Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Structural diversity and photocatalytic activities of six Co(II)/Ni(II) complexes with three flexible phenylenediacetate isomers

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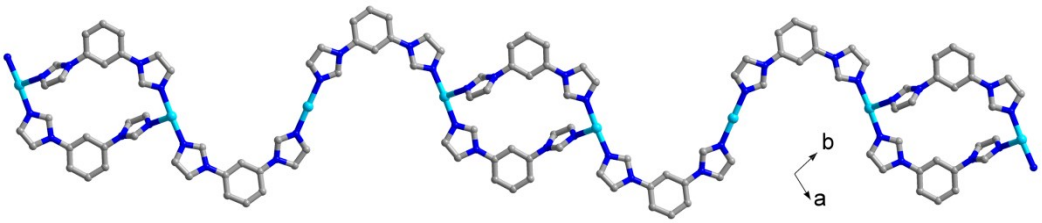


Fig. S1 View of the 1D loop containing polymer chain of **1** along *ab* plan.

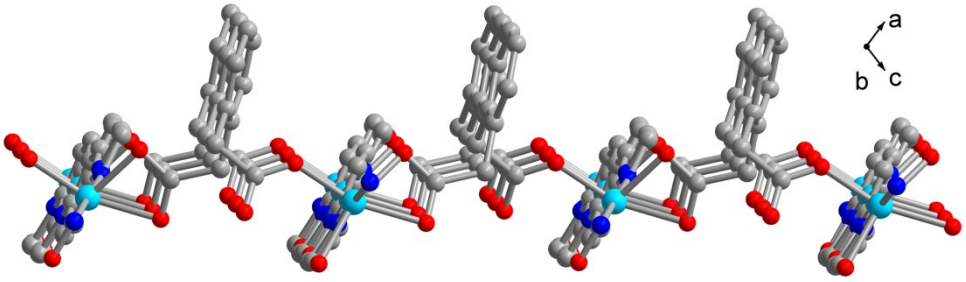


Fig. S2 Ball-and-stick view of 2D layer along *ac* plan in **4**.

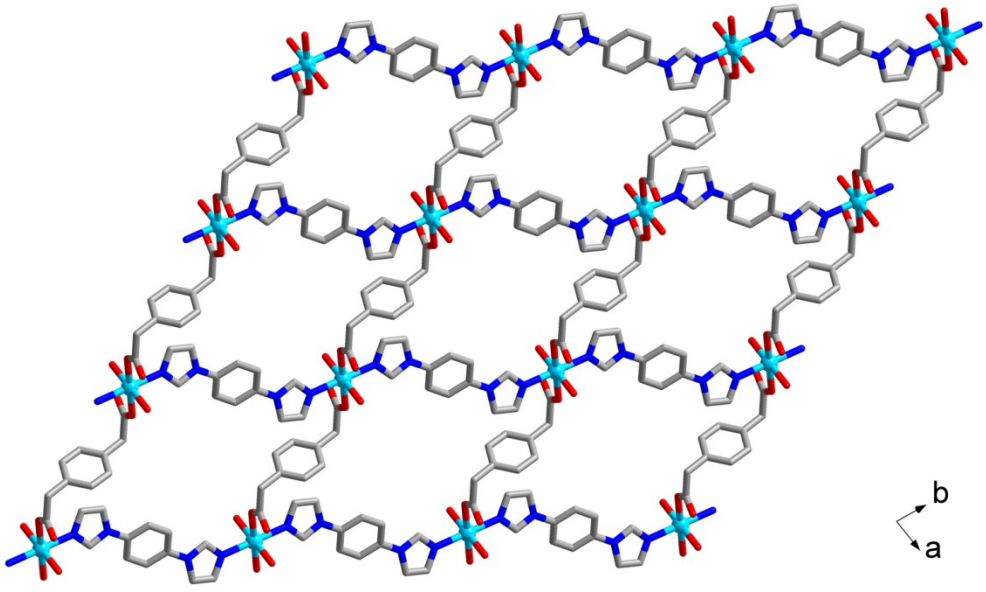
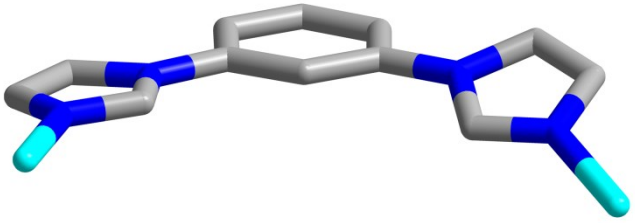
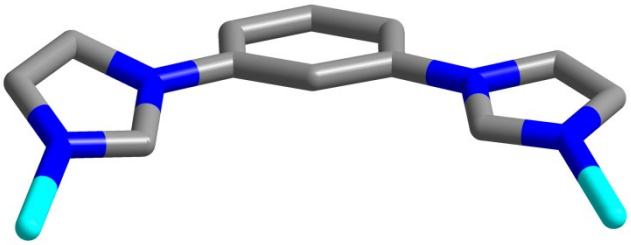


Fig. S3 Ball-and-stick view of 2D layer along *ab* plan in **6**.



(1)



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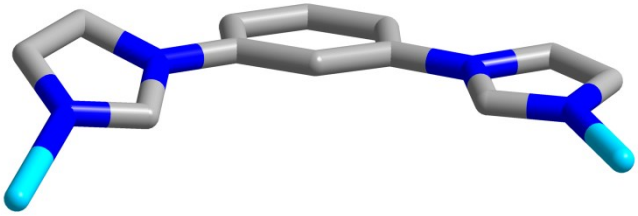

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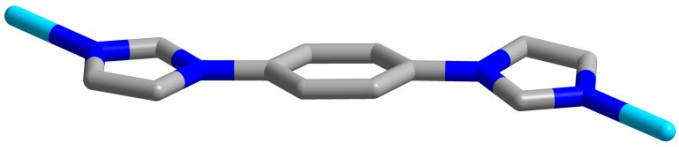

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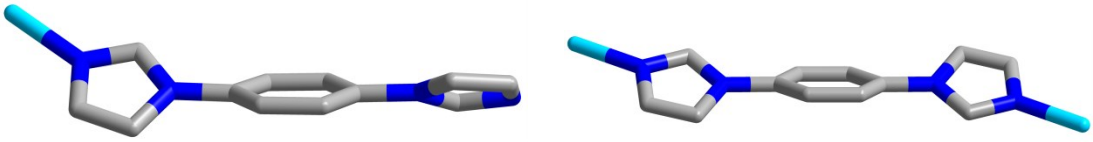
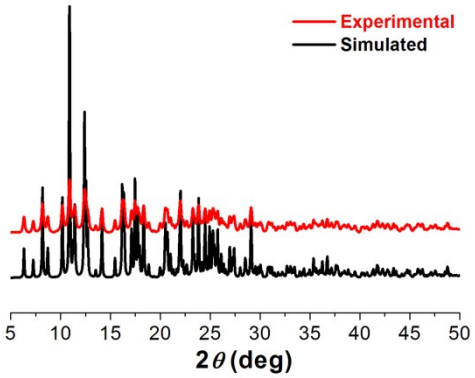
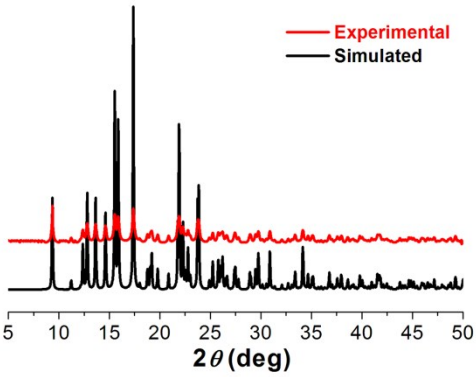


(5)

Fig. S4 Coordination modes and conformations of bis(1-imidazoly)benzene (bib) ligands in complexes **1**-**6**.



(1)



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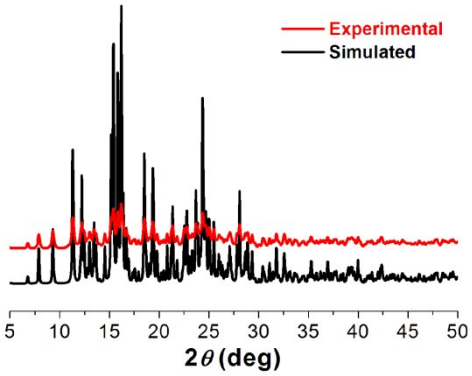

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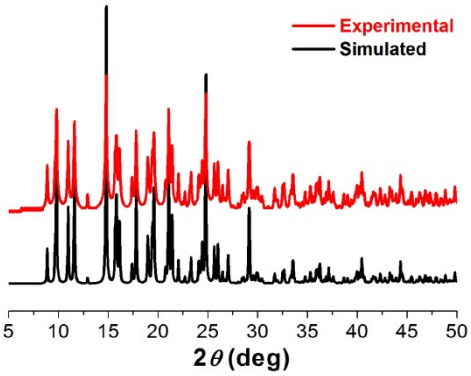

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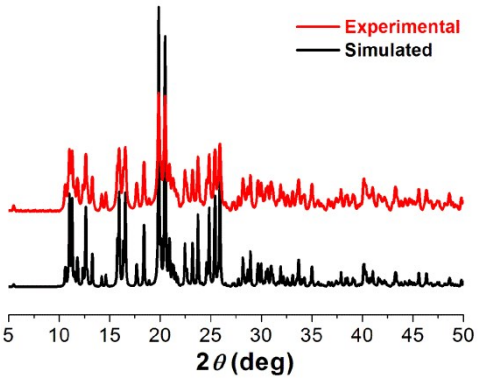

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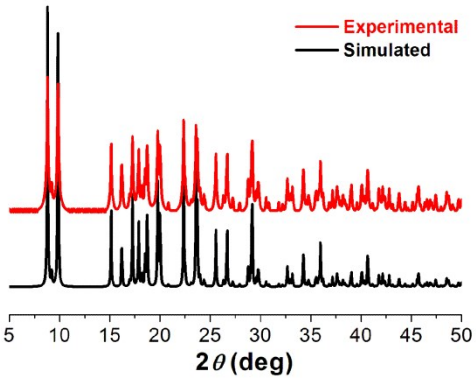


(6)

Fig. S5 PXRD patterns of complexes **1-6**.

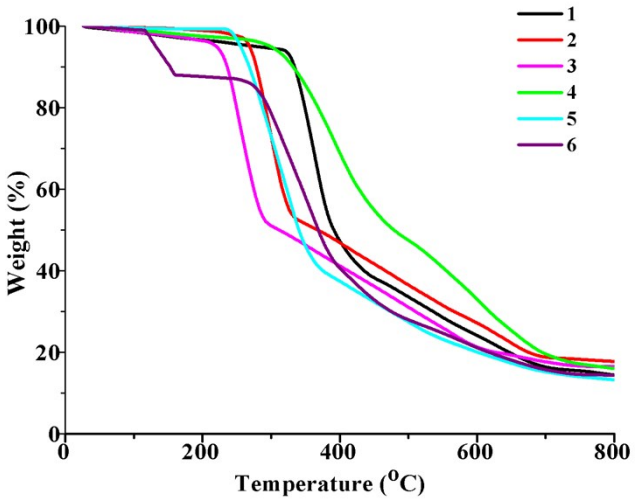


Fig. S6 Thermal gravimetric analysis (TGA) curves of complexes **1-6**.

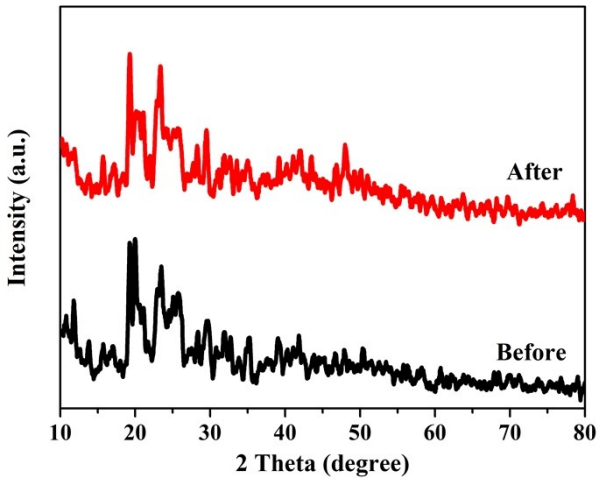


Fig. S7 The PXRD pattern of the complex 4 before and after photocatalytic reaction.

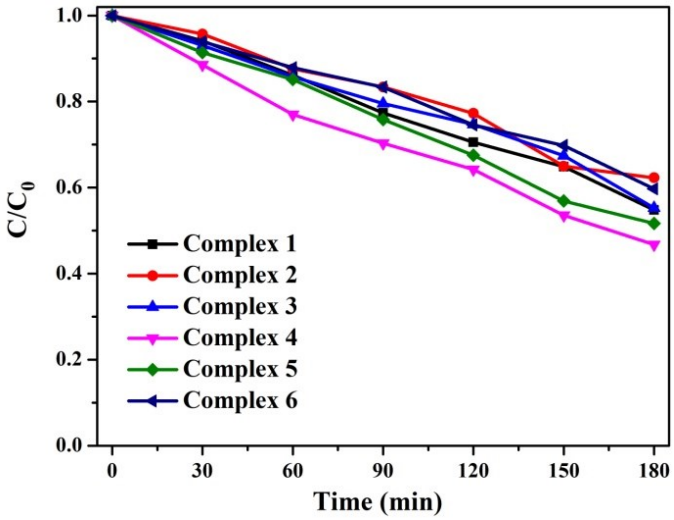


Fig. S8 Photocatalytic degradation of MB as a function of irradiation time for different samples without H_2O_2.

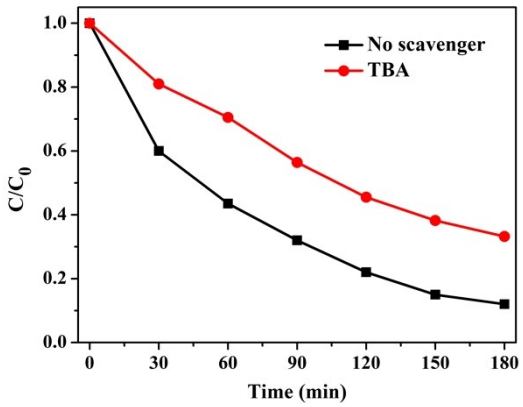
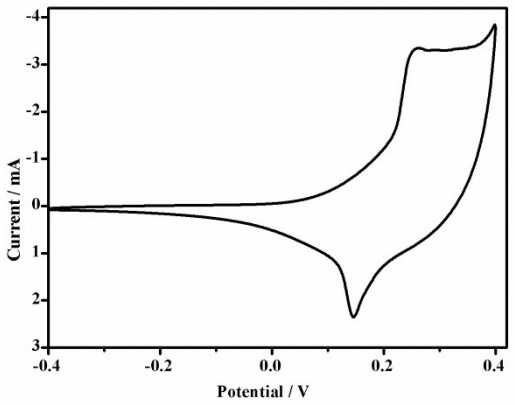
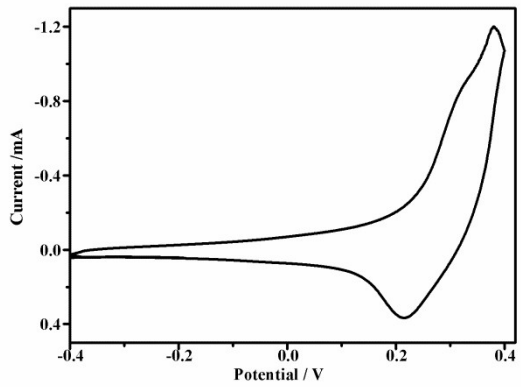


Fig. S9 Photodegradation efficiency of MB in the presence of TBA scavenger over complex 4.



(a)



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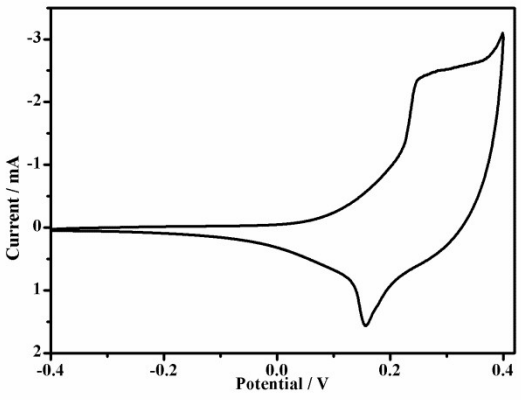

(c)

Fig. S10 Cyclic voltammograms of complexes **4**–**6 (a** for 4, **b** for 5, **c** for 6**)**.

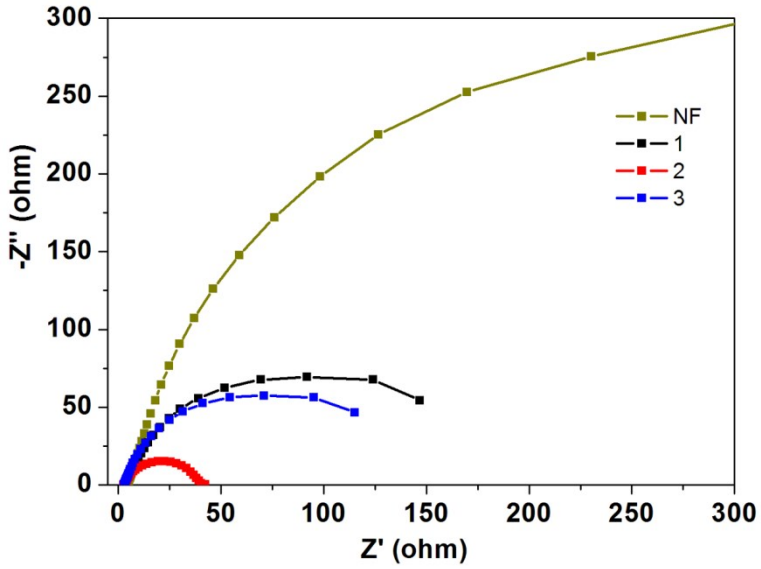

Fig. S11 Electrochemical impedance spectroscopy (EIS) Nyquist plots of complexes **1**–**3** and blank nickel foam tested in 0.1 M KOH.

Table S1. Selected Bond Lengths (Å) and Bond Angles (º) for Complexes **1-6**.

1

Bond	Dist.	Bond	Dist.	Bond	Dist.
Ni(1)-O(1)	2.068(2)	Ni(2)-O(3)	2.055(2)	Ni(1)-N(4B)	2.069(2)
Ni(1)-O(1A)	2.068(2)	Ni(2)-O(4)	2.073(2)	Ni(1)-N(4C)	2.069(2)
Ni(1)-O(8)	2.099(2)	Ni(2)-O(6)	2.128(2)	Ni(2)-N(5)	2.079(3)
Ni(1)-O(8A)	2.099(2)	Ni(2)-N(1)	2.069(2)	Ni(2)-N(8D)	2.081(2)
Angle	(°)	Angle	(°)	Angle	(°)
O(1A)-Ni(1)-O(1)	180.0	N(4C)-Ni(1)-O(8)	87.56(9)	O(4)-Ni(2)-O(6)	94.98(9)
O(1)-Ni(1)-O(8A)	88.09(9)	N(4C)-Ni(1)-O(8A)	92.44(9)	O(4)-Ni(2)-N(5)	87.07(10)
O(1)-Ni(1)-O(8)	91.91(9)	N(4B)-Ni(1)-O(8A)	87.56(9)	O(4)-Ni(2)-N(8D)	88.73(9)
O(1A)-Ni(1)-O(8A)	91.91(9)	N(4B)-Ni(1)-O(8)	92.44(9)	N(1)-Ni(2)-O(4)	92.99(9)
O(1A)-Ni(1)-O(8)	88.09(9)	N(4C)-Ni(1)-N(4B)	180.0	N(1)-Ni(2)-O(6)	89.48(10)
O(1A)-Ni(1)-N(4C)	88.67(9)	O(3)-Ni(2)-O(4)	174.62(8)	N(1)-Ni(2)-N(5)	176.11(10)
O(1)-Ni(1)-N(4C)	91.33(9)	O(3)-Ni(2)-O(6)	90.14(9)	N(1)-Ni(2)-N(8D)	94.17(9)
O(1)-Ni(1)-N(4B)	88.67(9)	O(3)-Ni(2)-N(1)	88.72(9)	N(5)-Ni(2)-O(6)	86.64(11)
O(1A)-Ni(1)-N(4B)	91.33(9)	O(3)-Ni(2)-N(5)	91.57(10)	N(5)-Ni(2)-N(8D)	89.72(10)
O(8)-Ni(1)-O(8A)	180.0	O(3)-Ni(2)-N(8D)	86.06(9)	N(8D)-Ni(2)-O(6)	174.66(9)

2

Bond	Dist.	Bond	Dist.	Bond	Dist.
Ni(1)-O(1A)	2.1186(16)	Ni(1)-O(2A)	2.136(2)	Ni(1)-O(3)	2.116(2)
Ni(1)-O(4)	2.1366(18)	Ni(1)-N(1)	2.041(2)	Ni(1)-N(4A)	2.025(3)
Angle	(°)	Angle	(°)	Angle	(°)
O(1A)-Ni(1)-O(2A)	61.61(7)	O(1A)-Ni(1)-O(4)	162.55(8)	O(2A)-Ni(1)-O(4)	105.46(8)
O(3)-Ni(1)-O(1A)	105.01(8)	O(3)-Ni(1)-O(2A)	91.97(10)	O(3)-Ni(1)-O(4)	61.86(7)
N(1)-Ni(1)-O(1A)	97.32(8)	N(1)-Ni(1)-O(2A)	94.92(10)	N(1)-Ni(1)-O(3)	157.26(8)
N(1)-Ni(1)-O(4)	95.41(8)	N(4A)-Ni(1)-O(1A)	95.27(8)	N(4A)-Ni(1)-O(2A)	156.37(8)
N(4A)-Ni(1)-O(3)	89.43(10)	N(4A)-Ni(1)-O(4)	95.98(9)	N(4A)-Ni(1)-N(1)	92.80(10)

3

Bond	Dist.	Bond	Dist.	Bond	Dist.
Ni(1)-O(1)	2.154(2)	Ni(1)-O(2)	2.091(2)	Ni(1)-O(3A)	2.083(2)
Ni(1)-O(4A)	2.153(2)	Ni(1)-N(1)	2.023(2)	Ni(1)-N(4B)	2.039(2)

Angle	(°)	Angle	(°)	Angle	(°)
O(2)-Ni(1)-O(1)	62.31(7)	O(2)-Ni(1)-O(4A)	100.32(9)	O(3A)-Ni(1)-O(1)	98.38(8)
O(3A)-Ni(1)-O(2)	155.68(8)	O(3A)-Ni(1)-O(4A)	62.21(8)	O(4A)-Ni(1)-O(1)	87.80(8)
N(1)-Ni(1)-O(1)	90.35(9)	N(1)-Ni(1)-O(2)	98.80(9)	N(1)-Ni(1)-O(3A)	95.77(9)
N(1)-Ni(1)-O(4A)	157.30(10)	N(1)-Ni(1)-N(4B)	96.97(10)	N(4B)-Ni(1)-O(1)	162.85(9)
N(4B)-Ni(1)-O(2)	101.12(8)	N(4B)-Ni(1)-O(3A)	96.29(9)	N(4B)-Ni(1)-O(4A)	91.23(9)

4

Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(4)	2.158(2)	Co(1)-O(2A)	1.996(2)	Co(1)-O(3)	2.273(3)
Co(1)-O(5)	2.149(3)	Co(1)-N(1)	2.118(3)	Co(1)-N(4B)	2.107(3)
Angle	(°)	Angle	(°)	Angle	(°)
O(1)-Co(1)-O(2)	59.63(9)	O(4A)-Co(1)-O(2)	160.99(11)	O(4A)-Co(1)-O(1)	101.37(10)
O(4A)-Co(1)-O(5)	93.95(12)	O(4A)-Co(1)-N(4B)	92.53(12)	O(4A)-Co(1)-N(1)	88.41(12)
O(5)-Co(1)-O(2)	104.93(11)	O(5)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(2)	88.88(11)
N(4B)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(5)	92.45(11)	N(4B)-Co(1)-N(1)	178.93(12)
N(1)-Co(1)-O(2)	90.39(11)	N(1)-Co(1)-O(1)	88.76(10)	N(1)-Co(1)-O(5)	86.98(11)

5

Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(2)	2.206(3)	Co(1)-O(1)	2.199(2)	Co(1)-O(4A)	2.042(3)
Co(1)-O(3A)	2.149(3)	Co(1)-N(1)	2.064(2)	Co(1)-N(5)	2.043(2)
Angle	(°)	Angle	(°)	Angle	(°)
O(4)-Co(1)-O(3)	58.14(7)	O(2A)-Co(1)-O(4)	94.97(8)	O(2A)-Co(1)-O(3)	145.43(9)
O(2A)-Co(1)-N(1)	121.76(9)	O(2A)-Co(1)-N(5)	96.95(8)	O(4)-Co(1)-N(1)	99.81(9)
N(1)-Co(1)-O(3)	86.62(8)	N(5)-Co(1)-O(4)	130.40(9)	N(5)-Co(1)-N(1)	113.69(11)
N(4B)-Co(1)-O(1)	163.98(11)	N(4B)-Co(1)-O(5)	92.45(11)	N(4B)-Co(1)-N(1)	178.93(12)
N(1)-Co(1)-O(2)	90.39(11)	N(1)-Co(1)-O(1)	88.76(10)	N(1)-Co(1)-O(5)	86.98(11)

6

Bond	Dist.	Bond	Dist.	Bond	Dist.
Co(1)-O(1)	2.1176(19)	Co(1)-O(1A)	2.1176(19)	Co(1)-N(1)	2.104(2)
Co(1)-N(1A)	2.104(2)	Co(1)-O(2)	2.1405(17)	Co(1)-N(2A)	2.1406(17)
Angle	(°)	Angle	(°)	Angle	(°)
N(1)-Co(1)-N(1A)	180.0	N(1)-Co(1)-O(1)	87.76(8)	N(1)-Co(1)-O(1A)	92.24(8)

N(1A)-Co(1)-O(1A)	92.24(9)	N(1A)-Co(1)-O(1)	87.76(8)	O(1)-Co(1)-O(1A)	180.0
N(1)-Co(1)-O(2)	89.23(8)	N(1)-Co(1)-O(2A)	90.77(8)	O(1)-Co(1)-O(2)	88.17(7)
O(1)-Co(1)-O(2A)	91.83(7)	N(1)-Co(1)-O(2)	90.775(8)	N(1)-Co(1)-O(2A)	89.23(8)
O(1A)-Co(1)-O(2)	91.83(7)	O(1A)-Co(1)-O(2A)	88.17(7)	O(2)-Co(1)-O(2A)	180.0

Symmetry code:

1 A: 1-x, -y, -z; B: 2-x, 1-y, 1-z; C: -1+x, -1+y, +z; D: 1-x, -y, 1-z.

2 A: -x+1/2, y-1/2, -z+1/2.

3 A: -x+3/2, y+1/2, z; B: -x+3/2, y-1/2, z.

4 A: x-1/2, -y+1/2, z-1/2; B: x, y-1, z; C: x+1/2, -y+1/2, +z; D: x, y+1, z.

5 A: x-1, y-1, z; B: -x-1, -y, -z+2; C: x+1, y+1, z.

6 A: x-1/2, -y+1/2, z-1/2; B: x, y-1, z; C: x+1/2, -y+1/2, +z; D: x, y+1, z.