Electronic Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry 2011

**Article title**: Construction of helical networks by using multiple V-shaped mixed ligand systems

**Authors:** Arijit Goswami, Satirtha Sengupta, Raju Mondal*

**Journal:** CrystEngComm

**Manuscript ID**: CE-ART-03-2011-005380

---

## Thermal analysis:

In order to characterize the compounds in terms of thermal stability, their thermal behaviors were studied by TGA. The experiment was performed on crystalline samples of **1**, **2**, **3**, **4** and **6** under nitrogen atmosphere with a heating rate of 10°C/min. Both of the

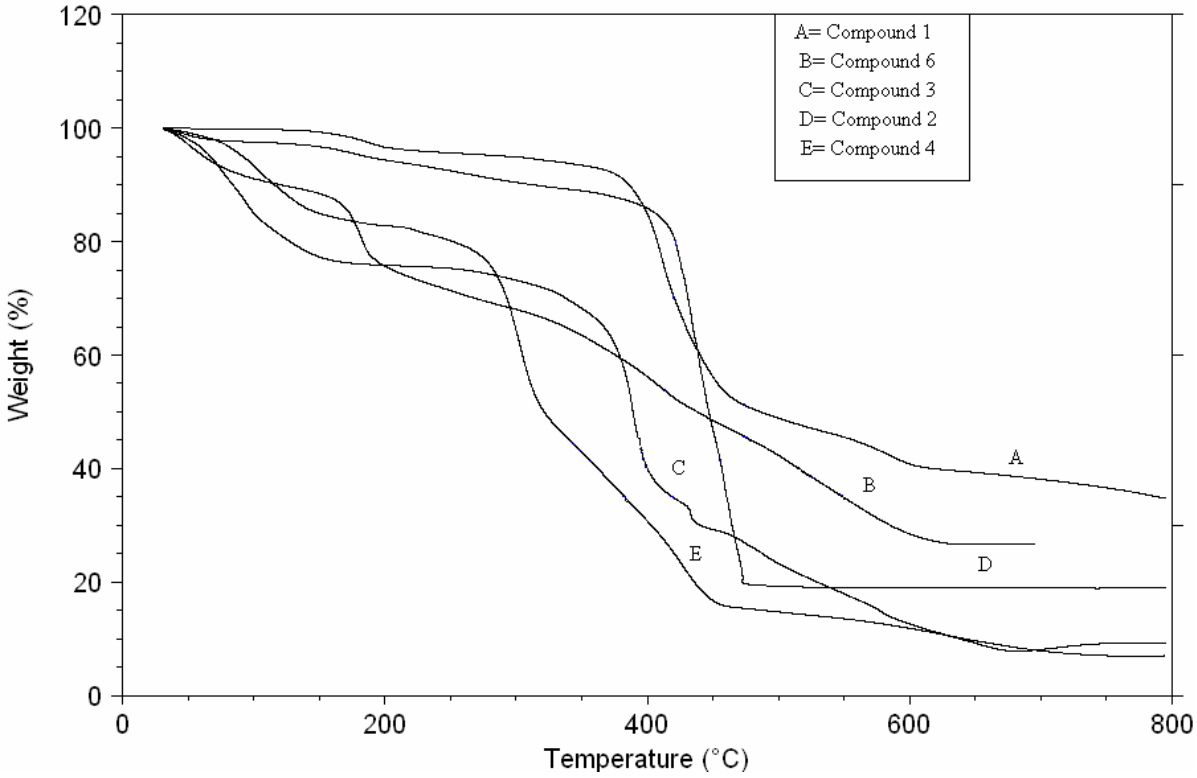


**Figure ESI 1**: TGA plot for compound **1,2,3,4** and **6**

This journal is © The Royal Society of Chemistry 2011

compounds **1** and **2** do not show any significant weight loss upto 400$^{o}$ C and 450$^{o}$ C, respectively. After that both the compounds start degrading rapidly. This is in good agreement with the crystal structure supporting the absence of any trapped solvent molecule inside the framework. Compound 3, however, shows almost 25% weight loss around 150$^{o}$ C indicating the removal of the solvent molecules. No further weight loss is observed upto 350$^{o}$ C and thereafter rapid degradation takes place. Compound **4** also shows an approximate 20% weight loss between room temperature and 275$^{o}$ C corresponding to the removal of the trapped solvent molecules and after that it starts degrading quickly. Compound **6** shows a 25% weight loss *ca*. 200$^{o}$ C corresponding to the removal of water molecules present in the framework and then shows a rapid degradation.

This journal is © The Royal Society of Chemistry 2011

## TOPOS data of Compound 1.

##################

1:C25 H24 N4 O5 Zn

##################

Structure consists of molecules (ZD1). The composition of molecule is Zn

Topology for ZD1

---

Atom ZD1 links by bridge ligands and has

| Common vertex with | | | | R(A-A) | f Total SA |
|---|---|---|---|---|---|
| ZD 1 | 1.3012 | 1.6988 | 0.9167 ( 1 1 0) | 9.649A | 1 23.72 |
| ZD 1 | -0.6988 | -0.3012 | 0.9167 (-1-1 0) | 9.649A | 1 23.72 |
| ZD 1 | 1.6988 | 1.3976 | 0.7500 ( 1 1-1) | 14.181A | 1 26.28 |
| ZD 1 | -0.3976 | -0.6988 | 1.0833 ( 0-1 0) | 14.181A | 1 26.28 |

---

Structural group analysis

---

---

Structural group No 1

---

Structure consists of 3D framework with ZD

Coordination sequences

---

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ZD1: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| Num | 4 | 12 | 36 | 72 | 122 | 188 | 264 | 354 | 456 | 570 |
| Cum | 5 | 17 | 53 | 125 | 247 | 435 | 699 | 1053 | 1509 | 2079 |

---

TD10=2079

Vertex symbols for selected sublattice

---

ZD1 Point (Schlafli) symbol:{7^5;9}

This journal is © The Royal Society of Chemistry 2011

Extended point symbol:[7(2).9(2).7(3).7(3).7(3).7(3)]

---

Point (Schlafli) symbol for net: {7^5;9}

4-c net; uninodal net

Topological type: qzd quartz-dual, "dense" net (topos&RCSR.ttd) {7^5;9} - VS [7(2).*.7(3).7(3).7(3).7(3)] (67371 types in 9 databases)

---

Non-equivalent circuits

---

Circuit No 1; Type=7a; Centroid: (0.787,0.213,0.917)

---

| Atom | x | y | z |
|---|---|---|---|
| ZD1 | 0.3012 | 0.6988 | 0.9167 |
| ZD1 | -0.3976 | -0.6988 | 1.0833 |
| ZD1 | -0.3976 | -1.6988 | 1.0833 |
| ZD1 | 0.3012 | -0.3012 | 0.9167 |
| ZD1 | 1.3012 | 0.6988 | 0.9167 |
| ZD1 | 2.6988 | 1.3976 | 0.7500 |
| ZD1 | 1.6988 | 1.3976 | 0.7500 |

Circuit No 2; Type=7b; Centroid: (0.215,0.785,0.917)

---

| Atom | x | y | z |
|---|---|---|---|
| ZD1 | 0.3012 | 0.6988 | 0.9167 |
| ZD1 | -0.3976 | -0.6988 | 1.0833 |
| ZD1 | -0.3976 | 0.3012 | 1.0833 |
| ZD1 | 0.3012 | 1.6988 | 0.9167 |
| ZD1 | -0.6988 | 0.6988 | 0.9167 |
| ZD1 | 0.6988 | 1.3976 | 0.7500 |

This journal is © The Royal Society of Chemistry 2011

ZD1 1.6988 1.3976 0.7500

Circuit No 3; Type=9a; Centroid: (0.679,0.321,0.917)

---

Atom x y z

---

ZD1 0.3012 0.6988 0.9167

ZD1 1.3012 1.6988 0.9167

ZD1 0.6024 0.3012 1.0833

ZD1 0.6024 -0.6988 1.0833

ZD1 1.3012 0.6988 0.9167

ZD1 0.3012 -0.3012 0.9167

ZD1 1.6988 0.3976 0.7500

ZD1 0.6988 0.3976 0.7500

ZD1 -0.6988 -0.3012 0.9167

Circuit No 4; Type=9b; Centroid: (0.234,0.766,0.917)

---

Atom x y z

---

ZD1 0.3012 0.6988 0.9167

ZD1 -0.6988 -0.3012 0.9167

ZD1 -1.3976 -1.6988 1.0833

ZD1 -1.3976 -0.6988 1.0833

ZD1 -0.6988 0.6988 0.9167

ZD1 0.3012 1.6988 0.9167

ZD1 1.6988 2.3976 0.7500

ZD1 2.6988 2.3976 0.7500

Elapsed time: 5.83 sec.

This journal is © The Royal Society of Chemistry 2011

**Table S-1: Selected Bond Lengths (A$^o$) and Angles ($^o$) for Compounds 1-9**

| Compound 1 | | | | Compound 2 | | | |
|---|---|---|---|---|---|---|---|
| $Zn_1$-$O_1$ | 1.939(5) | $O_1$-$Zn_1$-$O_1^i$ | 106.2(3) | $Co_1$-$O_1$ | 1.930(2) | $O_1$-$Co_1$-$O_1^i$ | 108.90(15) |
| $Zn_1$-$O_1^i$ | 1.939(5) | $O_1$-$Zn_1$-$N_1$ | 114.4(2) | $Co_1$-$O_1^i$ | 1.930(2) | $O_1$-$Co_1$-$N_1$ | 114.73(11) |
| $Zn_1$-$N_1$ | 1.974(5) | $O_1^i$-$Zn_1$-$N_1$ | 100.2(2) | $Co_1$-$N_1$ | 1.995(3) | $O_1^i$-$Co_1$-$N_1$ | 100.23(1) |
| $Zn_1$-$N_1^i$ | 1.974(5) | $O_1$-$Zn_1$-$N_1^i$ | 100.2(2) | $Co_1$-$N_1^i$ | 1.995(3) | $O_1$-$Co_1$-$N_1^i$ | 100.23(11) |
| | | $O_1^i$-$Zn_1$-$N_1^i$ | 114.4(2) | | | $O_1^i$-$Co_1$-$N_1^i$ | 114.73(11) |
| | | $N_1$-$Zn_1$-$N_1^i$ | 121.0(4) | | | $N_1$-$Co_1$-$N_1^i$ | 118.35(18) |
| Compound 3 | | | | Compound 4 | | | |

This journal is © The Royal Society of Chemistry 2011

| | | | |
|---|---|---|---|
| $Ni_1$-$O_3^{ii}$ 2.021(3) | $N_3^{iii}$-$Ni_1$-$O_2$ 89.10(15) | $Cu_1$-$O_3$ 1.969(3) | $O_4$-$Cu_1$-$N_1$ 94.21(14) |
| $Ni_1$-$N_3^{iii}$ 2.056(4) | $N_1$-$Ni_1$-$O_2$ 163.82(14) | $Cu_1$-$O_4$ 1.970(3) | $O_{3A}$-$Cu_1$-$N_1$ 94.31(14) |
| $Ni_1$-$N_1$ 2.059 (4) | $O_{1W}$-$Ni_1$-$O_2$ 87.06(14) | $Cu_1$-$O_{3A}$ 1.972(3) | $O_{4A}$-$Cu_1$-$N_1$ 98.50(14) |
| $Ni_1$-$O_{1W}$ 2.098(4) | $O_3^{ii}$-$Ni_1$-$O_1$ 155.47(13) | $Cu_1$-$O_{4A}$ 1.977(3) | $O_3$-$Cu_1$-$Cu_1^{iv}$ 82.27(10) |
| $Ni_1$-$O_2$ 2.117(3) | $N_3^{iii}$-$Ni_1$-$O_1$ 91.36(14) | $Cu_1$-$N_1$ 2.158(4) | $O_4$-$Cu_1$-$Cu_1^{iv}$ 84.75(10) |
| $Ni_1$-$O_1$ 2.148(3) | $N_1$-$Ni_1$-$O_1$ 101.89(14) | $Cu_1$-$Cu_1^{iv}$ 2.6935(11) | $O_{3A}$-$Cu_1$-$Cu_1^{iv}$ 80.77(10) |
| $Ni_1$-$C_{24}$ 2.476(5) | $O_{1W}$-$Ni_1$-$O_1$ 87.69(13) | $Cu_2$-$O_1$ 1.960(3) | $O_{4A}$-$Cu_1$-$Cu_1^{iv}$ 86.41(10) |
| $O_3^{ii}$-$Ni_1$-$N_3^{iii}$ 88.03(14) | $O_2$-$Ni_1$-$O_1$ 62.00(12) | $Cu_2$-$O_{2A}$ 1.971(3) | $N_1$-$Cu_1$-$Cu_1^{iv}$ 175.00(11) |
| $O_3^{ii}$-$Ni_1$-$N_1$ 102.63(15) | $O_3^{ii}$-$Ni_1$-$C_{24}$ 124.28(15) | $Cu_2$-$O_2$ 1.972(3) | $O_1$-$Cu_2$-$O_{2A}$ 88.90(14) |
| $N_3^{iii}$-$Ni_1$-$N_1$ 93.07(16) | $N_3^{iii}$-$Ni_1$-$C_{24}$ 89.99(16) | $Cu_2$-$O_{1A}$ 1.981(3) | $O_1$-$Cu_2$-$O_2$ 166.75(13) |
| $O_3^{ii}$-$Ni_1$-$O_{1W}$ 91.24(14) | $N_1$-$Ni_1$-$C_{24}$ 133.07(16) | $Cu_2$-$N_3$ 2.142(4) | $O_{2A}$-$Cu_2$-$O_2$ 88.22(14) |
| $N_3^{iii}$-$Ni_1$-$O_{1W}$ 176.04(16) | $O_{1W}$-$N_1$-$C_{24}$ 87.20(15) | $Cu_2$-$Cu_2^{v}$ 2.6824(11) | $O_1$-$Cu_2$-$O_{1A}$ 89.00(14) |
| $N_1$-$Ni_1$-$O_{1W}$ 90.88(16) | $O_2$-$Ni_1$-$C_{24}$ 30.82(14) | $O_3$-$Cu_1$-$O_4$ 167.00(13) | $O_{2A}$-$Cu_2$-$O_{1A}$ 167.26(14) |
| $O_3^{ii}$-$Ni_1$-$O_2$ 93.47(13) | $O_1$-$Ni_1$-$C_{24}$ 31.19(14) | $O_3$-$Cu_1$-$O_{3A}$ 90.62(14) | $O_2$-$Cu_2$-$O_{1A}$ 90.97(14) |
| | | $O_4$-$Cu_1$-$O_{3A}$ 88.02(13) | $O_1$-$Cu_2$-$N_3$ 97.23(14) |
| | | $O_3$-$Cu_1$-$O_{4A}$ 87.78(14) | $O_{2A}$-$Cu_2$-$N_3$ 99.88(15) |
| | | $O_4$-$Cu_1$-$O_{4A}$ 90.69(13) | $O_2$-$Cu_2$-$N_3$ 96.00(14) |
| | | $O_{3A}$-$Cu_1$-$O_{4A}$ 167.18(13) | $O_{1A}$-$Cu_2$-$N_3$ 92.85(15) |
| | | $O_3$-$Cu_1$-$N_1$ 98.78(14) | $O_1$-$Cu_2$-$Cu_2^{v}$ 85.76(10) |
| | | | $O_{2A}$-$Cu_2$-$Cu_2^{v}$ 89.11(10) |

This journal is © The Royal Society of Chemistry 2011

## Compound 5

| | | | |
|---|---|---|---|
| $Zn_1$-$O_1^{vi}$ | 1.898(3) | $O_1^{vi}$-$Zn_1$-$O_1$ | 110.6(2) |
| $Zn_1$-$O_1$ | 1.898(3) | $O_1^{vi}$-$Zn_1$-$N_1^{vi}$ | 109.41(12) |
| $Zn_1$-$N_1^{vi}$ | 1.982(3) | $O_1$-$Zn_1$-$N_1^{vi}$ | 108.23(11) |
| $Zn_1$-$N_1$ | 1.982(3) | $O_1^{vi}$-$Zn_1$-$N_1$ | 108.23(11) |
| | | $O_1$-$Zn_1$-$N_1$ | 109.41(12) |
| | | $N_1^{vi}$-$Zn_1$-$N_1$ | 110.99(16) |

## Compound 6

| | | | |
|---|---|---|---|
| $Co_1$-$O_1$ | 1.919(3) | $O_1$-$Co_1$-$O_1^{vii}$ | 110.8(2) |
| $Co_1$-$O_1$vii | 1.919(3) | $O_1$-$Co_1$-$N_1^{vii}$ | 107.85(12) |
| $Co_1$-$N_1$vii | 1.984(3) | $O_1^{vii}$-$Co_1$-$N_1^{vii}$ | 110.32(13) |
| $Co_1$-$N_1$ | 1.984(3) | $O_1$-$Co_1$-$N_1$ | 110.32(13) |
| | | $O_1^{vii}$-$Co_1$-$N_1$ | 107.85(12) |
| | | $N_1^{vii}$-$Co_1$-$N_1$ | 109.69(18) |

## Compound 7

| | | | |
|---|---|---|---|
| $Cd_1$-$O_2$ | 2.282(3) | $O_4$-$Cd_1$-$O_3$ | 54.16(10) |
| $Cd_1$-$N_1$ | 2.301(3) | $N_3$-$Cd_1$-$O_3$ | 78.22(9) |
| $Cd_1$-$O_4$ | 2.351(3) | $O_2$-$Cd_1$-$O_1$ | 96.04(9) |
| $Cd_1$-$N_3$ | 2.370(3) | $N_1$-$Cd_1$-$O_1$ | 82.35(9) |
| $Cd_1$-$O_3$ | 2.474(3) | $O_4$-$Cd_1$-$O_1$ | 74.97(10) |
| $Cd_1$-$O_1$ | 2.545(3) | $N_3$-$Cd_1$-$O_1$ | 176.88(9) |
| $Cd_1$-$C_{25}$ | 2.744(4) | $O_3$-$Cd_1$-$O_1$ | 104.57(8) |
| $O_2$-$Cd_1$-$N_1$ | 126.86(10) | $O_2$-$Cd_1$-$C_{25}$ | 111.31(12) |
| $O_2$-$Cd_1$-$O_4$ | 90.29(10) | $N_1$-$Cd_1$-$C_{25}$ | 121.77(11) |
| $N_1$-$Cd_1$-$O_4$ | 138.43(10) | $O_4$-$Cd_1$-$C_{25}$ | 26.99(11) |
| $O_2$-$Cd_1$-$N_3$ | 83.00(10) | $N_3$-$Cd_1$-$C_{25}$ | 93.21(11) |
| $N_1$-$Cd_1$-$N_3$ | 95.84(10) | $O_3$-$Cd_1$-$C_{25}$ | 27.18(11) |
| $O_4$-$Cd_1$-$N_3$ | 107.96(10) | $O_1$-$Cd_1$-$C_{25}$ | 89.90(11) |
| $O_2$-$Cd_1$-$O_3$ | 130.45(10) | | |
| $N_1$-$Cd_1$-$O_3$ | 100.55(9) | | |

## Compound 8

| | | | |
|---|---|---|---|
| $Ni_1$-$N_1$ | 2.100(3) | $O_1$-$Ni_1$-O1 | 172.87(16) |
| $Ni_1$-$O_1$ | 2.1034(15) | $N_1$-$Ni_1$-$N_3$ | 176.67(14) |
| $Ni_1$-$N_3$ | 2.110(3) | $N_1$-$Ni_1$-$N_3$ | 90.40(8) |
| $N_1$-$Ni_1$-$N_1$ | 92.92(16) | $O_1$-$Ni_1$-$N_3$ | 86.19(9) |
| $N_1$-$Ni_1$-$O_1$ | 93.73(9) | $O_1$-$Ni_1$-$N_3$ | 88.60(9) |
| $N_1$-$Ni_1$-$O_1$ | 91.18(9) | $N_3$-$Ni_1$-$N_3$ | 86.27(15) |

## Compound 9

| | | | |
|---|---|---|---|
| $Cu_1$-$O_1$ | 1.9730(15) | $N_1$-$Cu_1$-$O_4$ | 162.74(7) |
| $Cu_1$-$N_1$ | 1.9795(17) | $O_1$-$Cu_1$-$O_3$ | 145.57(7) |
| $Cu_1$-$O_4$ | 2.0108(17) | $N_1$-$Cu_1$-$O_3$ | 102.17(7) |
| $Cu_1$-$O_3$ | 2.0287(17) | $O_4$-$Cu_1$-$O_3$ | 64.57(7) |
| $Cu_1$-$N_3$ | 2.1911(18) | $O_1$-$Cu_1$-$N_3$ | 104.40(7) |
| $O_1$-$Cu_1$-$N_1$ | 90.47(7) | $N_1$-$Cu_1$-$N_3$ | 97.29(7) |
| $O_1$-$Cu_1$-$O_4$ | 95.25(7) | $O_4$-$Cu_1$-$N_3$ | 97.03(8) |
| | | $O_3$-$Cu_1$-$N_3$ | 105.53(7) |

This journal is © The Royal Society of Chemistry 2011

Symmetry operations: (i) -y+1, -x+1, -z+1/6; (ii) x+1/2, y-1/2, z; (iii) -x-1, y, -z+1/2; (iv) -x, -y, -z; (v) -x-1, -y+1, -z+1; (vi) -x+5/4, y, -z+1/4; (vii) -x+1/4, y, -z+1/4.