Electronic Supplementary Material (ESI) for CrystEngComm.

One-pot crystallization of 1,4-cyclohexanedicarboxylate based two tetranuclear Cu(II) compounds impacts on DNA binding affinities

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Supporting Information

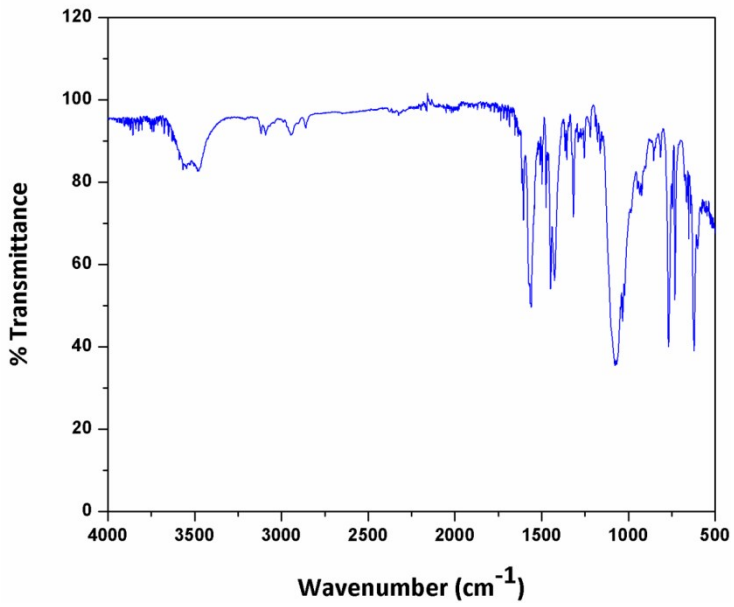

Fig. S1 FT-IR spectrum of compound **1**.

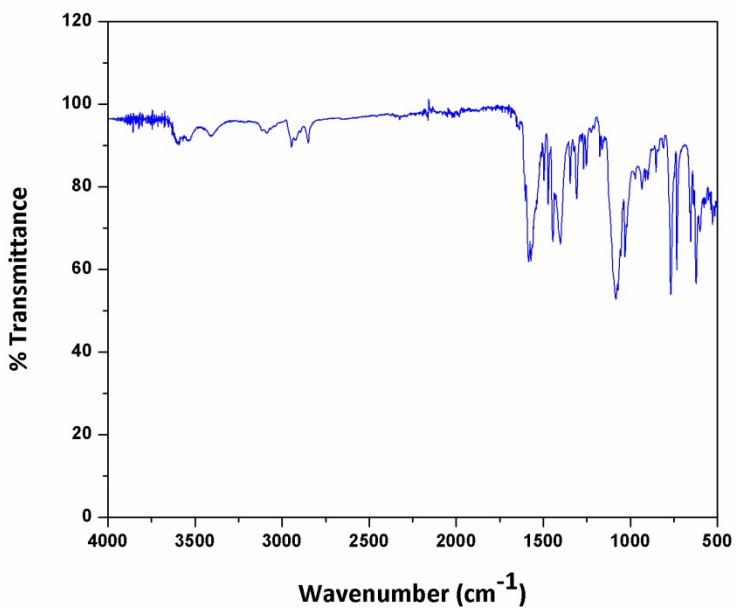

Fig. S2 FT-IR spectrum of compound **2**.

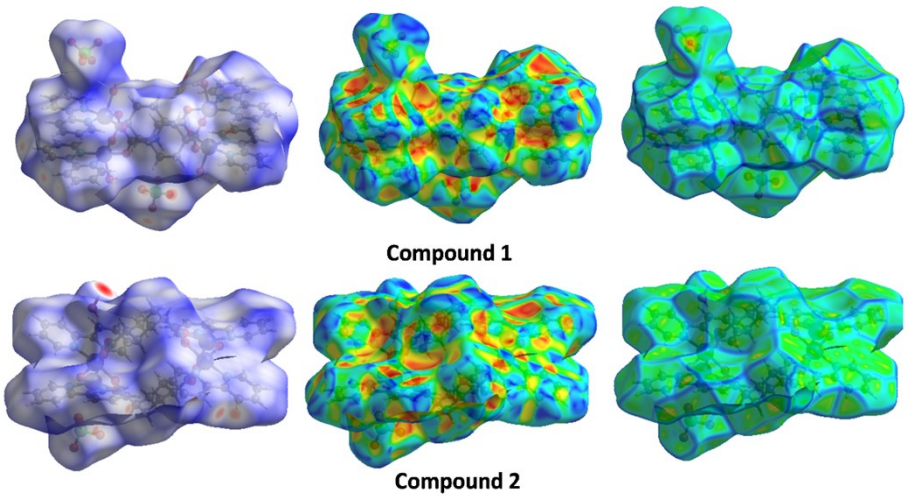

Fig. S3 Hirshfeld surfaces mapped with d*norm* (left), shape index (middle), curvedness (right) for compound **1** (above) and **2** (below).

Density functional study (DFT)

The electronic properties of compound **1** and **2** are determined by performing DFT study. DFT optimizations of the structure of the coordination motifs were explored for the calculation of difference in energy of the HOMO and LUMO (Fig. S4). The HOMO-LUMO gap is calculated as 1.36 eV for compound **1** and 2.09 eV for compound **2**. As the larger difference in the values of HOMO and LUMO points to the lower stability of the resulting molecule, it could be concluded that the compound **1** is more stable in comparison to **2**.

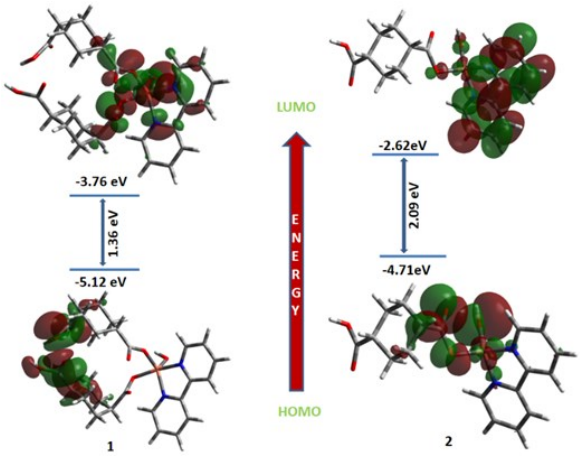

Fig. S4 DFT computed energy of MOs and the energy difference between HOMO and LUMO of compounds **1** and **2**.

Table S1 Crystal data and refinement parameters of compound **1** and **2**

Compound	**1**	**2**
Formula	$C_{56}H_{56}Cl_4Cu_4N_8O_{28}$	$C_{60}H_{68}Cu_4N_8O_{15}S_2$
fw	1685.09	1486.14
crystsyst	Monoclinic	Triclinic
space group	$P2_1/n$	$P\bar{1}$
a (Å)	9.5466(3)	9.3595(3)
b (Å)	17.6942(6)	12.4592(4)
c (Å)	20.2248(7)	14.5015(4)
α(deg)	90	87.821(1)
β(deg)	101.200(2)	72.827(1)
γ (deg)	90	68.258(1)
V (Å^3)	3351.3(2)	1495.86(8)
Z	2	1
D_{calcd}(g/cm^3)	1.670	1.650
μ(mm^{-1})	1.503	1.575
λ(Å)	0.71073	0.71073
GOF on F^2	1.052	1.047
data[$I>2\sigma(I)$]/params	8321/453	7353/412
final R indices [$I>2\sigma(I)$][a,b]	$R1 = 0.0533$ $wR2 = 0.1787$	$R1 = 0.0463$ $wR2 = 0.1356$

[a]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b]$wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) in **1** and **2**.

1	(Å)	**2**	(Å)
Cu(1)-O(2)	2.252(3)	Cu(1)-O(2)	1.987(3)
Cu(1)-O(3)	1.944(3)	Cu(1)-O(5)	1.924(3)
Cu(1)-N(1)	1.996(3)	Cu(1)-N(1)	2.010(3)
Cu(1)-N(2)	1.998(3)	Cu(1)-N(2)	2.033(3)
Cu(1)-O(6)a	1.926(3)	Cu(1)-O(3)a	2.161(3)
Cu(2)-O(1)	2.236(4)	Cu(2)-O(1)	1.961(3)
Cu(2)-O(4)	1.938(3)	Cu(2)-O(5)	1.933(2)
Cu(2)-N(3)	2.001(3)	Cu(2)-N(3)	2.030(3)
Cu(2)-N(4)	2.009(3)	Cu(2)-N(4)	2.023(2)
Cu(2)-O(5)a	1.950(3)	Cu(2)-O(4)a	2.163(3)

Symmetry transformations used to generate equivalent atoms: a = 1-x,1-y,1-z.

Table S3 Selected bond angles (°) in **1**.

O(2)-Cu(1)-O(3)	92.12(13)	O(1)-Cu(2)-O(4)	90.13(13)
O(2)-Cu(1)-N(1)	95.41(13)	O(1)-Cu(2)-N(3)	98.57(13)
O(2)-Cu(1)-N(2)	93.87(12)	O(1)-Cu(2)-N(4)	96.79(13)
O(2)-Cu(1)-O(6)a	93.64(13)	O(1)-Cu(2)-O(5)a	94.67(12)
O(3)-Cu(1)-N(1)	171.49(12)	O(4)-Cu(2)-N(3)	169.21(13)
O(3)-Cu(1)-N(2)	94.31(12)	O(4)-Cu(2)-N(4)	91.91(13)
O(3)-Cu(1)-O(6)a	91.11(12)	O(4)-Cu(2)-O(5)a	91.92(13)
N(1)-Cu(1)-N(2)	81.23(12)	N(3)-Cu(2)-N(4)	80.78(13)
O(6)a-Cu(1)-N(1)	92.38(12)	O(5)a-Cu(2)-N(3)	93.71(13)
O(6)a-Cu(1)-N(2)	170.57(13)	O(5)a-Cu(2)-N(4)	167.90(12)

Symmetry transformations used to generate equivalent atoms: a = 1-x,1-y,1-z.

Table S4 Selected bond angles (°) in **2**.

O(2)-Cu(1)-O(5)	93.83(11)	O(1)-Cu(2)-O(5)	93.27(10)
O(2)-Cu(1)-N(1)	89.60(11)	O(1)-Cu(2)-N(3)	90.49(11)
O(2)-Cu(1)-N(2)	151.19(10)	O(1)-Cu(2)-N(4)	161.47(12)
O(2)-Cu(1)-O(3)a	93.25(10)	O(1)-Cu(2)-O(4)a	97.40(10)
O(5)-Cu(1)-N(1)	169.92(10)	O(5)-Cu(2)-N(3)	163.62(11)
O(5)-Cu(1)-N(2)	92.60(11)	O(5)-Cu(2)-N(4)	92.21(10)
O(3)a-Cu(1)-O(5)	101.87(10)	O(4)a-Cu(2)-O(5)	103.27(11)
N(1)-Cu(1)-N(2)	79.98(11)	N(3)-Cu(2)-N(4)	79.58(11)
O(3)a-Cu(1)-N(1)	87.38(10)	O(4)a-Cu(2)-N(3)	92.03(10)
O(3)a-Cu(1)-N(2)	112.82(11)	O(4)a-Cu(2)-N(4)	98.54(10)

Symmetry transformations used to generate equivalent atoms: a = 1-x,1-y,1-z.

Table S5 Hydrogen bonding in compounds **1** and **2**

Compound	D—H···A	Distance (Å) D—H	Distance (Å) H···A	Distance (Å) D··A	Angle (°) ∠D—H···A	Symmetry
1	O(2)-H(2)···(O7)	0.8200	2.1000	2.826(8)	148.00	-
2	O(1AA)-H(1AA)···(O7)	0.86(8)	1.96(8)	2.804(9)	168(5)	r = 1+x, -1+y,z
2	O(1AA)-H(1AB)···(O4)	0.87(9)	2.14(9)	2.823(6)	136(11)	

Table S6 IR spectral data of compounds **1** and **2**

Compound	ν_{OH}	$\nu_{as}(COO^-)$	$\nu_{sys}(COO^-)$	$\Delta\nu$
1	3482	1561	1449	112
2	3475	1580	1446	134

Table S7 Docking score of **1**-DNA interaction

ΔG (kcal/mole)	**rmsd**	**ΔG_{conf}(kcal/mole)**
11.174747	11.14868	0
10.903216	11.098319	0
-4.0406713	9.287714	0.40000001
-9.2726345	7.2024074	0.40000001
-8.6024942	4.8537669	0.40000001

Table S8 Docking score of **2**-DNA interaction

ΔG (kcal/mole)	**rmsd**	**ΔG_{conf} (kcal/mole)**
10.702652	10.31814	0.39150268
-2.0227284	9.0111036	0.39150268
-6.5041547	6.7488694	0.39150268
-1.5231411	4.7725468	0.0029858467
-0.22762701	4.7634172	0.036107246
-1.2192179	4.7353959	0.16538859
0.025211502	4.7312188	0.34162697
0.13292329	4.7168374	0.49440539
-5.1104512	3.5182025	0.14538859

Table S9 Molecular descriptors of DNA, compounds and DNA bound compounds

Name	SASA ($^{O}A^{2}$)	ASA+ ($^{O}A^{2}$)	ASA- ($^{O}A^{2}$)	ASA_H ($^{O}A^{2}$)	ΔSASA ($^{O}A^{2}$)	ΔG kcal/mole	ΔG_{con} kcal/mole	ΔG_{hyd} kcal/mole
Free DNA	4754.21	1188.67	2051.83	1957.09				
1	765.23	352.95	267.04	596.27				
1-DNA	4934.2	2738.01	2196.19	2379.72	585.24	-8.60	0.4	-12.87
2	763.87	306.87	334.42	645.11				
2-DNA	4961.09	2716.38	2244.71	2445.23	562.99	-5.11	0.14	-12.38