Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

For

Preparation and characterisation of divalent hard and soft metal (M = Ca, Co, Cu, Zn, Cd, Hg, and Pb) complexes of 1,10-dithia-18-crown-6: structural versatility

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Table S1 Selected bond lengths (Å) and bond angles (°) for **1**, [Ca(**L**)$(ClO_4)_2$]

Ca1-O1	2.422(3)	Ca1-O2	2.520(2)
Ca1-O3	2.320(4)	Ca1···S1	3.0073(10)
O1-Ca1-O2	66.34(8)	O1-Ca1-O3	82.84(14)
O2-Ca1-O3	77.64(13)		

Table S2 Selected bond lengths (Å) and bond angles (°) for **2a**, [Co(**L**)$(H_2O)_3]_2(ClO_4)_4$

Co1-S2	2.4668(6)	Co1-O1	2.1136(14)
Co1-O2	2.1067(16)	Co1-O1W	2.0561(15)
Co1-O2W	2.0388(15)	Co1-O3W	2.0747(14)
Co2-S3	2.4852(6)	Co2-O5	2.0941(15)
Co2-O6	2.1414(14)	Co2-O4W	2.0732(14)
Co2-O5W	2.0289(15)	Co2-O6W	2.0751(15)
S2-Co1-O1	160.35(5)	S2-Co1-O2	83.53(4)
S2-Co1-O1W	102.56(4)	S2-Co1-O2W	92.74(5)
S2-Co1-O3W	93.68(4)	O1-Co1-O2	77.35(6)
O1-Co1-O1W	96.57(6)	O1-Co1-O2W	92.38(6)
O1-Co1-O3W	81.94(6)	O2-Co1-O1W	173.91(6)
O2-Co1-O2W	91.95(7)	O2-Co1-O3W	89.94(6)
O1W-Co1-O2W	87.99(6)	O1W-Co1-O3W	89.47(6)
O2W-Co1-O3W	173.47(6)	S3-Co2-O5	82.76(4)
S3-Co2-O6	160.16(4)	S3-Co2-O4W	92.44(4)
S3-Co2-O5W	93.27(5)	S3-Co2-O6W	101.86(4)
O5-Co2-O6	77.55(6)	O5-Co2-O4W	89.09(6)
O5-Co2-O5W	93.08(7)	O5-Co2-O6W	175.19(6)
O6-Co2-O4W	84.93(6)	O6-Co2-O5W	90.18(6)
O6-Co2-O6W	97.77(6)	O4W-Co2-O5W	174.11(6)
O4W-Co2-O6W	89.40(6)	O5W-Co2-O6W	87.99(6)

Table S3 Selected bond lengths (Å) and bond angles (°) for **2b**, $[Co(C_7H_5N)_4(H_2O)_2](ClO_4)_2$

Co1-N1	2.1022(15)	Co1-N2	2.1209(16)
Co1-O1W	2.0463(12)		
N1-Co1-N2	91.37(6)	N1-Co1- O1W	89.48(6)
N2-Co1- O1W	88.31(6)		

Table S4 Selected bond lengths (Å) and bond angles (°) for **3,** $[Cu(\mathbf{L})(ClO_4)_2]\cdot 2C_6H_5CN$

Cu1-S1	2.2991(11)	Cu1-S2	2.3083(9)
Cu1-O1	2.009(2)	Cu1-O2	1.991(2)
Cu1-O5	2.401(2)	Cu1-O9	2.396(2)
S1-Cu1-S2	106.10(4)	S1-Cu1-O1	85.74(8)
S1-Cu1-O2	167.72(6)	S1-Cu1-O5	95.87(7)
S1-Cu1-O9	90.61(8)	S2-Cu1-O1	168.07(8)
S2-Cu1-O2	86.08(7)	S2-Cu1-O5	95.65(6)
S2-Cu1-O9	94.80(9)	O1-Cu1-O2	82.05(9)
O1-Cu1-O5	84.38(8)	O1-Cu1-O9	83.38(10)
O2-Cu1-O5	84.22(9)	O2-Cu1-O9	86.75(10)
O5-Cu1-O9	165.68(10)		

Table S5 Selected bond lengths (Å) and bond angles (°) for **4,** $[Zn(\mathbf{L})(H_2O)_3]_2(ClO_4)_4$

Zn1-S2	2.4656(7)	Zn1-O1	2.1167(17)
Zn1-O2	2.1870(19)	Zn1-O1W	2.0319(18)
Zn1-O2W	2.0510(19)	Zn1-O3W	2.0973(17)
Zn2-S3	2.4882(7)	Zn2-O5	2.1681(19)
Zn2-O6	2.1436(17)	Zn2-O4W	2.0939(17)
Zn2-O5W	2.0448(18)	Zn2-O6W	2.0492(18)
S2-Zn1-O1	157.39(6)	S2-Zn1-O2	82.27(5)
S2-Zn1-O1W	105.72(6)	S2-Zn1O2W	94.04(6)
S2-Zn1-O3W	93.86(5)	O1-Zn1-O1W	96.52(7)
O1-Zn1-O2W	90.65(7)	O1-Zn1-O3W	81.65(7)
O2-Zn1-O1W	172.01(7)	O2-Zn1-O2W	91.17(8)
O2-Zn1-O3W	88.88(7)	O1-Zn1-O2	75.52(7)
O1W-Zn1-O2W	88.17(8)	O1W-Zn1-O3W	90.68(7)
O2W-Zn1-O3W	172.04(7)	S3-Zn2-O6	157.36(5)
S3-Zn2-O5	81.55(6)	S3-Zn2-O4W	92.79(5)
S3-Zn2-O5W	94.48(6)	S3-Zn2-O6W	104.74(5)
O5-Zn2-O6	75.93(7)	O5-Zn2-O4W	88.32(7)
O5-Zn2-O5W	92.30(8)	O5-Zn2-O6W	173.67(7)
O6-Zn2-O4W	84.37(7)	O6-Zn2-O5W	88.74(7)
O6-Zn2-O6W	97.76(7)	O4W-Zn2-O5W	172.72(7)
O4W-Zn2-O6W	90.65(7)	O5W-Zn2-O6W	87.94(8)

Table S6 Selected bond lengths (Å) and bond angles (°) for **5,** $[Cd(\mathbf{L})(ClO_4)_2]$

Cd1-S1	2.6273(6)	Cd1-S2	2.6351(6)
Cd1-O1	2.4016(15)	Cd1-O2	2.4982(15)
Cd1-O3	2.4500(15)	Cd1-O4	2.4792(15)
Cd1-O5	2.5339(15)	Cd1-O9	2.668(2)
S1-Cd1-S2	137.667(19)	S1-Cd1-O1	77.41(4)
S1-Cd1-O4	71.28(4)	S1-Cd1-O5	80.14(4)
S2-Cd1-O2	73.85(4)	S2-Cd1-O3	73.65(4)
S2-Cd1-O5	71.89(5)	O1-Cd1-O2	66.35(5)
O1-Cd1-O3	90.43(5)	O1-Cd1-O4	77.06(5)
O1-Cd1-O5	103.23(7)	O2-Cd1-O3	80.34(5)
O2-Cd1-O5	72.03(5)	O3-Cd1-O4	68.21(5)

Table S7 Selected bond lengths (Å) and bond angles (°) for **6,** $[Cd(\mathbf{L})(NO_3)]_2[Cd(NO_3)_4]$

Cd1-S1	2.5633(9)	Cd1-S2	2.6096(8)
Cd1-O2	2.5616(17)	Cd1-O3	2.4966(16)
Cd1-O4	2.5263(18)	Cd1-O5	2.2874(16)
Cd1-O6	2.4540(16)	Cd2-O8	2.370(3)
Cd2-O9	2.395(2)	Cd2-O11	2.415(2)
Cd2-O12	2.358(2)	Cd2-O14	2.4083(19)
Cd2-O15	2.385(2)		
S1-Cd1-S2	111.31(2)	S1-Cd1-O2	90.98(4)
S1-Cd1-O3	141.07(4)	S1-Cd1-O4	75.15(4)
S1-Cd1-O5	129.29(5)	S1-Cd1-O6	94.44(4)
S2-Cd1-O2	72.07(4)	S2-Cd1-O3	74.90(4)
S2-Cd1-O4	97.44(5)	S2-Cd1-O5	110.92(4)
S2-Cd1-O6	152.17(4)	O2-Cd1-O3	126.05(5)
O2-Cd1-O4	158.54(6)	O2-Cd1-O5	76.61(6)
O2-Cd1-O6	119.49(5)	O3-Cd1-O4	65.92(5)
O3-Cd1-O5	76.97(6)	O3-Cd1-O6	78.42(5)
O4-Cd1-O5	124.86(5)	O4-Cd1-O6	78.55(6)
O5-Cd1-O6	54.37(5)	O8-Cd2-O9	53.54(9)
O8-Cd2-O11	83.44(9)	O8-Cd2-O12	137.07(8)
O8-Cd2-O14	122.96(6)	O8-Cd2-O15	89.60(5)
O9-Cd2-O11	136.97(8)	O9-Cd2-O12	169.40(8)
O9-Cd2-O14	84.69(6)	O9-Cd2-O15	94.59(5)
O11-Cd2-O12	53.63(7)	O11-Cd2-O14	125.17(6)
O11-Cd2-O15	83.99(5)	O12-Cd2-O14	87.36(6)
O12-Cd2-O15	86.20(5)	O14-Cd2-O15	53.19(7)

Table S8 Selected bond lengths (Å) and bond angles (°) for **7,** $[Hg_2(\mathbf{L})_3](ClO_4)_4$

Hg1-S1	2.5255(15)	Hg1-S2	2.5404(15)
Hg1-S3	2.4758(14)	Hg1-O1	2.837(4)
Hg1-O2	2.679(4)	Hg1-O3	2.835(4)
Hg1-O4	2.838(4)		
S1-Hg1-S2	100.03(5)	S1-Hg1-S3	130.40(4)
S2-Hg1-S3	129.47(5)	S1-Hg1-O1	74.24(9)
S1-Hg1-O2	102.79(9)	S1-Hg1-O3	109.68(10)
S1-Hg1-O4	70.74(9)	S2-Hg1-O1	128.96(8)
S2-Hg1-O2	71.98(10)	S2-Hg1-O3	69.37(11)
S2-Hg1-O4	118.43(9)	S3-Hg1-O1	72.00(9)
S3-Hg1-O2	91.20(9)	S3-Hg1-O3	92.92(10)
S3-Hg1-O4	86.03(9)	O1-Hg1-O2	60.76(11)
O1-Hg1-O3	161.14(12)	O1-Hg1-O4	107.45(11)
O2-Hg1-O3	132.76(13)	O2-Hg1-O4	168.12(12)
O3-Hg1-O4	59.01(13)		

Table S9 Selected bond lengths (Å) and bond angles (°) for **8**, $[Hg(\mathbf{L})(NO_3)_2]\cdot 2H_2O$

Hg1-S1	2.4142(7)	Hg1-O1	2.9260(18)
Hg1-O2	2.8474 (19)	Hg1-O3	2.680(2)
S1-Hg1-O1	65.77(4)	S1-Hg1-O2	104.91(5)
S1-Hg1-O3	94.12(5)	O1-Hg1-O2	57.68(6)
O1-Hg1-O3	72.04(6)	O2-Hg1-O3	109.65(6)

Table S10 Selected bond lengths (Å) and bond angles (°) for **9**, $[Pb(\mathbf{L})(ClO_4)_2]$

Pb1-O1	2.6622(19)	Pb1-O2	2.744(2)
Pb1-O3	2.680(2)	Pb1···S1	3.0906(8)
O1-Pb1-O2	61.44(5)	O1-Pb1-O3	87.65(7)
O2-Pb1-O3	68.21(6)		

Table S11 Selected bond lengths (Å) and bond angles (°) for **10**, [Pb(**L**)$(NO_3)_2$]

Pb1-O1	2.863(12)	Pb1-O2	2.755(12)
Pb1-O3	2.879(11)	Pb1-O4	2.716(10)
Pb1-O5	2.680(12)	Pb1-O6	2.601(16)
Pb1-O8	2.877(16)	Pb1-O9	2.553(17)
Pb1···S1	3.114(6)	Pb1···S2	3.131(6)
O1-Pb1-O2	60.1(3)	O1-Pb1-O4	72.9(3)
O1-Pb1-O5	143.4(5)	O1-Pb1-O6	144.5(5)
O1-Pb1-O8	98.8(4)	O1-Pb1-O9	79.3(5)
O2-Pb1-O3	75.5(4)	O2-Pb1-O4	101.0(2)
O2-Pb1-O5	137.7(4)	O2-Pb1-O6	143.5(4)
O2-Pb1-O8	69.0(5)	O2-Pb1-O9	92.9(5)
O3-Pb1-O1	106.36(14)	O3-Pb1-O4	61.3(3)
O3-Pb1-O5	64.5(4)	O3-Pb1-O6	106.2(4)
O3-Pb1-O8	116.8(4)	O3-Pb1-O9	161.3(5)
O4-Pb1-O5	72.0(4)	O4-Pb1-O6	111.8(4)
O4-Pb1-O8	169.6(4)	O4-Pb1-O9	136.6(5)
O5-Pb1-O6	47.4(4)	O5-Pb1-O8	117.1(5)
O5-Pb1-O9	121.3(5)	O6-Pb1-O8	78.6(5)
O6-Pb1-O9	74.4(6)	O8-Pb1-O9	44.6(58)