4-C4	1.279(2)	C5-C6	1.522(3)
O5-C6	1.295(3)		

Bond angles		Bond angles	
O1-V-O2	105.11(6)	C6-O5-V	119.20(12)
O1-V-O5	103.68(7)	C5-N1-C3	115.03(15)
O2-V-O5	90.95(5)	C5-N1-C1	109.82(14)
O1-V-O4	102.00(7)	C3-N1-C1	113.12(15)
O2-V-O4	89.29(4)	C5-N1-V	103.45(10)
O5-V-O4	153.31(6)	C3-N1-V	104.70(10)
O1-V-O3	91.89(7)	C1-N1-V	110.08(11)
O2-V-O3	162.75(5)	N1-C1-C2	109.49(15)
O5-V-O3	87.76(6)	O3-C2-C1	105.0(2)
O4-V-O3	84.25(6)	N1-C3-C4	111.11(15)
O1-V-N1	166.87(7)	O7-C4-O4	122.8(2)
O2-V-N1	88.02(4)	O7-C4-C3	119.4(2)
O5-V-N1	75.61(6)	O4-C4-C3	117.7(2)
O4-V-N1	77.72(5)	N1-C5-C6	108.37(15)
O3-V-N1	74.99(6)	O6-C6-O5	123.4(2)
V-O2-V	180.0	O6-C6-C5	120.0(2)
C2-O3-V	117.26(12)	O5-C6-C5	116.6(2)
C4-O4-V	120.01(12)		

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

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

³ Symmetry transformations used to generate equivalent atoms: $x+1, -y, -z$.

Table S-4. Anisotropic Displacement Parameters (\AA^2). The Anisotropic Displacement Factor Exponent Takes the Form: $-2\pi^2(h^2a^2U_{11} + \dots + 2hka^*b^*U_{12})$.

For 1						
	U11	U22	U33	U23	U13	U12
V1	0.0207(6)	0.0224(6)	0.0262(6)	0.0026(5)	0.0032(5)	-0.0006(5)
N1	0.021(3)	0.020(3)	0.029(3)	-0.002(3)	0.003(3)	-0.001(3)
O1	0.028(3)	0.038(3)	0.049(3)	0.013(3)	0.009(3)	0.004(3)
O2	0.029(3)	0.022(3)	0.037(3)	0.000(3)	-0.006(3)	0.006(3)
O3	0.031(3)	0.043(3)	0.026(2)	0.005(3)	0.001(2)	0.001(3)
O4	0.021(2)	0.021(2)	0.032(3)	0.002(2)	0.003(2)	0.002(2)
O5	0.032(3)	0.022(2)	0.025(2)	-0.002(2)	0.005(2)	0.003(2)
O6	0.038(3)	0.019(2)	0.036(2)	-0.006(2)	0.004(3)	0.005(3)
O7	0.028(3)	0.021(3)	0.052(3)	-0.012(3)	0.006(2)	-0.001(3)
C1	0.033(4)	0.033(4)	0.038(4)	0.000(4)	-0.007(4)	0.000(4)
C2	0.037(4)	0.048(5)	0.035(4)	0.001(4)	-0.008(4)	0.008(5)
C3	0.029(4)	0.022(3)	0.037(4)	0.000(3)	0.010(3)	-0.003(4)
C4	0.021(4)	0.022(3)	0.030(4)	0.000(3)	-0.006(3)	-0.002(3)
C5	0.033(4)	0.018(3)	0.026(3)	0.002(3)	0.001(3)	0.001(3)
C6	0.029(4)	0.028(4)	0.021(3)	-0.002(3)	-0.004(3)	-0.002(3)

For 2						
	U11	U22	U33	U23	U13	U12
V1	0.018(1)	0.012(1)	0.008(1)	-0.001(1)	0.004(1)	0.001(1)
N1	0.021(2)	0.009(1)	0.010(1)	-0.001(1)	0.004(1)	-0.003(1)
O1	0.021(1)	0.019(1)	0.013(1)	-0.003(1)	0.005(1)	0.002(1)
O2	0.024(2)	0.021(1)	0.016(1)	0.000(1)	0.004(1)	-0.003(1)
O3	0.024(2)	0.013(1)	0.014(1)	-0.004(1)	0.005(1)	-0.004(1)
O4	0.018(1)	0.015(1)	0.012(1)	-0.001(1)	0.002(1)	0.003(1)

O5	0.028(2)	0.014(1)	0.011(1)	0.001(1)	0.002(1)	0.002(1)
O6	0.052(2)	0.015(2)	0.020(2)	0.003(1)	0.007(1)	0.010(2)
O7	0.029(2)	0.017(1)	0.012(1)	0.000(1)	-0.002(1)	0.001(1)
C1	0.028(2)	0.012(2)	0.015(2)	-0.002(1)	0.011(2)	0.001(2)
C2	0.021(2)	0.014(2)	0.018(2)	-0.001(1)	0.009(2)	-0.005(2)
C3	0.024(2)	0.016(2)	0.010(2)	-0.002(1)	0.002(1)	0.001(2)
C4	0.016(2)	0.014(2)	0.013(2)	-0.001(1)	0.002(1)	-0.001(1)
C5	0.029(2)	0.009(2)	0.014(2)	-0.001(1)	0.006(2)	0.001(2)
C6	0.026(2)	0.011(2)	0.014(2)	0.000(1)	0.005(2)	-0.002(2)
Na1	0.026(1)	0.013(1)	0.013(1)	0.000(1)	0.003(1)	0.001(1)
W8	0.050(3)	0.036(2)	0.094(4)	0.015(2)	0.041(3)	-0.005(2)
W9	0.035(2)	0.051(2)	0.026(2)	0.007(2)	0.003(2)	-0.011(2)
W10	0.031(2)	0.016(1)	0.014(1)	0.001(1)	0.003(1)	-0.001(1)
W11	0.030(2)	0.034(2)	0.015(1)	0.003(1)	0.007(1)	0.000(2)

For 3

	U11	U22	U33	U23	U13	U12
V	0.0276(2)	0.0125(2)	0.0222(2)	-0.00178(10)	0.00664(12)	-0.00121(11)
O1	0.0473(9)	0.0150(6)	0.0395(8)	-0.0008(6)	0.0193(7)	-0.0032(6)
O2	0.0317(10)	0.0212(8)	0.0200(8)	-0.0023(7)	0.0086(7)	0.0000(7)
O3	0.0384(8)	0.0209(6)	0.0293(7)	0.0043(6)	0.0167(6)	0.0014(6)
O4	0.0327(7)	0.0193(6)	0.0208(6)	0.0021(5)	0.0043(5)	0.0049(5)
O5	0.0286(7)	0.0259(7)	0.0265(7)	-0.0009(5)	0.0029(5)	-0.0061(6)
O6	0.0333(8)	0.0452(10)	0.0265(7)	0.0025(7)	-0.0033(6)	0.0025(7)
O7	0.0294(7)	0.0348(8)	0.0363(8)	-0.0141(7)	-0.0071(6)	0.0104(6)
N1	0.0227(7)	0.0154(6)	0.0177(6)	0.0004(5)	0.0033(5)	0.0006(5)
N2	0.0259(13)	0.045(2)	0.049(2)	0.000	0.0088(12)	0.000
C1	0.0308(9)	0.0209(8)	0.0252(8)	0.0006(7)	0.0098(7)	0.0072(7)

C2	0.0391(11)	0.0249(9)	0.0258(9)	0.0007(7)	0.0144(8)	0.0069(8)
C3	0.0261(9)	0.0158(7)	0.0285(9)	-0.0013(7)	0.0010(7)	-0.0030(7)
C5	0.0284(9)	0.0182(8)	0.0222(8)	0.0049(6)	0.0044(7)	0.0011(7)
C6	0.0252(8)	0.0291(9)	0.0220(8)	-0.0003(7)	0.0055(7)	0.0005(7)

Table S-5. Hydrogen Atom Coordinates and Isotropic Thermal Displacement Coefficients (\AA^2).

For 1				
	x	y	z	U(eq)
H21	0.8466(141)	0.7238(92)	0.7609(46)	0.018(27)
H3	1.1403(118)	0.5525(83)	0.9909(43)	0.019(19)
H1A	1.5185(13)	0.7448(8)	0.8782(4)	0.034(22)
H1B	1.3573(13)	0.8253(8)	0.9179(4)	0.030(22)
H2A	1.4119(12)	0.5351(11)	0.9213(4)	0.048
H2B	1.4341(12)	0.6328(11)	0.9887(4)	0.048
H3A	1.3174(11)	0.6622(7)	0.7292(4)	0.046(27)
H3B	1.4834(11)	0.6266(7)	0.7823(4)	0.012(16)
H5A	1.3163(11)	0.9190(7)	0.8063(4)	0.051(28)
H5B	1.1723(11)	0.8496(7)	0.7534(4)	0.033(24)
For 2				
	x	y	z	U(eq)
H1B	0.3514(8)	0.3469(2)	-0.1298(4)	0.0021
H1C	0.4587(8)	0.3227(2)	0.0002(4)	0.0021
H2B	0.4860(7)	0.4448(2)	-0.0037(4)	0.0020
H2C	0.2372(7)	0.4525(2)	-0.0606(4)	0.0020
H3A	-0.1528(7)	0.2933(2)	-0.1500(3)	0.0020
H3B	0.0068(7)	0.3373(2)	-0.2095(3)	0.0020
H5A	0.2646(7)	0.2186(2)	-0.0646(3)	0.0021
H5B	0.0371(7)	0.2110(2)	-0.0316(3)	0.0021
H3	0.3731(5)	0.4502(2)	0.1744(2)	0.0021

For 3

	x	y	z	U(eq)
H31	0.1293(18)	0.1649(46)	0.6865(21)	0.047(9)
H21	-0.0184(26)	0.2811(61)	0.1987(28)	0.091(15)
H22	0.0305(21)	0.1438(58)	0.2465(29)	0.076(13)
H1B	0.07688(11)	0.5539(3)	0.59108(12)	0.027(6)
H1A	0.13601(11)	0.6698(3)	0.65635(12)	0.029(6)
H2A	0.17679(13)	0.4214(3)	0.74503(13)	0.038(7)
H2B	0.09101(13)	0.4253(3)	0.72578(13)	0.027(6)
H3B	0.25319(11)	0.6758(2)	0.66328(13)	0.033(7)
H3A	0.28095(11)	0.6077(2)	0.58612(13)	0.033(7)
H5B	0.19300(11)	0.5865(2)	0.46662(12)	0.028(6)
H5A	0.12866(11)	0.6886(2)	0.48929(12)	0.031(7)