Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Trinuclear nickel and cobalt complexes containing unsymmetrical tripodal tetradentate ligands: syntheses, structural, magnetic, and catalytic properties

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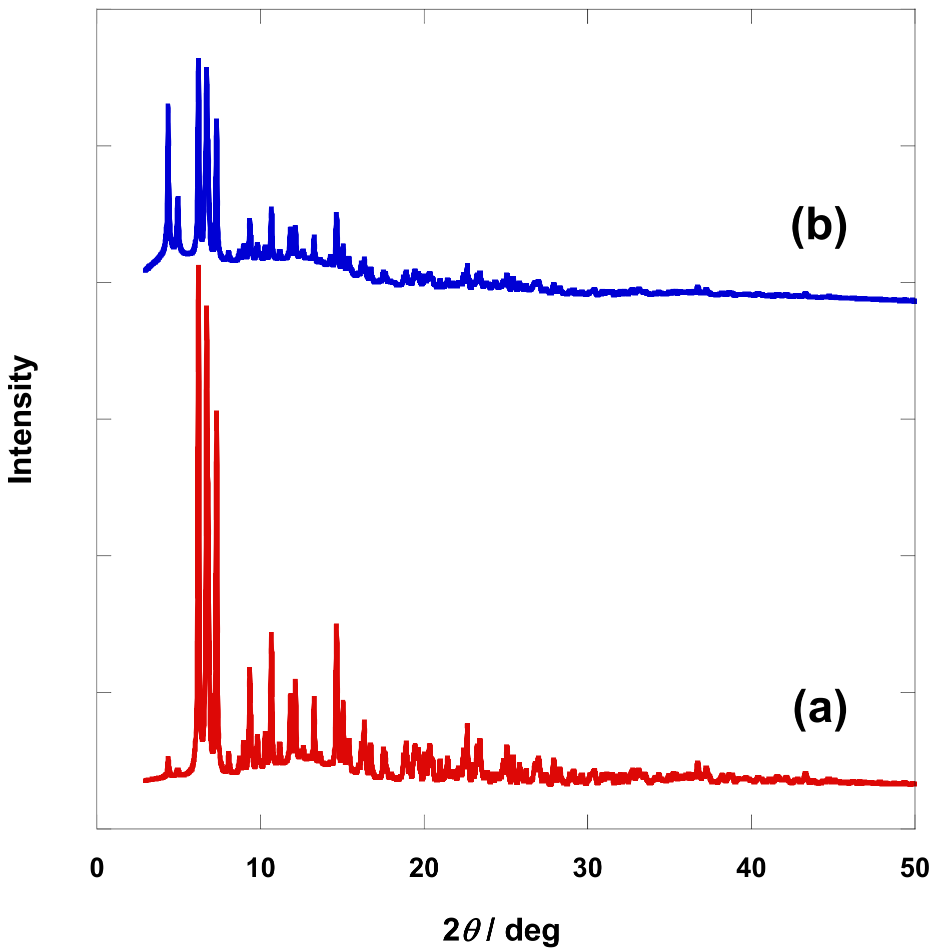


Fig. S1 The XRPD patterns of (a) original compound $[(Hpmide)_2Co_3(CH_3COO)_4]$ (**2**) and (b) solid obtained after the reaction of **2**/MCPBA and cyclohexene.

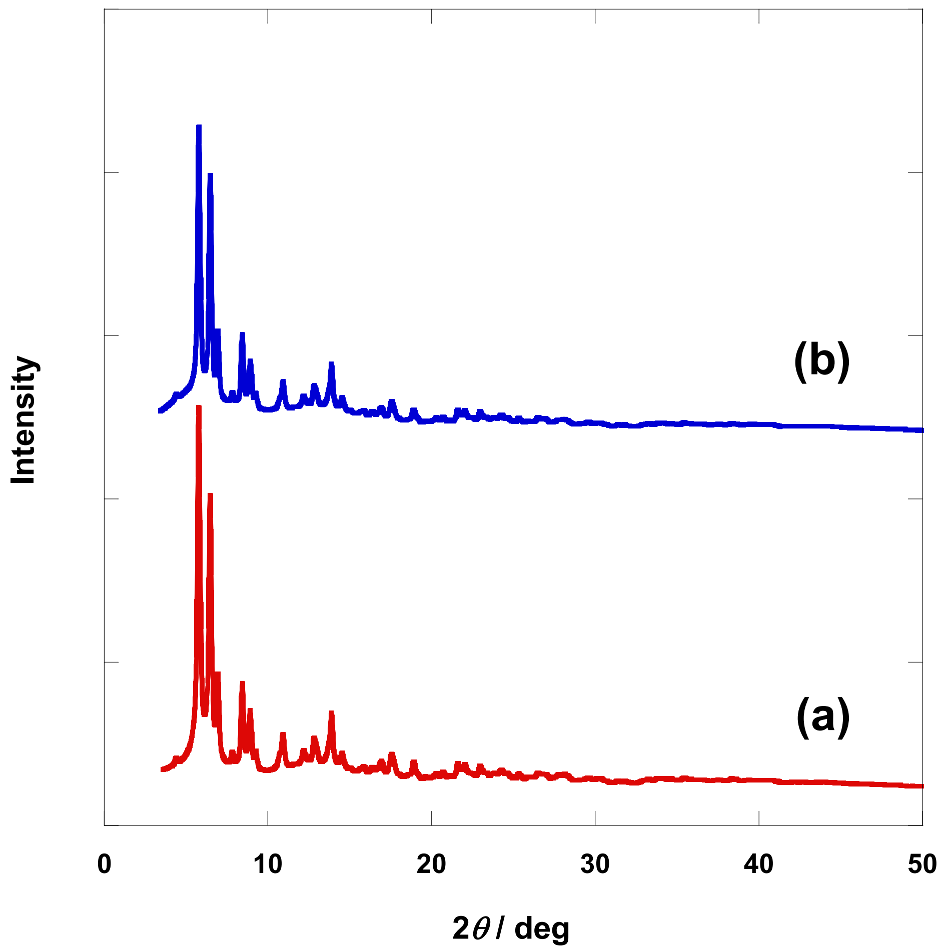


Fig. S2 The XRPD patterns of (a) original compound [(pmidip)$_2$Co$_3$(CH$_3$COO)$_4$] (**3**) and (b) solid obtained after the reaction of **3**/MCPBA and cyclohexene.

Table S1 Selected bond distances (Å) and angles (°) for **1**

Ni1−N1	2.0651(10)	Ni2−O1	2.0244(8)
Ni1−N2	2.1211(10)	Ni2−O4	2.0415(8)
Ni1−O1	2.0036(9)	Ni2−O6	2.1535(9)
Ni1−O2	2.1524(9)	Ni1•••Ni2	3.0895(6)
Ni1−O3	2.0236(8)	Ni1•••Ni1^{i}	6.1790(12)
Ni1−O6	2.1451(9)		
N1−Ni1−N2	80.97(4)	O2−Ni1−O3	94.15(3)
N1−Ni1−O1	102.28(4)	O2−Ni1−O6	87.85(4)
N1−Ni1−O2	88.53(4)	O3−Ni1−O6	88.14(3)
N1−Ni1−O3	94.58(3)	O1−Ni2−O4	87.16(3)
N1−Ni1−O6	175.62(3)	O1−Ni2−O4^{i}	92.84(3)
N2−Ni1−O1	85.07(3)	O1−Ni2−O6	79.94(4)
N2−Ni1−O2	82.06(3)	O1−Ni2−O6^{i}	100.06(4)
N2−Ni1−O3	174.20(3)	O4−Ni2−O6	88.19(3)
N2−Ni1−O6	96.07(3)	O4−Ni2−O6^{i}	91.81(3)
O1−Ni1−O2	161.70(3)	Ni1−O1−Ni2	100.17(4)
O1−Ni1−O3	99.58(3)	Ni1−O6−Ni2	91.90(4)
O1−Ni1−O6	80.61(4)		

Symmetry transformations used to generate equivalent atoms: (i) −x+1, −y, −z.

Table S2 Selected bond distances (Å) and angles (°) for **2**

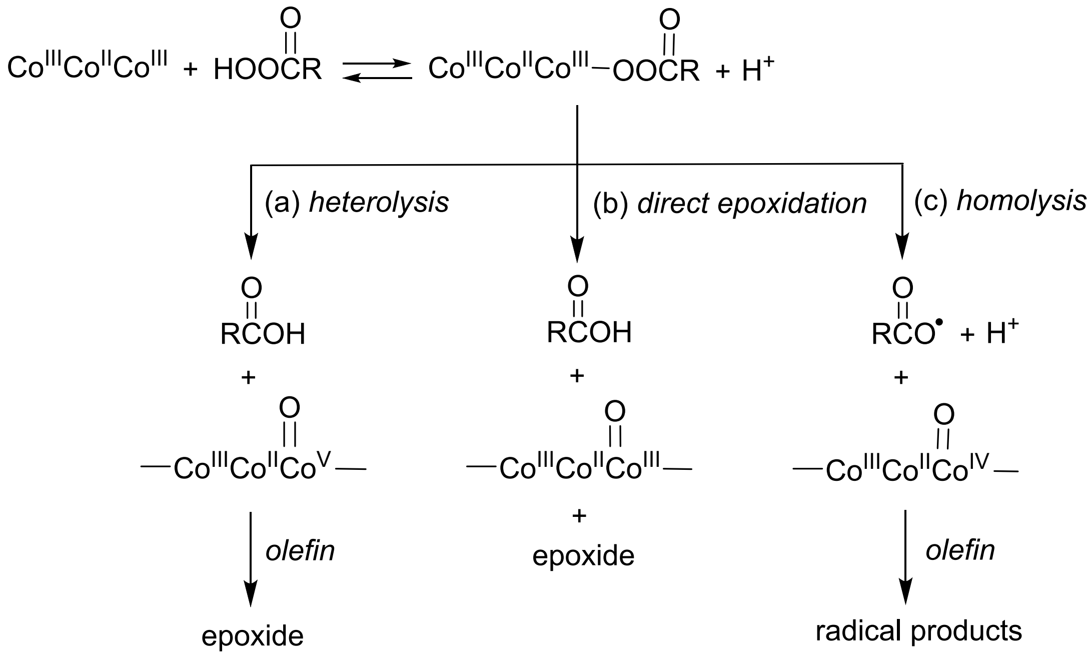
Co1-N1	2.150(4)	Co2−O1	2.016(4)
Co1-N2	2.250(4)	Co2−O4	2.110(4)
Co1-O1	1.987(4)	Co2−O6	2.196(4)
Co1−O2	2.196(4)	Co1•••Co2	3.1314(2)
Co1−O3	2.115(5)	Co1•••Co1^{i}	6.2627(4)
Co1−O6	2.016(4)		
N1−Co1−N2	78.74(17)	O2−Co1−O3	98.01(15)
N1−Co1−O1	105.05(17)	O2−Co1−O6	83.80(14)
N1−Co1−O2	90.32(16)	O3−Co1−O6	86.71(15)
N1−Co1−O3	96.89(17)	O1−Co2−O4	87.47(16)
N1−Co1−O6	173.49(17)	O1−Co2−O4^{i}	92.54(16)
N2−Co1−O1	82.15(16)	O1−Co2−O6	80.14(15)
N2−Co1−O2	79.99(15)	O1−Co2−O6^{i}	99.86(15)
N2−Co1−O3	175.14(16)	O4−Co2−O6	86.91(15)
N2−Co1−O6	97.43(16)	O4−Co2−O6^{i}	93.09(15)
O1−Co1−O2	153.63(16)	Co1−O1−Co2	102.92(17)
O1−Co1−O3	101.17(15)	Co1−O6−Co2	89.56(14)
O1−Co1−O6	79.44(15)		

Symmetry transformations used to generate equivalent atoms: (i) −x+2, −y+1, −z.

Table S3 Selected bond distances (Å) and angles (°) for **3**

Co1-N1	1.9441(17)	Co2−O1	2.0719(14)
Co1-N2	1.9380(19)	Co2−O2	2.1621(14)
Co1-O1	1.8999(14)	Co2−O4	2.0980(17)
Co1−O2	1.8904(14)	Co1•••Co2	3.0045(6)
Co1−O3	1.9152(16)	Co1•••Co1^{i}	6.0090(11)
Co1−O5	1.9375(15)		
N1−Co1−N2	85.25(8)	O2−Co1−O3	91.58(6)
N1−Co1−O1	171.21(7)	O2−Co1−O5	177.00(7)
N1−Co1−O2	92.47(7)	O3−Co1−O5	91.39(7)
N1−Co1−O3	89.33(7)	O1−Co2−O4	86.99(6)
N1−Co1−O5	87.93(7)	O1−Co2−O4^{i}	93.00(6)
N2−Co1−O1	86.09(7)	O1−Co2−O2	75.02(5)
N2−Co1−O2	88.17(7)	O1−Co2−O2^{i}	104.98(5)
N2−Co1−O3	174.56(7)	O2−Co2−O4	83.57(6)
N2−Co1−O5	88.90(7)	O2−Co2−O4^{i}	96.43(6)
O1−Co1−O2	85.76(6)	Co1−O1−Co2	98.21(6)
O1−Co1−O3	99.31(6)	Co1−O2−Co2	95.47(6)
O1−Co1−O5	93.40(6)		

Symmetry transformations used to generate equivalent atoms: (i) −x, −y+1, −z+1.



Scheme S1 Plausible olefin epoxidation mechanism catalyzed by **3** with peracids.