Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary material.

Table S1. Structural geometric parameters of compounds **1**, **2** and **3**.

Compound	Center	τ[a]	Angle[b]	Distance[c]
1	Cu1	2.80	79.00	0.2521
2	Cu	18.7	85.34	-0.1967
3	Cu1	23.9	78.00	-0.0806
	Cu2	14.3	83.95	-0.1628

[a] τ (%) The ideal value for Square pyramid (C_4v symmetry) is 0 and for a Trigonal bipyramid (D_3h symmetry) is 100.
[b] Dihedral angle between the equatorial plane around Cu(II) and the apex of the pyramid (°).
[c] Perpendicular distance between the basal plane and Cu(II) (Å).

Table S2. Hydrogen Bonds (Å, °), for **1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symm*
C3" --H3"..O3	0.9300	2.2900	3.21(2)	171.00	-x,y,1/2-z
C5 --H5…O5	0.9300	2.4000	3.18(3)	141.00	1/2-x,-1/2+y,1/2-z
C5'-- H5'… O6	0.9300	2.5200	3.28(2)	139.00	-x,y,1/2-z
C6 -- H6 … O1	0.9300	2.5600	3.03(1)	112.00	
C6" -- H6" … O2	0.9300	2.3000	3.12(1)	148.00	-x,-y,-z

* Symmetry transformations used to generate equivalent atoms:

Table S3 - Hydrogen Bonds (Å, °) for **3**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symm*
C11-- H11…F2	0.9300	2.4400	3.2396(2)	144.00	-1/2+x,1/2-y,1/2+z
C15-- H15…O9	0.9300	2.4000	3.2269(2)	148.00	-1+x,y,1+z
C17-- H17…O5	0.9300	2.5000	3.3157(2)	147.00	-x,-y,2-z
C20-- H20…O6	0.9300	2.4900	3.3858(2)	161.00	-x,-y,-z
C22-- H22…O10	0.9300	2.5500	3.3426(2)	144.00	3_656
C26-- H26…O7	0.9300	2.5800	3.3124(2)	136.00	1/2-x,-1/2+y,3/2-z
C31-- H31…O9	0.9300	2.5600	3.2216(2)	128.00	3/2-x,-1/2+y,1/2-z
C38-- H38…O4	0.9300	2.5200	3.1131(2)	122.00	.

* Symmetry transformations used to generate equivalent atoms:

Table S4. Hydrogen bonds for **2** (Å , °).

...D-HA	d(D-H)	...d(HA)	...d(DA)	<(DHA)	Symm*
O(5)-H(5A)...O(4)#2	0.85	2.13	2.848(6)	142.2	x+1,y+1,z
O(5)-H(5A)...F(2)#3	0.85	2.59	3.145(7)	124.4	x+1,y,z
O(5)-H(5B)...O(6)#4	0. 85	1.93	2.782(7)	179.2	-x+1,-y+1,-z+1
O(6)-H(6A)...O(2)	0.85	2.22	3.068(5)	174.6	
O(6)-H(6B)...O(5)	0.85	1.95	2.805(7)	178.9	
O(7)-H(7A)...O(1)#5	0.85	2.24	3.085(4)	175.9	x,y+1,z
O(7)-H(7B)...O(6)#4	0.85	1.95	2.805(6)	178.2	-x+1,-y+1,-z+1

* Symmetry transformations used to generate equivalent atoms:

Table SXX. Analysis of Short Ring-Interactions

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).

Compound **1**

Cg(I) - Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp
Cg(1)- Cg(5)	-x,y,1/2-z	3.615(4)	2.8(3)	15.6	15.6	3.482(3)	3.481(3)
Cg(1)- Cg(2)	-x,y,1/2-z	3.984(5)	2.6(3)	29.0	30.8	3.420(3)	3.485(3)
Cg(2)- Cg(2)	-x,y,1/2-z	3.455(4)	1.9(3)	2.7	2.7	3.450(3)	3.451(3)
Cg(4)- Cg(4)	-x,y,1/2-z	3.877(6)	1.5(4)	25.2	25.2	3.508(3)	3.509(3)

(1) Cu(1)-N(1) -C(2) -C(2')-N(1')
(2) Cu(1)-N(1')-C(6')-C(2'')-N(1'')
(4) N(1')-C(2')-C(3')-C(4')-C(5')-C(6')
(5) N(1'')-C(2'')-C(3'')-C(4'')-C(5'')-C(6'')

Compound **2**

Cg(I) - Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp
Cg(4) - Cg(5)	-x,-y,2-z	3.655(2)	6.64(17)	16.6	22.6	-3.3758(14)	-3.5026(15)
Cg(4) - Cg(7)	x,y,z	3.7019(19)	6.63(16)	30.7	24.2	-3.3767(14)	3.1827(13)
Cg(5) - Cg(6)	1-x,-y,2-z	3.7910(19)	4.98(16)	25.9	22.2	3.5109(14)	3.4100(13)

(4) N(1) - C(2) - C(3) - C(4) - C(5) - C(6)
(5) N(7) - C(8) - C(9) - C(10) - C(11) - C(12)
(6) N(13) - C(14) - C(15) - C(16) - C(17) - C(18)
(7) C(19) - C(20) - C(21) - C(22) - C(23) - C(24)

Table SX. interactions between rings in 3

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp
Cg(6)	Cg(9)	1-x,-y,2-z	3.587(2)	7.0(2)	13.1	9.4	3.5388(17)	3.4933(18)
Cg(8)	Cg(12)	1-x,-y,2-z	3.571(2)	9.6(2)	13.3	12.5	3.4863(18)	3.4751(16)
Cg(10)	Cg(12)	1-x,-y,1-z	3.814(2)	8.9(2)	11.8	14.3	-3.6953(19)	-3.7336(16)

(6) N(1) - C(9) - C(10) - C(11) - C(12) - C(13)
(8) N(3) - C(19) - C(20) - C(21) - C(22) - C(23)
(9) N(4) - C(24) - C(25) - C(26) - C(27) - C(28)
(10) N(5) - C(29) - C(30) - C(31) - C(32) - C(33)
(12) C(1) - C(2) - C(3) - C(4) - C(5) - C(6)