

Supplementary information for

New topology of CN-bridged clusters: dodecanuclear face-sharing defective cubes based on octacyanomethylates(IV) and nickel(II) with diimine ligands

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Additional elemental analysis results for compound 2

Sample in form of crystals analysed within 2 days after removal from solution.

Found: C, 34.90; H, 3.64; N, 16.84; calc. for C₁₁₆H₁₄₀N₄₈O₃₄Ni₈W₄: C, 35.22; H, 3.57; N, 17.00

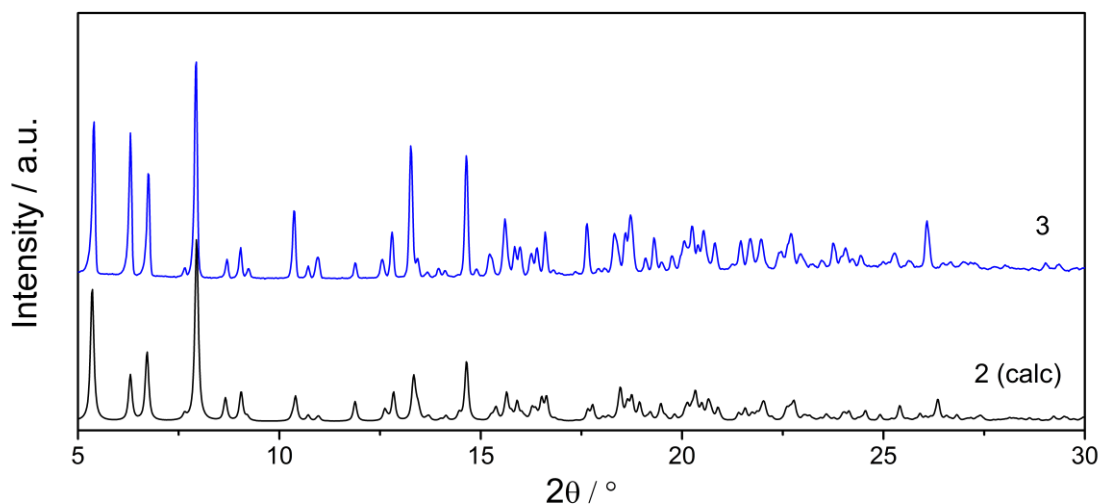


Figure S1. Powder X-ray diffraction pattern for **3** (blue line) in comparison to the pattern calculated for **2** (black line).

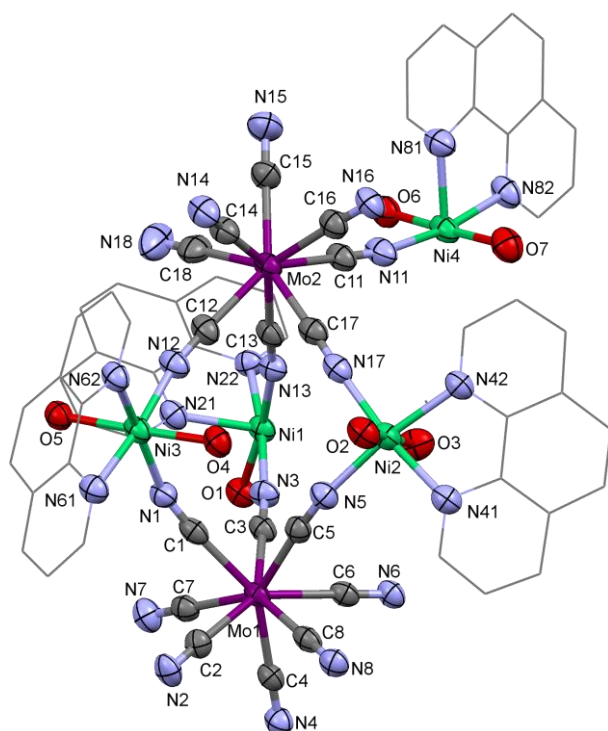


Figure S2. Asymmetric unit of **1** with selected atoms numbering. Thermal ellipsoids at 40% probability. Hydrogen atoms and crystallisation solvent omitted for clarity; phen ligands depicted as sticks.

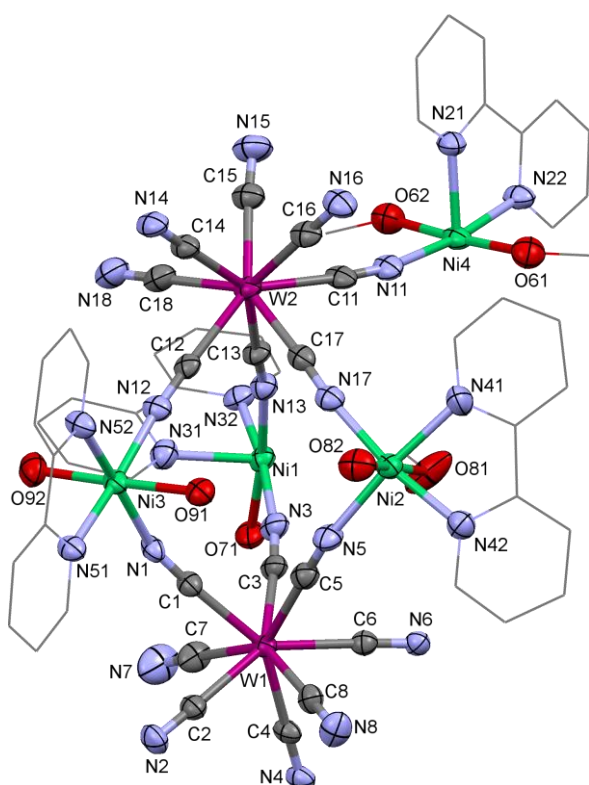


Figure S3. Asymmetric unit of **2** with selected atoms numbering. Thermal ellipsoids at 40% probability. Hydrogen atoms and crystallisation solvent omitted for clarity; bpy ligands depicted as sticks.

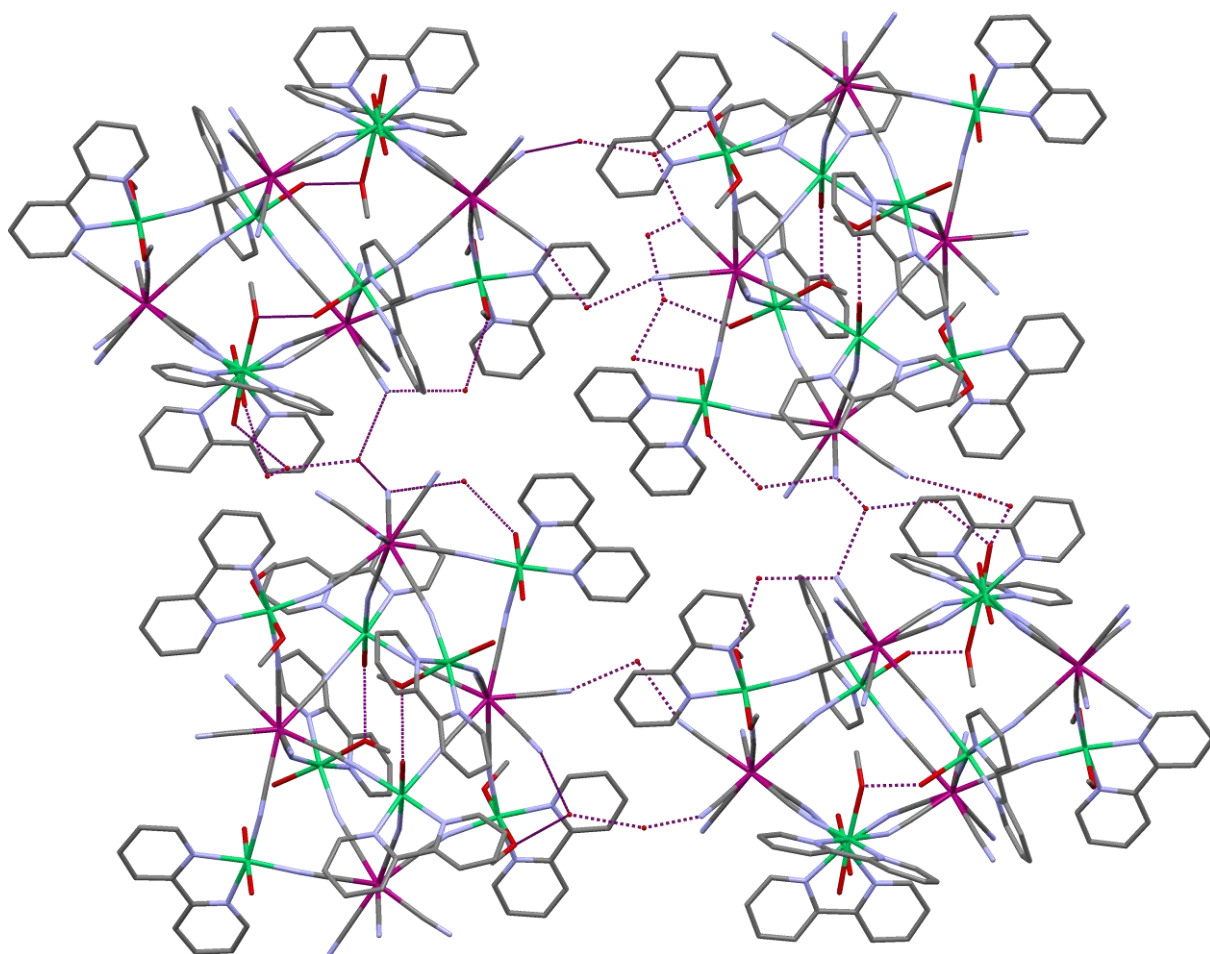


Figure S4. Hydrogen bonds in the structure of **2**.

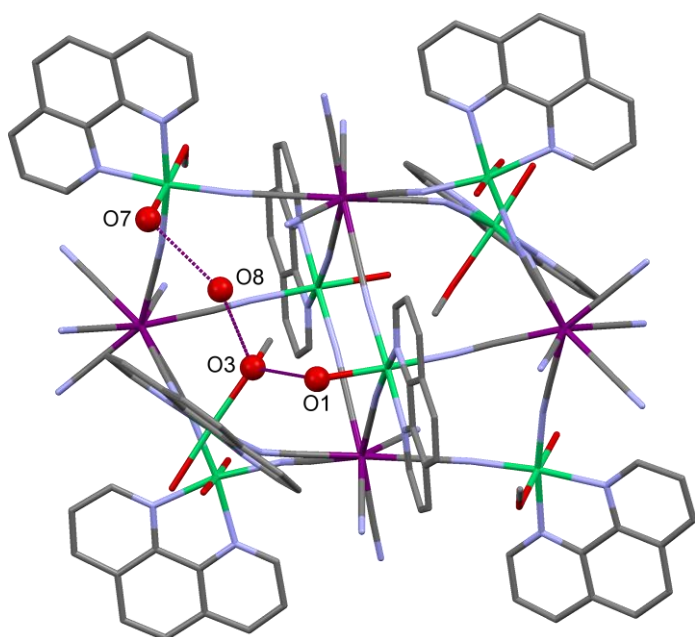


Figure S4. Hydrogen bonds in the structure of **1**.

Table S1. Selected bond angles (°) in the structures of **1** and **2**.

Angles of bridging CN ligands					
	1	2		1	2
Ni1-N3-C3	175.0(5)	170.7(8)	M1-C1-N1	175.0(4)	175.4(6)
Ni1-N6-C6	174.6(4)	178.9(7)	M1-C3-N3	178.8(5)	174.9(8)
Ni1-N13-C13	169.1(5)	167.3(7)	M1-C4-N4	179.4(5)	178.9(8)
Ni2-N5-C5	159.7(4)	157.6(7)	M1-C5-N5	175.2(5)	176.9(7)
Ni2-N17-C17	166.5(5)	169.1(6)	M1-C6-N6	176.9(5)	176.6(7)
Ni3-N1-C1	153.4(5)	156.9(6)	M2-C11-N11	178.2(5)	174.8(8)
Ni3-N12-C12	164.6(5)	168.2(7)	M2-C12-N12	175.7(6)	177.3(8)
Ni4-N4-C4	175.5(5)	171.2(6)	M2-C13-N13	176.6(4)	177.3(8)
Ni4-N11-C11	169.7(6)	164.8(8)	M2-C17-N17	178.4(5)	176.2(7)
Angles at M ^{IV} centres					
	1	2		1	2
C1-M1-C2	76.16(19)	74.4(3)	C11-M2-C12	140.8(2)	136.6(3)
C1-M1-C3	76.19(19)	78.5(3)	C11-M2-C13	68.85(19)	70.2(3)
C1-M1-C4	145.75(19)	145.9(3)	C11-M2-C14	144.5(2)	142.4(3)
C1-M1-C5	70.5(2)	71.7(3)	C11-M2-C15	77.3(2)	73.4(3)
C1-M1-C6	136.85(18)	140.1(3)	C11-M2-C16	74.1(2)	72.0(3)
C1-M1-C7	75.7(2)	77.9(3)	C11-M2-C17	87.9(2)	78.1(3)
C1-M1-C8	119.3(2)	114.8(3)	C11-M2-C18	105.3(3)	123.4(4)
C2-M1-C3	144.4(2)	141.7(3)	C12-M2-C13	74.12(19)	78.1(3)
C2-M1-C4	83.6(2)	81.5(3)	C12-M2-C14	73.0(2)	75.8(3)
C2-M1-C5	109.14(19)	115.4(3)	C12-M2-C15	135.9(2)	144.3(3)
C2-M1-C6	142.7(2)	141.7(3)	C12-M2-C16	127.6(2)	123.9(3)
C2-M1-C7	78.58(19)	76.3(4)	C12-M2-C17	72.7(2)	69.5(3)
C2-M1-C8	71.81(19)	72.8(3)	C12-M2-C18	76.5(3)	73.5(3)
C3-M1-C4	107.96(19)	108.5(3)	C13-M2-C14	146.61(18)	147.0(3)
C3-M1-C5	81.97(19)	80.0(3)	C13-M2-C15	122.1(2)	103.1(3)
C3-M1-C6	72.0(2)	74.5(3)	C13-M2-C16	133.4(2)	139.8(3)
C3-M1-C7	73.17(19)	71.9(4)	C13-M2-C17	79.1(2)	83.6(3)
C3-M1-C8	142.61(19)	144.5(3)	C13-M2-C18	75.1(2)	75.4(3)
C4-M1-C5	143.3(2)	141.8(3)	C14-M2-C15	79.5(2)	87.0(3)
C4-M1-C6	73.30(19)	71.8(3)	C14-M2-C16	73.9(2)	72.7(3)
C4-M1-C7	73.3(2)	73.1(3)	C14-M2-C17	96.6(2)	105.5(3)
C4-M1-C8	78.7(2)	79.4(3)	C14-M2-C18	91.5(3)	78.0(3)
C5-M1-C6	76.8(2)	75.2(3)	C15-M2-C16	73.9(2)	78.2(4)
C5-M1-C7	141.9(2)	142.0(3)	C15-M2-C17	145.5(2)	146.1(4)
C5-M1-C8	73.4(2)	74.3(3)	C15-M2-C18	70.3(3)	72.4(4)
C6-M1-C7	120.2(2)	119.3(3)	C16-M2-C17	72.2(2)	75.8(3)
C6-M1-C8	75.20(18)	75.6(3)	C16-M2-C18	143.2(2)	139.2(3)
C7-M1-C8	141.05(19)	141.1(3)	C17-M2-C18	144.1(2)	140.4(3)

Angles at Ni ^{II} centres (in rows corresponding angles for 1 and 2)			
1		2	
N3 Ni1 N13	92.70(18)	N3 Ni1 N13	93.4(3)
N3 Ni1 N6	94.39(19)	N3 Ni1 N6	91.2(3)
N13 Ni1 N6	96.91(19)	N6 Ni1 N13	97.3(3)
N3 Ni1 N21	94.31(18)	N3 Ni1 N31	95.7(3)
N13 Ni1 N21	86.77(19)	N13 Ni1 N31	85.6(3)
N13 Ni1 N22	89.57(18)	N13 Ni1 N32	91.6(3)
N6 Ni1 N22	91.40(18)	N6 Ni1 N32	94.1(3)
N21 Ni1 N22	79.71(18)	N31 Ni1 N32	78.7(3)
N3 Ni1 O1	87.15(17)	N3 Ni1 O71	87.9(3)
N6 Ni1 O1	88.70(17)	N6 Ni1 O71	88.0(2)
N21 Ni1 O1	87.64(17)	N31 Ni1 O71	89.0(3)
N22 Ni1 O1	89.98(17)	N32 Ni1 O71	86.6(3)
N17 Ni2 N5	93.62(19)	N17 Ni2 N5	93.2(3)
N5 Ni2 N41	93.03(19)	N42 Ni2 N5	95.3(3)
N17 Ni2 N42	92.94(19)	N17 Ni2 N41	91.8(3)
N41 Ni2 N42	79.90(19)	N42 Ni2 N41	79.5(3)
N17 Ni2 O2	94.46(19)	N17 Ni2 O82	93.8(3)
N5 Ni2 O2	93.35(17)	N5 Ni2 O82	91.9(3)
N41 Ni2 O2	89.83(19)	N42 Ni2 O82	88.1(3)
N42 Ni2 O2	93.25(17)	N41 Ni2 O82	92.1(3)
N17 Ni2 O3	89.53(19)	N17 Ni2 O81	90.6(3)
N5 Ni2 O3	86.78(18)	N5 Ni2 O81	88.3(4)
N41 Ni2 O3	86.16(19)	N42 Ni2 O81	87.5(3)
N42 Ni2 O3	86.15(18)	N41 Ni2 O81	87.3(4)
N12 Ni3 N1	95.89(18)	N12 Ni3 N1	93.4(2)
N12 Ni3 N62	93.90(18)	N12 Ni3 N52	93.6(3)
N1 Ni3 N61	91.16(18)	N1 Ni3 N51	93.9(2)
N62 Ni3 N61	79.36(18)	N51 Ni3 N52	78.9(3)
N12 Ni3 O5	90.49(18)	N12 Ni3 O92	90.0(3)
N1 Ni3 O5	94.98(18)	N1 Ni3 O92	93.8(3)
N62 Ni3 O5	92.98(18)	N52 Ni3 O92	92.1(3)
N61 Ni3 O5	87.25(18)	N51 Ni3 O92	92.0(3)
N12 Ni3 O4	87.97(18)	N12 Ni3 O91	88.7(3)
N1 Ni3 O4	85.82(18)	N1 Ni3 O91	86.8(2)
N62 Ni3 O4	86.49(18)	N52 Ni3 O91	87.5(3)
N61 Ni3 O4	94.20(18)	N51 Ni3 O91	89.2(3)
N11 Ni4 N4	95.98(19)	N4 Ni4 N11	93.9(3)
N4 Ni4 N82	92.80(19)	N4 Ni4 N22	92.3(2)
N11 Ni4 N81	91.16(19)	N11 Ni4 N21	94.9(3)
N82 Ni4 N81	80.1(2)	N22 Ni4 N21	78.9(3)
N4 Ni4 O6	90.8(2)	N4 Ni4 O62	92.3(3)
N11 Ni4 O6	91.4(2)	N11 Ni4 O62	91.1(3)
O6 Ni4 N82	85.9(2)	N22 Ni4 O62	84.1(3)
O6 Ni4 N81	89.7(2)	N21 Ni4 O62	88.1(3)
N11 Ni4 O7	90.8(2)	N4 Ni4 O61	89.9(3)
N4 Ni4 O7	89.6(2)	N11 Ni4 O61	91.1(3)
N82 Ni4 O7	91.9(2)	N22 Ni4 O61	93.5(3)
N81 Ni4 O7	89.6(2)	N21 Ni4 O61	89.4(3)