Supplementary Material for CrystEngComm

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For

Syntheses and Structures of $Cu^{II}Bi^{III}$, $Cu^{II}Ba^{II}Cu^{II}$, $[Cu^{II}Pb^{II}]_2$ and Cocrystallized $(U^{VI}O_2)_2.4Cu^{II}$ Complexes: Structural Diversity of the Coordination Compounds Derived from *N*,*N*′-Ethylenebis(3-Ethoxysalicylaldiimine)

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Table S1

Bond angles (°) in the coordination environments of the bismuth(III) in **1** and barium(II) in **2**.

Compound 1		**Compound 2**	
O(1)–Bi(1)–O(2)	62.93(6)	O(1)–Ba(1)–O(2)	54.29(7)
O(1)–Bi(1)–O(3)	122.99(6)	O(1)–Ba(1)–O(3)	107.58(7)
O(1)–Bi(1)–O(4)	154.98(6)	O(1)–Ba(1)–O(4)	125.62(7)
O(1)–Bi(1)–O(5)	70.11(6)	O(1)–Ba(1)–O(5)	64.83(7)
O(1)–Bi(1)–O(7)	114.15(6)	O(1)–Ba(1)–O(6)	110.74(7)
O(1)–Bi(1)–O(8)	122.06(6)	O(1)–Ba(1)–O(7)	167.48(7)
O(1)–Bi(1)–O(10)	78.84(6)	O(1)–Ba(1)–O(8)	136.61(6)
O(1)–Bi(1)–O(11)	76.24(6)	O(1)–Ba(1)–O(9A)	94.5(6)
O(1)–Bi(1)–O(13)	77.24(6)	O(1)–Ba(1)–O(10A)	68.61(14)
O(2)–Bi(1)–O(3)	65.43(6)	O(1)–Ba(1)–O(12A)	73.83(11)
O(2)–Bi(1)–O(4)	125.60(6)	O(2)–Ba(1)–O(3)	56.25(6)
O(2)–Bi(1)–O(5)	74.29(6)	O(2)–Ba(1)–O(4)	99.18(6)
O(2)–Bi(1)–O(7)	73.71(6)	O(2)–Ba(1)–O(5)	63.75(7)
O(2)–Bi(1)–O(8)	138.91(6)	O(2)–Ba(1)–O(6)	73.32(7)
O(2)–Bi(1)–O(10)	135.08(7)	O(2)–Ba(1)–O(7)	118.65(7)
O(2)–Bi(1)–O(11)	123.06(6)	O(2)–Ba(1)–O(8)	163.17(6)
O(2)–Bi(1)–O(13)	81.82(6)	O(2)–Ba(1)–O(9A)	124.9(6)
O(3)–Bi(1)–O(4)	60.23(6)	O(2)–Ba(1)–O(10A)	121.20(15)
O(3)–Bi(1)–O(5)	116.52(6)	O(2)–Ba(1)–O(12A)	102.20(10)
O(3)–Bi(1)–O(7)	70.97(6)	O(3)–Ba(1)–O(4)	51.75(6)
O(3)–Bi(1)–O(8)	112.28(6)	O(3)–Ba(1)–O(5)	100.62(6)
O(3)–Bi(1)–O(10)	158.00(6)	O(3)–Ba(1)–O(6)	64.27(7)
O(3)–Bi(1)–O(11)	115.59(6)	O(3)–Ba(1)–O(7)	70.29(6)
O(3)–Bi(1)–O(13)	73.17(6)	O(3)–Ba(1)–O(8)	108.02(6)
O(4)–Bi(1)–O(5)	133.21(6)	O(3)–Ba(1)–O(9A)	142.7(2)
O(4)–Bi(1)–O(7)	90.64(6)	O(3)–Ba(1)–O(10A)	174.5(2)
O(4)–Bi(1)–O(8)	69.17(5)	O(3)–Ba(1)–O(12A)	103.73(9)
O(4)–Bi(1)–O(10)	99.05(6)	O(4)–Ba(1)–O(5)	151.31(6)
O(4)–Bi(1)–O(11)	80.53(6)	O(4)–Ba(1)–O(6)	102.37(6)
O(4)–Bi(1)–O(13)	80.87(6)	O(4)–Ba(1)–O(7)	63.39(6)
O(5)–Bi(1)–O(7)	51.34(6)	O(4)–Ba(1)–O(8)	64.17(6)
O(5)–Bi(1)–O(8)	71.09(6)	O(4)–Ba(1)–O(9A)	133.7(7)
O(5)–Bi(1)–O(10)	71.02(6)	O(4)–Ba(1)–O(10A)	126.8(3)
O(5)–Bi(1)–O(11)	127.37(6)	O(4)–Ba(1)–O(12A)	66.77(10)
O(5)–Bi(1)–O(13)	145.69(6)	O(5)–Ba(1)–O(6)	52.06(7)
O(7)–Bi(1)–O(8)	67.62(6)	O(5)–Ba(1)–O(7)	103.08(7)
O(7)–Bi(1)–O(10)	104.26(6)	O(5)–Ba(1)–O(8)	129.99(6)
O(7)–Bi(1)–O(11)	163.16(7)	O(5)–Ba(1)–O(9A)	61.8(6)
O(7)–Bi(1)–O(13)	142.51(6)	O(5)–Ba(1)–O(10A)	81.5(3)
O(8)–Bi(1)–O(10)	48.49(6)	O(5)–Ba(1)–O(12A)	136.66(10)

O(8)–Bi(1)–O(11)	95.73(6)	O(6)–Ba(1)–O(7)	56.94(7)
O(8)–Bi(1)–O(13)	138.64(6)	O(6)–Ba(1)–O(8)	106.60(7)
O(10)–Bi(1)–O(11)	63.53(6)	O(6)–Ba(1)–O(9A)	80.05(18)
O(10)–Bi(1)–O(13)	113.11(6)	O(6)–Ba(1)–O(10A)	120.5(3)
O(11)–Bi(1)–O(13)	50.38(6)	O(6)–Ba(1)–O(12A)	167.83(9)
		O(7)–Ba(1)–O(8)	53.22(6)
		O(7)–Ba(1)–O(9A)	81.6(6)
		O(7)–Ba(1)–O(10A)	114.34(15)
		O(7)–Ba(1)–O(12A)	118.68(11)
		O(8)–Ba(1)–O(9A)	70.8(7)
		O(8)–Ba(1)–O(10A)	73.88(17)
		O(8)–Ba(1)–O(12A)	74.30(10)
		O(9A)–Ba(1)–O(10A)	42.7(3)
		O(9A)–Ba(1)–O(12A)	111.3(2)
		O(10A)–Ba(1)–O(12A)	71.6(3)

Table S2

Bond angles (°) in the coordination environments of the lead(II) in **3** and uranium(VI) in **4**.

Compound 3		**Compound 4**	
O(1A)–Pb(1)–O(2)	61.0(2)	O(17)–U(1)–O(18)	175.72(9)
O(1A)–Pb(1)–O(3)	125.6(2)	O(11)–U(1)–O(15)	161.15(6)
O(1A)–Pb(1)–O(4)	172.06(15)	O(12)–U(1)–O(19G)	178.75(6)
O(1A)–Pb(1)–O(5)	114.52(12)	O(14)–U(1)–O(19)	176.22(6)
O(1A)–Pb(1)–O(6)	72.07(14)	O(17)–U(1)–O(11)	89.87(8)
O(1A)–Pb(1)–O(7C)	74.5(2)	O(17)–U(1)–O(12)	89.54(8)
O(1A)–Pb(1)–O(8)	76.46(17)	O(17)–U(1)–O(14)	88.05(8)
O(1A)–Pb(1)–O(9)	100.21(12)	O(17)–U(1)–O(15)	89.63(8)
O(2)–Pb(1)–O(3)	65.14(9)	O(17)–U(1)–O(19)	93.59(8)
O(2)–Pb(1)–O(4)	125.30(8)	O(17)–U(1)–O(19G)	90.26(8)
O(2)–Pb(1)–O(5)	86.74(10)	O(18)–U(1)–O(11)	90.30(8)
O(2)–Pb(1)–O(6)	82.18(10)	O(18)–U(1)–O(12)	87.30(9)
O(2)–Pb(1)–O(7C)	133.76(9)	O(18)–U(1)–O(14)	87.90(8)
O(2)–Pb(1)–O(8)	69.29(10)	O(18)–U(1)–O(15)	88.83(8)
O(2)–Pb(1)–O(9)	114.93(10)	O(18)–U(1)–O(19)	90.37(8)
O(3)–Pb(1)–O(4)	60.21(8)	O(18)–U(1)–O(19G)	92.84(8)
O(3)–Pb(1)–O(5)	68.27(9)	O(11)–U(1)–O(12)	49.85(6)
O(3)–Pb(1)–O(6)	108.11(9)	O(11)–U(1)–O(14)	111.05(6)
O(3)–Pb(1)–O(7C)	159.53(9)	O(11)–U(1)–O(19)	65.59(6)
O(3)–Pb(1)–O(8)	78.38(10)	O(11)–U(1)–O(19G)	131.38(6)
O(3)–Pb(1)–O(9)	95.22(9)	O(12)–U(1)–O(14)	61.22(6)
O(4)–Pb(1)–O(5)	72.03(9)	O(12)–U(1)–O(15)	111.30(6)
O(4)–Pb(1)–O(6)	112.34(9)	O(12)–U(1)–O(19)	115.35(6)
O(4)–Pb(1)–O(7C)	100.19(9)	O(14)–U(1)–O(15)	50.10(6)
O(4)–Pb(1)–O(8)	100.80(10)	O(14)–U(1)–O(19G)	117.54(6)
O(4)–Pb(1)–O(9)	73.04(9)	O(15)–U(1)–O(19)	133.24(6)
O(5)–Pb(1)–O(6)	46.64(9)	O(15)–U(1)–O(19G)	67.46(6)
O(5)–Pb(1)–O(7C)	101.51(9)	O(19)–U(1)–O(19G)	65.89(7)
O(5)–Pb(1)–O(8)	144.98(10)		
O(5)–Pb(1)–O(9)	145.05(9)		
O(6)–Pb(1)–O(7C)	72.30(9)		
O(6)–Pb(1)–O(8)	145.01(11)		
O(6)–Pb(1)–O(9)	155.65(10)		
O(7C)–Pb(1)–O(8)	113.51(10)		
O(7C)–Pb(1)–O(9)	83.40(9)		
O(8)–Pb(1)–O(9)	45.70(10)		

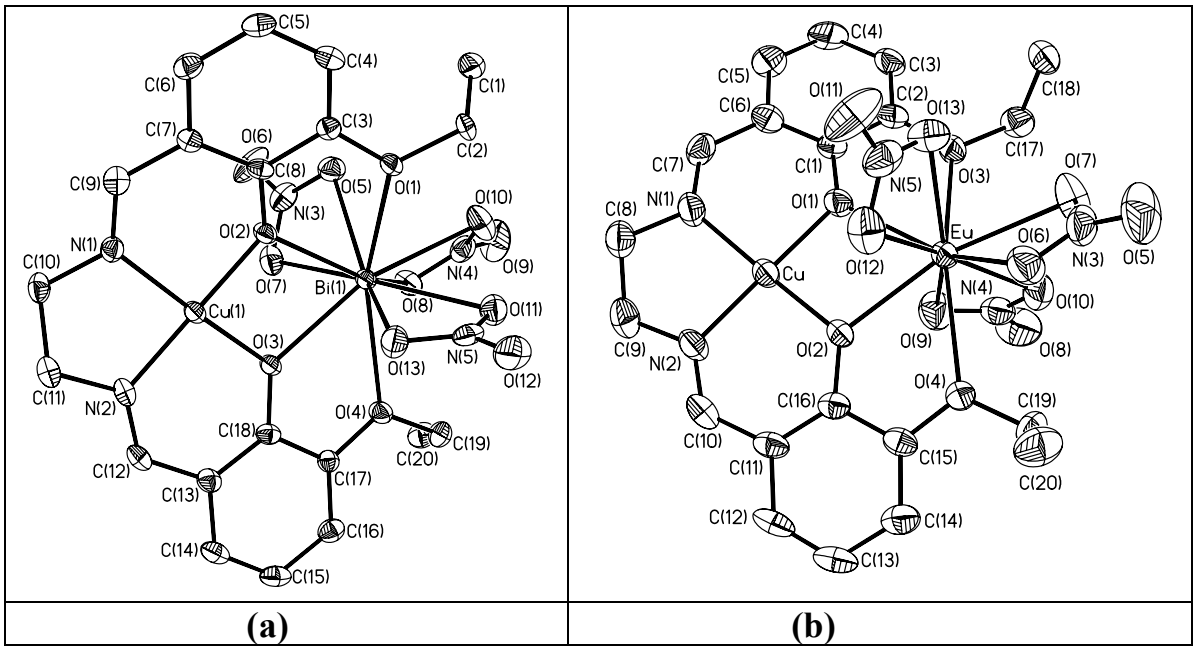


Fig. S1 Crystal structures of (a) $[Cu^{II}L^{1}Bi^{III}(NO_3)_3]$ and (b) a $Cu^{II}Ln^{III}$ compound, $[Cu^{II}L^{1}Eu^{III}(NO_3)_3]$.

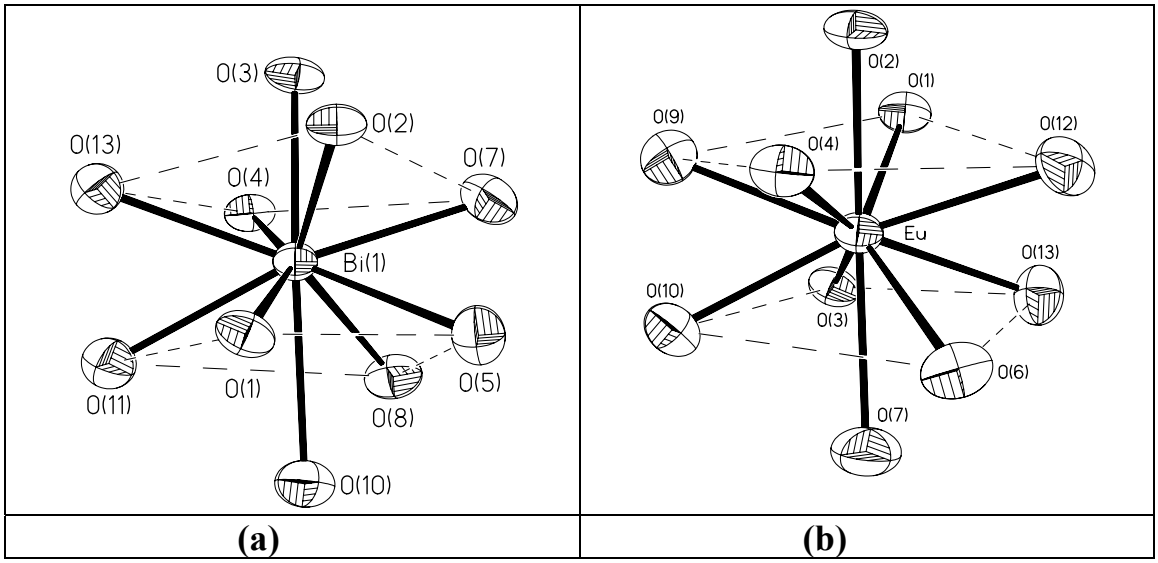
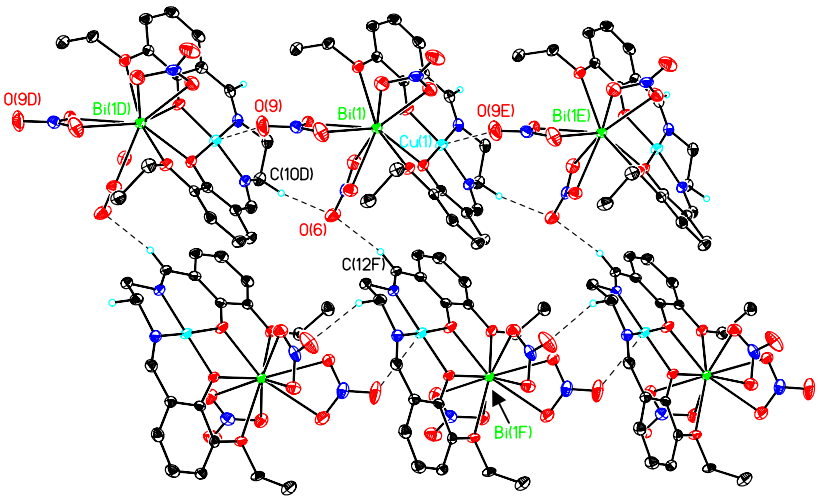
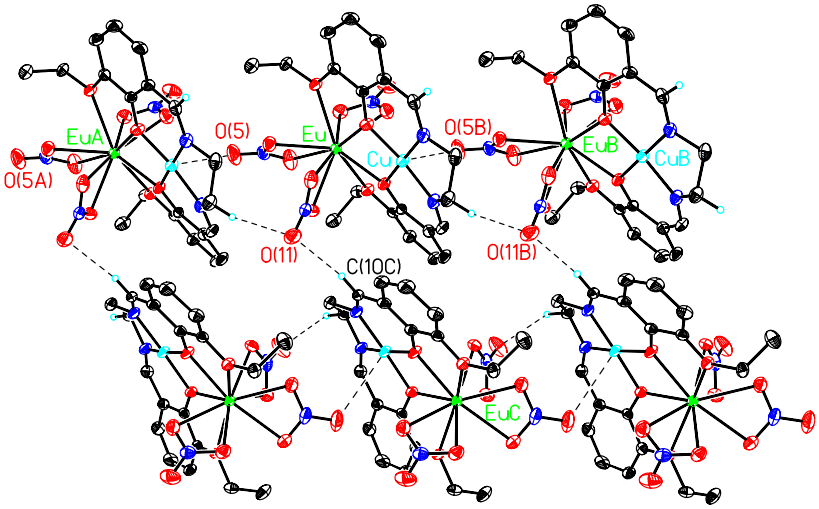


Fig. S2 Distorted bi-capped square-antiprismitic coordination environment of (a) bismuth(III) in $[Cu^{II}L^{1}Bi^{III}(NO_3)_3]$ and (b) europium(III) in $[Cu^{II}L^{1}Eu^{III}(NO_3)_3]$.



(a)



(b)

Fig. S3 Perspective view to illustrate the two-dimensional structure of (a) $[Cu^{II}L^{1}Bi^{III}(NO_3)_3]$ and (b) $[Cu^{II}L^{1}Eu^{III}(NO_3)_3]$. Except two hydrogens participating in hydrogen bonds, the hydrogens are omitted for clarity. Symmetry: D, 1+x, y, z; E, x-1, y, z; F, 3-x, -0.5y, 1.5-z. for (a) and A, 1+x, y, z; B, x-1, y, z; C, 1-x, 0.5+y, 0.5-z. for (b).