Supporting Information for

Structural Diversity in Copper(II)/Isophthalato/9-methyladenine System. From 1D to 3D Metal-biomolecule Frameworks.

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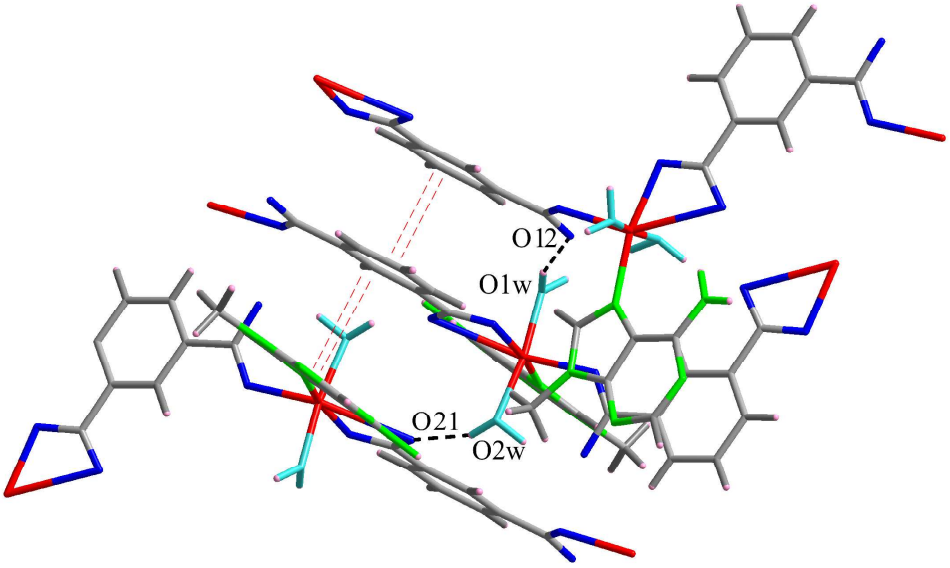


Figure S.1. Hydrogen bonding and π-π interactions involving the aromatic rings of isophthalato and 9-methyladenine between the chains of compound **1**.

Table S.1. Structural parameters (Å, °) of non-covalent interactions in compound **1**. [a]

Hydrogen bonding interactions

D–H···A[b]	H···A	D···A	D–H···A
N6–H6A···N1a	2.15	2.990(4)	166
N6–H6B···O21	2.04	2.841(4)	154
O1w–H11w···O12b	1.77	2.598(3)	157
O1w–H12w···N3c	1.93	2.787(3)	171
O2w–H22w···O12	1.80	2.625(3)	147
O2w–H21w···O21d	1.82	2.656(3)	157

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
p–is(e)	9.3	3.79	18.5	3.37–3.60	–
h–is(e)	9.9	3.72	15.1	3.59–3.71	–
is–is(f)	0.0	3.78	23.7	3.46–3.46	1.52

[a] Symmetry codes: (a) –x+1, –y, –z+2; (b) –x+2, y+1/2, –z+3/2; (c) –x+1, y+1/2, –z+3/2; (d) –x+2, –y, –z+2; (e) –x, y–1/2, –z+1/2; (f) –x, –y, –z+1. [b] D : donor; A : acceptor. [c] Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å), [d] p: pentagonal ring of the 9-methyladenine; h: hexagonal ring of the 9-methyladenine; is: isophthalato ligand.

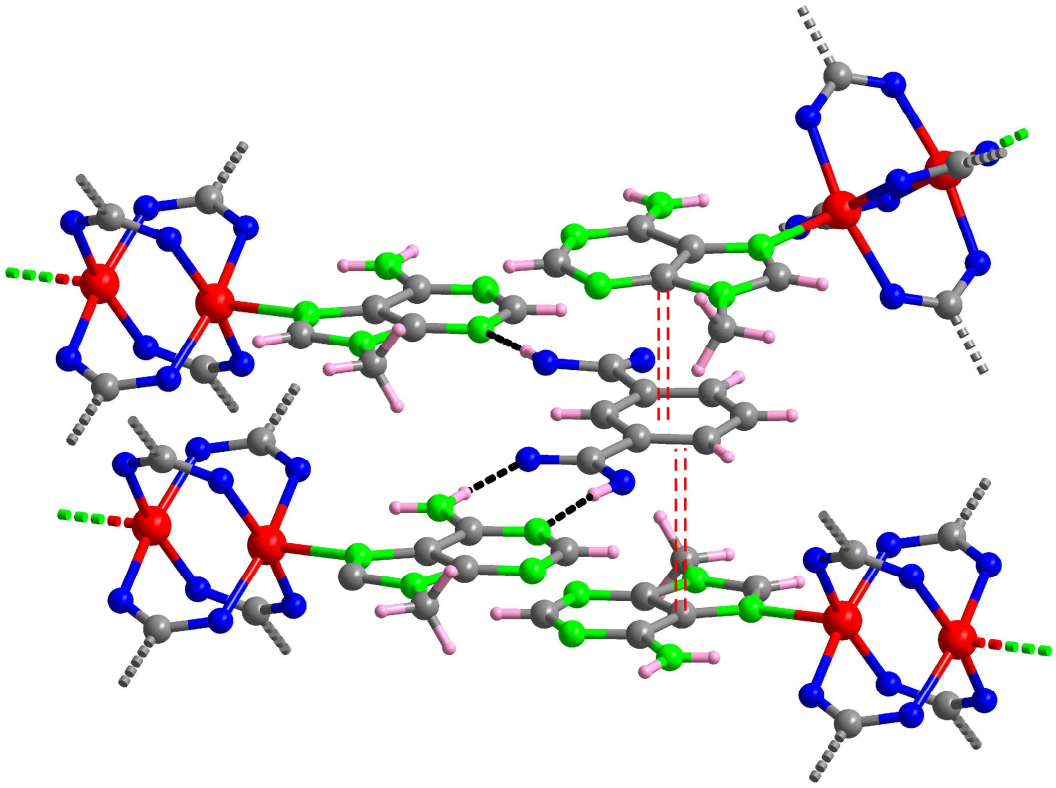


Figure S.2. Supramolecular interactions of the isophthalic acid sited among the layers of compound **3**.

Table S.2. Structural parameters (Å, °) of non-covalent interactions in compound **3**. [a]

Hydrogen bonding interactions

D–H···A[b]	H···A	D···A	D–H···A
N6–H6A···O31a	1.90	2.75(2)	172
N6–H6B···O12a	2.07	2.88(2)	157
O42–H42···N3	1.90	2.71(1)	171
O32–H32···N1a	1.94	2.75(1)	172

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
p–is(d)	4.3	3.63	18.7	3.35–3.44	–
p–is(c)	3.4	3.57	17.9	3.36–3.40	–
h–is(c)	2.5	3.55	16.9	3.40–3.40	–

[a] Symmetry codes: (a) –x, –y+1, –z; (c) x–1/2, –y+1/2, z–1; (d) x, y, z–1. [b] D : donor; A : acceptor. [c] Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å), [d] p: pentagonal ring of the 9-methyladenine; h: hexagonal ring of the 9-methyladenine; is: isophthalato ligand.

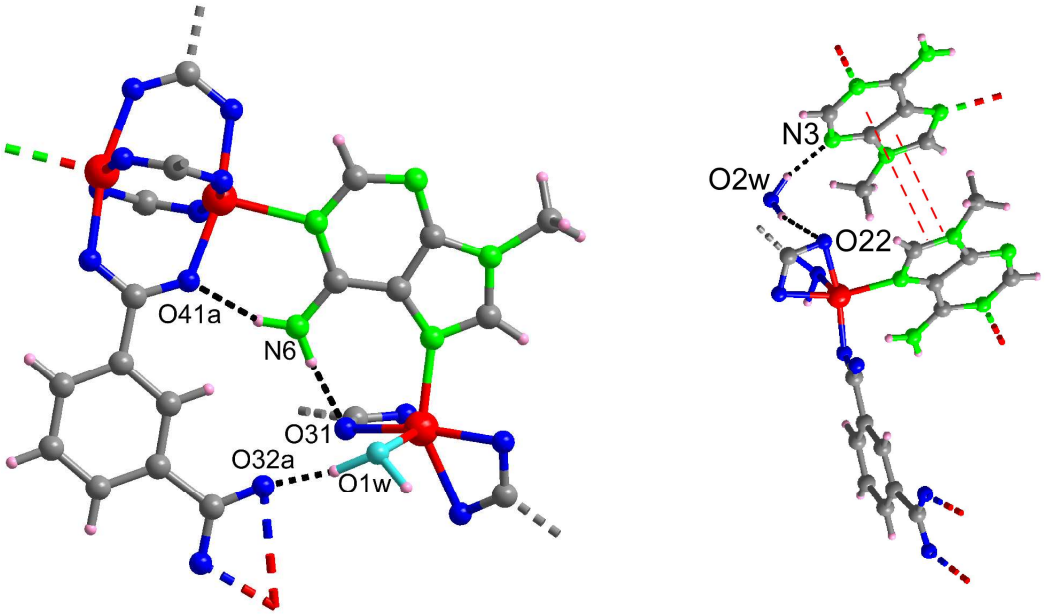


Figure S.3. Non-covalent interactions in compound **4**: **(a)** hydrogen bonds of the exocyclic amino group and **(b)** π-π interactions.

Table S.3. Structural parameters (Å, °) of non-covalent interactions in compound **4**. [a]

Hydrogen bonding interactions

D–H···A[b]	H···A	D···A	D–H···A
N6–H6A···O31	2.00	2.833(5)	162
N6–H6B···O41b	2.14	2.878(5)	144
O1w–H11w···O2w	1.83	2.769(4)	146
O1w–H12w···O32a	1.62	2.666(5)	165
O2w ···N3e		2.758(5)	
O2w ···O22d		3.336(4)	

π-π interactions [c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
h–is(f)	12.5	3.67	15.3	3.25–3.54	–

[a] Symmetry codes: (a) –x+3, –y+1, –z+2; (b) x+1/2, –y+1/2, z; (d) x–1/2, –y+1/2, z–1; (e) –x+2, –y+1, –z+1; (f) x–1/2, y–1/2, z. [b] D : donor; A : acceptor. [c] Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å), [d] p: pentagonal ring of the 9-methyladenine; h: hexagonal ring of the 9-methyladenine; is: isophthalato ligand.

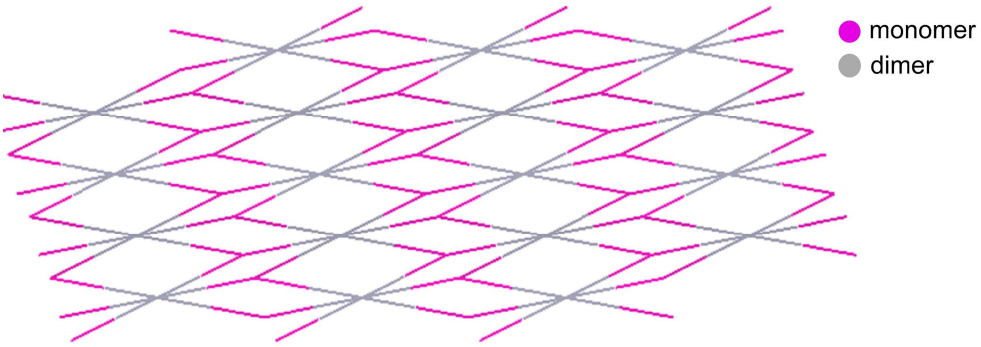


Figure S.4. Rutile type network of compound **4**.

Table S.4. Structural parameters (Å, °) of non-covalent interactions in compound **5**. [a]

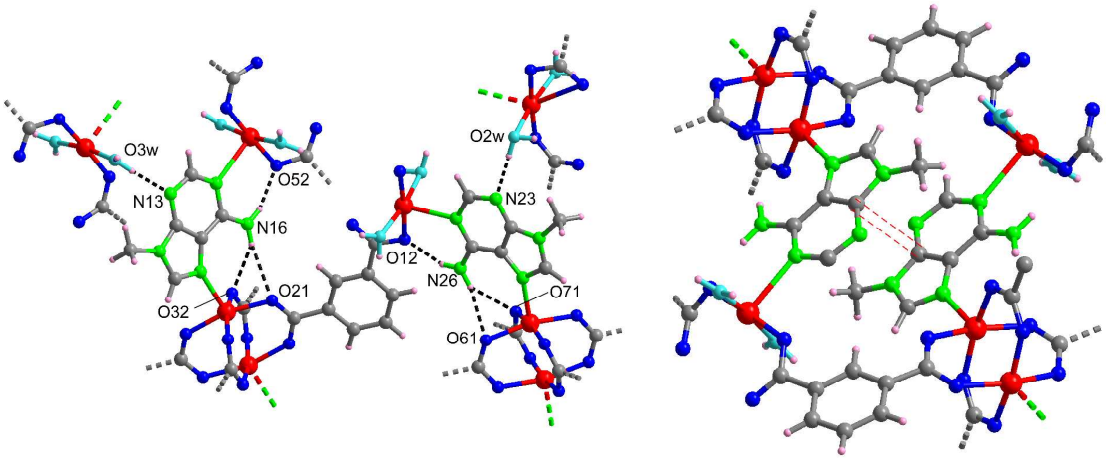
Hydrogen bonding interactions

D–H···A[b]	H···A	D···A	D–H···A
N16–H16A···O52f	2.01	2.843(7)	162
N16–H16B···O32a	2.50	3.222(7)	142
N16–H16B···O21	2.60	3.372(7)	150
N26–H26A···O12	2.00	2.828(6)	160
N26–H26B···O71	2.40	3.142(6)	145
N26–H26B···O61	2.50	3.243(6)	146
O1w–H11w···O42e	2.07	2.915(7)	162
O1w–H12w···O51	1.90	2.761(6)	174
O2w–H21w···O5wd	2.57	3.417(6)	176
O2w–H22w···N23g	1.96	2.810(6)	176
O3w–H31w···N13h	1.95	2.799(6)	176
O3w–H32w···O21e	2.53	3.388(7)	175
O4w–H41w···O5w	1.76	2.609(6)	170
O4w–H42w···O7w	1.91	2.749(10)	165

π-π interactions [c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
p–h(d)	0.5	3.88	28.6	3.40–3.41	–
p–h(i)	0.2	3.95	32.7	3.33–3.33	

[a] Symmetry codes: (a) –x+1, –y, –z+1; (d) –x+1, –y+1, –z+1; (e) –x+2, –y+1, –z+1; (f) x–1, y, z; (g) –x+1, –y+1, –z; (h) x+1, y, z; (i) –x+2, –y+1, –z. [b] D : donor; A : acceptor. [c] Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å), [d] p: pentagonal ring of the 9-methyladenine; h: hexagonal ring of the 9-methyladenine; is: isophthalato ligand.



(a) **(b)**

Figure S.5. Non-covalent interactions in compound **5**: **(a)** hydrogen bonding interactions established by 9-methyladenine and **(b)** π-π interactions.

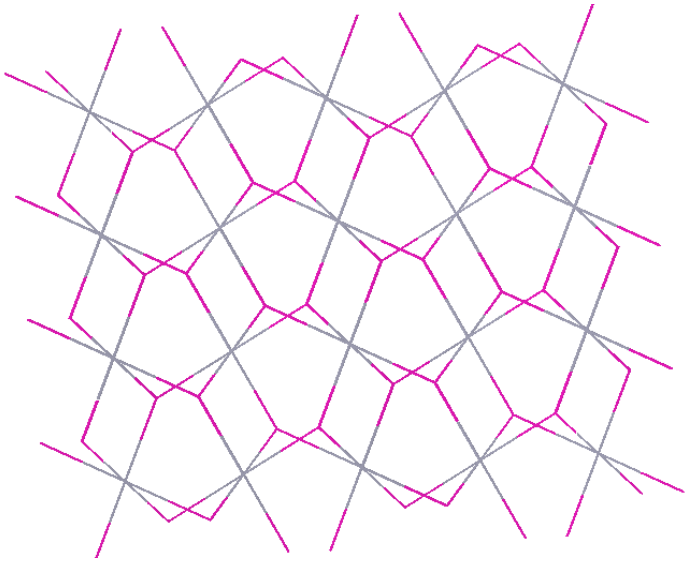


Figure S.6. Rutile type network of compound **5**.