

One-Pot Self-Assembly of Dinuclear, Tetranuclear, and H-Bonding-Directed Polynuclear Cobalt(II), Cobalt(III), and Mixed-Valence Co(II)/Co(III) Complexes of Schiff Base Ligands with Incomplete Double Cubane Core

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Table S1. Bond lengths [Å] and angles [°] for **1**.

Bond Lengths	[Å]	Bond Angles	[°]
		N4 Co1 O3	88.5(2)
		N4 Co1 O6	95.5(3)
		O3 Co1 O5	80.7(2)
		O6 Co1 O5	94.8(2)
		N4 Co1 O5	167.5(2)
		N5 Co1 O4	171.3(3)
		O6 Co1 O3	173.6(2)
Co(1)-N(4)	1.848(6)		
Co(1)-N(5)	1.939(7)		
Co(1)-O(3)	1.897(5)	N2 Co2 N3	93.3(3)
Co(1)-O(4)	1.968(5)	N2 Co2 O3	95.5(2)
Co(1)-O(5)	1.943(5)	O4 Co2 N3	89.0(2)
Co(1)-O(6)	1.874(5)	O4 Co2 O3	80.8(2)
Co(2)-N(2)	1.869(6)	N2 Co2 O4	170.8(3)
Co(2)-N(3)	1.934(6)	N3 Co2 O3	167.0(2)
Co(2)-O(2)	1.907(5)	O5 Co2 O2	176.3(2)
Co(2)-O(3)	1.943(5)		
Co(2)-O(4)	1.890(5)	Co1 O3 Co2	82.93(18)
Co(2)-O(5)	1.881(5)	C20 O3 Co1	108.9(4)
Co(1)-Co(2)	2.543	C20 O3 Co2	120.9(4)
		Co2 O4 Co1	82.45(19)
		C17 O4 Co1	120.6(4)
		C17 O4 Co2	109.8(4)
		Co2 O5 Co1	83.36(19)
		C14 O5 Co1	118.7(4)
		C14 O5 Co2	108.6(4)

Table S2. Bond lengths [Å] and angles [°] for **2**.

Bond Lengths	[Å]	Bond Angles	[°]
		N(6A)-Co(1)-N(1)	96.98(9)
		N(6A)-Co(1)-N(3)	91.96(9)
		O(1)-Co(1)-N(1)	87.91(8)
		O(1)-Co(1)-N(3)	81.82(8)
		O(1)-Co(1)-N(6A)	169.59(8)
		N(1)-Co(1)-N(3)	167.06(8)
		N(3A)-Co(1)-Cl(1)	168.56(6)
Co(1)-N(1)	2.082(2)		
Co(1)-N(3)	2.188(2)	O(2)-Co(2)-N(3)	106.43(8)
Co(1)-N(3A)	2.248(2)	N(2)-Co(2)-O(1)	91.39(9)
Co(1)-N(6A)	2.079(2)	N(2)-Co(2)-O(2)	79.17(9)
Co(1)-O(1)	2.0674(17)	O(1)-Co(2)-N(3)	83.55(8)
Co(1)-Cl(1)	2.4751(8)	O(1)-Co(2)-O(2)	168.99(8)
Co(2)-N(3)	2.137(2)	N(6)-Co(2)-O(3)	165.63(8)
Co(2)-N(6)	2.118(2)	N(2)-Co(2)-N(3)	172.05(9)
Co(2)-N(2)	2.016(2)		
Co(2)-O(1)	2.0468(19)	Co(2)-N(3)-Co(1)	93.85(9)
Co(2)-O(3)	2.1410(19)	Co(1)-N(3)-Co(1A)	99.66(9)
Co(2)-O(2)	2.131(2)	Co(2)-N(3)-Co(1A)	97.29(8)
Co(1)-Co(2)	3.160		
Co(1)-Co(2A)	3.293	Co(1A)-N(6)-Co(2)	103.36(9)
		N(7)-N(6)-Co(1A)	130.40(19)
		N(7)-N(6)-Co(2)	123.55(18)
		Co(2)-O(1)-Co(1)	100.36(8)
		C(3)-O(1)-Co(1)	130.73(17)
		C(3)-O(1)-Co(2)	126.02(16)

Table S3. Bond lengths [Å] and angles [°] for **3**.

Bond Lengths	[Å]	Bond Angles	[°]
		O(2)-Co(1)-O(3)	95.97(14)
		O(1)-Co(1)-O(3)	85.98(14)
Co(1)-Co(1A)	2.9288(16)	N(1)-Co(1)-O(2)	84.84(15)
Co(1)-Co(2)	2.948	N(1)-Co(1)-O(1)	92.96(16)
Co(2)-Co(1A)	3.071	N(1)-Co(1)-O(3)	177.08(16)
Co(1)-O(2)	1.891(3)	O(3A)-Co(1)-O(5)	170.67(15)
Co(1)-O(1)	1.895(3)	O(2)-Co(1)-O(1)	174.43(14)
Co(1)-O(5)	1.908(3)	O(1)-Co(2)-O(3)	79.37(13)
Co(1)-O(3A)	1.892(3)	O(1)-Co(2)-N(2)	88.39(15)
Co(1)-O(3)	1.928(3)	O(3)-Co(2)-O(4)	112.36(14)
Co(1)-N(1)	1.873(4)	N(2)-Co(2)-O(4)	79.75(16)
Co(2)-O(2A)	2.089(3)	N(2)-Co(2)-O(3)	167.75(16)
Co(2)-O(1)	2.000(3)	O(2A)-Co(2)-O(6)	156.22(11)
Co(2)-O(4)	2.099(4)	O(1)-Co(2)-O(4)	165.74(13)
Co(2)-O(6)	2.131(3)	Co(1)-O(2)-Co(2A)	100.86(13)
Co(2)-O(3)	2.081(3)	C(10)-O(2)-Co(1)	106.7(3)
Co(2)-N(2)	2.036(4)	C(10)-O(2)-Co(2A)	126.1(3)
		Co(1)-O(1)-Co(2)	98.35(15)
		C(5)-O(1)-Co(1)	129.4(3)

C(5)-O(1)-Co(2)	132.0(3)
Co(1A)-O(3)-Co(1)	100.12(16)
Co(1A)-O(3)-Co(2)	101.12(14)
Co(1)-O(3)-Co(2)	94.63(15)

Table S4. Bond lengths [Å] and angles [°] for 3.

Bond Lengths	[Å]	Bond Angles	[°]
		O(1)-Co(1)-O(3)	75.84(11)
		O(2)-Co(1)-O(1)	88.29(12)
		O(2)-Co(1)-O(6A)	100.20(14)
		O(3)-Co(1)-O(6A)	95.70(14)
		O(4A)-Co(1)-O(7)	168.41(15)
		O(1)-Co(1)-O(6A)	171.51(14)
		O(2)-Co(1)-O(3)	162.99(12)
Co(1)-O(1)	2.049(3)	O(1)-Co(2)-O(3)	84.07(12)
Co(1)-O(2)	2.036(3)	O(4)-Co(2)-O(3)	94.78(12)
Co(1)-O(3)	2.108(3)	N(1)-Co(2)-O(1)	95.49(14)
Co(1)-O(4A)	2.014(3)	N(1)-Co(2)-O(4)	85.59(14)
Co(1)-O(6A)	2.118(4)	N(2)-Co(2)-O(3A)	165.50(16)
Co(1)-O(7)	2.037(4)	O(4)-Co(2)-O(1)	177.50(13)
Co(2)-Co(2A)	2.9522(11)	N(1)-Co(2)-O(3)	178.16(14)
Co(2)-O(1)	1.897(3)		
Co(2)-O(3A)	1.977(3)	Co(2)-O(1)-Co(1)	101.38(13)
Co(2)-O(3)	1.919(3)	C(5)-O(1)-Co(1)	130.7(3)
Co(2)-O(4)	1.877(3)	C(5)-O(1)-Co(2)	126.7(3)
Co(2)-N(1)	1.867(4)		
Co(2)-N(2)	1.925(4)	Co(2A)-O(3)-Co(1)	94.96(12)
		Co(2)-O(3)-Co(1)	98.58(12)
		Co(2)-O(3)-Co(2A)	98.52(13)
		C(15)-O(3)-Co(1)	117.2(3)
		C(15)-O(3)-Co(2)	108.3(3)
		C(15)-O(3)-Co(2A)	133.2(3)
		Co(2)-O(4)-Co(1A)	101.39(13)
		C(11)-O(4)-Co(1A)	114.6(3)
		C(11)-O(4)-Co(2)	110.8(3)

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