Electronic Supplementary Information

For

Syntheses, crystal structures and supramolecular topologies of nickel(II)–s/p/d^{10}/NH_4^+ complexes derived from a compartmental ligand

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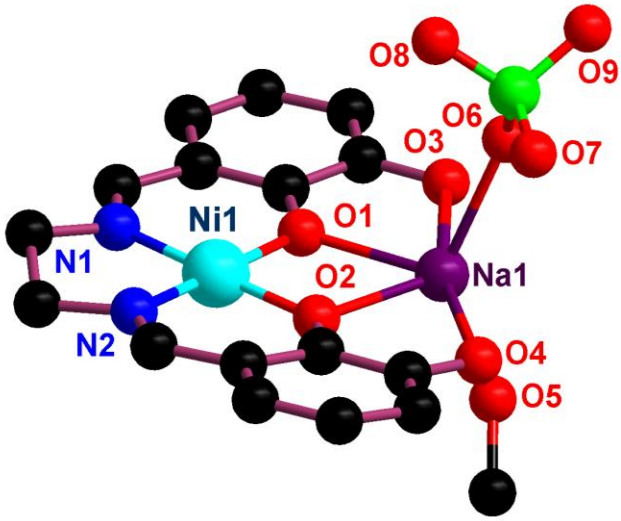

Fig. S1 Crystal structure of $[Ni^{II}LNa^{I}(ClO_4)(CH_3OH)]$ (**2**). Hydrogen atoms and the ethoxy carbon atoms are not shown for clarity.

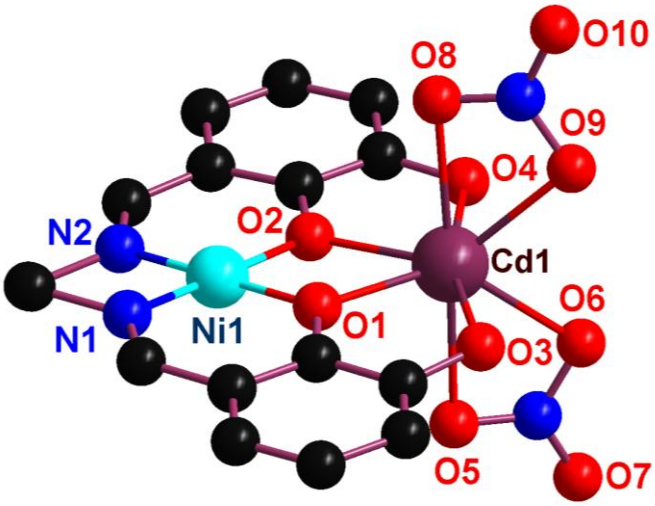

Fig. S2 Crystal structure of $[Ni^{II}LCd^{II}(NO_3)_2]\cdot CH_3CN$ (**8**). Hydrogen atoms are omitted. The acetonitrile molecule of crystallization and the ethoxy carbon atoms are also not shown for clarity.

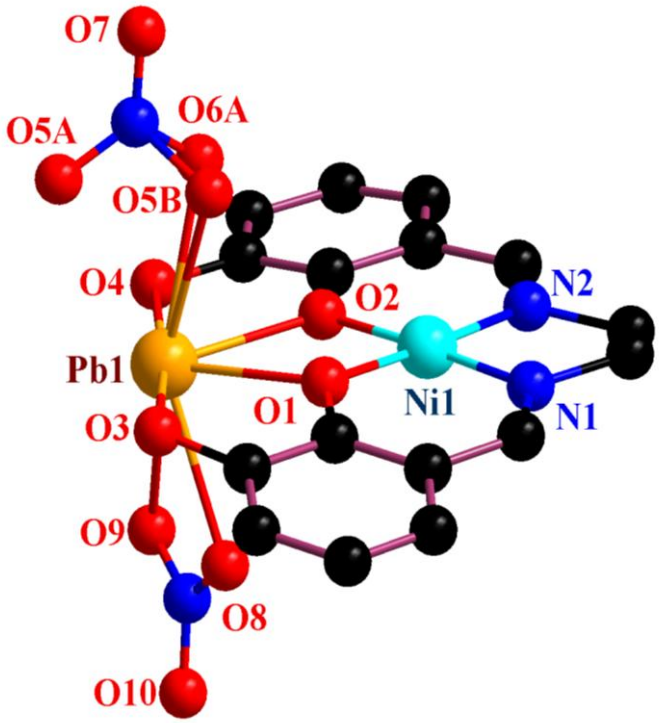

Fig. S3 Crystal structure of [$Ni^{II}LPb^{II}(NO_3)_2$] (**9**). Hydrogen atoms and the ethoxy carbon atoms are not shown for clarity. Of the one disordered positions of one oxygen atom of one nitrate anion, one is shown.

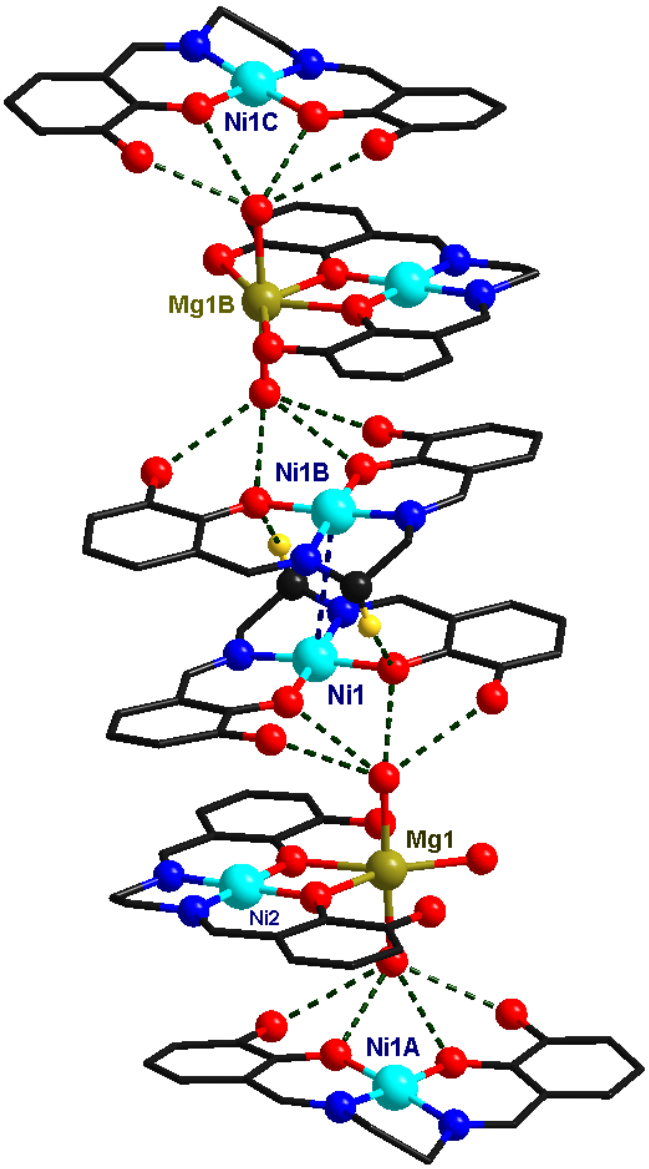

Fig. S4 Perspective view of $[\{Ni^{II}LMg^{II}(H_2O)_3\}\{Ni^{II}L\}_2](ClO_4)_2$ (**6**) demonstrating the one-dimensional supramolecular topology generated due to Ni···Ni weak interaction and C–H···O hydrogen bond. Hydrogen atoms, except those participating in hydrogen bonds, are omitted. The perchlorate anion and ethoxy carbon atoms are also not shown for clarity. Symmetry codes: A, 1–x, y, 0.5–z; B, 1.5–x, 0.5–y, –z; C, 0.5+x, 0.5–y, –0.5+z.

Table S1 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and lithium(I) centres in **1**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.840(3)	N(1)–Ni(1)–O(2)	178.52(16)
Ni(1)–O(2)	1.851(3)	O(1)–Ni(1)–N(2)	178.14(16)
Ni(1)–N(1)	1.847(4)	N(1)–Ni(1)–O(1)	94.41(19)
Ni(1)–N(2)	1.836(5)	N(1)–Ni(1)–N(2)	85.9(2)
		N(2)–Ni(1)–O(2)	94.56(19)
		O(1)–Ni(1)–O(2)	85.20(15)
Ni(2)–O(5)	1.829(3)	N(3)–Ni(2)–O(6)	177.8(2)
Ni(2)–O(6)	1.836(3)	O(5)–Ni(2)–N(4)	177.4(2)
Ni(2)–N(3)	1.827(5)	N(3)–Ni(2)–O(5)	95.4(2)
Ni(2)–N(4)	1.834(5)	N(3)–Ni(2)–N(4)	87.1(3)
		N(4)–Ni(2)–O(6)	95.0(2)
		O(5)–Ni(2)–O(6)	82.48(15)
Ni(3)–O(11)	1.841(3)	N(5)–Ni(3)–O(12)	178.29(17)
Ni(3)–O(12)	1.839(3)	O(11)–Ni(3)–N(6)	178.99(17)
Ni(3)–N(5)	1.834(5)	N(5)–Ni(3)–O(11)	94.52(19)
Ni(3)–N(6)	1.840(5)	N(5)–Ni(3)–N(6)	85.9(2)
		N(6)–Ni(3)–O(12)	94.8(2)
		O(11)–Ni(3)–O(12)	84.87(16)
Li(1)–O(5)	2.024(10)	O(5)–Li(1)–O(6)	73.6(3)
Li(1)–O(6)	2.008(9)	O(5)–Li(1)–O(9)	104.1(4)
Li(1)–O(9)	1.983(9)	O(5)–Li(1)–O(10)	101.6(4)
Li(1)–O(10)	1.993(9)	O(6)–Li(1)–O(9)	100.2(4)
		O(6)–Li(1)–O(10)	102.3(4)
		O(9)–Li(1)–O(10)	149.7(5)
		Ni(2)–O(5)–Li(1)	101.7(3)
		Ni(2)–O(6)–Li(1)	102.1(3)

Table S2 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and sodium(I) centres in **2**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.8480(13)	N(1)–Ni(1)–O(2)	178.75(7)
Ni(1)–O(2)	1.8355(13)	O(1)–Ni(1)–N(2)	177.27(7)
Ni(1)–N(1)	1.8450(16)	N(1)–Ni(1)–O(1)	94.82(7)
Ni(1)–N(2)	1.8404(16)	N(1)–Ni(1)–N(2)	86.87(8)
		N(2)–Ni(1)–O(2)	94.37(7)
		O(1)–Ni(1)–O(2)	83.93(5)
Na(1)–O(1)	2.3027(14)	O(3)–Na(1)–O(4)	166.48(6)
Na(1)–O(2)	2.3182(15)	O(1)–Na(1)–O(2)	64.42(5)
Na(1)–O(3)	2.5610(14)	O(1)–Na(1)–O(3)	64.58(5)
Na(1)–O(4)	2.5312(15)	O(1)–Na(1)–O(4)	128.82(5)
Na(1)–O(5)	2.3471(19)	O(1)–Na(1)–O(5)	106.28(7)
Na(1)–O(6)	2.365(2)	O(1)–Na(1)–O(6)	106.21(9)
		O(2)–Na(1)–O(3)	128.99(5)
		O(2)–Na(1)–O(4)	64.40(5)
		O(2)–Na(1)–O(5)	110.17(7)
		O(2)–Na(1)–O(6)	108.58(8)
		O(3)–Na(1)–O(5)	85.20(6)
		O(3)–Na(1)–O(6)	84.33(6)
		O(4)–Na(1)–O(5)	91.52(6)
		O(4)–Na(1)–O(6)	89.26(7)
		O(5)–Na(1)–O(6)	137.23(10)
		Ni(1)–O(1)–Na(1)	105.89(6)
		Ni(1)–O(2)–Na(1)	105.71(6)

Table S3 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and sodium(I) centres in **3**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.827(2)	N(1)–Ni(1)–O(2)	175.13(11)
Ni(1)–O(2)	1.840(2)	O(1)–Ni(1)–N(2)	174.90(12)
Ni(1)–N(1)	1.844(3)	N(1)–Ni(1)–O(1)	94.40(12)
Ni(1)–N(2)	1.840(3)	N(1)–Ni(1)–N(2)	87.07(15)
		N(2)–Ni(1)–O(2)	94.47(12)
		O(1)–Ni(1)–O(2)	84.47(9)
Ni(2)–O(5)	1.838(2)	N(3)–Ni(2)–O(6)	178.32(12)
Ni(2)–O(6)	1.8346(19)	O(5)–Ni(2)–N(4)	178.24(11)
Ni(2)–N(3)	1.824(3)	N(3)–Ni(2)–O(5)	94.74(12)
Ni(2)–N(4)	1.836(3)	N(3)–Ni(2)–N(4)	86.45(13)
		N(4)–Ni(2)–O(6)	94.75(11)
		O(5)–Ni(2)–O(6)	84.09(9)
Na(1)–O(1)	2.409(2)	O(3)–Na(1)–O(4)	170.91(8)
Na(1)–O(2)	2.424(2)	O(7)–Na(1)–O(8)	172.42(8)
Na(1)–O(3)	2.531(2)	O(1)–Na(1)–O(2)	61.34(7)
Na(1)–O(4)	2.580(2)	O(1)–Na(1)–O(3)	63.11(7)
Na(1)–O(5)	2.414(2)	O(1)–Na(1)–O(4)	122.28(8)
Na(1)–O(6)	2.443(2)	O(1)–Na(1)–O(5)	138.75(8)
Na(1)–O(7)	2.505(2)	O(1)–Na(1)–O(6)	136.06(8)
Na(1)–O(8)	2.579(2)	O(1)–Na(1)–O(7)	88.78(8)
		O(1)–Na(1)–O(8)	89.14(7)
		O(2)–Na(1)–O(3)	124.44(8)
		O(2)–Na(1)–O(4)	61.60(7)
		O(2)–Na(1)–O(5)	139.29(8)
		O(2)–Na(1)–O(6)	137.35(8)
		O(2)–Na(1)–O(7)	88.20(7)
		O(2)–Na(1)–O(8)	84.41(7)
		O(3)–Na(1)–O(5)	86.76(8)
		O(3)–Na(1)–O(6)	85.47(7)
		O(3)–Na(1)–O(7)	91.56(8)
		O(3)–Na(1)–O(8)	93.99(7)
		O(4)–Na(1)–O(5)	84.83(7)
		O(4)–Na(1)–O(6)	93.44(7)
		O(4)–Na(1)–O(7)	81.54(8)
		O(4)–Na(1)–O(8)	93.43(8)
		O(5)–Na(1)–O(6)	60.84(7)
		O(5)–Na(1)–O(7)	63.12(7)
		O(5)–Na(1)–O(8)	122.31(8)
		O(6)–Na(1)–O(7)	123.96(8)
		O(6)–Na(1)–O(8)	61.74(7)
		Ni(1)–O(1)–Na(1)	107.54(9)
		Ni(1)–O(2)–Na(1)	106.48(9)
		Ni(2)–O(5)–Na(1)	107.96(9)
		Ni(2)–O(6)–Na(1)	106.93(9)

Table S4 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and rubidium(I) centres in **4**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.835(3)	N(1)–Ni(1)–O(2)	176.83(12)
Ni(1)–O(2)	1.839(2)	O(1)–Ni(1)–N(2)	176.65(12)
Ni(1)–N(1)	1.838(3)	N(1)–Ni(1)–O(1)	95.04(13)
Ni(1)–N(2)	1.847(3)	N(1)–Ni(1)–N(2)	86.04(15)
		N(2)–Ni(1)–O(2)	94.53(13)
		O(1)–Ni(1)–O(2)	84.56(10)
Ni(2)–O(5)	1.845(2)	N(3)–Ni(2)–O(6)	176.36(13)
Ni(2)–O(6)	1.829(2)	O(5)–Ni(2)–N(4)	176.60(13)
Ni(2)–N(3)	1.820(3)	N(3)–Ni(2)–O(5)	94.88(14)
Ni(2)–N(4)	1.849(3)	N(3)–Ni(2)–N(4)	86.61(16)
		N(4)–Ni(2)–O(6)	94.07(13)
		O(5)–Ni(2)–O(6)	84.63(10)
Ni(3)–O(9)	1.841(2)	N(5)–Ni(3)–O(10)	178.52(11)
Ni(3)–O(10)	1.830(2)	O(9)–Ni(3)–N(6)	177.81(12)
Ni(3)–N(5)	1.834(3)	N(5)–Ni(3)–O(9)	94.68(11)
Ni(3)–N(6)	1.834(3)	N(5)–Ni(3)–N(6)	87.34(12)
		N(6)–Ni(3)–O(10)	94.13(11)
		O(9)–Ni(3)–O(10)	83.84(9)
Ni(4)–O(13)	1.828(2)	N(7)–Ni(4)–O(14)	175.85(12)
Ni(4)–O(14)	1.838(2)	O(13)–Ni(4)–N(8)	176.73(12)
Ni(4)–N(7)	1.838(3)	N(7)–Ni(4)–O(13)	94.84(12)
Ni(4)–N(8)	1.833(3)	N(7)–Ni(4)–N(8)	86.61(14)
		N(8)–Ni(4)–O(14)	94.49(12)
		O(13)–Ni(4)–O(14)	84.27(9)
Rb(1)–O(1)	2.855(2)	O(1)–Rb(1)–O(2)	51.10(7)
Rb(1)–O(2)	2.875(2)	O(1)–Rb(1)–O(3)	51.57(7)
Rb(1)–O(3)	3.101(3)	O(1)–Rb(1)–O(4)	97.80(7)
Rb(1)–O(4)	2.960(3)	O(1)–Rb(1)–O(5)	109.59(7)
Rb(1)–O(5)	2.833(2)	O(1)–Rb(1)–O(6)	77.40(7)
Rb(1)–O(6)	2.798(2)	O(1)–Rb(1)–O(7)	155.48(7)
Rb(1)–O(7)	3.102(3)	O(1)–Rb(1)–O(8)	83.81(7)
Rb(1)–O(8)	3.064(2)	O(2)–Rb(1)–O(3)	94.57(7)
		O(2)–Rb(1)–O(4)	52.27(7)
		O(2)–Rb(1)–O(5)	158.57(7)
		O(2)–Rb(1)–O(6)	109.05(7)
		O(2)–Rb(1)–O(7)	150.01(6)
		O(2)–Rb(1)–O(8)	74.42(7)
		O(3)–Rb(1)–O(4)	114.46(8)
		O(3)–Rb(1)–O(5)	74.78(7)
		O(3)–Rb(1)–O(6)	83.73(7)
		O(3)–Rb(1)–O(7)	104.61(7)

		O(3)–Rb(1)–O(8)	124.61(7)
		O(4)–Rb(1)–O(5)	149.10(7)
		O(4)–Rb(1)–O(6)	152.90(7)
		O(4)–Rb(1)–O(7)	98.28(7)
		O(4)–Rb(1)–O(8)	100.93(7)
		O(5)–Rb(1)–O(6)	52.12(7)
		O(5)–Rb(1)–O(7)	51.26(7)
		O(5)–Rb(1)–O(8)	96.09(7)
		O(6)–Rb(1)–O(7)	95.98(7)
		O(6)–Rb(1)–O(8)	52.25(7)
		O(7)–Rb(1)–O(8)	111.02(7)
		Ni(1)–O(1)–Rb(1)	104.98(10)
		Ni(1)–O(2)–Rb(1)	104.14(10)
		Ni(2)–O(5)–Rb(1)	101.61(10)
		Ni(2)–O(6)–Rb(1)	103.34(10)
Rb(2)–O(9)	2.842(2)	O(9)– Rb(2)–O(10)	51.10(6)
Rb(2)–O(10)	2.844(2)	O(9)–Rb(2)–O(11)	51.31(6)
Rb(2)–O(11)	3.134(2)	O(9)–Rb(2)–O(12)	95.02(6)
Rb(2)–O(12)	3.003(2)	O(9)–Rb(2)–O(13)	176.55(6)
Rb(2)–O(13)	2.886(2)	O(9)–Rb(2)–O(14)	130.28(6)
Rb(2)–O(14)	2.772(2)	O(9)–Rb(2)–O(15)	127.27(6)
Rb(2)–O(15)	2.977(2)	O(9)–Rb(2)–O(16)	86.76(6)
Rb(2)–O(16)	2.993(2)	O(10)–Rb(2)–O(11)	93.86(6)
		O(10)–Rb(2)–O(12)	51.86(6)
		O(10)–Rb(2)–O(13)	126.66(6)
		O(10)–Rb(2)–O(14)	172.31(6)
		O(10)–Rb(2)–O(15)	82.60(6)
		O(10)–Rb(2)–O(16)	132.30(6)
		O(11)–Rb(2)–O(12)	108.20(7)
		O(11)–Rb(2)–O(13)	128.52(6)
		O(11)–Rb(2)–O(14)	83.90(6)
		O(11)–Rb(2)–O(15)	175.00(6)
		O(11)–Rb(2)–O(16)	68.65(6)
		O(12)–Rb(2)–O(13)	81.76(6)
		O(12)–Rb(2)–O(14)	121.90(7)
		O(12)–Rb(2)–O(15)	66.83(7)
		O(12)–Rb(2)–O(16)	174.13(7)
		O(13)–Rb(2)–O(14)	51.48(6)
		O(13)–Rb(2)–O(15)	52.53(6)
		O(13)–Rb(2)–O(16)	96.33(6)
		O(14)–Rb(2)–O(15)	99.15(7)
		O(14)–Rb(2)–O(16)	53.53(6)
		O(15)–Rb(2)–O(16)	116.36(7)
		Ni(3)–O(9)–Rb(2)	102.51(9)
		Ni(3)–O(10)–Rb(2)	102.75(9)
		Ni(4)–O(13)–Rb(2)	103.17(9)
		Ni(4)–O(14)–Rb(2)	107.20(10)

Table S5 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and cesium(I) centres in **5**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.853(3)	N(1)–Ni(1)–O(2)	176.39(15)
Ni(1)–O(2)	1.849(3)	O(1)–Ni(1)–N(2)	177.04(14)
Ni(1)–N(1)	1.839(5)	N(1)–Ni(1)–O(1)	94.67(19)
Ni(1)–N(2)	1.848(5)	N(1)–Ni(1)–N(2)	85.7(2)
		N(2)–Ni(1)–O(2)	93.95(19)
		O(1)–Ni(1)–O(2)	85.91(14)
Ni(2)–O(5)	1.855(3)	N(3)–Ni(2)–O(6)	177.17(13)
Ni(2)–O(6)	1.846(3)	O(5)–Ni(2)–N(4)	177.14(13)
Ni(2)–N(3)	1.846(4)	N(3)–Ni(2)–O(5)	93.94(15)
Ni(2)–N(4)	1.838(4)	N(3)–Ni(2)–N(4)	86.53(18)
		N(4)–Ni(2)–O(6)	94.39(16)
		O(5)–Ni(2)–O(6)	85.28(12)
Cs(1)–O(1)	3.021(3)	O(2)–Cs(1)–O(7)	163.00(9)
Cs(1)–O(2)	2.988(3)	O(4)–Cs(1)–O(5)	163.54(9)
Cs(1)–O(3)	3.119(3)	O(1)–Cs(1)–O(2)	49.64(9)
Cs(1)–O(4)	3.170(4)	O(1)–Cs(1)–O(3)	50.67(9)
Cs(1)–O(5)	3.047(3)	O(1)–Cs(1)–O(4)	92.72(9)
Cs(1)–O(6)	2.963(3)	O(1)–Cs(1)–O(5)	101.79(8)
Cs(1)–O(7)	3.180(3)	O(1)–Cs(1)–O(6)	71.71(8)
Cs(1)–O(8)	3.183(3)	O(1)–Cs(1)–O(7)	146.79(9)
		O(1)–Cs(1)–O(8)	83.94(9)
		O(2)–Cs(1)–O(3)	95.09(9)
		O(2)–Cs(1)–O(4)	50.14(10)
		O(2)–Cs(1)–O(5)	146.32(8)
		O(2)–Cs(1)–O(6)	99.23(8)
		O(2)–Cs(1)–O(8)	71.21(9)
		O(3)–Cs(1)–O(5)	70.57(8)
		O(3)–Cs(1)–O(4)	114.46(10)
		O(3)–Cs(1)–O(6)	80.00(8)
		O(3)–Cs(1)–O(7)	98.48(9)
		O(3)–Cs(1)–O(8)	122.46(10)
		O(4)–Cs(1)–O(6)	145.20(10)
		O(4)–Cs(1)–O(7)	114.18(10)
		O(4)–Cs(1)–O(8)	98.74(10)
		O(5)–Cs(1)–O(6)	49.29(7)
		O(5)–Cs(1)–O(7)	49.55(8)
		O(5)–Cs(1)–O(8)	90.56(8)
		O(6)–Cs(1)–O(7)	93.19(8)
		O(6)–Cs(1)–O(8)	49.94(8)
		O(7)–Cs(1)–O(8)	109.24(9)
		Ni(1)–O(1)–Cs(1)	104.03(13)
		Ni(1)–O(2)–Cs(1)	105.36(13)
		Ni(2)–O(5)–Cs(1)	103.08(11)
		Ni(2)–O(6)–Cs(1)	106.41(11)

Table S6 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and magnesium(II) centres in **6**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.855(4)	N(1)–Ni(1)–O(2)	176.14(18)
Ni(1)–O(2)	1.840(3)	O(1)–Ni(1)–N(2)	176.29(18)
Ni(1)–N(1)	1.844(5)	N(1)–Ni(1)–O(1)	94.0(2)
Ni(1)–N(2)	1.837(5)	N(1)–Ni(1)–N(2)	86.1(2)
		N(2)–Ni(1)–O(2)	94.74(19)
		O(1)–Ni(1)–O(2)	85.40(16)
Ni(2)–N(3)	1.828(5)	N(3)–Ni(2)–O(5A)	177.74(19)
Ni(2)–O(5)	1.838(4)	N(3)–Ni(2)–O(5)	95.38(18)
		N(3)–Ni(2)–N(3A)	86.7(3)
		O(5)–Ni(2)–O(5A)	82.6(2)
Mg(1)–O(5)	2.191(4)	O(7)–Mg(1)–O(7A)	178.0(3)
Mg(1)–O(7)	2.112(4)	O(5)–Mg(1)–O(7)	90.27(15)
Mg(1)–O(8)	2.108(9)	O(5)–Mg(1)–O(7A)	91.39(15)
		O(5)–Mg(1)–O(8)	146.40(10)
		O(5)–Mg(1)–O(5A)	67.2(2)
		O(7)–Mg(1)–O(8)	89.00(13)
		Ni(2)–O(5)–Mg(1)	105.13(16)

Table S7 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and calcium(II) centres in **7**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.830(2)	N(1)–Ni(1)–O(2)	178.16(13)
Ni(1)–O(2)	1.844(2)	O(1)–Ni(1)–N(2)	178.09(13)
Ni(1)–N(1)	1.827(3)	N(1)–Ni(1)–O(1)	95.70(14)
Ni(1)–N(2)	1.825(3)	N(1)–Ni(1)–N(2)	85.92(16)
		N(2)–Ni(1)–O(2)	95.21(14)
		O(1)–Ni(1)–O(2)	83.19(11)
Ca(1)–O(1)	2.367(3)	O(1)–Ca(1)–O(2)	61.98(8)
Ca(1)–O(2)	2.370(2)	O(1)–Ca(1)–O(3)	63.71(8)
Ca(1)–O(3)	2.502(3)	O(1)–Ca(1)–O(4)	125.04(9)
Ca(1)–O(4)	2.519(3)	O(1)–Ca(1)–O(5)	114.65(10)
Ca(1)–O(5)	2.578(3)	O(1)–Ca(1)–O(6)	80.22(12)
Ca(1)–O(6)	2.490(4)	O(1)–Ca(1)–O(8B)	78.3(2)
Ca(1)–O(8B)	2.690(8)	O(1)–Ca(1)–O(9A)	84.1(2)
Ca(1)–O(9A)	2.292(9)	O(1)–Ca(1)–O(11)	146.89(10)
Ca(1)–O(11)	2.355(3)	O(2)–Ca(1)–O(3)	125.69(8)
		O(2)–Ca(1)–O(4)	63.38(8)
		O(2)–Ca(1)–O(5)	124.81(9)
		O(2)–Ca(1)–O(6)	78.55(10)
		O(2)–Ca(1)–O(8B)	101.0(2)
		O(2)–Ca(1)–O(9A)	81.0(2)
		O(2)–Ca(1)–O(11)	143.66(10)
		O(3)–Ca(1)–O(4)	169.13(9)
		O(3)–Ca(1)–O(5)	78.15(10)
		O(3)–Ca(1)–O(6)	91.95(14)
		O(3)–Ca(1)–O(8B)	68.31(17)
		O(3)–Ca(1)–O(9A)	94.3(3)
		O(3)–Ca(1)–O(11)	87.47(10)
		O(4)–Ca(1)–O(5)	91.62(10)
		O(4)–Ca(1)–O(6)	83.92(14)
		O(4)–Ca(1)–O(8B)	117.97(17)
		O(4)–Ca(1)–O(9A)	93.2(3)
		O(4)–Ca(1)–O(11)	85.75(10)
		O(5)–Ca(1)–O(6)	48.97(9)
		O(5)–Ca(1)–O(8B)	133.6(2)
		O(5)–Ca(1)–O(9A)	152.63(18)
		O(5)–Ca(1)–O(11)	71.37(10)
		O(6)–Ca(1)–O(8B)	155.7(2)
		O(6)–Ca(1)–O(9A)	158.40(18)
		O(6)–Ca(1)–O(11)	118.83(11)
		O(8B)–Ca(1)–O(9A)	26.7(3)
		O(8B)–Ca(1)–O(11)	75.9(2)
		O(9A)–Ca(1)–O(11)	82.13(19)
		Ni(1)–O(1)–Ca(1)	107.69(11)
		Ni(1)–O(2)–Ca(1)	107.04(10)

Table S8 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and cadmium(II) centres in **8**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.836(5)	N(1)–Ni(1)–O(2)	177.7(3)
Ni(1)–O(2)	1.828(5)	O(1)–Ni(1)–N(2)	178.4(3)
Ni(1)–N(1)	1.830(7)	N(1)–Ni(1)–O(1)	94.7(3)
Ni(1)–N(2)	1.828(7)	N(1)–Ni(1)–N(2)	86.6(3)
		N(2)–Ni(1)–O(2)	95.0(3)
		O(1)–Ni(1)–O(2)	83.7(2)
Cd(1)–O(1)	2.291(5)	O(5)–Cd(1)–O(8)	175.8(2)
Cd(1)–O(2)	2.288(5)	O(1)–Cd(1)–O(2)	64.54(18)
Cd(1)–O(3)	2.524(6)	O(1)–Cd(1)–O(3)	64.84(18)
Cd(1)–O(4)	2.544(6)	O(1)–Cd(1)–O(4)	129.60(18)
Cd(1)–O(5)	2.445(7)	O(1)–Cd(1)–O(5)	88.1(2)
Cd(1)–O(6)	2.343(7)	O(1)–Cd(1)–O(6)	135.9(2)
Cd(1)–O(8)	2.467(7)	O(1)–Cd(1)–O(8)	91.0(2)
Cd(1)–O(9)	2.357(7)	O(1)–Cd(1)–O(9)	123.7(2)
		O(2)–Cd(1)–O(3)	129.15(19)
		O(2)–Cd(1)–O(4)	65.17(18)
		O(2)–Cd(1)–O(5)	89.8(2)
		O(2)–Cd(1)–O(6)	125.9(2)
		O(2)–Cd(1)–O(8)	86.1(2)
		O(2)–Cd(1)–O(9)	135.5(2)
		O(3)–Cd(1)–O(4)	165.54(18)
		O(3)–Cd(1)–O(5)	84.0(2)
		O(3)–Cd(1)–O(6)	88.8(2)
		O(3)–Cd(1)–O(8)	99.3(2)
		O(3)–Cd(1)–O(9)	79.2(2)
		O(4)–Cd(1)–O(5)	94.9(2)
		O(4)–Cd(1)–O(6)	79.2(2)
		O(4)–Cd(1)–O(8)	82.5(2)
		O(4)–Cd(1)–O(9)	90.8(2)
		O(5)–Cd(1)–O(6)	52.8(2)
		O(5)–Cd(1)–O(9)	131.0(2)
		O(6)–Cd(1)–O(8)	129.4(2)
		O(6)–Cd(1)–O(9)	81.0(3)
		O(8)–Cd(1)–O(9)	52.5(2)
		Ni(1)–O(1)–Cd(1)	105.7(2)
		Ni(1)–O(2)–Cd(1)	106.1(2)

Table S9 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) and lead(II) centres in **9**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.859(4)	N(1)–Ni(1)–O(2)	177.0(3)
Ni(1)–O(2)	1.862(5)	O(1)–Ni(1)–N(2)	177.3(3)
Ni(1)–N(1)	1.833(6)	N(1)–Ni(1)–O(1)	95.0(3)
Ni(1)–N(2)	1.826(6)	N(1)–Ni(1)–N(2)	85.3(3)
		N(2)–Ni(1)–O(2)	94.8(3)
		O(1)–Ni(1)–O(2)	85.1(2)
Pb(1)–O(1)	2.478(5)	O(3)–Pb(1)–O(4)	174.09(19)
Pb(1)–O(2)	2.448(5)	O(1)–Pb(1)–O(2)	61.42(14)
Pb(1)–O(3)	2.699(5)	O(1)–Pb(1)–O(3)	61.22(16)
Pb(1)–O(4)	2.684(6)	O(1)–Pb(1)–O(4)	123.02(16)
Pb(1)–O(5A)	2.940(12)	O(1)–Pb(1)–O(5A)	105.8(3)
Pb(1)–O(6A)	2.640(16)	O(1)–Pb(1)–O(6A)	80.5(4)
Pb(1)–O(8)	2.631(6)	O(1)–Pb(1)–O(8)	69.61(18)
Pb(1)–O(9)	2.763(8)	O(1)–Pb(1)–O(9)	108.7(2)
		O(2)–Pb(1)–O(3)	122.61(16)
		O(2)–Pb(1)–O(4)	61.66(15)
		O(2)–Pb(1)–O(5A)	113.1(3)
		O(2)–Pb(1)–O(6A)	72.3(4)
		O(2)–Pb(1)–O(8)	88.79(19)
		O(2)–Pb(1)–O(9)	86.3(2)
		O(3)–Pb(1)–O(5A)	80.9(3)
		O(3)–Pb(1)–O(6A)	96.8(4)
		O(3)–Pb(1)–O(8)	73.4(2)
		O(3)–Pb(1)–O(9)	113.5(2)
		O(4)–Pb(1)–O(5A)	93.6(3)
		O(4)–Pb(1)–O(6A)	80.5(4)
		O(4)–Pb(1)–O(8)	111.6(2)
		O(4)–Pb(1)–O(9)	69.92)
		O(5A)–Pb(1)–O(6A)	41.5(4)
		O(5A)–Pb(1)–O(8)	152.8(3)
		O(5A)–Pb(1)–O(9)	145.4(3)
		O(6A)–Pb(1)–O(8)	149.7(4)
		O(6A)–Pb(1)–O(9)	149.3(4)
		O(8)–Pb(1)–O(9)	46.3(2)
		Ni(1)–O(1)–Pb(1)	106.0(2)
		Ni(1)–O(2)–Pb(1)	107.13(19)

Table S10 Bond lengths (Å) and bond angles (°) in the coordination environments of the nickel(II) centres in **10**

Bond lengths		**Bond angles**	
Ni(1)–O(1)	1.8404(13)	O(1)–Ni(1)–N(2)	177.31(6)
Ni(1)–O(2)	1.8443(14)	O(2)–Ni(1)–N(1)	177.31(6)
Ni(1)–N(1)	1.8447(17)	O(1)–Ni(1)–O(2)	84.86(6)
Ni(1)–N(2)	1.8478(16)	O(1)–Ni(1)–N(1)	94.23(7)
		O(2)–Ni(1)–N(2)	94.48(7)
		N(1)–Ni(1)–N(2)	86.55(8)
Ni(2)–O(5)	1.8331(14)	O(5)–Ni(2)–N(4)	177.00(8)
Ni(2)–O(6)	1.8409(13)	O(6)–Ni(2)–N(3)	178.13(8)
Ni(2)–N(3)	1.8390(19)	O(5)–Ni(2)–O(6)	84.79(6)
Ni(2)–N(4)	1.839(2)	O(5)–Ni(2)–N(3)	94.25(8)
		O(6)–Ni(2)–N(4)	94.11(8)
		N(3)–Ni(2)–N(4)	86.93(10)