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Supporting Information for

Supramolecular architectures based on various macrocyclic metallic tectons with 1,3,5-triazine-2,4,6-triamine hexaacetic acid ligand

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Supporting Information Table 1: Selected bond lengths (Å) and angles (°) for the compound **4**-**12**.

Compound **4**		Compound **5**		Compound **6**	
Cu(1)-N(4)	1.9976(18)	N(1)-Ni	1.915(2)	N(1)-Ni(1)	1.912(3)
Cu(1)-N(2)	2.0073(18)	N(2)-Ni	1.9406(18)	N(2)-Ni(1)	1.937(3)
Cu(1)-N(1)	2.0111(18)	N(3)-Ni	1.911(2)	N(3)-Ni(1)	1.916(3)
Cu(1)-N(3)	2.0183(19)	N(4)-Ni	1.9322(18)	N(4)-Ni(1)	1.940(3)
N(4)-Cu(1)-N(2)	176.91(8)	O(1)-Ni	3.2220(15)	O(1)-Ni(1)	3.2089(33)
N(4)-Cu(1)-N(1)	86.57(7)	O(11)-Ni	2.9639(15)	O(4)-Ni(1)	2.9563(32)
N(2)-Cu(1)-N(1)	92.21(8)	N(1)-Ni-N(2)	93.37(9)	N(3)-Ni(1)-N(4)	93.44(14)
N(4)-Cu(1)-N(3)	95.07(8)	N(4)-Ni-N(2)	178.44(7)	N(2)-Ni(1)-N(4)	178.36(13)
N(2)-Cu(1)-N(3)	86.56(8)	N(3)-Ni-N(1)	179.42(8)	N(1)-Ni(1)-N(3)	179.50(14)
N(1)-Cu(1)-N(3)	171.37(8)	N(3)-Ni-N(4)	93.06(10)	N(1)-Ni(1)-N(2)	93.16(16)
		N(1)-Ni-N(4)	86.78(9)	N(3)-Ni(1)-N(2)	86.53(15)
		N(3)-Ni-N(2)	86.77(9)	N(1)-Ni(1)-N(4)	86.86(15)
		O(1)-Ni-O(11)	176.657	O(1)-Ni(1)-O(4)	176.676(82)

Compound **7**[a]		Compound **8**		Compound **9**	
N(1)-Ni(1)	1.927(6)	N(7)-Ni(1)	1.921(3)	Cu(1)-N(4)	2.007(4)
N(2)-Ni(1)	1.939(6)	N(8)-Ni(1)	1.931(3)	Cu(1)-N(2)	2.009(4)
Ni(1)-N(1)#1	1.927(6)	N(9)-Ni(1)	1.938(3)	Cu(1)-N(3)	2.015(4)
Ni(1)-N(2)#1	1.939(6)	N(10)-Ni(1)	1.910(3)	Cu(1)-N(1)	2.018(4)
Ni(1)-O6	3.0189(5)	O(1)-Ni(1)	2.6897(23)	Cu(1)-O(12)	2.373(3)
Ni(1)-O6#1	3.0189(5)	O(4)-Ni(1)	3.0488(28)	N(4)-Cu(1)-N(2)	177.23(19)
N(1)-Ni(1)-N(1)#1	86.4(4)	N(10)-Ni(1)-N(7)	87.84(14)	N(4)-Cu(1)-N(3)	86.16(19)
N(1)-Ni(1)-N(2)#1	175.0(2)	N(10)-Ni(1)-N(8)	176.22(12)	N(2)-Cu(1)-N(3)	96.05(19)
N(1)#1-Ni(1)-N(2)#1	93.3(3)	N(7)-Ni(1)-N(8)	94.57(13)	N(4)-Cu(1)-N(1)	92.0(2)
N(1)-Ni(1)-N(2)	93.3(3)	N(10)-Ni(1)-N(9)	92.75(14)	N(2)-Cu(1)-N(1)	85.5(2)
N(1)#1-Ni(1)-N(2)	175.0(2)	N(7)-Ni(1)-N(9)	172.67(11)	N(3)-Cu(1)-N(1)	166.92(16)
N(2)#1-Ni(1)-N(2)	87.4(3)	N(8)-Ni(1)-N(9)	85.24(13)	N(4)-Cu(1)-O(12)	94.59(14)
O(6)-Ni(1)-O6#1	146.407(117)	O(1)-Ni-O(4)	157.494	N(2)-Cu(1)-O(12)	86.53(13)
				N(3)-Cu(1)-O(12)	103.32(14)
				N(1)-Cu(1)-O(12)	89.73(13)

Compound **10**		Compound **11**[b]		Compound **12**[c]	
N(1)-Ni(1)	1.930(3)	Ni(1)-N(1)	1.923(4)	Ni(1)-N(1)	1.927(4)
N(2)-Ni(1)	1.923(3)	Ni(1)-N(1)#1	1.923(4)	Ni(1)-N(1)#1	1.927(4)
N(3)-Ni(1)	1.926(3)	Ni(1)-N(3)#1	1.932(4)	Ni(1)-N(3)	1.929(4)
N(4)-Ni(1)	1.937(3)	Ni(1)-N(3)	1.932(4)	Ni(1)-N(3)#1	1.929(4)
O(6)-Ni(1)	3.0017(36)	Ni(1)-O(5)	2.9372(33)	Ni(1)-O(5)	2.9476(33)
O(7)-Ni(1)	3.0698(36)	Ni(1)-O(5)#1	2.9372(33)	Ni(1)-O(5)#1	2.9476(33)
N(2)-Ni(1)-N(3)	87.29(11)	N(1)#1-Ni(1)-N(1)	87.0(3)	N(1)-Ni(1)-N(1)#1	86.4(3)
N(2)-Ni(1)-N(1)	93.43(12)	N(1)#1-Ni(1)-N(3)#1	93.01(18)	N(1)-Ni(1)-N(3)	93.27(18)
N(3)-Ni(1)-N(1)	173.66(11)	N(1)#1-Ni(1)-N(3)#1	174.27(17)	N(1)#1-Ni(1)-N(3)	174.04(15)
N(2)-Ni(1)-N(4)	174.85(11)	N(1) -Ni(1)-N(3)	174.27(17)	N(1)-Ni(1)-N(3)#1	174.04(15)
N(3)-Ni(1)-N(4)	93.00(12)	N(1) -Ni(1)-N(3)	93.01(18)	N(1)#1-Ni(1)-N(3)#1	93.27(18)
N(1)-Ni(1)-N(4)	86.86(13)	N(3)#1-Ni(1)-N(3)	87.6(2)	N(3)-Ni(1)-N(3)#1	87.7(2)
O(6)-Ni(1)-O(7)	151.119	O(5)-Ni(1)-O(5)#1	152.278(87)	O(5)-Ni(1)-O(5)#1	150.435

Symmetry transformations used to generate equivalent atoms:

a: #1 -x+1,y,-z+3/2 b: #1 -x+1,y,-z+1/2 c: #1 -x,y,-z+3/2

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Supporting Information Table 2: Selected hydrogen bond Geometry lengths (Å) and angles (°) for the compounds.

Compounds	D-H···A	*d* (D-H)	*d* (H···A)	*d* (D···A)	∠D-H···A
5	N3-H···O3	0.912	1.922	2.831	174.7
	N1-H···O9	0.858	2.003	2.856	172.8
7	N1-H···O4	0.859	2.193	2.979	152.1
8	N8-H···O7	1.019	2.262	3.211	154.3
	N9-H···O4	0.918	2.309	3.145	151.3
9	N1-H···O9	0.850	2.306	3.052	146.1
10	N1-H···O1	0.896	2.369	3.142	144.6
	N4-H···O10	0.892	2.203	3.061	161.2
12	N1-H···O4	0.910	2.091	2.939	154.7