Supplementary Materials

Fig. S1 A view of the asymmetric unit and some symmetry-related atoms in the structure of 1. H atoms are omitted for clarity.

Fig. S2 A view of the asymmetric unit and some symmetry-related atoms in the structure of 2. H atoms are omitted for clarity.

Fig. S3 A view of the asymmetric unit and some symmetry-related atoms in the structure of 3. The $[Co(en)_3]^{2+}$ is disorder.

Fig. S4 XPS spectrum for V in compound 1.

Fig. S5 XPS spectrum for V in compound 2.

Fig. S6 XPS spectrum for V in compound 3.

Fig. S7XPS spectrum for Ni in compound 2.

Fig. S8 XPS spectrum for Co in compound 3

Fig. S9 Emission spectrum of HTMA ligand in DMF solution at room temperature.

Fig. S10 TG curve for compound 1

Fig. S11 TG curve for compound 2

Fig. S12 TG curve for compound 3

Fig. S13 IR spectrum for compound 1

Fig. S14 IR spectrum for compound 2

Fig. S15 IR spectrum for compound 3

Table S1 Bond lengths and angles for 1-3.



Fig. S1 A view of the asymmetric unit and some symmetry-related atoms in the structure of 1. H atoms are omitted for



Fig. S2 A view of the asymmetric unit and some symmetry-related atoms in the structure of 2. H atoms are omitted for clarity.



Fig. S3 A view of the asymmetric unit and some symmetry-related atoms in the structure of 3. The $[Co(en)_3]^{2+}$ is disorder.



Fig. S4 XPS spectrum for V in compound 1.



Fig. S5 XPS spectrum for V in compound 2.



Fig. S6 XPS spectrum for V in compound 3.



Fig. S7XPS spectrum for Ni in compound 2.



Fig. S8 XPS spectrum for Co in compound 3.



Fig. S9 .Emission spectrum of HTMA ligand in DMF solution at room temperature.



Fig. S10 TG curve for compound 1 $\,$



Fig. S11 TG curve for compound $\mathbf{2}$



Fig. S12 TG curve for compound 3



Fig. S13 IR spectrum for compound 1.



Fig. S14 IR spectrum for compound 2.



Fig. S15 IR spectrum for compound 3.

| Table S1 | Bond | lengths | and | angles | for | 1-3. |
|----------|------|---------|-----|--------|-----|------|
| | | | | | | |

| Compound 1 | | | |
|-------------|------------|-------------|------------|
| V(1)-O(7) | 1.689(3) | V(2)-O(6) | 1.611(2) |
| V(1)-O(9) | 1.695(3) | V(2)-O(4) | 1.799(2) |
| V(1)-O(1)#1 | 1.9298(19) | V(2)-O(5) | 1.901(2) |
| V(1)-O(1) | 1.9298(19) | V(2)-O(1)#3 | 1.9553(19) |
| V(1)-O(3) | 2.099(3) | V(2)-O(1) | 2.023(2) |
| V(1)-O(3)#2 | 2.138(2) | V(2)-O(3) | 2.2525(7) |
| V(1)-V(4)#2 | 3.0741(15) | V(2)-V(2)#3 | 3.0174(16) |
| V(1)-V(3) | 3.0850(16) | V(2)-V(4) | 3.1125(9) |
| V(1)-V(2)#2 | 3.1454(7) | V(2)-V(1)#2 | 3.1454(7) |
| V(1)-V(2)#3 | 3.1454(7) | V(4)-O(10) | 1.603(3) |
| V(3)-O(8) | 1.603(3) | V(4)-O(2) | 1.861(3) |
| V(3)-O(2) | 1.796(3) | V(4)-O(4) | 1.891(2) |
| V(3)-O(5)#1 | 1.908(2) | V(4)-O(4)#1 | 1.891(2) |
| V(3)-O(5) | 1.908(2) | V(4)-O(9)#2 | 2.004(3) |
| V(3)-O(7) | 2.063(3) | V(4)-O(3) | 2.320(3) |
| V(3)-O(3) | 2.315(3) | V(4)-V(1)#2 | 3.0741(15) |
| V(3)-V(4) | 3.0665(11) | V(4)-V(2)#1 | 3.1125(9) |
| O(1)-V(2)#3 | 1.9553(19) | O(3)-V(2)#1 | 2.2524(7) |
| O(3)-V(1)#2 | 2.138(2) | O(9)-V(4)#2 | 2.004(3) |
| N(1)-C(4) | 1.471(4) | C(2)-N(2)#4 | 1.488(4) |
| N(1)-C(1) | 1.474(4) | C(2)-H(2A) | 0.9700 |
| N(1)-C(3) | 1.482(4) | C(2)-H(2B) | 0.9700 |
| N(2)-C(2) | 1.488(4) | C(3)-N(1)#4 | 1.482(4) |
| N(2)-C(4)#4 | 1.497(4) | C(3)-H(3A) | 0.9700 |
| N(2)-C(1) | 1.492(4) | C(3)-H(3B) | 0.9700 |

| C(1)-H(1A) | 0.9700 | C(4)-N(2)#4 | 1.497(4) |
|--------------------|------------|--------------------|------------|
| C(1)-H(1B) | 0.9700 | C(4)-H(4A) | 0.9700 |
| C(4)-H(4B) | 0.9700 | | |
| | | | |
| O(7)-V(1)-O(9) | 107.99(14) | O(7)-V(3)-V(4) | 122.44(8) |
| O(7)-V(1)-O(1)#1 | 97.45(6) | O(3)-V(3)-V(4) | 48.65(7) |
| O(9)-V(1)-O(1)#1 | 96.32(6) | O(8)-V(3)-V(1) | 130.59(13) |
| O(7)-V(1)-O(1) | 97.45(6) | O(2)-V(3)-V(1) | 125.21(9) |
| O(9)-V(1)-O(1) | 96.32(6) | O(5)#1-V(3)-V(1) | 78.80(6) |
| O(1)#1-V(1)-O(1) | 156.43(11) | O(5)-V(3)-V(1) | 78.80(6) |
| O(7)-V(1)-O(3) | 87.47(12) | O(7)-V(3)-V(1) | 30.92(8) |
| O(9)-V(1)-O(3) | 164.54(12) | O(3)-V(3)-V(1) | 42.86(6) |
| O(1)#1-V(1)-O(3) | 81.26(6) | V(4)-V(3)-V(1) | 91.52(3) |
| O(1)-V(1)-O(3) | 81.26(6) | O(10)-V(4)-O(2) | 104.16(16) |
| O(7)-V(1)-O(3)#2 | 165.95(12) | O(10)-V(4)-O(4) | 102.15(6) |
| O(9)-V(1)-O(3)#2 | 86.06(12) | O(2)-V(4)-O(4) | 90.08(6) |
| O(1)#1-V(1)-O(3)#2 | 80.56(6) | O(10)-V(4)-O(4)#1 | 102.15(6) |
| O(1)-V(1)-O(3)#2 | 80.56(6) | O(2)-V(4)-O(4)#1 | 90.08(6) |
| O(3)-V(1)-O(3)#2 | 78.47(11) | O(4)-V(4)-O(4)#1 | 154.89(12) |
| O(7)-V(1)-V(4)#2 | 145.13(10) | O(10)-V(4)-O(9)#2 | 100.28(15) |
| O(9)-V(1)-V(4)#2 | 37.14(9) | O(2)-V(4)-O(9)#2 | 155.56(12) |
| O(1)#1-V(1)-V(4)#2 | 89.08(6) | O(4)-V(4)-O(9)#2 | 84.77(6) |
| O(1)-V(1)-V(4)#2 | 89.08(6) | O(4)#1-V(4)-O(9)#2 | 84.77(6) |
| O(3)-V(1)-V(4)#2 | 127.39(8) | O(10)-V(4)-O(3) | 174.97(14) |
| O(3)#2-V(1)-V(4)#2 | 48.92(7) | O(2)-V(4)-O(3) | 80.87(11) |
| O(7)-V(1)-V(3) | 38.88(10) | O(4)-V(4)-O(3) | 77.62(6) |
| O(9)-V(1)-V(3) | 146.87(9) | O(4)#1-V(4)-O(3) | 77.62(6) |

| O(1)#1-V(1)-V(3) | 90.11(6) | O(9)#2-V(4)-O(3) | 74.69(10) |
|--------------------|------------|--------------------|-------------|
| O(1)-V(1)-V(3) | 90.11(6) | O(10)-V(4)-V(3) | 136.53(12) |
| O(3)-V(1)-V(3) | 48.60(7) | O(2)-V(4)-V(3) | 32.37(9) |
| O(3)#2-V(1)-V(3) | 127.07(7) | O(4)-V(4)-V(3) | 83.38(6) |
| V(4)#2-V(1)-V(3) | 175.99(3) | O(4)#1-V(4)-V(3) | 83.38(6) |
| O(7)-V(1)-V(2)#2 | 133.66(2) | O(9)#2-V(4)-V(3) | 123.19(8) |
| O(9)-V(1)-V(2)#2 | 84.17(7) | O(3)-V(4)-V(3) | 48.50(6) |
| O(1)#1-V(1)-V(2)#2 | 36.21(5) | O(10)-V(4)-V(1)#2 | 130.98(12) |
| O(1)-V(1)-V(2)#2 | 126.21(6) | O(2)-V(4)-V(1)#2 | 124.86(9) |
| O(3)-V(1)-V(2)#2 | 85.02(5) | O(4)-V(4)-V(1)#2 | 79.68(6) |
| O(3)#2-V(1)-V(2)#2 | 45.713(15) | O(4)#1-V(4)-V(1)#2 | 79.68(6) |
| V(4)#2-V(1)-V(2)#2 | 60.044(18) | O(9)#2-V(4)-V(1)#2 | 30.70(8) |
| V(3)-V(1)-V(2)#2 | 117.63(2) | O(3)-V(4)-V(1)#2 | 43.99(7) |
| O(7)-V(1)-V(2)#3 | 133.66(2) | V(3)-V(4)-V(1)#2 | 92.49(3) |
| O(9)-V(1)-V(2)#3 | 84.17(7) | O(10)-V(4)-V(2)#1 | 133.742(18) |
| O(1)#1-V(1)-V(2)#3 | 126.21(6) | O(2)-V(4)-V(2)#1 | 82.47(6) |
| O(1)-V(1)-V(2)#3 | 36.22(5) | O(4)-V(4)-V(2)#1 | 123.81(7) |
| O(3)-V(1)-V(2)#3 | 85.02(5) | O(4)#1-V(4)-V(2)#1 | 31.59(6) |
| O(3)#2-V(1)-V(2)#3 | 45.713(15) | O(9)#2-V(4)-V(2)#1 | 80.68(6) |
| V(4)#2-V(1)-V(2)#3 | 60.044(18) | O(3)-V(4)-V(2)#1 | 46.197(16) |
| V(3)-V(1)-V(2)#3 | 117.63(2) | V(3)-V(4)-V(2)#1 | 61.655(19) |
| V(2)#2-V(1)-V(2)#3 | 91.10(3) | V(1)#2-V(4)-V(2)#1 | 61.11(2) |
| O(6)-V(2)-O(4) | 103.46(10) | O(10)-V(4)-V(2) | 133.741(17) |
| O(6)-V(2)-O(5) | 100.81(10) | O(2)-V(4)-V(2) | 82.47(6) |
| O(4)-V(2)-O(5) | 93.19(10) | O(4)-V(4)-V(2) | 31.59(6) |
| O(6)-V(2)-O(1)#3 | 101.13(10) | O(4)#1-V(4)-V(2) | 123.82(7) |
| O(4)-V(2)-O(1)#3 | 92.28(9) | O(9)#2-V(4)-V(2) | 80.68(6) |

| O(5)-V(2)-O(1)#3 | 155.45(9) | O(3)-V(4)-V(2) | 46.197(16) |
|--------------------|------------|--------------------|------------|
| O(6)-V(2)-O(1) | 99.59(10) | V(3)-V(4)-V(2) | 61.656(18) |
| O(4)-V(2)-O(1) | 156.25(9) | V(1)#2-V(4)-V(2) | 61.11(2) |
| O(5)-V(2)-O(1) | 87.99(9) | V(2)#1-V(4)-V(2) | 92.34(3) |
| O(1)#3-V(2)-O(1) | 77.63(9) | V(1)-O(1)-V(2)#3 | 108.11(9) |
| O(6)-V(2)-O(3) | 175.11(10) | V(1)-O(1)-V(2) | 107.19(9) |
| O(4)-V(2)-O(3) | 81.25(9) | V(2)#3-O(1)-V(2) | 98.63(9) |
| O(5)-V(2)-O(3) | 80.05(9) | V(3)-O(2)-V(4) | 113.94(15) |
| O(1)#3-V(2)-O(3) | 77.17(9) | V(1)-O(3)-V(1)#2 | 101.53(11) |
| O(1)-V(2)-O(3) | 75.60(9) | V(1)-O(3)-V(2)#1 | 93.92(6) |
| O(6)-V(2)-V(2)#3 | 90.04(8) | V(1)#2-O(3)-V(2)#1 | 91.49(6) |
| O(4)-V(2)-V(2)#3 | 133.79(7) | V(1)-O(3)-V(2) | 93.92(6) |
| O(5)-V(2)-V(2)#3 | 127.83(7) | V(1)#2-O(3)-V(2) | 91.49(6) |
| O(1)#3-V(2)-V(2)#3 | 41.53(6) | V(2)#1-O(3)-V(2) | 170.89(13) |
| O(1)-V(2)-V(2)#3 | 39.84(6) | V(1)-O(3)-V(3) | 88.54(9) |
| O(3)-V(2)-V(2)#3 | 85.68(7) | V(1)#2-O(3)-V(3) | 169.94(13) |
| O(6)-V(2)-V(4) | 136.76(8) | V(2)#1-O(3)-V(3) | 87.78(6) |
| O(4)-V(2)-V(4) | 33.40(7) | V(2)-O(3)-V(3) | 87.78(6) |
| O(5)-V(2)-V(4) | 84.01(7) | V(1)-O(3)-V(4) | 171.38(13) |
| O(1)#3-V(2)-V(4) | 87.51(6) | V(1)#2-O(3)-V(4) | 87.09(9) |
| O(1)-V(2)-V(4) | 123.61(6) | V(2)#1-O(3)-V(4) | 85.78(6) |
| O(3)-V(2)-V(4) | 48.03(7) | V(2)-O(3)-V(4) | 85.78(6) |
| V(2)#3-V(2)-V(4) | 120.89(2) | V(3)-O(3)-V(4) | 82.84(9) |
| O(6)-V(2)-V(1)#2 | 136.26(8) | V(2)-O(4)-V(4) | 115.00(10) |
| O(4)-V(2)-V(1)#2 | 78.85(7) | V(2)-O(5)-V(3) | 112.47(10) |
| O(5)-V(2)-V(1)#2 | 122.82(7) | V(1)-O(7)-V(3) | 110.20(14) |
| O(1)#3-V(2)-V(1)#2 | 35.67(6) | V(1)-O(9)-V(4)#2 | 112.16(14) |

| O(1)-V(2)-V(1)#2 | 80.61(6) | C(4)-N(1)-C(1) | 109.4(3) |
|--------------------|------------|-------------------|----------|
| O(3)-V(2)-V(1)#2 | 42.80(6) | C(4)-N(1)-C(3) | 108.9(2) |
| V(2)#3-V(2)-V(1)#2 | 62.136(19) | C(1)-N(1)-C(3) | 109.0(2) |
| V(4)-V(2)-V(1)#2 | 58.84(3) | C(2)-N(2)-C(4)#4 | 109.0(2) |
| O(8)-V(3)-O(2) | 104.20(16) | C(2)-N(2)-C(1) | 109.4(2) |
| O(8)-V(3)-O(5)#1 | 101.18(6) | C(4)#4-N(2)-C(1) | 109.0(3) |
| O(2)-V(3)-O(5)#1 | 92.26(7) | N(1)-C(1)-N(2) | 110.1(2) |
| O(8)-V(3)-O(5) | 101.18(6) | N(1)-C(1)-H(1A) | 109.6 |
| O(2)-V(3)-O(5) | 92.26(7) | N(2)-C(1)-H(1A) | 109.6 |
| O(5)#1-V(3)-O(5) | 155.33(12) | N(1)-C(1)-H(1B) | 109.6 |
| O(8)-V(3)-O(7) | 99.66(15) | N(2)-C(1)-H(1B) | 109.6 |
| O(2)-V(3)-O(7) | 156.14(12) | H(1A)-C(1)-H(1B) | 108.2 |
| O(5)#1-V(3)-O(7) | 83.05(7) | N(2)-C(2)-N(2)#4 | 109.4(3) |
| O(5)-V(3)-O(7) | 83.05(7) | N(2)-C(2)-H(2A) | 109.8 |
| O(8)-V(3)-O(3) | 173.45(14) | N(2)#4-C(2)-H(2A) | 109.8 |
| O(2)-V(3)-O(3) | 82.35(11) | N(2)-C(2)-H(2B) | 109.8 |
| O(5)#1-V(3)-O(3) | 78.30(6) | N(2)#4-C(2)-H(2B) | 109.8 |
| O(5)-V(3)-O(3) | 78.30(6) | H(2A)-C(2)-H(2B) | 108.2 |
| O(7)-V(3)-O(3) | 73.79(10) | N(1)#4-C(3)-N(1) | 110.9(3) |
| O(8)-V(3)-V(4) | 137.90(13) | N(1)#4-C(3)-H(3A) | 109.5 |
| O(2)-V(3)-V(4) | 33.70(9) | N(1)-C(3)-H(3A) | 109.5 |
| O(5)#1-V(3)-V(4) | 85.20(6) | N(1)#4-C(3)-H(3B) | 109.5 |
| O(5)-V(3)-V(4) | 85.20(6) | N(1)-C(3)-H(3B) | 109.5 |
| N(2)#4-C(4)-H(4A) | 109.6 | H(3A)-C(3)-H(3B) | 108.0 |
| N(1)-C(4)-H(4B) | 109.6 | N(1)-C(4)-N(2)#4 | 110.3(2) |
| N(2)#4-C(4)-H(4B) | 109.6 | N(1)-C(4)-H(4A) | 109.6 |
| H(4A)-C(4)-H(4B) | 108.1 | | |

| Compound 2 | | | |
|---------------------|------------|--------------------|------------|
| Ni(1)-N(1) | 2.112(7) | V(3)-O(7) | 1.577(9) |
| Ni(1)-N(1)#1 | 2.112(7) | V(3)-O(6)#5 | 1.987(5) |
| Ni(1)-N(1)#2 | 2.112(7) | V(3)-O(6) | 1.987(5) |
| Ni(1)-N(2)#2 | 2.117(8) | V(3)-O(3)#5 | 2.024(6) |
| Ni(1)-N(2)#1 | 2.117(7) | V(3)-O(3) | 2.024(6) |
| Ni(1)-N(2) | 2.117(7) | V(3)-V(2)#5 | 3.0197(14) |
| V(1)-O(2) | 1.606(6) | C(1)-C(2) | 1.455(13) |
| V(1)-O(1) | 1.822(3) | C(1)-N(1) | 1.501(11) |
| V(1)-O(6)#3 | 1.895(6) | C(1)-C(3) | 1.517(12) |
| V(1)-O(3) | 1.898(6) | C(2)-N(2) | 1.481(13) |
| V(1)-O(4)#3 | 2.043(6) | O(1)-V(1)#5 | 1.822(3) |
| V(1)-V(2)#3 | 2.940(2) | O(4)-V(2)#4 | 1.887(6) |
| V(1)-V(2) | 2.9402(19) | O(4)-V(1)#4 | 2.043(5) |
| V(2)-O(5) | 1.598(5) | O(6)-V(1)#4 | 1.895(6) |
| V(2)-O(4)#3 | 1.887(6) | V(2)-O(6) | 1.917(5) |
| V(2)-O(4) | 1.895(6) | V(2)-V(1)#4 | 2.939(2) |
| V(2)-O(3) | 1.911(6) | V(2)-V(3) | 3.0197(14) |
| | | | |
| N(1)-Ni(1)-N(1)#1 | 92.0(3) | O(7)-V(3)-O(6)#5 | 105.4(3) |
| N(1)-Ni(1)-N(1)#2 | 92.0(3) | O(7)-V(3)-O(6) | 105.4(3) |
| N(1)#1-Ni(1)-N(1)#2 | 92.0(3) | O(6)#5-V(3)-O(6) | 95.6(3) |
| N(1)-Ni(1)-N(2)#2 | 97.3(3) | O(7)-V(3)-O(3)#5 | 106.1(3) |
| N(1)#1-Ni(1)-N(2)#2 | 168.4(3) | O(6)#5-V(3)-O(3)#5 | 76.7(2) |
| N(1)#2-Ni(1)-N(2)#2 | 80.8(3) | O(6)-V(3)-O(3)#5 | 148.5(2) |
| N(1)-Ni(1)-N(2)#1 | 168.4(3) | O(7)-V(3)-O(3) | 106.1(3) |
| N(1)#1-Ni(1)-N(2)#1 | 80.8(3) | O(6)#5-V(3)-O(3) | 148.5(2) |
| N(1)#2-Ni(1)-N(2)#1 | 97.3(3) | O(6)-V(3)-O(3) | 76.7(2) |
| N(2)#2-Ni(1)-N(2)#1 | 91.1(3) | O(3)#5-V(3)-O(3) | 94.0(3) |
| N(1)-Ni(1)-N(2) | 80.8(3) | O(7)-V(3)-V(2)#5 | 114.25(4) |
| N(1)#1-Ni(1)-N(2) | 97.3(3) | O(6)#5-V(3)-V(2)#5 | 38.50(16) |
| N(1)#2-Ni(1)-N(2) | 168.4(3) | O(6)-V(3)-V(2)#5 | 124.60(18) |
| N(2)#2-Ni(1)-N(2) | 91.1(3) | O(3)#5-V(3)-V(2)#5 | 38.53(16) |
| N(2)#1-Ni(1)-N(2) | 91.1(3) | O(3)-V(3)-V(2)#5 | 123.43(18) |
| O(2)-V(1)-O(1) | 103.6(4) | O(7)-V(3)-V(2) | 114.24(4) |
| O(2)-V(1)-O(6)#3 | 110.9(3) | O(6)#5-V(3)-V(2) | 124.60(18) |
| O(1)-V(1)-O(6)#3 | 90.5(3) | O(6)-V(3)-V(2) | 38.50(16) |
| O(2)-V(1)-O(3) | 111.7(3) | O(3)#5-V(3)-V(2) | 123.43(18) |
| O(1)-V(1)-O(3) | 90.1(3) | O(3)-V(3)-V(2) | 38.53(16) |
| O(6)#3-V(1)-O(3) | 135.9(3) | V(2)#5-V(3)-V(2) | 131.51(8) |
| O(2)-V(1)-O(4)#3 | 104.9(3) | C(2)-C(1)-N(1) | 108.0(7) |
| O(1)-V(1)-O(4)#3 | 151.5(3) | C(2)-C(1)-C(3) | 111.3(8) |
| O(6)#3-V(1)-O(4)#3 | 79.6(2) | N(1)-C(1)-C(3) | 113.5(8) |

| O(3)-V(1)-O(4)#3 | 79.2(2) | C(1)-C(2)-N(2) | 109.0(7) |
|--------------------|------------|--------------------|------------|
| O(2)-V(1)-V(2)#3 | 113.0(2) | C(1)-N(1)-Ni(1) | 108.8(5) |
| O(1)-V(1)-V(2)#3 | 125.6(3) | C(2)-N(2)-Ni(1) | 108.5(5) |
| O(6)#3-V(1)-V(2)#3 | 39.82(16) | V(1)#5-O(1)-V(1) | 139.8(5) |
| O(3)-V(1)-V(2)#3 | 110.57(18) | V(1)-O(3)-V(2) | 101.0(3) |
| O(4)#3-V(1)-V(2)#3 | 39.82(16) | V(1)-O(3)-V(3) | 137.8(3) |
| O(2)-V(1)-V(2) | 113.7(3) | V(2)-O(3)-V(3) | 100.2(3) |
| O(1)-V(1)-V(2) | 125.1(3) | V(2)#4-O(4)-V(2) | 140.2(3) |
| O(6)#3-V(1)-V(2) | 110.65(17) | V(2)#4-O(4)-V(1)#4 | 96.8(2) |
| O(3)-V(1)-V(2) | 39.65(17) | V(2)-O(4)-V(1)#4 | 96.5(2) |
| O(4)#3-V(1)-V(2) | 39.59(16) | V(1)#4-O(6)-V(2) | 100.9(2) |
| V(2)#3-V(1)-V(2) | 74.41(6) | V(1)#4-O(6)-V(3) | 137.5(3) |
| O(5)-V(2)-O(4)#3 | 106.5(3) | V(2)-O(6)-V(3) | 101.3(3) |
| O(5)-V(2)-O(4) | 107.1(3) | O(5)-V(2)-V(1) | 112.0(2) |
| O(4)#3-V(2)-O(4) | 93.6(3) | O(4)#3-V(2)-V(1) | 43.62(17) |
| O(5)-V(2)-O(3) | 106.7(3) | O(4)-V(2)-V(1) | 128.08(17) |
| O(4)#3-V(2)-O(3) | 82.9(2) | O(3)-V(2)-V(1) | 39.31(18) |
| O(4)-V(2)-O(3) | 145.6(2) | O(6)-V(2)-V(1) | 114.88(17) |
| O(5)-V(2)-O(6) | 107.4(3) | V(1)#4-V(2)-V(1) | 133.83(6) |
| O(4)#3-V(2)-O(6) | 145.5(2) | O(5)-V(2)-V(3) | 116.9(2) |
| O(4)-V(2)-O(6) | 82.9(2) | O(4)#3-V(2)-V(3) | 115.36(17) |
| O(3)-V(2)-O(6) | 81.1(2) | O(4)-V(2)-V(3) | 114.55(16) |
| O(5)-V(2)-V(1)#4 | 112.8(2) | O(3)-V(2)-V(3) | 41.26(19) |
| O(4)#3-V(2)-V(1)#4 | 128.18(17) | O(6)-V(2)-V(3) | 40.18(17) |
| O(4)-V(2)-V(1)#4 | 43.66(17) | V(1)#4-V(2)-V(3) | 74.76(5) |
| O(3)-V(2)-V(1)#4 | 115.01(19) | V(1)-V(2)-V(3) | 75.72(5) |
| O(6)-V(2)-V(1)#4 | 39.28(16) | | |
| Compound 3 | | | |
| V(1)-O(6) | 1.607(13) | Co(1)-N(1)#7 | 1.952(10) |
| V(1)-O(1)#1 | 1.972(6) | Co(1)-N(1)#5 | 1.952(10) |
| V(1)-O(1)#2 | 1.972(6) | Co(1)-N(1)#6 | 1.953(10) |
| V(1)-O(1) | 1.972(6) | Co(1)-N(1)#4 | 1.953(10) |
| V(1)-O(1)#3 | 1.972(6) | Co(1)-N(1) | 1.953(10) |
| V(1)-V(3)#1 | 2.9924(17) | Co(1)-N(1)#3 | 1.953(10) |
| V(1)-V(3) | 2.9925(17) | Co(1)-N(2)#3 | 1.974(9) |
| V(2)-O(5) | 1.597(8) | Co(1)-N(2) | 1.974(9) |
| V(2)-O(4) | 1.842(5) | Co(1)-N(2)#4 | 1.974(9) |
| V(2)-O(1)#4 | 1.895(7) | Co(1)-N(2)#6 | 1.974(9) |
| V(2)-O(1) | 1.895(7) | Co(1)-N(2)#5 | 1.974(9) |
| V(2)-O(2) | 2.055(7) | Co(1)-N(2)#7 | 1.974(9) |
| V(2)-V(3)#5 | 2.9337(17) | C(1)-N(1)#3 | 1.493(14) |
| V(2)-V(3) | 2.9338(17) | C(1)-N(1) | 1.493(14) |
| V(3)-O(3) | 1.614(6) | C(1)-C(2) | 1.511(15) |

| V(3)-O(2)#6 | 1.893(2) | C(2)-N(2) | 1.536(13) |
|--------------------|------------|---------------------|-----------|
| V(3)-O(2) | 1.893(2) | C(2)-N(2)#3 | 1.536(13) |
| V(3)-O(1) | 1.925(5) | O(2)-V(3)#5 | 1.893(2) |
| V(3)-O(1)#3 | 1.925(5) | O(4)-V(2)#1 | 1.842(5) |
| V(3)-V(2)#6 | 2.9337(17) | | |
| | | | |
| O(6)-V(1)-O(1)#1 | 105.97(16) | N(1)#5-Co(1)-N(2)#3 | 173.2(4) |
| O(6)-V(1)-O(1)#2 | 105.97(16) | N(1)#6-Co(1)-N(2)#3 | 94.0(4) |
| O(1)#1-V(1)-O(1)#2 | 78.3(3) | N(1)#4-Co(1)-N(2)#3 | 129.6(4) |
| O(6)-V(1)-O(1) | 105.97(16) | N(1)-Co(1)-N(2)#3 | 84.5(4) |
| O(1)#1-V(1)-O(1) | 93.0(3) | N(1)#3-Co(1)-N(2)#3 | 69.2(4) |
| O(1)#2-V(1)-O(1) | 148.1(3) | N(1)#7-Co(1)-N(2) | 173.2(4) |
| O(6)-V(1)-O(1)#3 | 105.97(16) | N(1)#5-Co(1)-N(2) | 133.2(5) |
| O(1)#1-V(1)-O(1)#3 | 148.1(3) | N(1)#6-Co(1)-N(2) | 129.6(4) |
| O(1)#2-V(1)-O(1)#3 | 93.0(3) | N(1)#4-Co(1)-N(2) | 94.0(4) |
| O(1)-V(1)-O(1)#3 | 78.3(3) | N(1)-Co(1)-N(2) | 69.2(4) |
| O(6)-V(1)-V(3)#1 | 114.15(5) | N(1)#3-Co(1)-N(2) | 84.5(4) |
| O(1)#1-V(1)-V(3)#1 | 39.26(16) | N(2)#3-Co(1)-N(2) | 40.2(6) |
| O(1)#2-V(1)-V(3)#1 | 39.26(16) | N(1)#7-Co(1)-N(2)#4 | 129.6(4) |
| O(1)-V(1)-V(3)#1 | 123.31(18) | N(1)#5-Co(1)-N(2)#4 | 84.5(4) |
| O(1)#3-V(1)-V(3)#1 | 123.31(18) | N(1)#6-Co(1)-N(2)#4 | 173.2(4) |
| O(6)-V(1)-V(3) | 114.15(5) | N(1)#4-Co(1)-N(2)#4 | 69.2(4) |
| O(1)#1-V(1)-V(3) | 123.31(18) | N(1)-Co(1)-N(2)#4 | 94.0(4) |
| O(1)#2-V(1)-V(3) | 123.31(18) | N(1)#3-Co(1)-N(2)#4 | 133.2(4) |
| O(1)-V(1)-V(3) | 39.26(16) | N(2)#3-Co(1)-N(2)#4 | 90.4(4) |
| O(1)#3-V(1)-V(3) | 39.26(16) | N(2)-Co(1)-N(2)#4 | 56.4(6) |
| V(3)#1-V(1)-V(3) | 131.70(10) | N(1)#7-Co(1)-N(2)#6 | 84.5(4) |
| O(5)-V(2)-O(4) | 104.3(5) | N(1)#5-Co(1)-N(2)#6 | 129.6(4) |
| O(5)-V(2)-O(1)#4 | 112.09(16) | N(1)#6-Co(1)-N(2)#6 | 69.2(4) |
| O(4)-V(2)-O(1)#4 | 89.8(2) | N(1)#4-Co(1)-N(2)#6 | 173.2(4) |
| O(5)-V(2)-O(1) | 112.10(16) | N(1)-Co(1)-N(2)#6 | 133.2(4) |
| O(4)-V(2)-O(1) | 89.8(2) | N(1)#3-Co(1)-N(2)#6 | 94.0(4) |
| O(1)#4-V(2)-O(1) | 134.4(3) | N(2)#3-Co(1)-N(2)#6 | 56.4(6) |
| O(5)-V(2)-O(2) | 102.5(4) | N(2)-Co(1)-N(2)#6 | 90.4(4) |
| O(4)-V(2)-O(2) | 153.2(4) | N(2)#4-Co(1)-N(2)#6 | 109.4(5) |
| O(1)#4-V(2)-O(2) | 80.11(16) | N(1)#7-Co(1)-N(2)#5 | 94.0(4) |
| O(1)-V(2)-O(2) | 80.11(16) | N(1)#5-Co(1)-N(2)#5 | 69.2(4) |
| O(5)-V(2)-V(3)#5 | 111.8(3) | N(1)#6-Co(1)-N(2)#5 | 133.2(4) |
| O(4)-V(2)-V(3)#5 | 126.1(2) | N(1)#4-Co(1)-N(2)#5 | 84.5(4) |
| O(1)#4-V(2)-V(3)#5 | 40.20(15) | N(1)-Co(1)-N(2)#5 | 129.6(5) |
| O(1)-V(2)-V(3)#5 | 110.74(17) | N(1)#3-Co(1)-N(2)#5 | 173.2(4) |
| O(2)-V(2)-V(3)#5 | 39.93(6) | N(2)#3-Co(1)-N(2)#5 | 109.4(5) |
| O(5)-V(2)-V(3) | 111.8(3) | N(2)-Co(1)-N(2)#5 | 90.4(4) |
| O(4)-V(2)-V(3) | 126.1(2) | N(2)#4-Co(1)-N(2)#5 | 40.2(6) |

| O(1)#4-V(2)-V(3) | 110.74(17) | N(2)#6-Co(1)-N(2)#5 | 90.4(4) |
|---------------------|------------|---------------------|-----------|
| O(1)-V(2)-V(3) | 40.20(15) | N(1)#7-Co(1)-N(2)#7 | 69.2(4) |
| O(2)-V(2)-V(3) | 39.93(6) | N(1)#5-Co(1)-N(2)#7 | 94.0(4) |
| V(3)#5-V(2)-V(3) | 74.64(7) | N(1)#6-Co(1)-N(2)#7 | 84.5(4) |
| O(3)-V(3)-O(2)#6 | 106.3(2) | N(1)#4-Co(1)-N(2)#7 | 133.2(4) |
| O(3)-V(3)-O(2) | 106.3(2) | N(1)-Co(1)-N(2)#7 | 173.2(4) |
| O(2)#6-V(3)-O(2) | 92.6(4) | N(1)#3-Co(1)-N(2)#7 | 129.6(5) |
| O(3)-V(3)-O(1) | 107.7(2) | N(2)#3-Co(1)-N(2)#7 | 90.4(4) |
| O(2)#6-V(3)-O(1) | 145.5(2) | N(2)-Co(1)-N(2)#7 | 109.4(5) |
| O(2)-V(3)-O(1) | 83.6(3) | N(2)#4-Co(1)-N(2)#7 | 90.4(4) |
| O(3)-V(3)-O(1)#3 | 107.7(2) | N(2)#6-Co(1)-N(2)#7 | 40.2(6) |
| O(2)#6-V(3)-O(1)#3 | 83.6(3) | N(2)#5-Co(1)-N(2)#7 | 56.4(6) |
| O(2)-V(3)-O(1)#3 | 145.5(2) | N(1)#3-C(1)-N(1) | 59.0(9) |
| O(1)-V(3)-O(1)#3 | 80.6(4) | N(1)#3-C(1)-C(2) | 103.4(7) |
| O(3)-V(3)-V(2)#6 | 112.10(5) | N(1)-C(1)-C(2) | 103.4(7) |
| O(2)#6-V(3)-V(2)#6 | 44.18(19) | C(1)-C(2)-N(2) | 104.0(7) |
| O(2)-V(3)-V(2)#6 | 128.10(19) | C(1)-C(2)-N(2)#3 | 104.0(7) |
| O(1)-V(3)-V(2)#6 | 114.87(17) | N(2)-C(2)-N(2)#3 | 52.4(8) |
| O(1)#3-V(3)-V(2)#6 | 39.45(19) | C(1)-N(1)-Co(1) | 109.4(6) |
| O(3)-V(3)-V(2) | 112.10(5) | C(2)-N(2)-Co(1) | 108.7(6) |
| O(2)#6-V(3)-V(2) | 128.10(19) | V(2)-O(1)-V(3) | 100.4(2) |
| O(2)-V(3)-V(2) | 44.18(19) | V(2)-O(1)-V(1) | 139.8(3) |
| O(1)-V(3)-V(2) | 39.45(19) | V(3)-O(1)-V(1) | 100.3(3) |
| O(1)#3-V(3)-V(2) | 114.87(17) | V(3)#5-O(2)-V(3) | 140.0(3) |
| V(2)#6-V(3)-V(2) | 134.55(8) | V(3)#5-O(2)-V(2) | 95.90(19) |
| O(3)-V(3)-V(1) | 117.0(2) | V(3)-O(2)-V(2) | 95.90(19) |
| O(2)#6-V(3)-V(1) | 115.78(18) | V(2)#1-O(4)-V(2) | 136.2(7) |
| O(2)-V(3)-V(1) | 115.78(18) | N(1)#6-Co(1)-N(1)#4 | 111.4(6) |
| O(1)-V(3)-V(1) | 40.41(18) | N(1)#7-Co(1)-N(1) | 111.4(6) |
| O(1)#3-V(3)-V(1) | 40.41(18) | N(1)#5-Co(1)-N(1) | 91.5(4) |
| V(2)#6-V(3)-V(1) | 75.58(4) | N(1)#6-Co(1)-N(1) | 91.5(4) |
| V(2)-V(3)-V(1) | 75.58(4) | N(1)#4-Co(1)-N(1) | 53.5(6) |
| N(1)#7-Co(1)-N(1)#5 | 53.5(6) | N(1)#7-Co(1)-N(1)#3 | 91.5(4) |
| N(1)#7-Co(1)-N(1)#6 | 44.2(7) | N(1)#5-Co(1)-N(1)#3 | 111.4(6) |
| N(1)#5-Co(1)-N(1)#6 | 91.5(4) | N(1)#6-Co(1)-N(1)#3 | 53.5(6) |
| N(1)#7-Co(1)-N(1)#4 | 91.5(4) | N(1)#4-Co(1)-N(1)#3 | 91.5(4) |
| N(1)#5-Co(1)-N(1)#4 | 44.2(7) | N(1)-Co(1)-N(1)#3 | 44.2(7) |
| N(1)#7-Co(1)-N(2)#3 | 133.2(5) | | |

Symmetry transformations used to generate equivalent atoms: #1 x,-y,z; #2 -x,-y,-z+1; #3 -x,y,-z+1; #4 -x+1,y,-z for **1.** #1 -y+1,x-y,z; #2 -x+y+1,-x+1,z; #3 -y+1,x-y+1,z; #4 -x+y,-x+1,z; #5 x,y,-z+3/2 for **2.** #1 x,y,-z+1/2; #2 -y+1,-x+1,-z+1/2; #3 -y+1,-x+1,z; #4 x,x-y+1,z; #5 -y+1,x-y+1,z; #6 -x+y,-x+1,z; #7 -x+y,y,z for **3.**