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Supplementary Material

Supplementary Table 1. π-π and C-H...π interactions in **1**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	3.881(2)	22.37(18)	3.7460(16)
R(1)→ R(7)^{ii}	3.899(2)	21.72(19)	3.7453(16)
R(2)→ R(4)^{iii}	3.839(2)	21.16(18)	3.7032(15)
R(2)→ R(8)^{iv}	3.886(2)	21.55(18)	3.7320(16)
R(3)→ R(1)^{i}	3.881(2)	22.37(18)	3.2910(15)
R(3)→ R(7)^{v}	4.585(2)	38.29(19)	4.3307(17)
R(4)→ R(2)^{vi}	3.839(2)	21.16(18)	3.2613(14)
R(5)→ R(6)^{v}	4.335(2)	23.1(2)	3.2265(16)
R(6)→ R(1)^{vii}	3.899(2)	21.72(19)	3.2859(15)
R(6)→ R(5)^{viii}	4.335(2)	23.1(2)	4.0335(17)
R(7)→ R(3)^{viii}	4.584(2)	38.29(19)	2.7296(16)
R(8)→ R(2)^{ix}	3.886(2)	21.55(18)	3.2763(15)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(19)-H(19) → R(8)^{x}	2.85	143	3.636(6)

Symmetry code: (i) = x,y,z (ii) = 1/2+x,1/2+y,z (iii) = x,-1+y,z (iv) = 1/2+x,-1/2+y,z; (v) = 1/2+x,1/2-y,-1/2+z; (vi) = x,1+y,z; (vii) = -1/2+x,-1/2+y,z;(viii) = -1/2+x,1/2-y,1/2+z (ix) = -1/2 +x, 1/2+ y, z; (x)= x,1-y,-1/2+z; R(i)/R(j) denotes the ith/jth rings: R(1) = N(2)/C(6)/C(7)/C(8)/ C(9)/C(10);R(2)=N(3)/C(46)/C(47)/C(48)/C(49)/C(50);R(3)= C(11)/C(12)/C(62)/C(63)/C(15)/ C(16);R(4)=C(23)/C(24)/C(25)/C(26)/C(27)/C(28);R(5)= C(29)/C(30)/C(31)/C(32)/C(33)/C(34); R(6) = C(35)/C(36)/C(37)/C(38)/C(39)/C(40); R(7) = C(41)/C(42)/C(43)/C(44)/C(45)/C(66); R(8) = C(55)/C(56)/C(57)/C(58)/C(59)/C(60).

Supplementary Table 2: Hydrogen bonding interactions of complex 2, 5, 6 and 9 (Å, °)

Complex	D-H…A	D-H	H….A	D….A	∟D-H…A
2	O1S-H1SA…O3^{i}	0.82	2.09	2.894(5)	165.00
	O2W-H2WB…O8^{iii}	0.85	2.01	2.826(6)	161.00
5	O1W-H1W…O3	0.98	1.86	2.831(9)	171.00
6	O1W-H1W… O7	0.85	1.98	2.821(17)	171.00
9	O1W-H1W... O2	0.83	2.01	2.834(16)	169.00

Symmetry Code : (i) = x,1+y,z; (ii) = 1-x,2-y,1-z; (iii) = x,2-y,-1/2+z.

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Supplementary Table 3. π-π and C-H...π interactions in **2**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(2)^{i}	4.544(2)	70.40(19)	3.8185(17)
R(2)→ R(3)^{i}	4.603(2)	62.3(2)	3.0337(17)
R(3)→ R(2)^{i}	4.603(2)	62.3(2)	2.6110(18)
R(4)→ R(5)^{ii}	4.469(4)	65.8(3)	3.292(2)
R(5)→ R(4)^{iii}	4.468(4)	65.8(3)	3.1664(19)
R(5)→ R(9)^{iii}	4.672(4)	63.1(3)	3.837(2)
R(6)→ R(1)^{iv}	4.597(2)	70.9(2)	4.5682(16)
R(9)→ R(5)^{ii}	4.672(4)	63.1(3)	3.982(3)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(1)-H(1) → R(6)^{iv}	2.69	136	3.418(4))
C(10)-H(10) → R(6)^{vi}	2.95	129	3.605(4)
C(18)-H(18) → R(7)^{iv}	2.96	148	3.777(4)
C(19)-H(19A) → R(1)^{vii}	2.79	138	3.568(5)
C(26)-H(26) → R(9)^{iii}	2.64	153	3.490(5)

Symmetry code: (i) = 1/2-x,3/2-y,-z (ii) = x,1+y,z (iii) = x,-1+y,z; (iv) = x,y,z; (v) = x, 1+y,z; (vi)=1/2-x,1/2-y,-z; (vii)= x,1-y,1/2+z ; R(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(1)/C(2)/C(3)/ C(4)/C(5); R(2) = N(2)/C(9)/C(10)/C(11)/C(12)/C(13); R(3) = N(3)/C(14)/C(15)/C(16)/C(17)/C(18); R(4) = N(4)/C(22)/C(23)/C(24)/C(25)/C(26); R(5) = N(6)/C(35)/C(36)/C(37)/C(38)/C(39); R(6) = C(40)/C(41)/C(42)/C(43)/C(44)/C(45); R(7) = C(46)/C(47)/C(48)/C(49)/C(50)/C(51); R(8) = C(52)/C(53)/C(54)/C(55)/C(56)/C(57); R(9) = C(58)/C(59)/C(60)/C(61)/C(62)/C(63).

Supplementary Table 4. π-π and C-H...π interactions in **3**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	4.821(3)	58.7(3)	4.601(3)
R(1)→ R(5)^{ii}	4.841(4)	57.2(3)	4.722(3)
R(2)→ R(4)^{iii}	4.706(7)	32.9(6)	4.489(3)
R(2)→ R(6)^{iii}	4.667(7)	37.0(6	4.458(2)
R(3)→ R(1)^{ii}	4.760(3	58.7(3)	4.7405(19)
R(4)→ R(2)^{iv}	4.705(7)	32.9(6)	4.529(7)
R(5)→ R(1)^{v}	4.625(4)	57.2(3)	4.613(2)
R(6)→ R(2)^{iv}	4.667(7)	37.0(6)	4.390(7)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(36)-H(36) → R(1)^{ii}	2.87	139	3.623(8)

Symmetry code: (i) = 1+x,y,z (ii) = x,y,z (iii) = 3/2-x,-y,1/2+z (iv) = 3/2-x,-y,-1/2+z (v) = -1+x,y,z r(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(1)/C(2)/C(3)/ C(4)/C(5); R(2) = N(1A)/C(11A)/C(13B)/C(9)/C(10A)/C(12A); R(3) = C(14)/C(15)/ C(16)/C(17)/C(18)/C(19); R(4) = C(25)/C(26)/C(27)/C(28)/C(29)/C(30)

Supplementary Table 5. π-π and C-H...π interactions in **4**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(2)^{i}	4.4894(15)	53.38(13)	2.8083(11)
R(1)→ R(5)^{ii}	4.271(2)	37.60(19)	3.391(2)
R(2)→ R(1)^{i}	4.4896(15)	53.38(13)	4.4829(10)
R(2)→ R(2)^{iii}	3.9492(16)	0	3.6484(11)
R(3)→ R(3)^{iv}	4.0174(18)	0	3.6655(14)
R(4)→ R(4)^{v}	3.8959(17)	0	3.7480(12)
R(5)→ R(1)^{ii}	4.271(2)	37.60(19)	4.2691(11)
R(5)→ R(5)^{vi}	4.271(3)	0	3.289(2)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(36)-H(36) → R(6)^{vii}	2.97	143	3.755(5)

Symmetry code: (i) = 2-x,2-y,1-z (ii) = 1-x,2-y,1-z (iii) = 2-x,3-y,1-z (iv) = 2-x,2-y,2-z (v) = 1-x,1-y,1-z ; (vi) = = 1-x,2-y,-z; (vii) = x, y , z R(i)/R(j) denotes the ith/jth rings: R(1) = N(2)/C(8)/C(9)/C(10)/ C(11)/C(12); R(2) = C(13)/C(14)/C(15)/C(16)/C(17)/C(18); R(3) = C(19)/C(20)/ C(21)/C(22)/C(23)/C(24); R(4) = C(25)/C(26)/C(27)/C(28)/C(29)/C(30); R(5) = C(31)/C(32)/ C(33)/C(34)/C(35)/C(36). R(6) = N(1)/C(1)/ C(2)/C(3)/C(4)/C(5).

Supplementary Table 6. π-π and C-H...π interactions in **5**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(4)^{i}	4.2205(12)	25.14(10)	3.1734(10)
R(3)→ R(2)^{ii}	4.7868(10)	88.16(8)	4.6959(6)
R(3)→ R(4)^{iii}	4.6841(13)	44.62(10)	2.4994(9)
R(4)→ R(1)^{i}	4.2205(12)	25.14(10)	3.7531(6)
R(4)→ R(3)^{iii}	4.6842(13)	44.62(10)	4.4968(8)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(3)-H(3) → R(4)^{iii}	2.99	124	3.595(2)
C(15)-H(15) → R(3)^{iv}	2.70	160	3.5911(16)
C(26)-H(26) → R(3)^{v}	2.94	135	3.660(2)

Symmetry code: (i) = -x,-y,1-z (ii) = -1/2-x,1/2+y,1/2-z (iii) = -1-x,-y,1-z (iv) = -1/2-x,1/2-y,1-z (v) = -1/2-x,1/2+y,1/2-z; R(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(14)/C(15)/C(16)/ C(17)/C(18); R(2) = N(2)/C(22)/C(23)/C(24)/C(26)/C(27); R(3) = C(1)/C(2)/ C(3)/C(4)/C(5)/C(6); R(4) = C(7)/C(8)/C(9)/C(10)/C(11)/C(12).

Supplementary Table 7. π-π and C-H...π interactions in **6**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	4.2804(13)	26.67(11)	3.1631(11)
R(2)→ R(3)^{ii}	4.6773(14)	44.88(11)	2.5061(11)
R(3)→ R(1)^{iii}	4.2802(13)	26.67(11)	3.7524(7)
R(3)→ R(2)^{ii}	4.6774(14)	44.88(11)	4.4809(9)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(13)-H(13) → R(2)^{iv}	2.71	162	3.6083(19)
C(16)-H(16) → R(3)^{ii}	2.99	124	3.589(3)

Symmetry code: (i) = -1/2+x,-1/2-y,-1/2+z (ii) = 1-x,-y,1-z (iii) = 1/2+x,-1/2-y,1/2+z (iv) = x,-y,-1/2+z; R(i)/R(j) denotes the ith/jth rings: R(1) = N(2)/C(9)/C(10)/C(11)/ C(12)/C(13); R(2) = C(14)/C(15)/C(16)/C(17)/C(18)/C(19); R(3) = C(20)/C(21)/C(22)/C(23)/C(24)/C(25).

Supplementary Table 8. π-π and C-H...π interactions in **7**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	3.945(4)	1.31(12)	3.5943(10)
R(2)→ R(2)^{ii}	4.807(4)	59.0	4.6176(11)
R(3)→ R(1)^{i}	3.945(4)	1.31(12)	3.5566(10)
R(3)→ R(3)^{iii}	4.827(4)	59.0	4.6328(10)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(2)-H(2) → R(2)^{iv}	2.88	135	3.596(4)
C(10)-H(10) → R(3)^{v}	2.97	132	3.653(4)

Symmetry code: (i) = 1-x,-1+y,2-z (ii) = 3/2-x,-1/2+y,2-z (iii) = 3/2-x,-1/2+y,3-z (iv) = 3/2-x,1/2+y,2-z (v) = 3/2-x,1/2+y,3-z; R(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(13)/C(14)/C(15)/ C(16)/C(17); R(2) = C(1)/C(2)/C(3)/C(4)/C(5)/C(6); R(3) = C(7)/C(8)/ C(9)/C(10)/C(11)/C(12).

Supplementary Table 9. π-π and C-H...π interactions in **9**

ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	4.2603(12)	25.75(10)	3.1477(10)
R(2)→ R(3)^{ii}	4.6844(14)	44.33(11)	2.5140(10)
R(3)→ R(1)^{i}	4.2604(12)	25.75(10)	3.7714(7)
R(3)→ R(2)^{ii}	4.6843(14)	44.33(11)	4.4963(9)
C-H→ ring(j)			
C(2)-H(2) → R(2)^{iii}	2.71	161	3.6035(18)
C(12)-H(12) → R(2)^{ii}	2.97	135	3.680(2)
C(18)-H(18) → R(3)^{ii}	3.00	124	3.598(3)

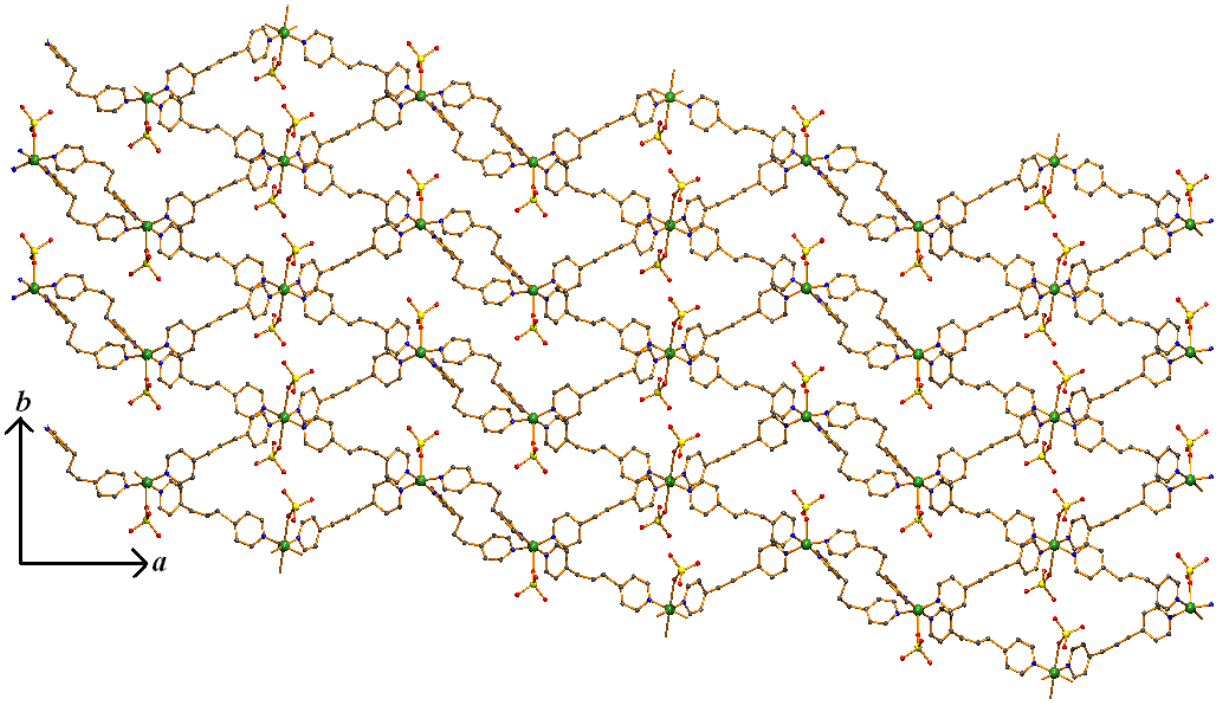
Symmetry code: (i) = 2-x,-y,1-z (ii) = 3-x,-y,1-z (iii) = 5/2-x,-1/2-y,1-z (iv) = 5/2-x,-1/2+y,3/2-z; R(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(1)/C(2)/C(3)/ C(4)/C(5); R(2) = C(14)/C(15)/C(16)/C(17)/C(18)/C(19); R(3) = C(20)/C(21)/C(22)/C(23)/C(24)/C(25).

Supplementary Table 10. π-π and C-H...π interactions in **10**

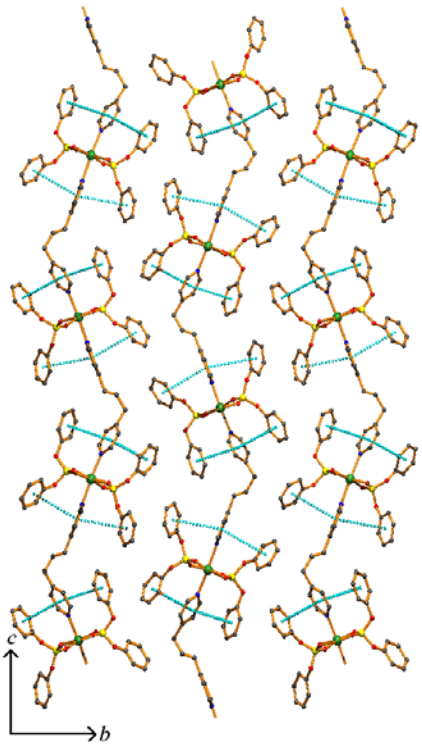
ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	distance between the (i,j) ring centroids,(Å)
R(1)→ R(3)^{i}	4.122(2)	23.26(18)	3.3028(16)
R(3)→ R(1)^{ii}	4.122(2)	23.26(18)	3.7398(14)
C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
C(13)-H(13) → R(3)^{iv}	2.85	158	3.722(4)

Symmetry code: (i) = x,y,1+z (ii) = x,y,-1+z (iii) = -1+x,y,z; iv = 2-x,-y,1-z ; r(i)/R(j) denotes the ith/jth rings: R(1) = N(2)/C(9)/C(10)/C(11)/ C(12)/C(13); R(2) = C(14)/C(15)/C(16)/C(17)/C(18)/C(19); R(3) = C(40)/C(41)/ C(42)/C(43)/C(44)/C(45).

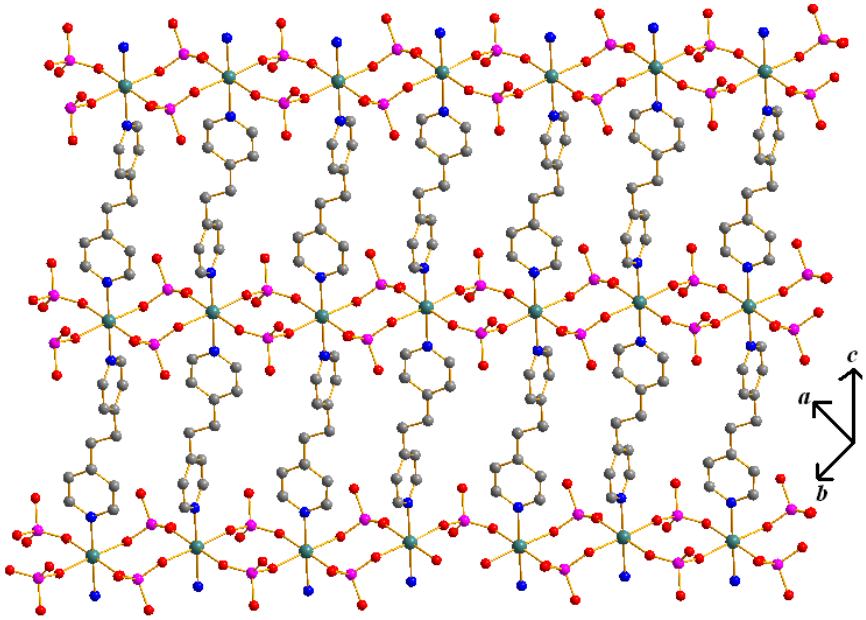
Figures:



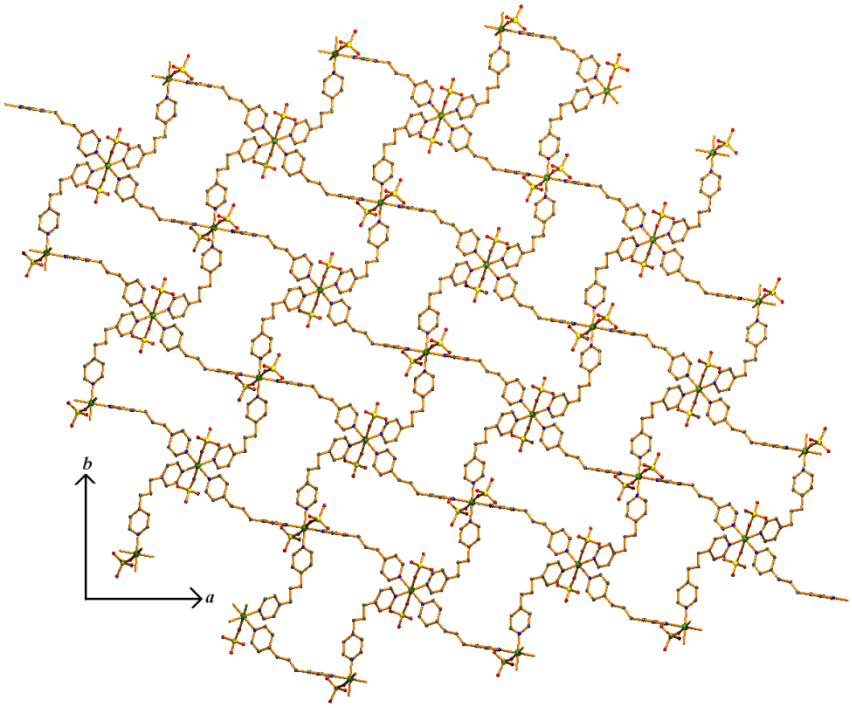
Supplementary Figure 1: 2D sheet arrangement in **2** (phenyl rings are omitted for clarity; Colour Code: Cu: Green, N: Blue, O: Red, P: Yellow, C: Gray)



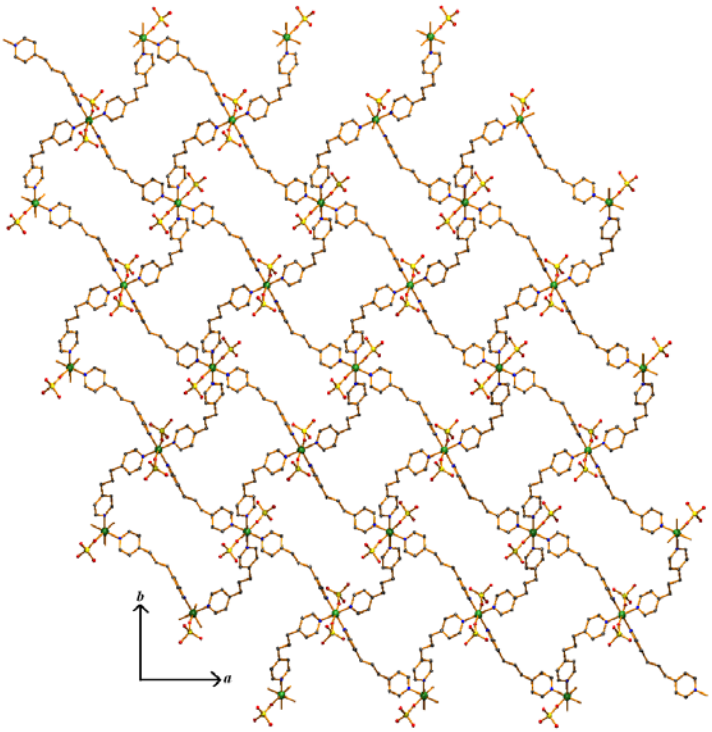
Supplementary Figure 2: Disposition of sheets in **3** showing a *zig-zag* arrangement (Colour Code: Mn: Green, N: Blue, O: Red, P: Yellow, C: Gray, π-π interaction: Cyan dotted lines)



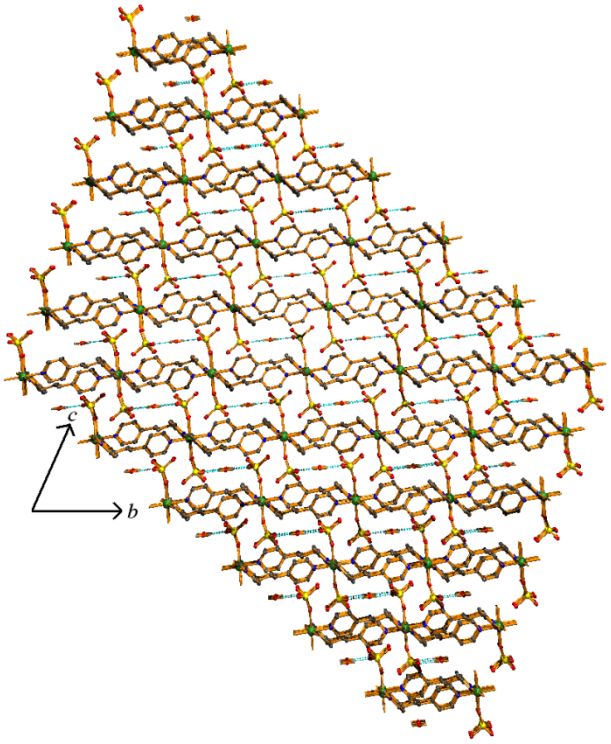
Supplementary Figure 3: Formation of 2D arrangement in **4** (phenyl rings are omitted for clarity; Colour Code: Mn: Green, N: Blue, O: Red, P: Pink, C: Gray)



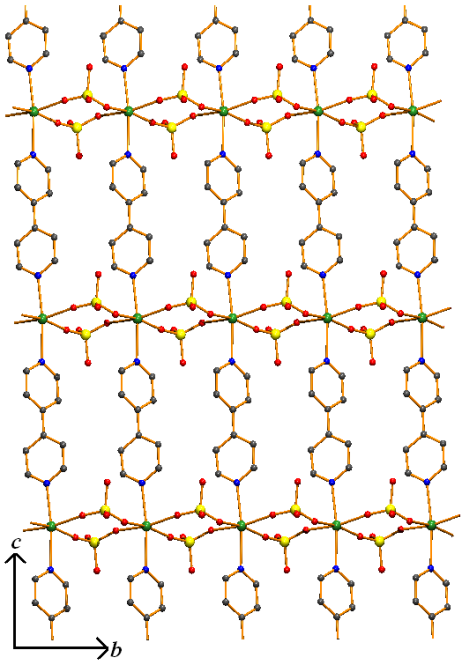
Supplementary Figure 4: 2D (4,4) net arrangement of **5** (phenyl rings are omitted for clarity; Colour Code: Co: Green, N: Blue, O: Red, P: Yellow, C: Gray)



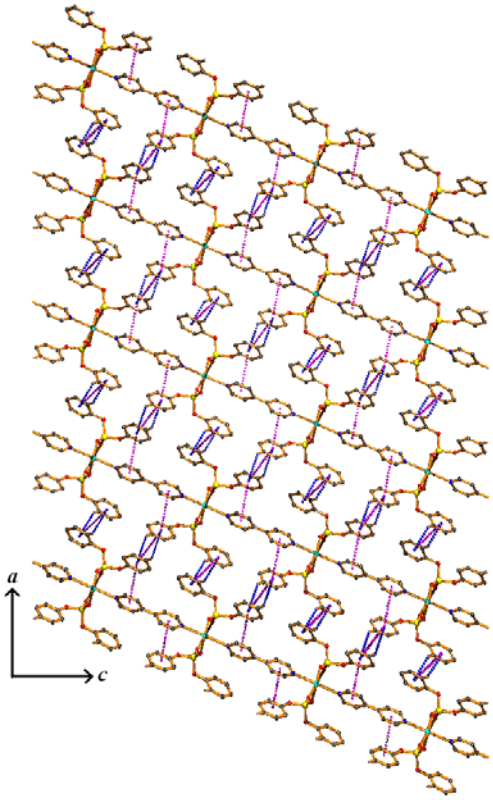
Supplementary Figure 5: 2D (4,4) net arrangement of **6** (phenyl rings are omitted for clarity; Colour Code: Ni: Green, N: Blue, O: Red, P: Yellow, C: Gray)



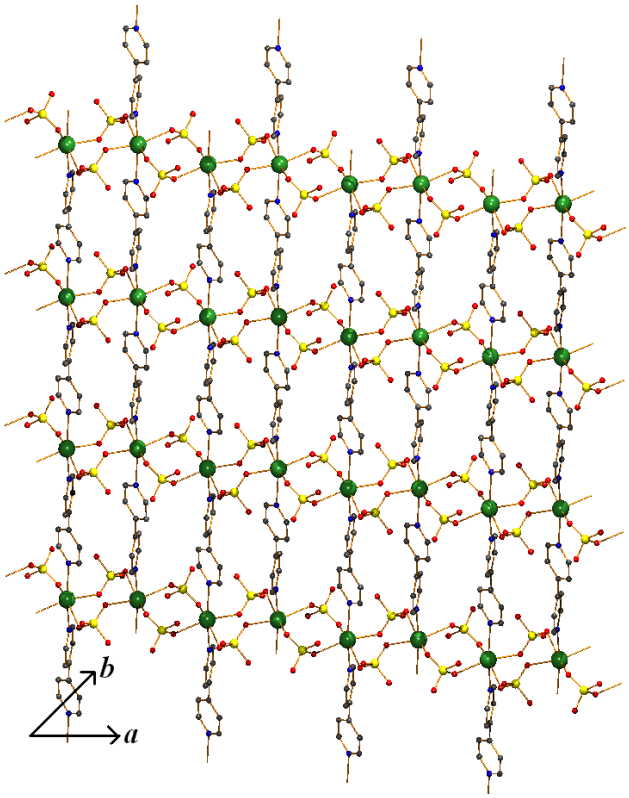
Supplementary Figure 6: Supramolecular 3D arrangement in **6** by locking of 2D sheets by H-bonding (Colour Code: Ni: Green, N: Blue, O: Red, P: Yellow, C: Gray, H-bonding: Cyan dotted lines)



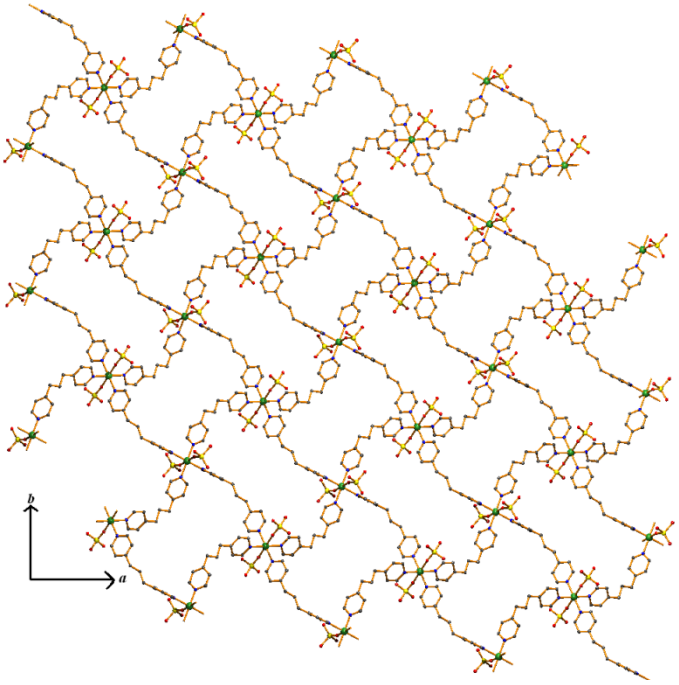
Supplementary Figure 7: Formation of 2D arrangement in **7** (phenyl rings are omitted for clarity; Colour Code: Ca: Green, N: Blue, O: Red, P: Yellow, C: Gray)



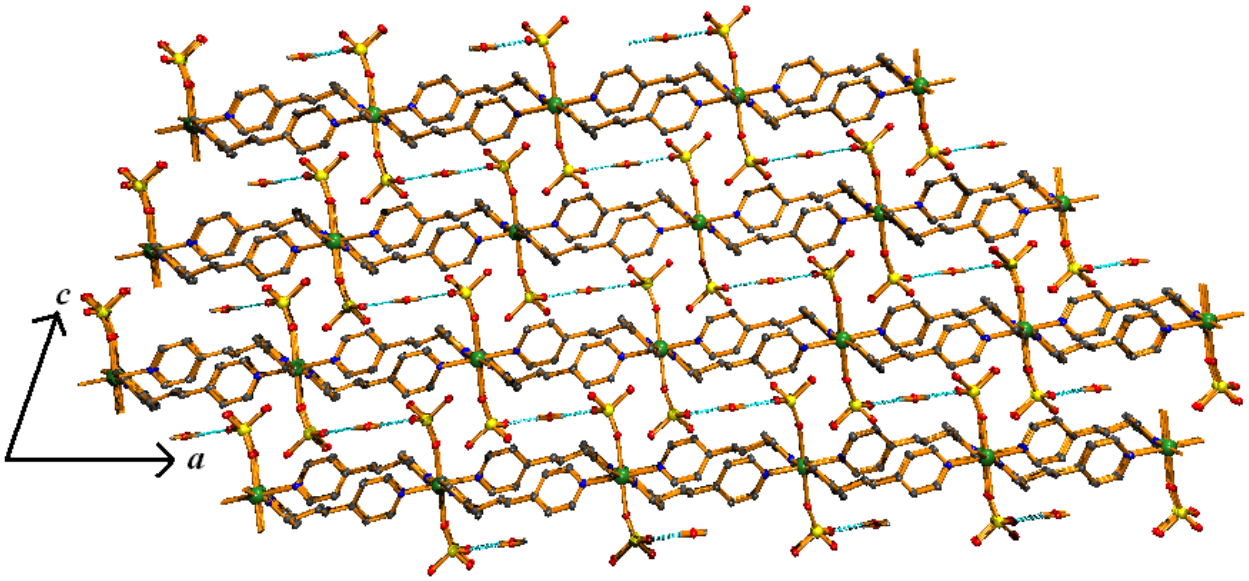
Supplementary Figure 8: Formation of supramolecular 3D structure in **7** by π-π and C-H…π interaction (Colour Code: Ca: Green, N: Blue, O: Red, P: Yellow, C: Gray, π-π interaction: Pink dotted lines, C-H…π interaction: Blue dotted lines)



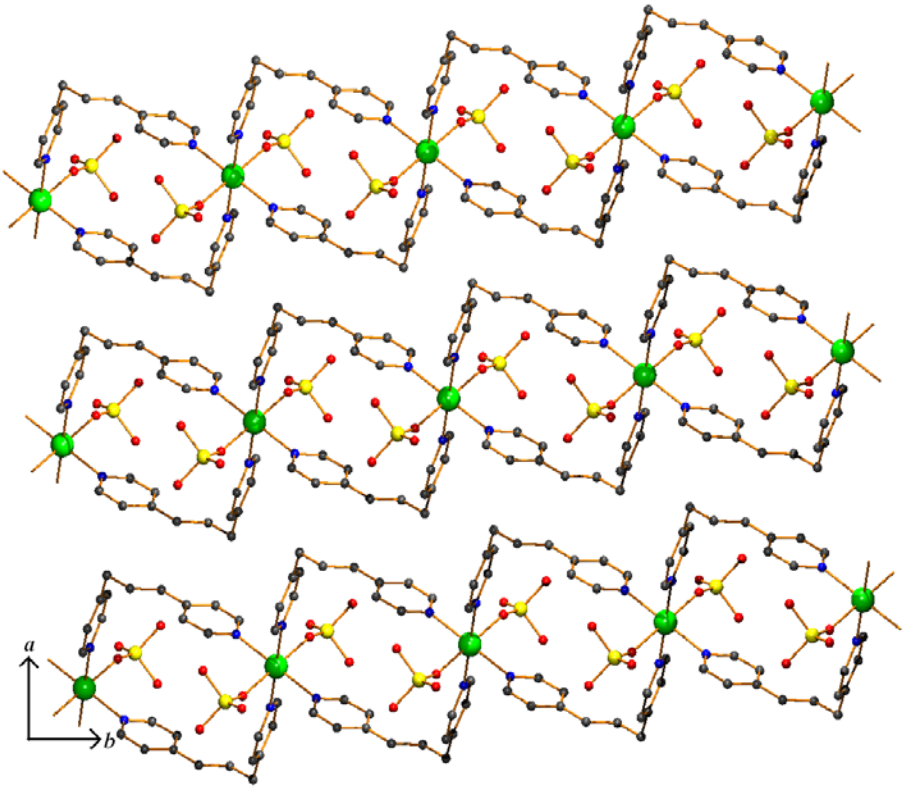
Supplementary Figure 9: Formation of 2D arrangement in **8** (phenyl rings are omitted for clarity; Colour Code: Pb: Green, N: Blue, O: Red, P: Yellow, C: Gray)



Supplementary Figure 10: 2D (4,4) net arrangement of **9** (phenyl rings are omitted for clarity; Colour Code: Zn: Green, N: Blue, O: Red, P: Yellow, C: Gray))



Supplementary Figure 11: Supramolecular 3D arrangement in **9** by locking of 2D sheets by H-bonding (Colour Code: Zn: Green, N: Blue, O: Red, P: Yellow, C: Gray, H-bonding: Cyan dotted lines)



Supplementary Figure 12: Disposition of sheets in **10** (Colour Code: Cd: Green, N: Blue, O: Red, P: Yellow, C: Gray)