Electronic Supplementary Material for CrystEngComm


# Electronic Supporting Information

**For**

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

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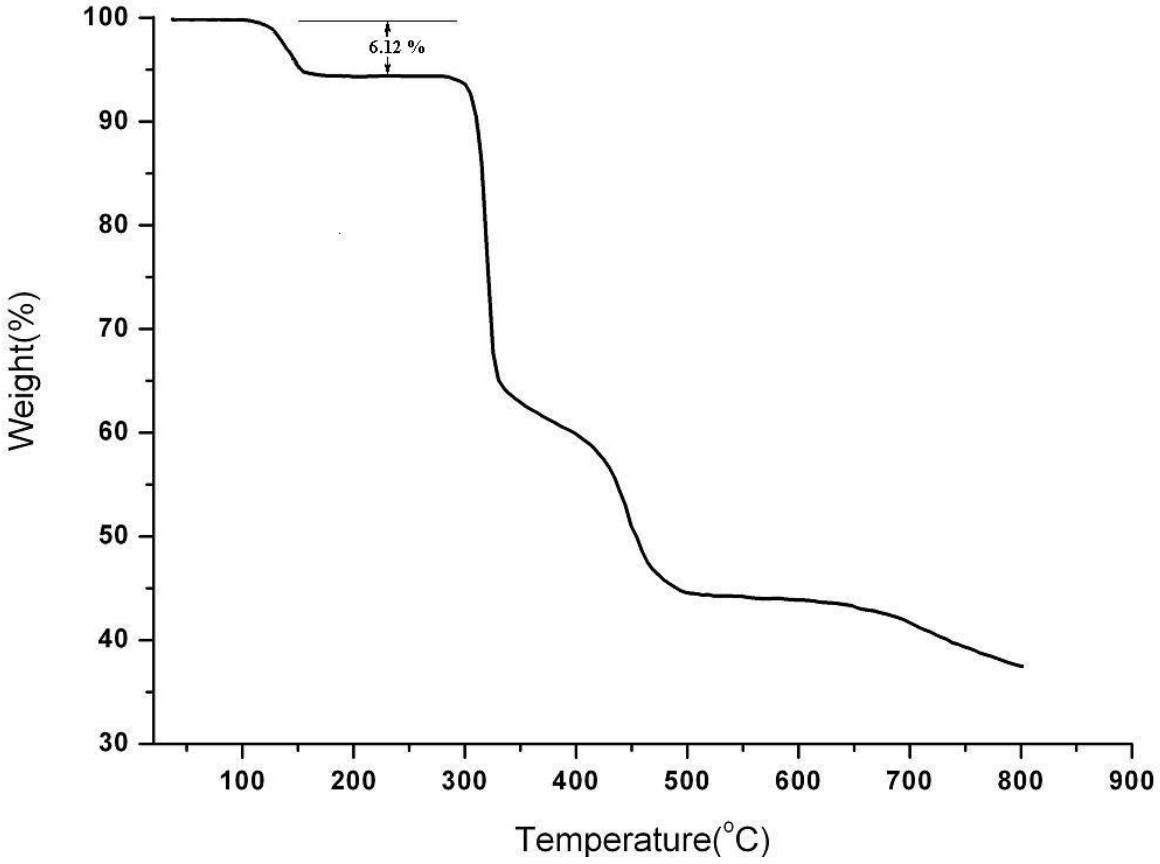
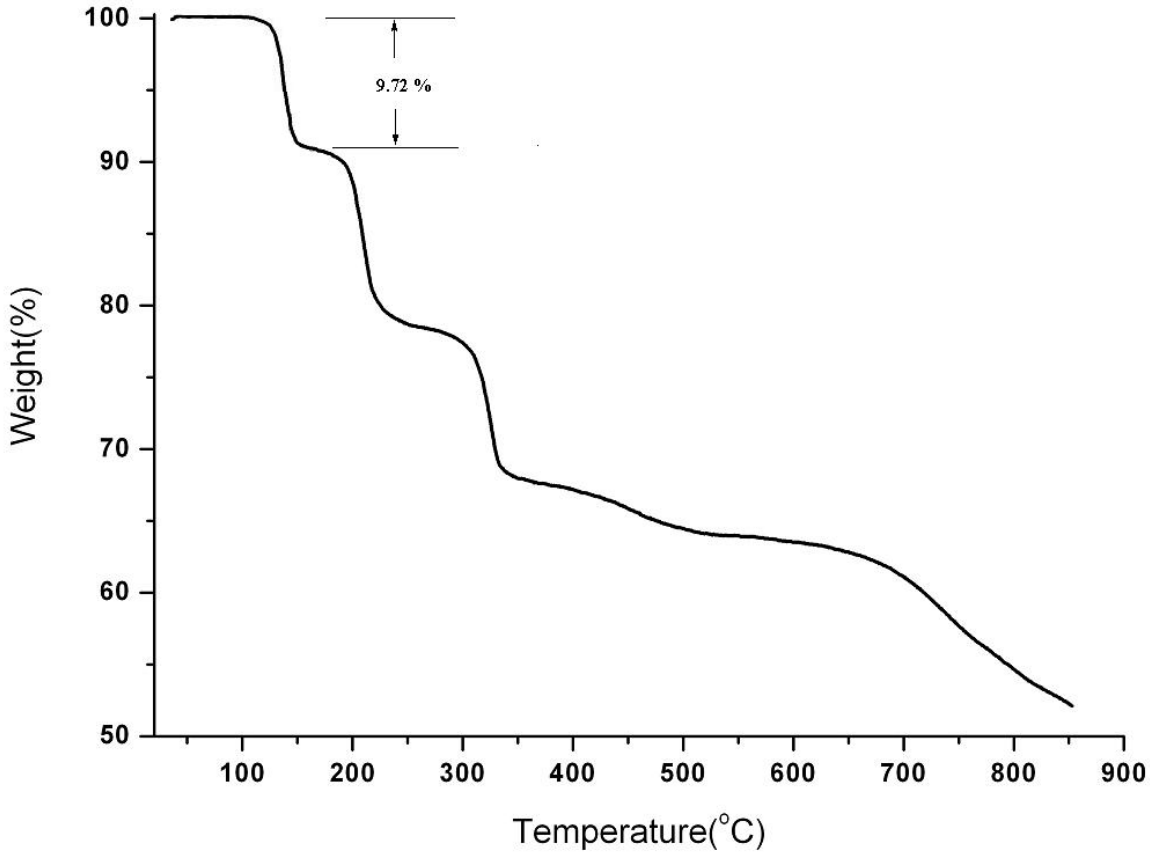
# Contents

# Fig. S1

(**a**) for compound **1**



**(b)** for compound **2**



**(c)** for compound **5**

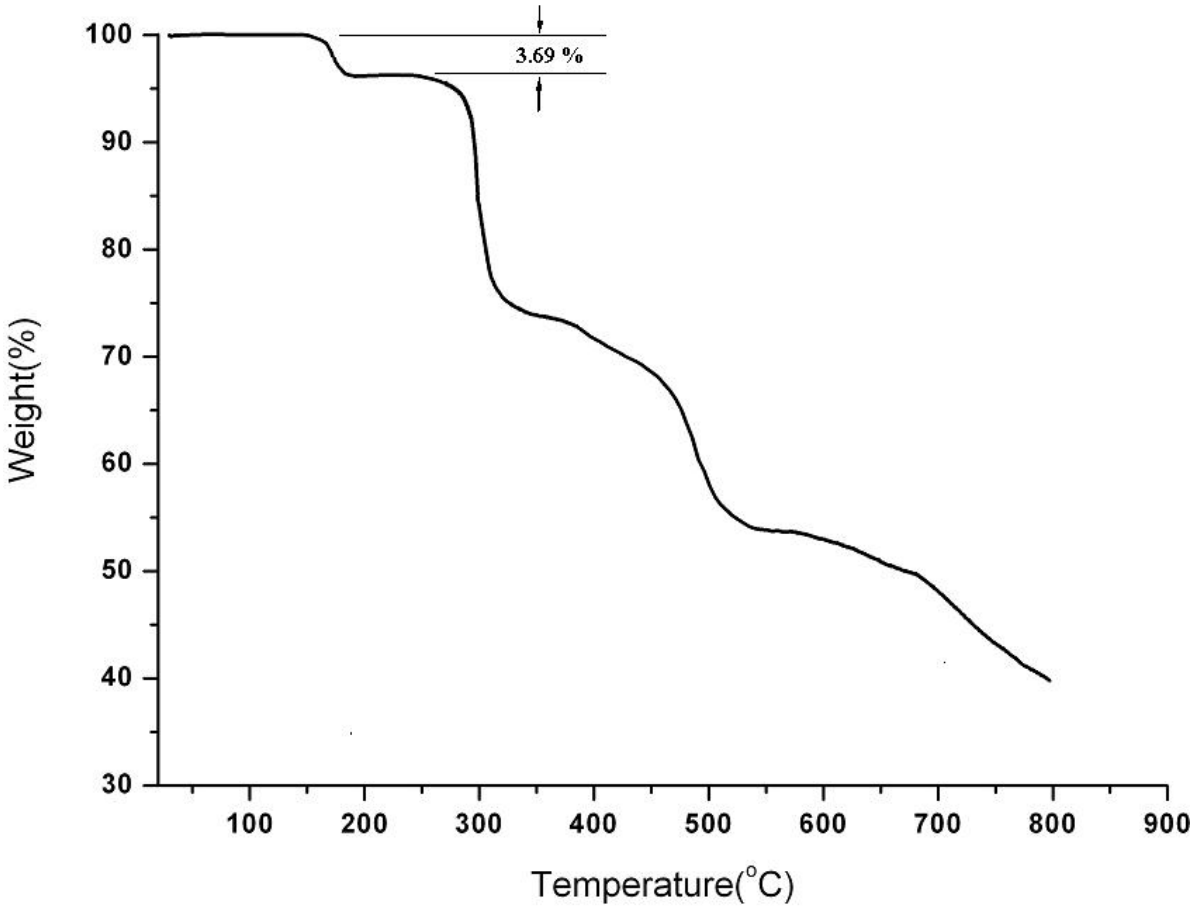


**Table S2**

Selected bond distances (Å) and bond angles (°) 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) |

[a]Symmetry 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 S3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1**, **2** and **5**[b]

| D-H···A | d(H···A) | d(D···A) | ∠D-H···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 | |

[b]Symmetry 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 (benzimidale), Cg1a (pyridine) and Cg2 respectively denote the centroids of six-membered and five-membered rings in the asymmetrical ligand HL.

**Fig. S4**

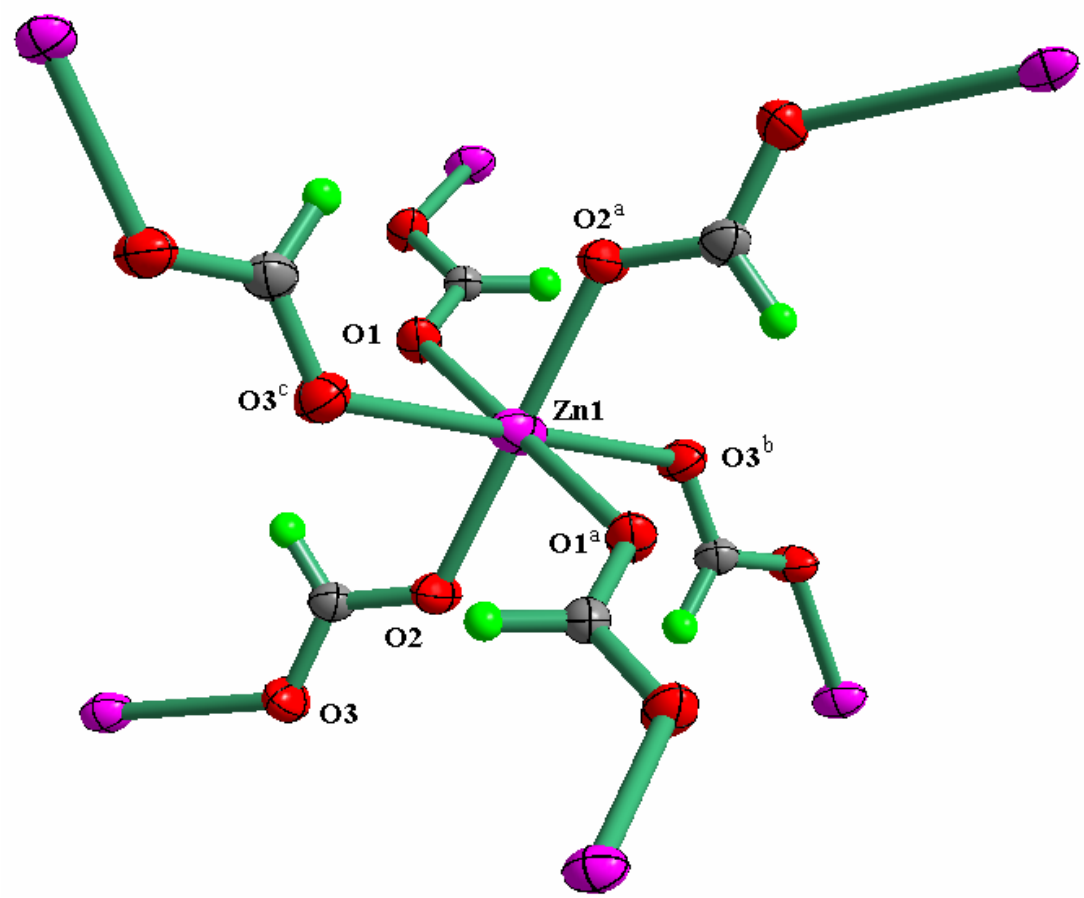


**Fig. S5**

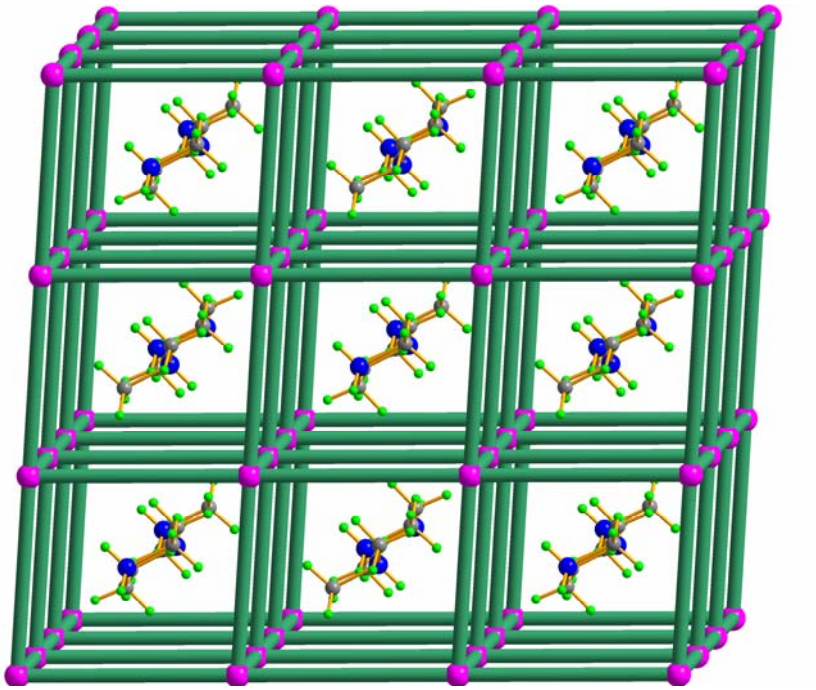


**Fig. S6**

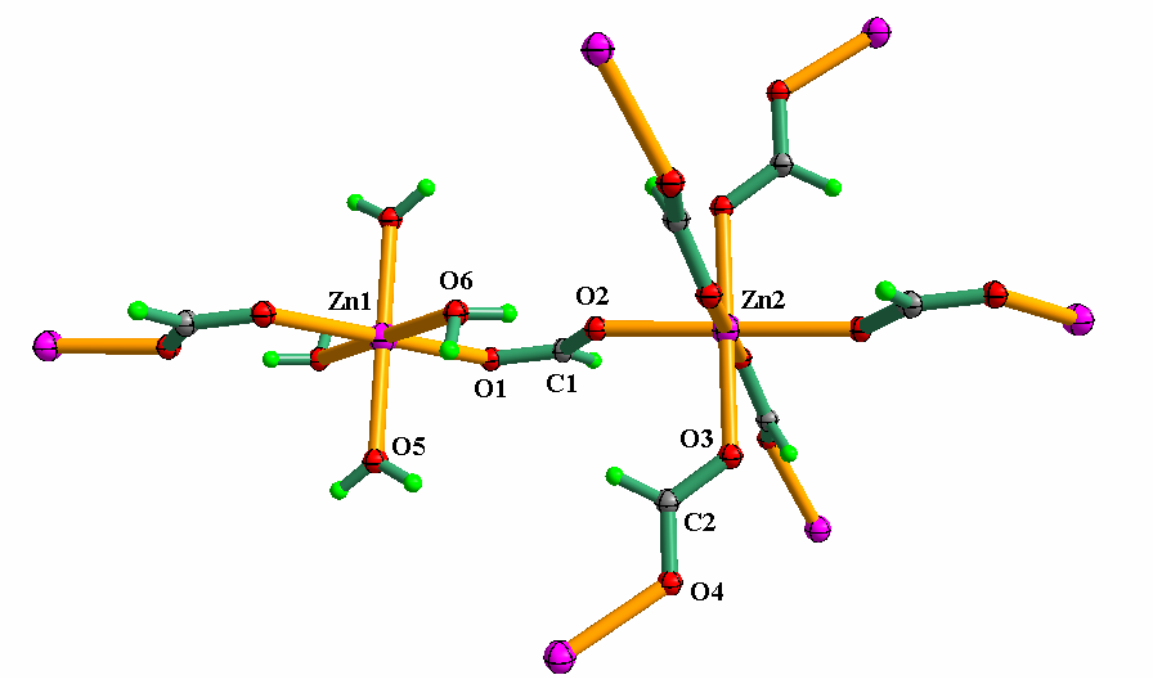


**Fig. 7**

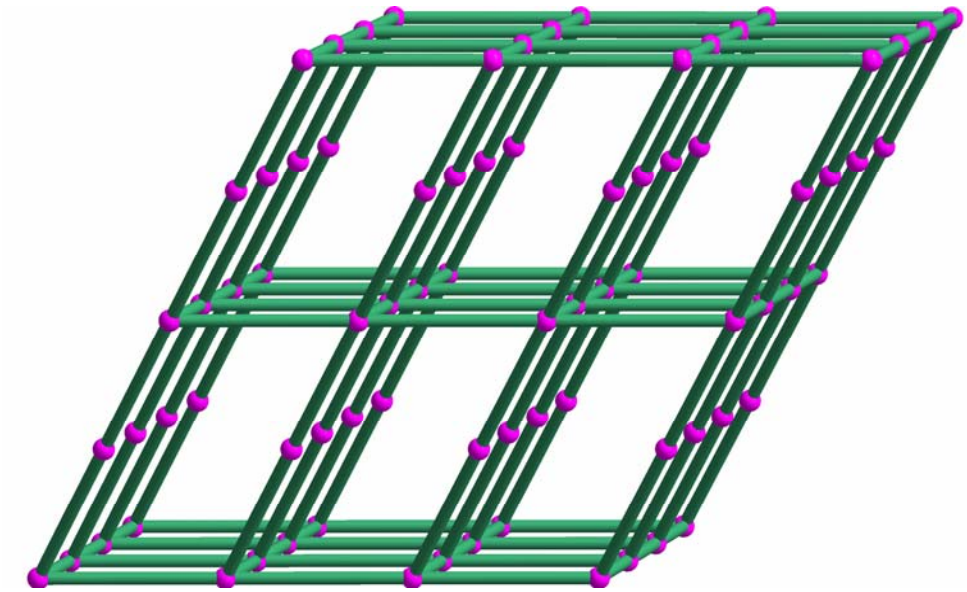


**Fig. S8**

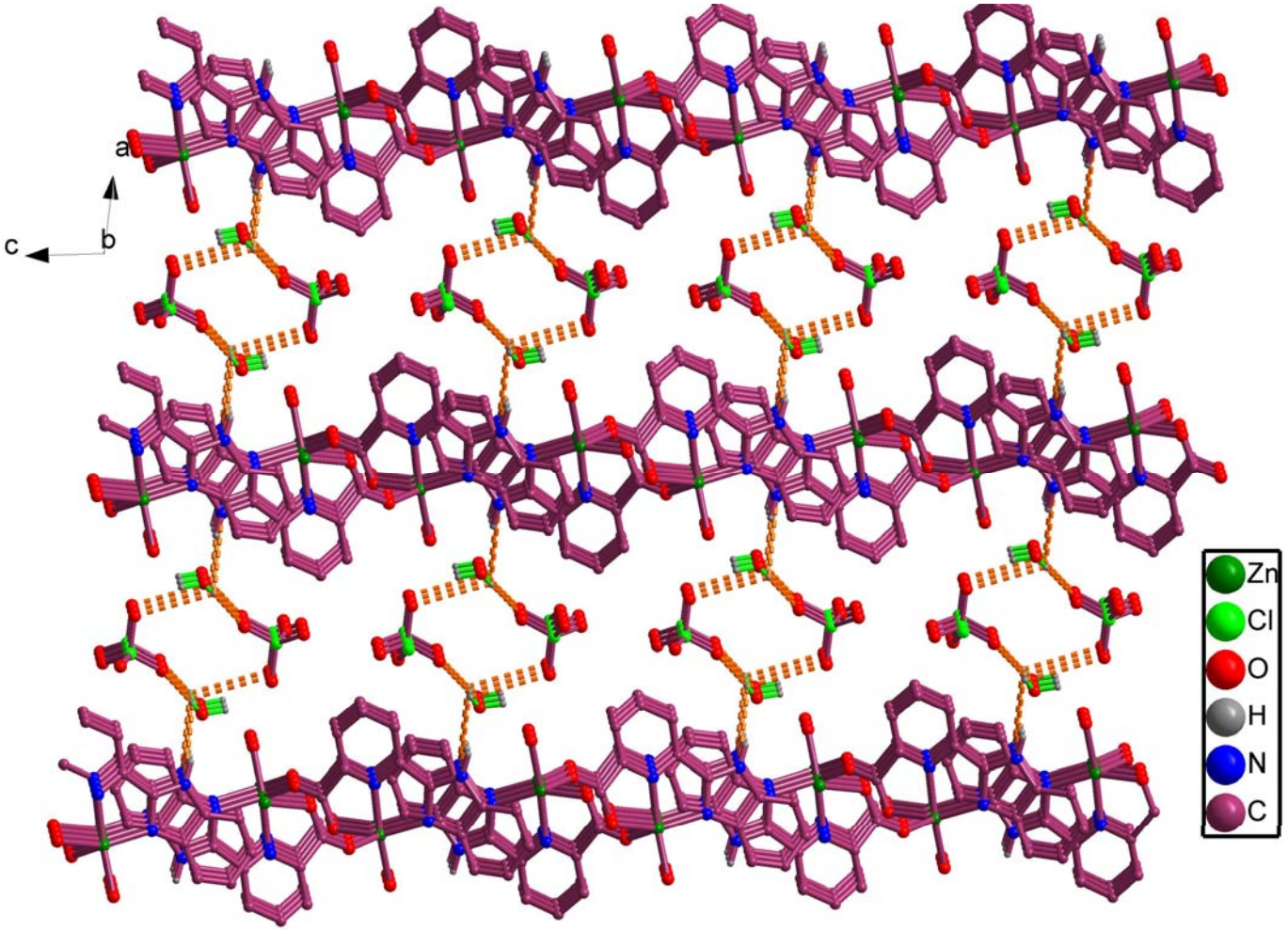
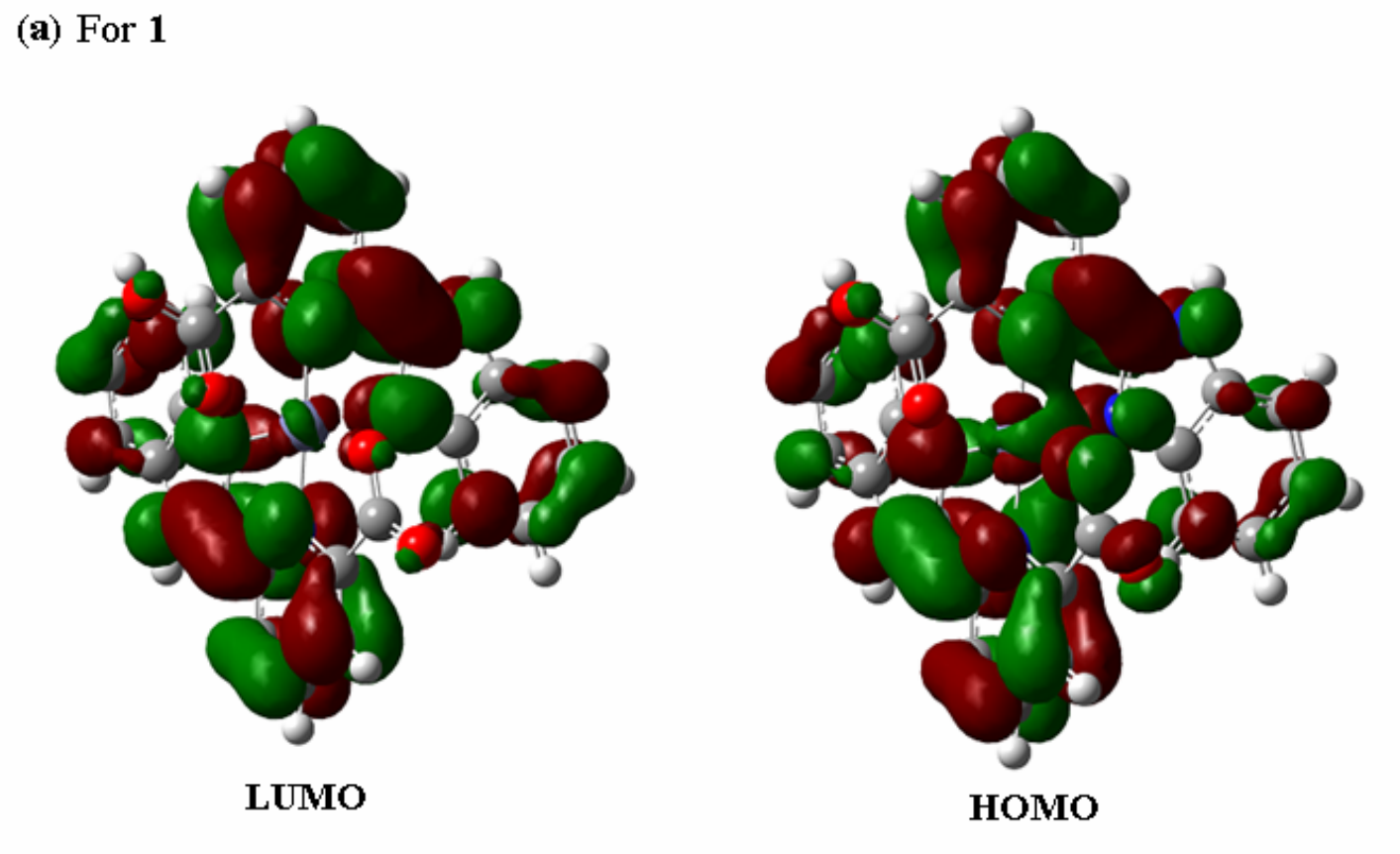
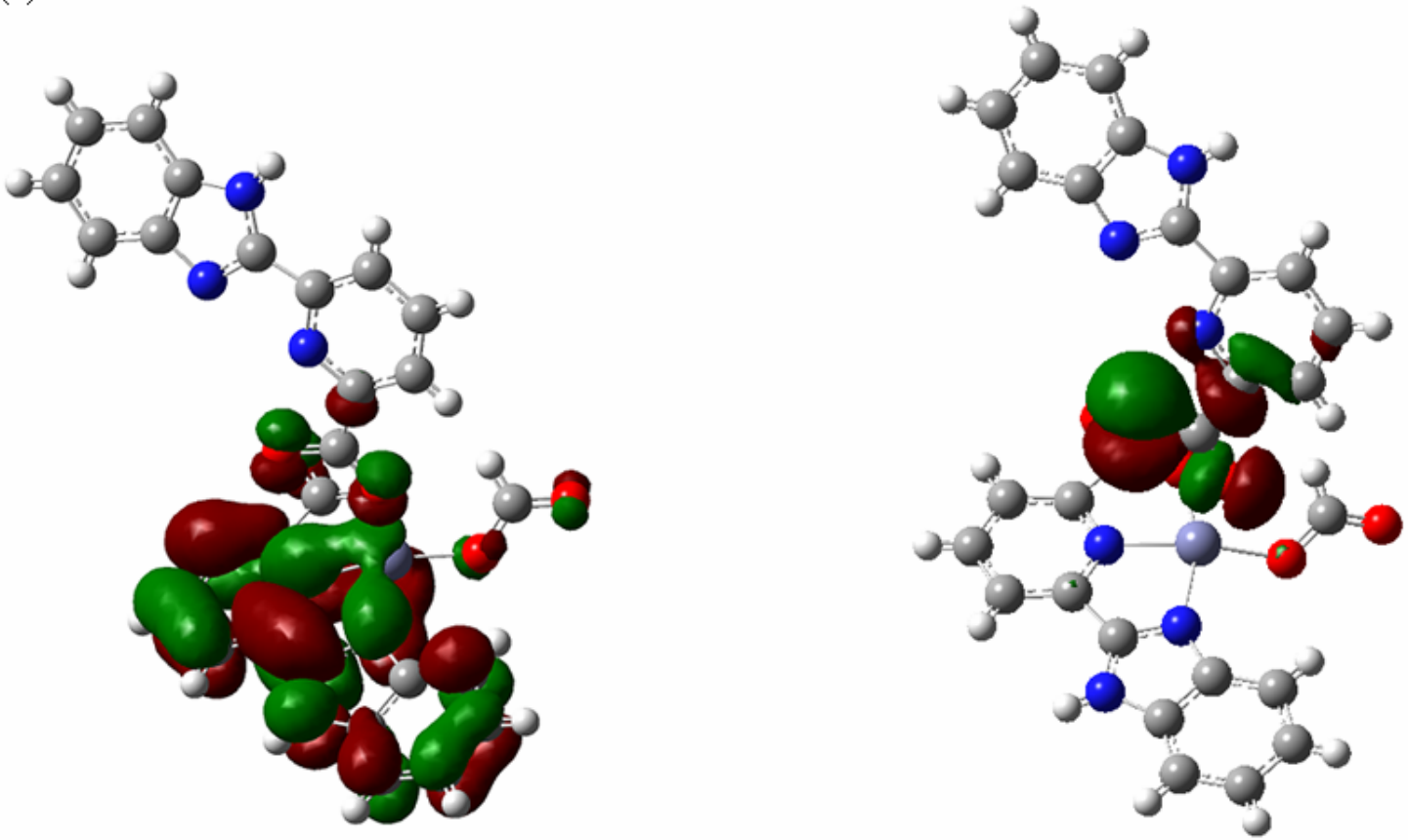


**Fig. S9**



**(b) for 2**



**(c) for 5**