

Electronic Supporting Information

For

Temperature- and solvent-controlled dimensionality in a zinc 6-(1H-benzoimidazol-2-yl)pyridinecarboxylate system

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Contents

Fig.**S1** The thermal analyses (N2) of the crystalline **1**, **2** and **5** (TG curves)

Table **S2**. Selected bond distances (\AA) and bond angles ($^{\circ}$) for three complexes **1**, **2** and **5**.

Table **S3** Table **3** Distances (\AA) and angles ($^{\circ}$) of hydrogen bonds for compounds **1**, **2** and **5**

Fig.**S4** ORTEP plot of coordination environment of Zn(II) center in complex **3** with

partial atomic labels, and guest molecules $[\text{H}_2\text{N}(\text{CH}_3)_2]^+$ are omitted for clarity.

Symmetry code a: 0.5-x, 0.5-y, 1-z; b: 0.5-x, 0.5+y, 1-z; c: x, -y, 0.5+z.

Fig. **S5** 3D metal-organic framework with 3D channels containing the guest motifs

$[\text{H}_2\text{N}(\text{CH}_3)_2]^+$ in complex **3**.

Fig. **S6** ORTEP plot of two coordination geometries of Zn(II) centers in complex **4** with

atomic labels.

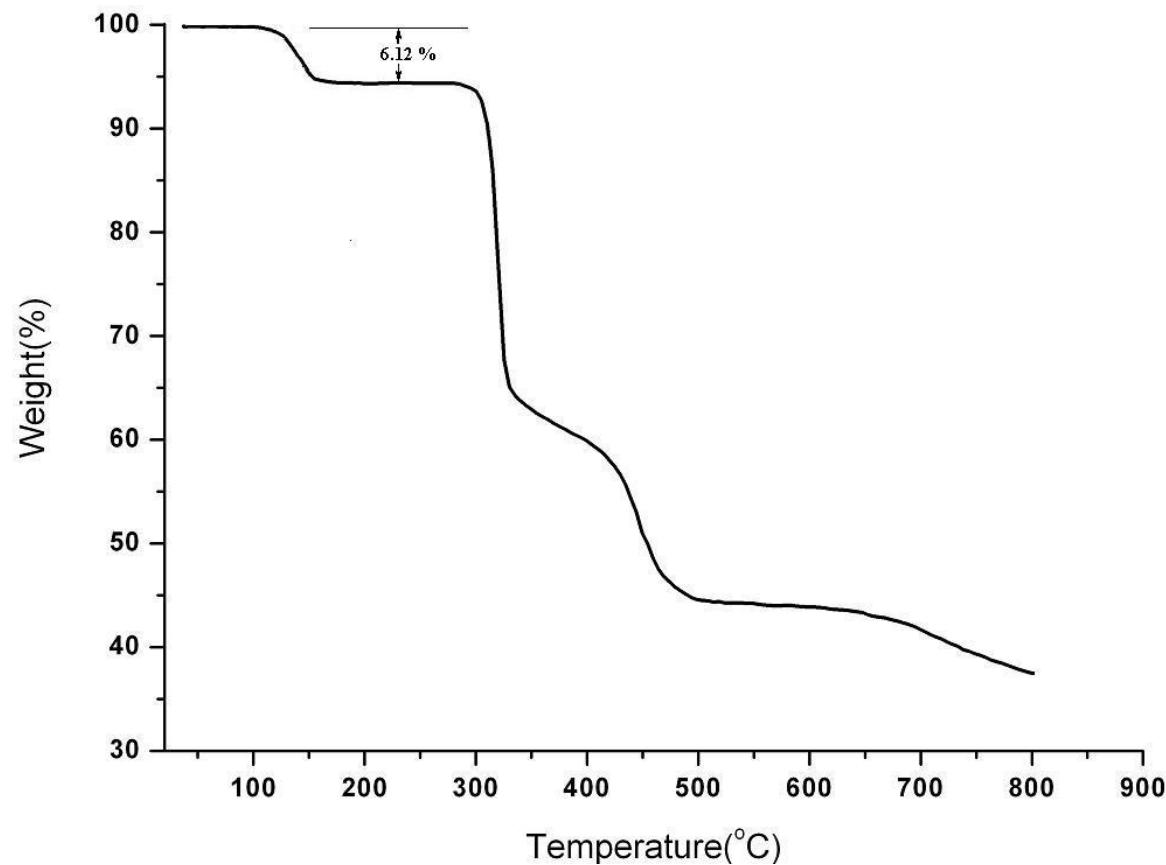
Fig. **S7** 3D metal-organic framework with 3D channels in **4**.

Fig. **S8** 3D network in **5** constructed by $\pi \cdots \pi$ stacking and O-H \cdots O hydrogen bonding interactions in *ac* plane.

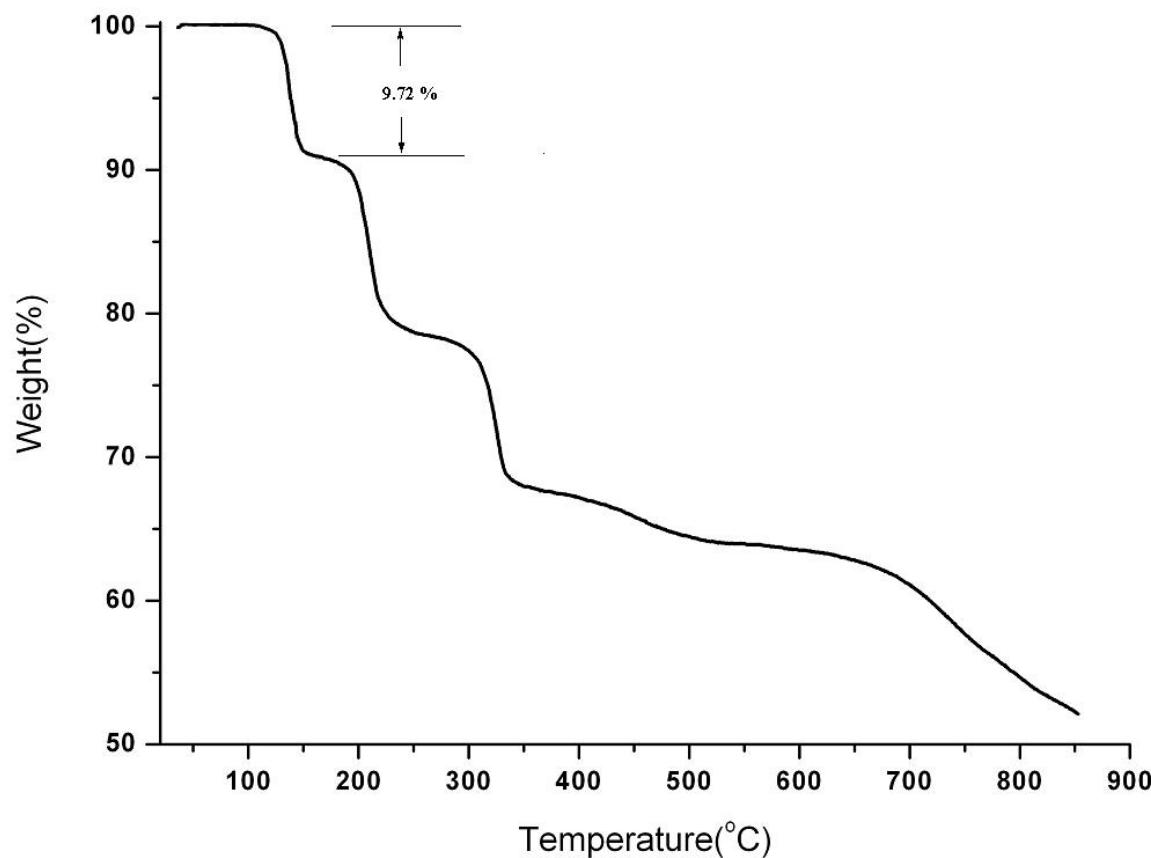
Fig. **S9** HOMO and LUMO diagrams for **1**, **2** and **5**.

Fig. S1

(a) for compound 1



(b) for compound 2



(c) for compound 5

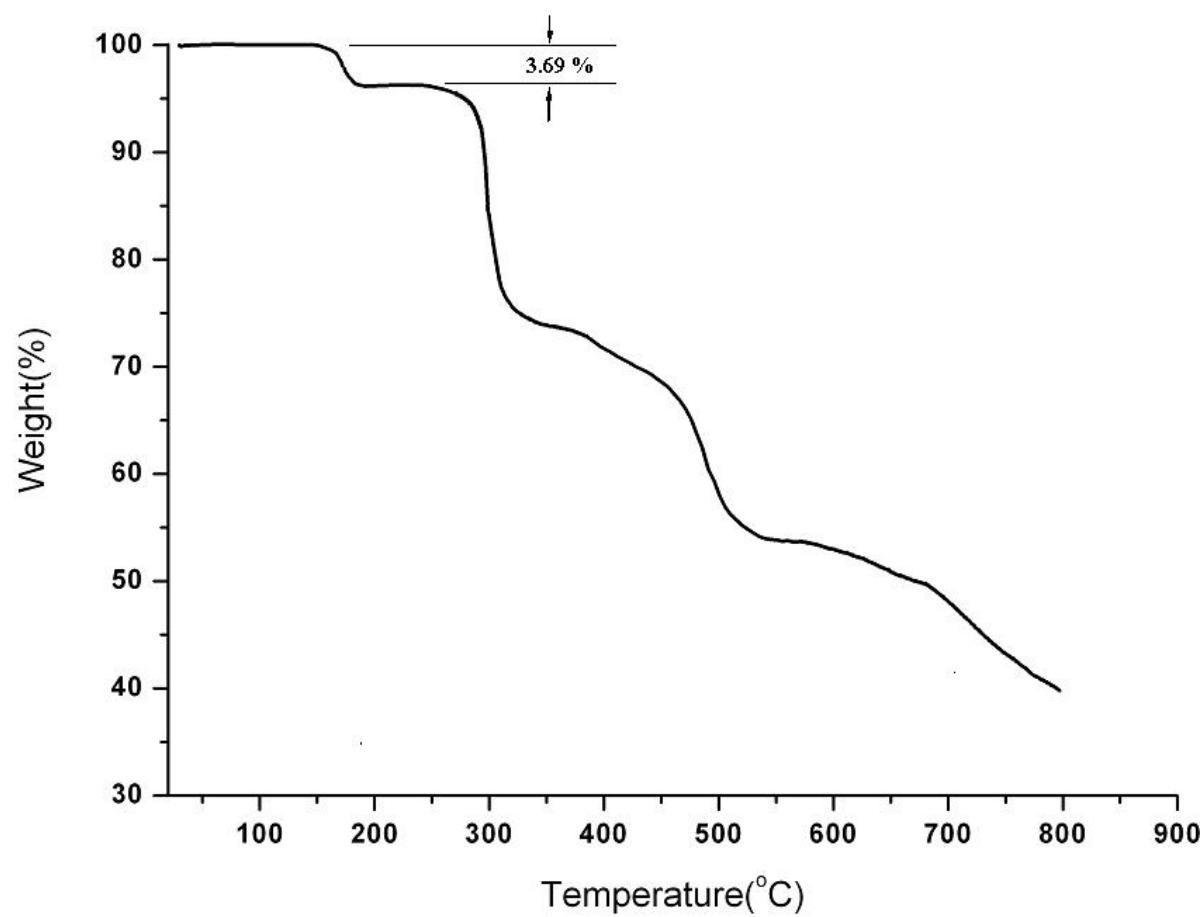


Table S2Electronic Supplementary Material for CrystEngComm
This journal is (c) The Royal Society of Chemistry 2009Selected bond distances (\AA) and bond angles ($^\circ$) for three complexes **1**, **2** and **5**^a

	1		
Zn(1)-N(1)	2.2093(15)	N(6)-Zn(1)-N(3)	178.57(5)
Zn(1)-N(3)	1.9725(13)	N(6)-Zn(1)-N(4)	79.12(5)
Zn(1)-N(4)	2.1188(12)	N(3)-Zn(1)-N(4)	99.84(5)
Zn(1)-N(6)	1.9481(13)	N(6)-Zn(1)-O(3)	78.81(5)
Zn(1)-O(1)	2.2891(14)	N(3)-Zn(1)-O(3)	102.14(5)
Zn(1)-O(3)	2.1304(12)	N(4)-Zn(1)-O(3)	157.48(5)
N(6)-Zn(1)-N(1)	102.62(6)	N(3)-Zn(1)-N(1)	78.45(6)
N(4)-Zn(1)-N(1)	96.81(5)	O(3)-Zn(1)-N(1)	92.32(5)
N(6)-Zn(1)-O(1)	102.44(5)	N(3)-Zn(1)-O(1)	76.55(5)
N(4)-Zn(1)-O(1)	91.28(5)	O(3)-Zn(1)-O(1)	89.12(5)
N(1)-Zn(1)-O(1)	154.69(5)		
	2		
Zn(1)-N(1)	2.040(2)	O(3)-Zn(1)-N(3)	161.02(9)
Zn(1)-N(3)	1.933(2)	O(3)-Zn(1)-O(1)	97.46(8)
Zn(1)-O(1)	2.0370(18)	N(3)-Zn(1)-O(1)	80.12(8)
Zn(1)-O(3)	1.9040(18)	O(3)-Zn(1)-N(1)	99.12(8)
Zn(1)-O(2)#1	2.2993(19)	N(3)-Zn(1)-N(1)	80.02(8)
O(3)-Zn(1)-O(2)#1	92.05(8)	O(1)-Zn(1)-N(1)	159.04(8)
O(1)-Zn(1)-O(2)#1	96.53(7)	N(3)-Zn(1)-O(2)#1	106.91(8)
N(1)-Zn(1)-O(2)#1	95.61(7)		
	5		
Zn(1)-N(1)	1.927(3)	N(1)-Zn(1)-O(3)	168.81(12)
Zn(1)-N(2)	2.048(3)	N(1)-Zn(1)-N(2)	80.16(11)
Zn(1)-O(1)	2.050(2)	O(3)-Zn(1)-N(2)	99.09(11)
Zn(1)-O(2)#2	2.242(2)	N(1)-Zn(1)-O(1)	79.90(10)
Zn(1)-O(3)	1.934(3)	O(3)-Zn(1)-O(1)	98.61(11)
O(2)-Zn(1)#3	2.242(2)	N(1)-Zn(1)-O(2)#2	97.28(10)
N(2)-Zn(1)-O(1)	157.87(10)	N(2)-Zn(1)-O(2)#2	100.35(10)
O(3)-Zn(1)-O(2)#2	93.84(11)	O(1)-Zn(1)-O(2)#2	91.60(9)

^aSymmetry transformations used to generate equivalent atoms: #1 -x+1,y-1/2,-z+1/2; #2 -x+1,y-1/2,-z+3/2; #3 -x+1,y+1/2,-z+3/2.

Table S3Electronic Supplementary Material for CrystEngComm
This journal is (c) The Royal Society of Chemistry 2009**Table S3** Distances (\AA) and angles ($^\circ$) of hydrogen bonds for compounds **1**, **2** and **5^b**

D-H…A	d(H…A)	d(D…A)	$\angle D\text{-H}\cdots A$
1			
O(1W)-H(1WA)…O(2)#1	2.067(9)	2.753(3)	138.1(13)
O(2W)-H(2WB)…O(3W)	2.168(13)	2.927(7)	150.7(17)
O(3W)-H(3WA)…O(2W)	2.245(13)	2.927(7)	138.6(11)
N(2)-H(2)…O(3)#2	2.132(12)	2.8839(18)	145.3(12)
N(5)-H(5)…O(1)#3	2.101(12)	2.8291(16)	142.0(12)
C(16)-H(16)…O(2W)	2.668(12)	3.436(7)	140.4(11)
C(23)-H(23)…O(3W)	2.528(13)	3.330(7)	144.7(12)
2			
O(1W)-H(1WA)…O(4)#4	1.923(13)	2.752(3)	168(3)
O(1W)-H(1WB)…O(2)#5	2.204(19)	3.001(3)	158(4)
O(2W)-H(2WB)…O(1W)#6	1.934(14)	2.762(3)	167(3)
O(2W)-H(2WA)…O(4)#7	2.07(2)	2.842(3)	153(3)
O(2W)-H(2WA)…O(3)#7	2.61(3)	3.209(3)	129(4)
N(2)-H(2)…O(2W)#1	1.91(3)	2.767(3)	171.6
Cg1…Cg2		3.582	
Cg1…Cg1a		3.782	
5			
O(8)-H(8A)…O(7)#1	2.31(8)	2.950(6)	170(10)
O(8)-H(8B)…O(4)#8	2.05(7)	2.870(5)	154(7)
N(3)-H(3)…O(8)#9	1.90(7)	2.754(4)	177(6)
C(5)-H(5)…O(5)#10	2.56(6)	3.182(5)	135(7)
Cg1…Cg2		3.510	
Cg1…Cg1a		3.867	

^bSymmetry transformation used to generate equivalent atoms: #1 x,y,z-1; #2 -x+1,-y+2,-z+1; #3 -x+2,-y+2,-z+2; #4 x-1,y,z; #5 x,y,z; #6 x,-y+1/2,z+1/2; #7 -x+1,-y+1,-z+1; #8 -x,-y+1,-z+1; #9 x,y,z+; #10 x,2+y,z. Cg1 (benzimidazole), Cg1a (pyridine) and Cg2 respectively denote the centroids of six-membered and five-membered rings in the asymmetrical ligand HL.

Fig S4

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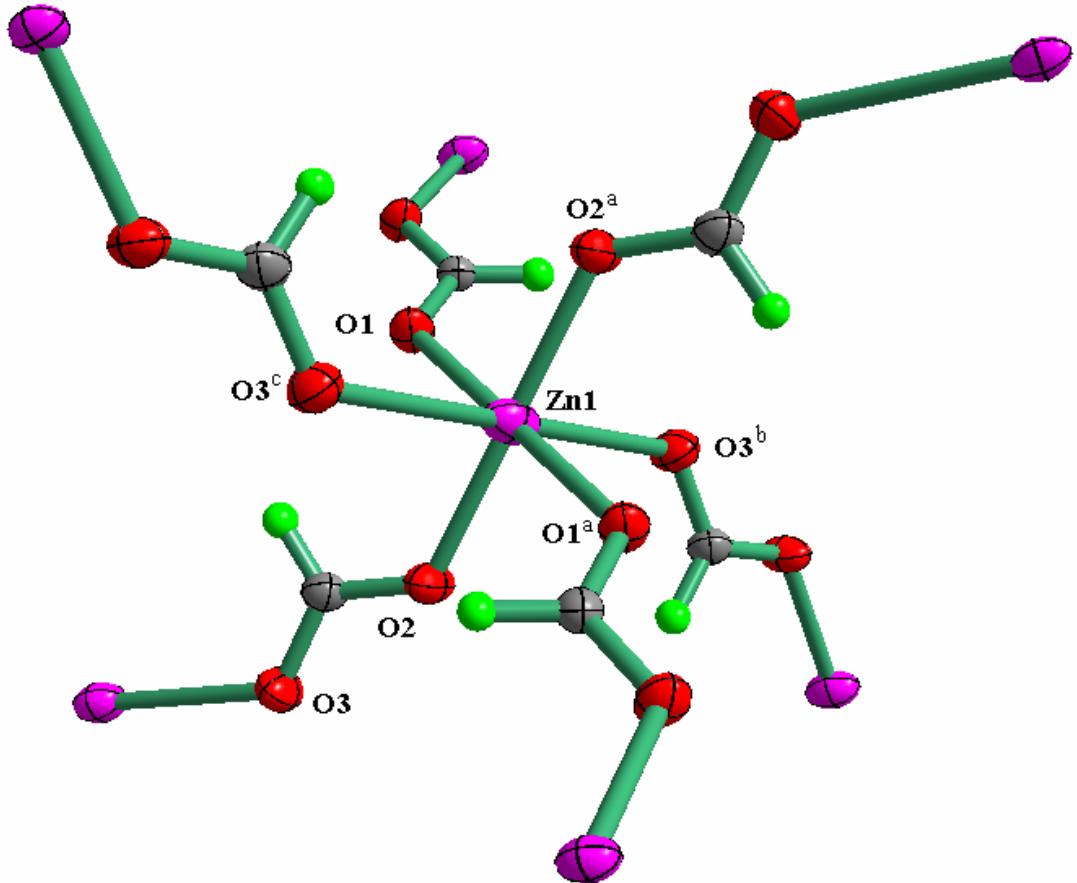
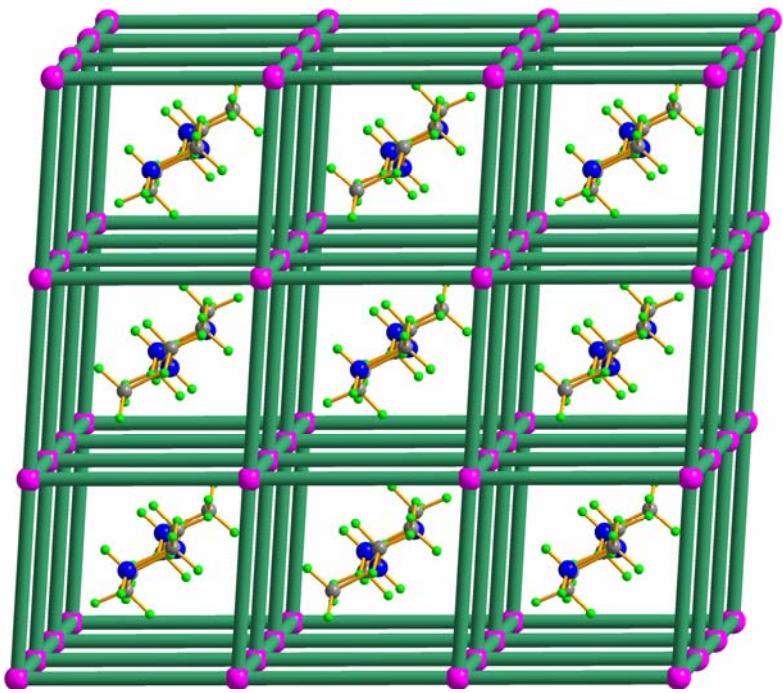
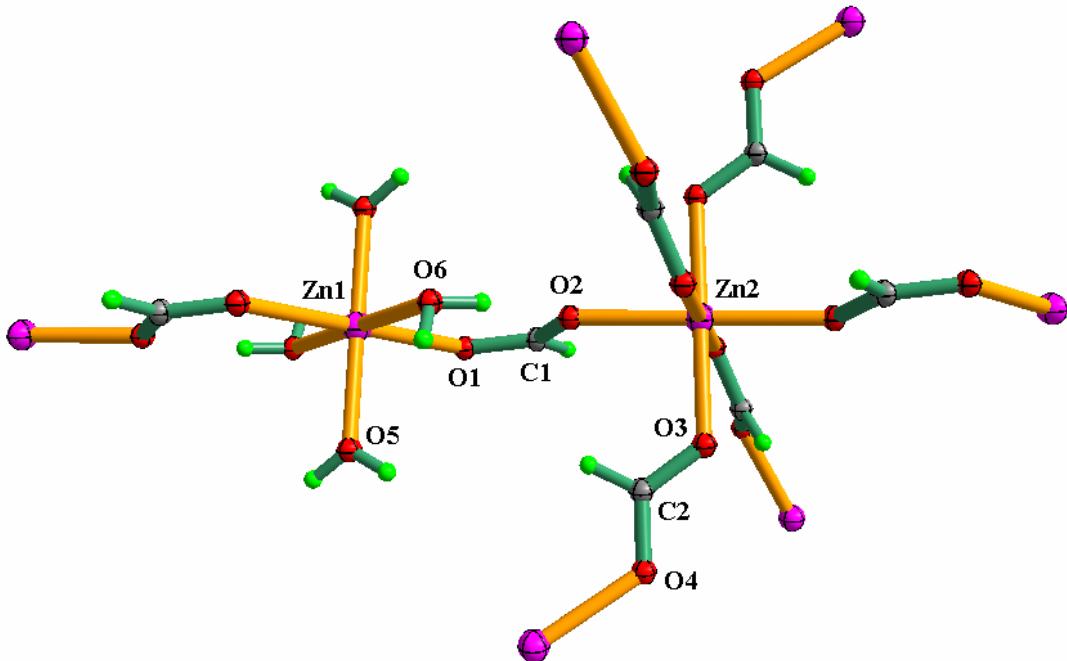


Fig S5

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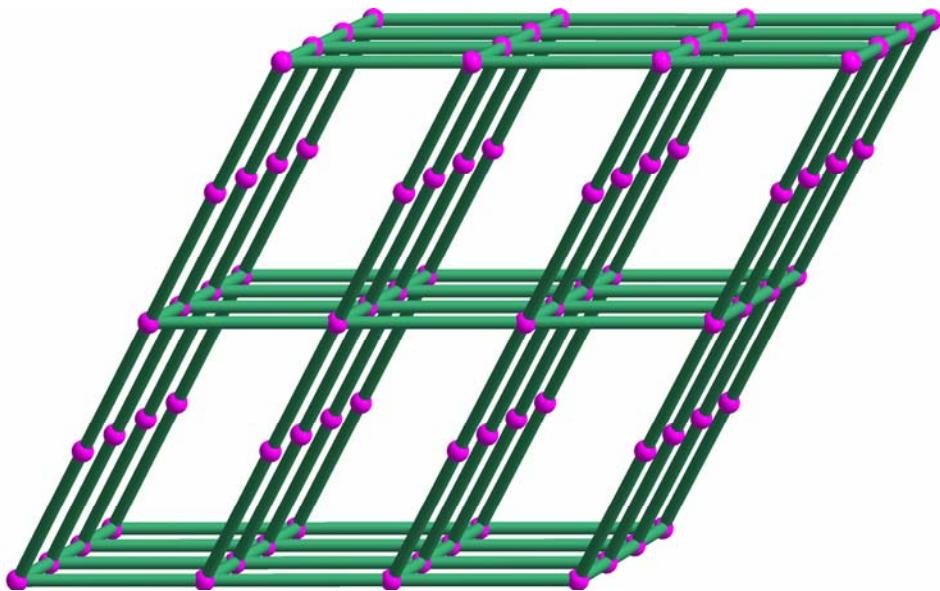


Fig. S8

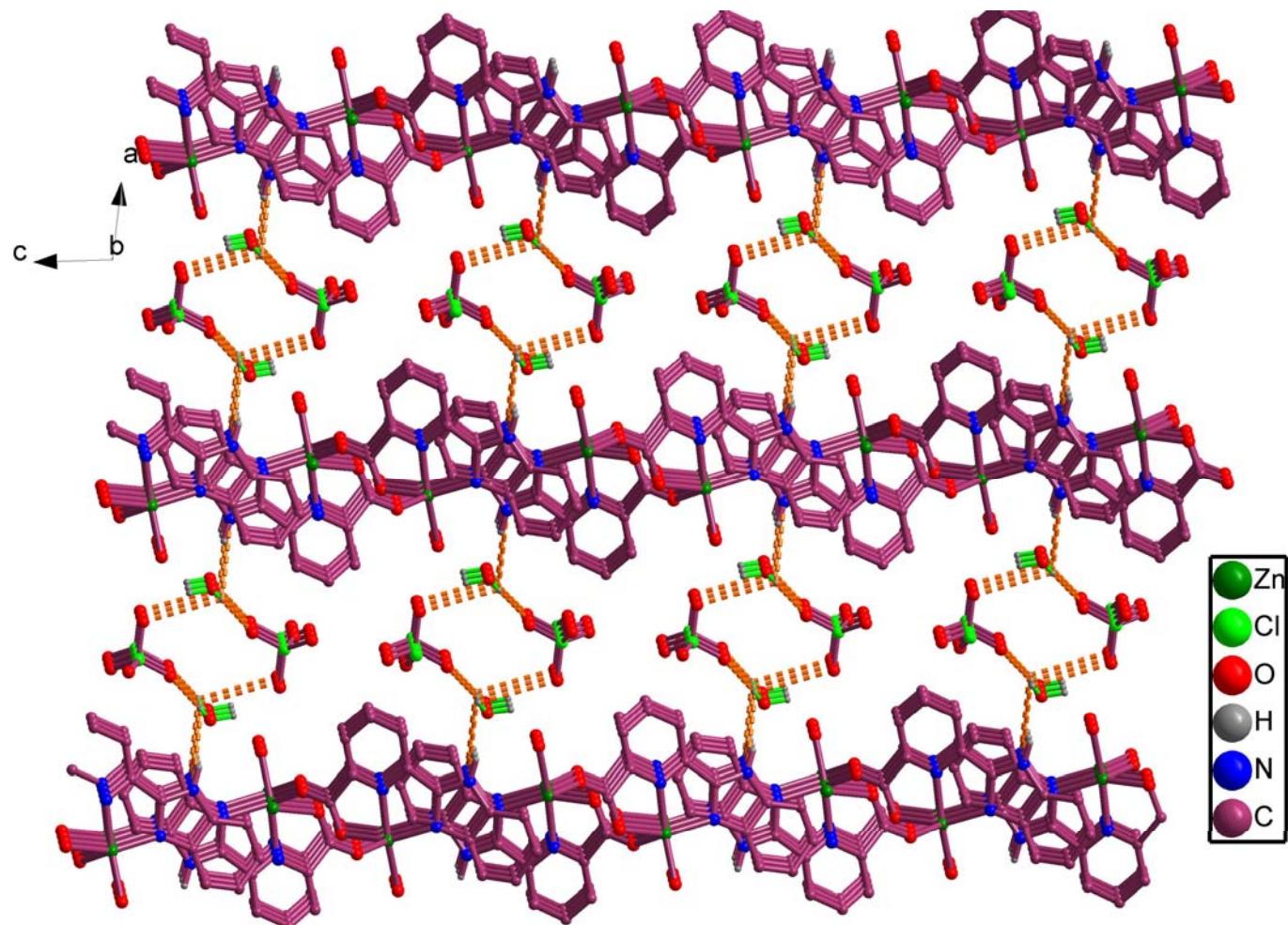
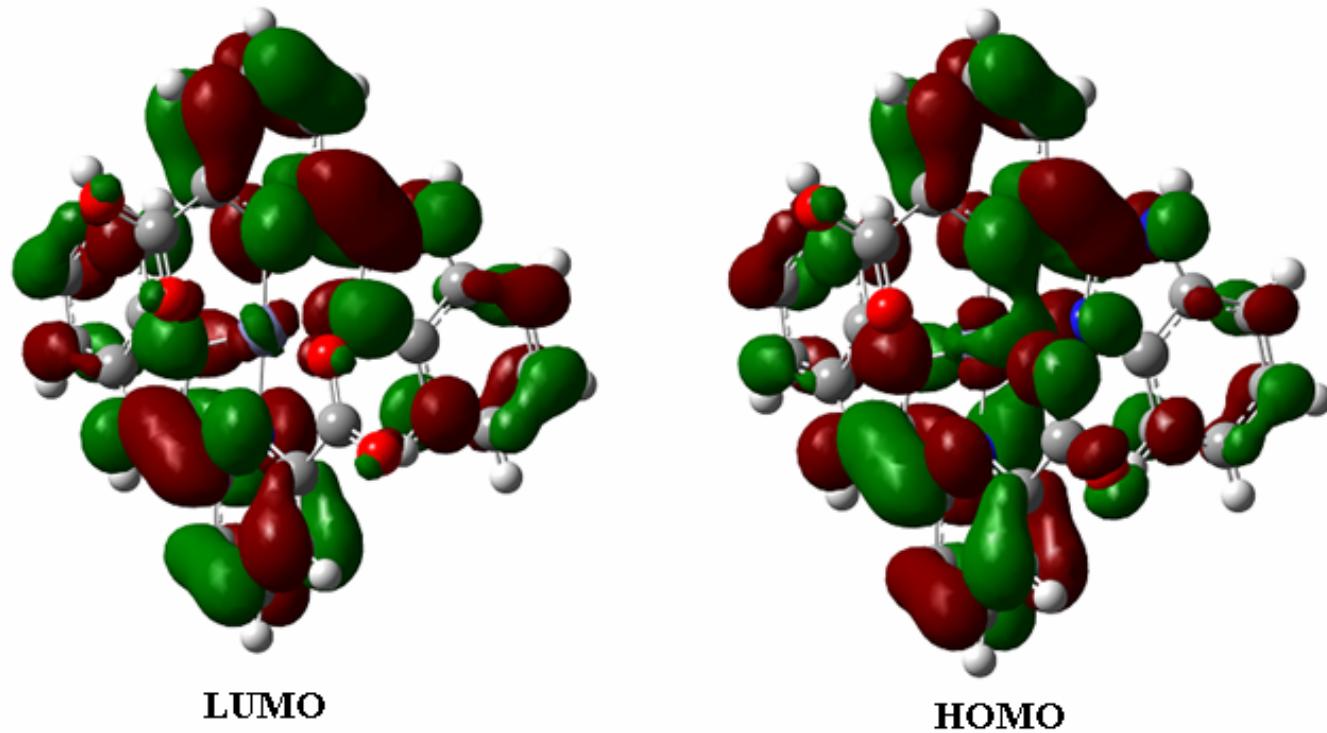
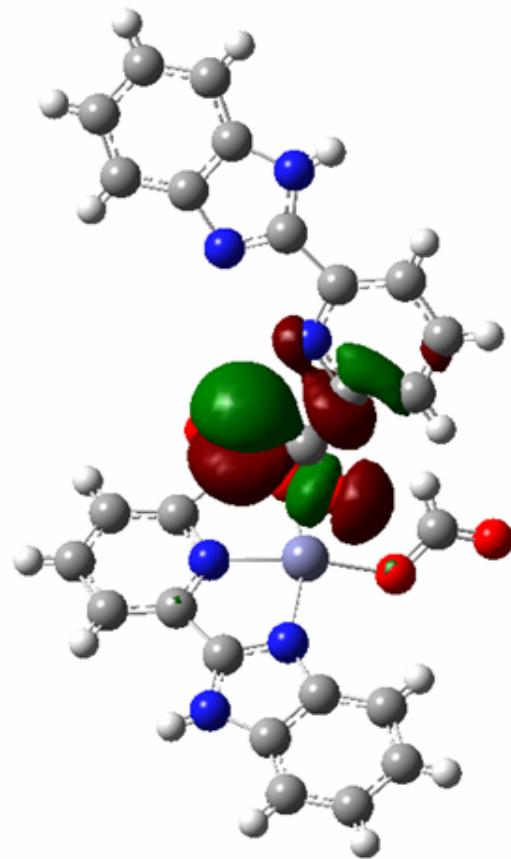
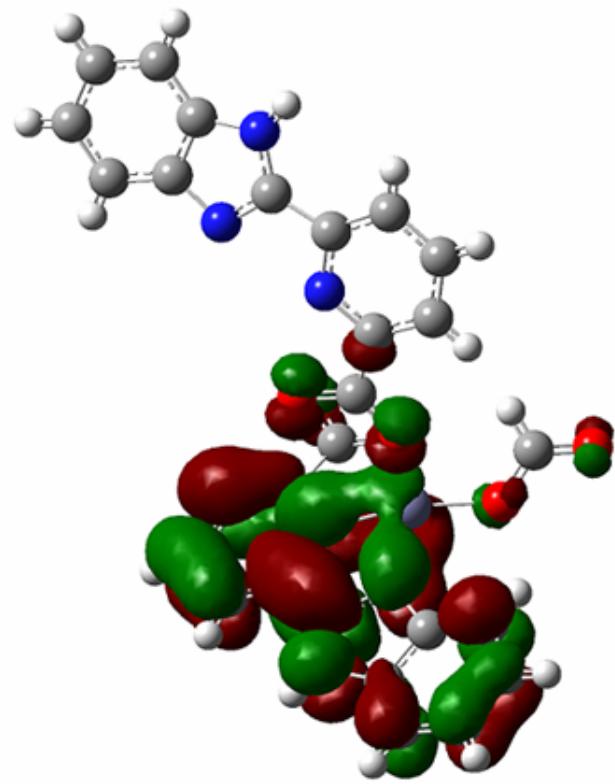


Fig. S9

(a) For **1**



(b) for 2



(c) for 5

