Electronic Supporting Information

For

Construction of 3D metal-organic frameworks with helical character through coordinative and supramolecular interactions

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Contents

Table S1. Crystallographic Data and Structure Refinements for **L**·4H_2O

Complex	**L**·4H_2O
Empirical formula	$C_{22}H_{26}N_4O_4$
Formula weight	410.47
Temperature/K	298(2)
Crystal system	Monoclinic
Space group	$P2_1/n$
a /Å	4.8087(17)
b /Å	12.043(4)
c /Å	18.482(6)
β /deg	91.160(8)
V /(Å^3)	1070.1(6)
Z	2
Dc /g cm^{-3}	1.274
μ /mm^{-1}	0.089
F (000)	436
θ range/deg	2.02-27.61
Measured refln.	6843
Unique refln.	2471 (R_{int} = 0.0477)
Refinement method	Full-matrix least-squares on F^2
Parameters refined	148
GOF on F^2	1.089
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0606, wR_2 = 0.1570
R indices (all data)	R_1 = 0.1311, wR_2 = 0.1878
Largest diff. peak and hole /e.Å^{-3}	0.225 and -0.226

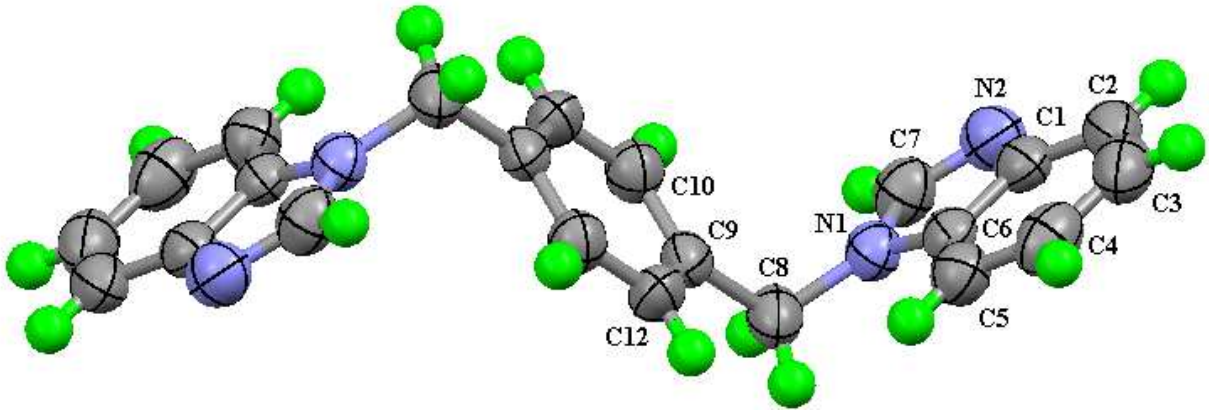
*R= $\Sigma||F_o|-|F_c||/S|F_o|$. $wR = [\Sigma w(|F_o|^2-|F_c|^2)^2/\Sigma w(F_o^2)^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (0.0988P)^2+0.0119P]$ for **L**·4H_2O. $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Selected bond distances (Å) and bond angles (°)for complexes **1-6**[a]

		1	
Zn(1)-O(2)	2.081(3)	O(2)-Zn(1)-O(1)	87.00(11)
Zn(1)-N(1)	2.126(3)	O(2)-Zn(1)-N(1)	87.96(11)
Zn(1)-O(1)	2.156(3)	N(1)-Zn(1)-O(1)	87.77(11)
O(2)-Zn(1)-N(1)#1	92.04(11)	N(1)-Zn(1)-N(1)#1	180.00(6)
O(1)#1-Zn(1)-O(1)	180.00(14)	O(2)-Zn(1)-O(1)#1	93.00(11)
N(1)-Zn(1)-O(1)#1	92.23(11)	O(2)-Zn(1)-O(2)#1	180.0
		2	
Co(1)-O(2)	2.091(2)	O(2)-Co(1)-N(1)	87.69(8)
Co(1)-N(1)	2.121(2)	O(2)-Co(1)-O(1)	87.49(7)
Co(1)-O(1)	2.159(2)	N(1)-Co(1)-O(1)	87.99(7)
O(2)#1-Co(1)-O(2)	180.00(10)	O(2)-Co(1)-N(1)#1	92.31(8)
N(1)#1-Co(1)-N(1)	180.00(14)	O(2)-Co(1)-O(1)#1	92.51(7)
O(1)#1-Co(1)-O(1)	180.00(12)	N(1)-Co(1)-O(1)#1	92.01(7)
		3	
Zn(1)-N(1)	2.020(2)	N(1)-Zn(1)-N(4)#2	103.96(11)
Zn(1)-N(4)#2	2.001(3)	Cl(1)-Zn(1)-N(4)#2	112.10(9)
Zn(1)-Cl(1)	2.208(1)	N(1)-Zn(1)-Cl(1)	112.52(8)
Zn(1)-Cl(2)	2.242(1)	Cl(2)-Zn(1)-N(4)#2	109.55(7)
Cl(1)-Zn(1)-Cl(2)	111.27(4)	N(1)-Zn(1)-Cl(2)	107.09(8)
		4	
Co(1)-N(1)	2.004(4)	N(1)-Co(1)-N(4)#3	104.00(14)
Co(1)-N(4)#3	2.013(3)	N(1)-Co(1)-Cl(1)	111.85(12)
Co(1)-Cl(1)	2.222(2)	Cl(1)-Co(1)-N(4)#3	110.54(11)
Co(1)-Cl(2)	2.246(1)	N(1)-Co(1)-Cl(2)	109.47(10)
Cl(1)-Co(1)-Cl(2)	112.27(6)	Cl(2)-Co(1)-N(4)#3	108.35(11)
		5	
Zn(1)-N(1)	1.983(1)	N(1)-Zn(1)-N(3)	107.82(5)
Zn(1)-N(3)	2.004(1)	N(1)-Zn(1)-N(5)	106.11(5)
Zn(1)-N(5)	2.004(1)	N(3)-Zn(1)-N(5)	116.96(5)
Zn(1)-N(7)	2.011(1)	N(1)-Zn(1)-N(7)	115.44(5)
N(5)-Zn(1)-N(7)	105.70(5)	N(3)-Zn(1)-N(7)	105.20(5)
		6	
Co(1)-O(3)	2.166(2)	O(3)-Co(1)-N(1)	87.28(5)
Co(1)-N(1)	2.247(2)	O(3)-Co(1)-N(1)#4	92.72(5)
N(1)#5-Co(1)-N(1)	90.51(9)	N(1)-Co(1)-N(1)#4	89.75(9)

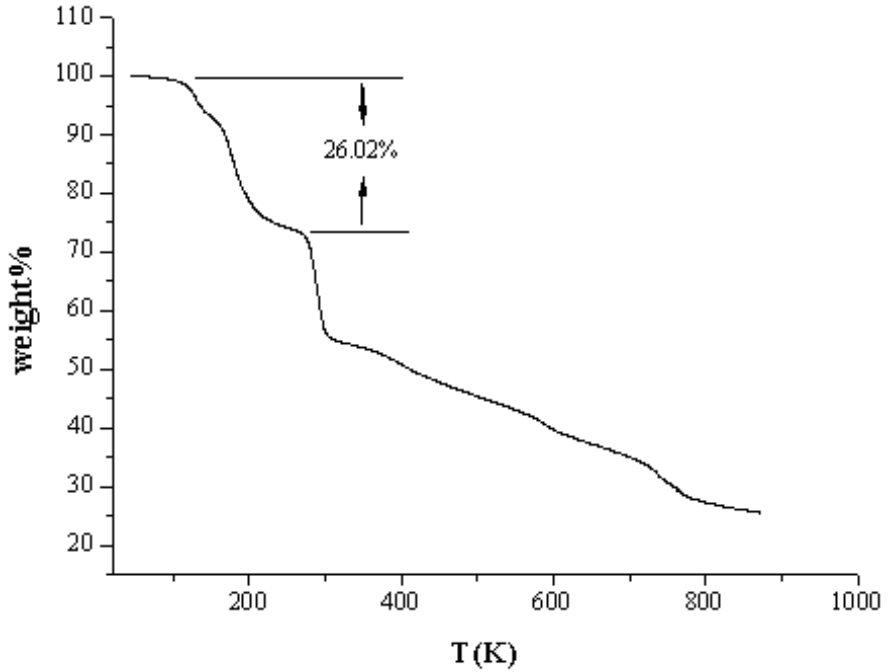
[a]Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z; #2 -x+3/2,y+1/2,-z+3/2; #3 -x+1/2,y-1/2,-z+3/2; #4 -x+5/4,y,-z+5/4; #5 x,-y+5/4,-z+5/4.

2. Fig. **S1**

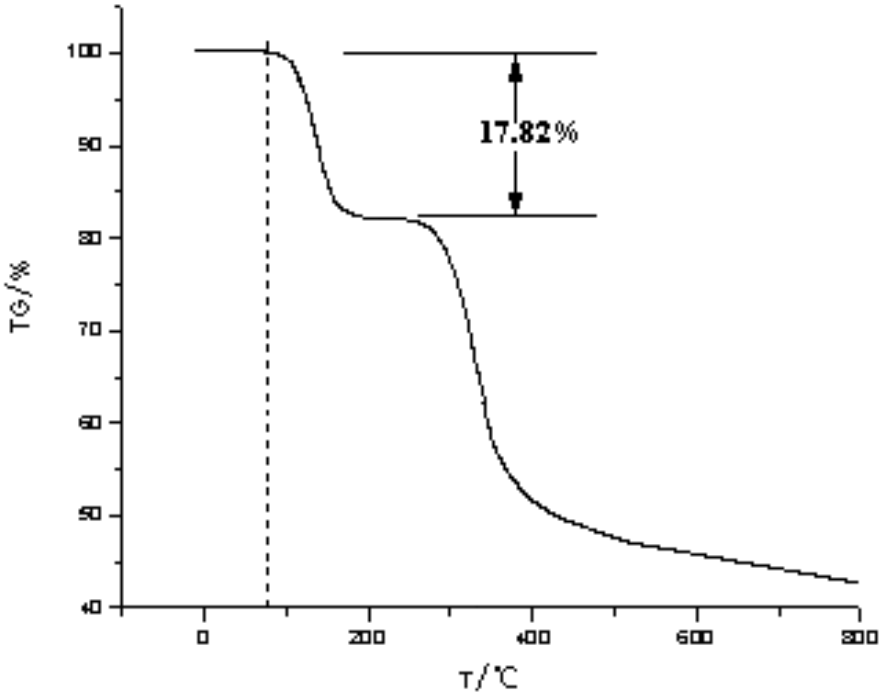


3. Fig. **S2**

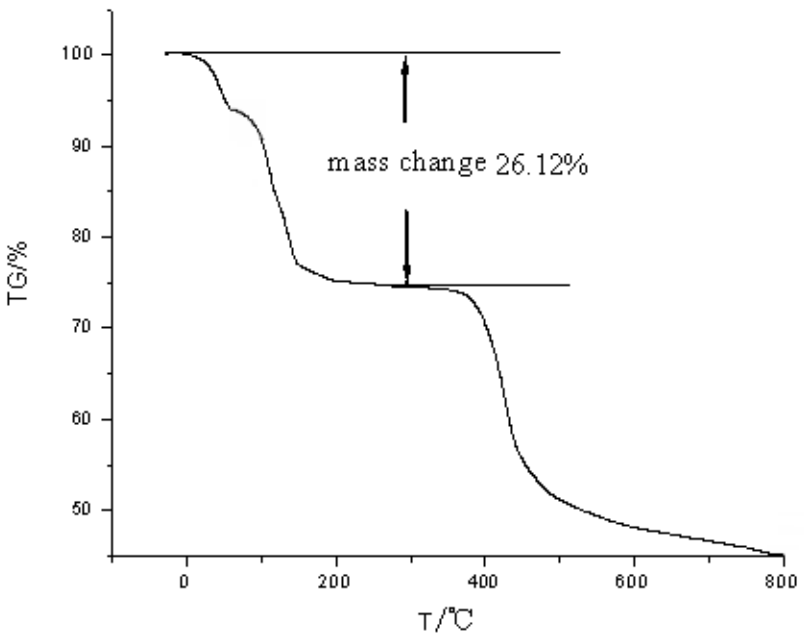
(**1**) for **2**



(**2**) for **3**



(3) for **5**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TG/%
T/℃
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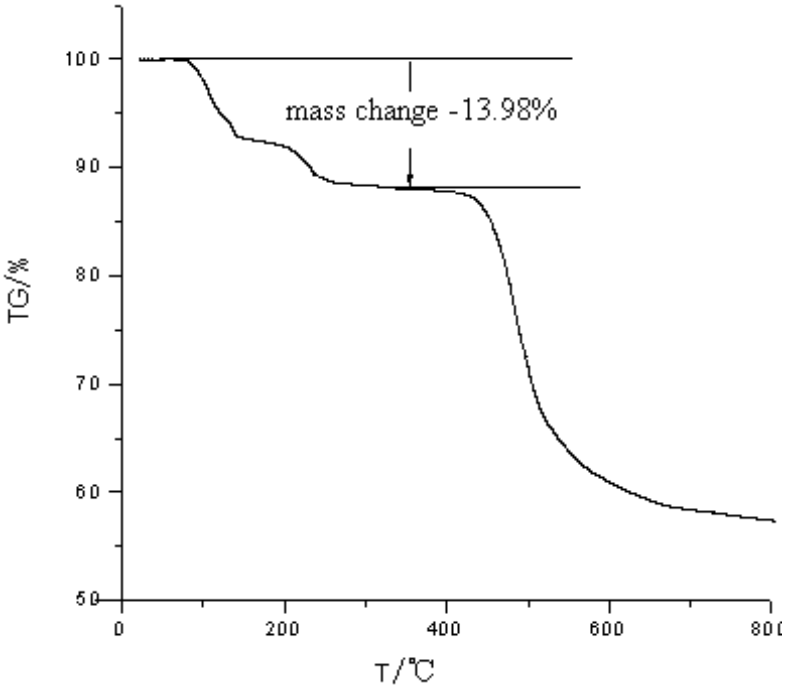
90
80
70
60
50
0
200
400
600
800

(4) for **6**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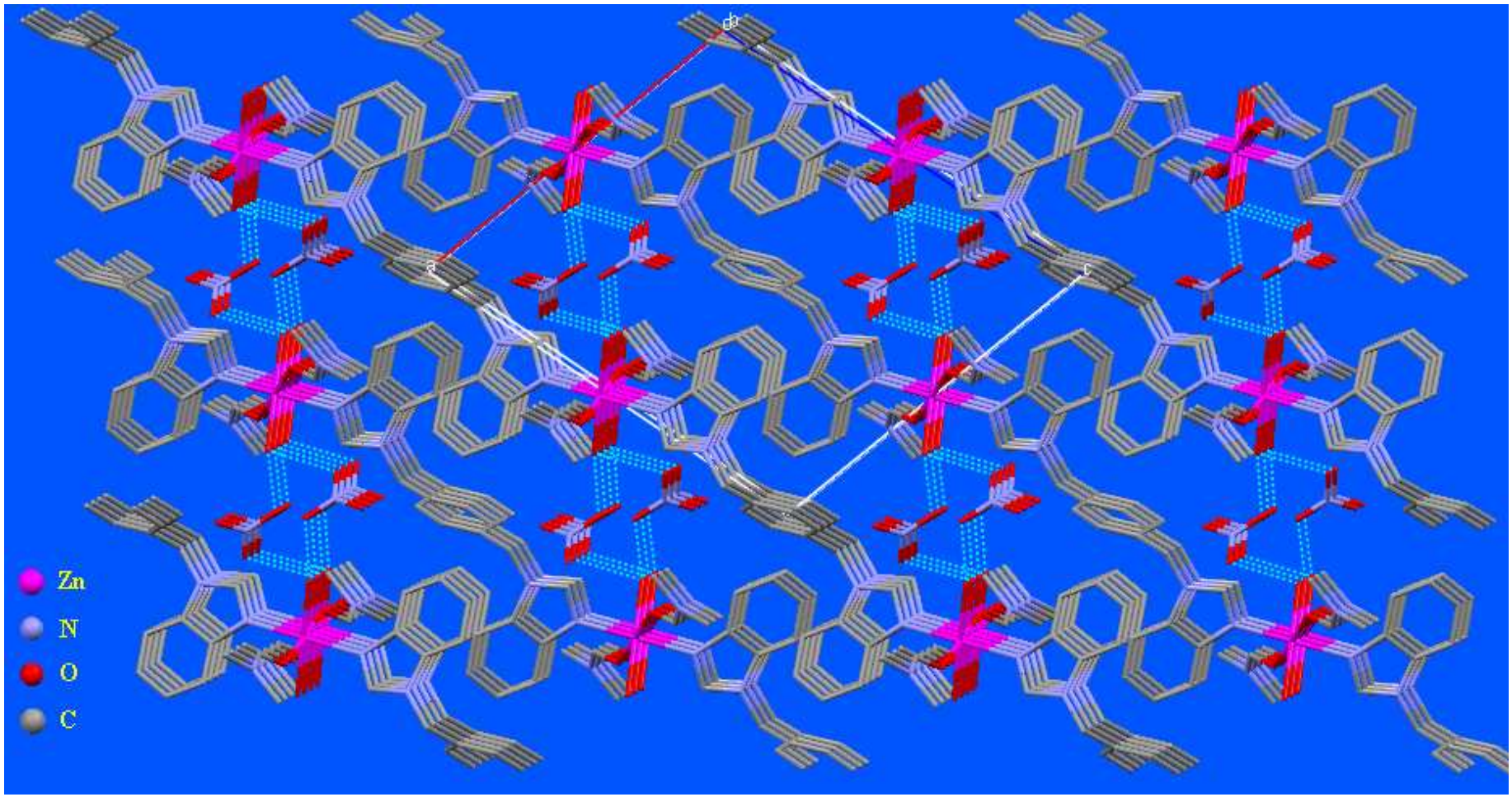
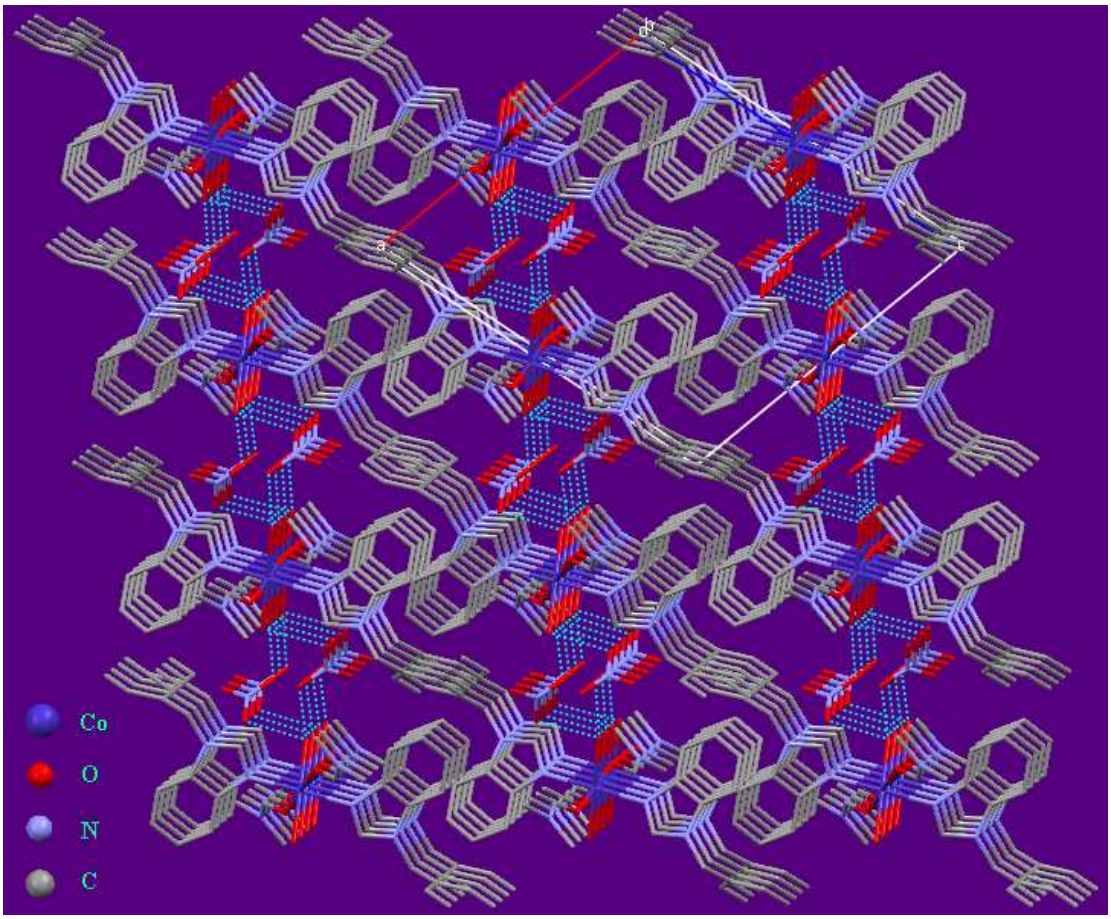
TG/%
T/℃
100
90
80
70
60
50
0
200
400
600

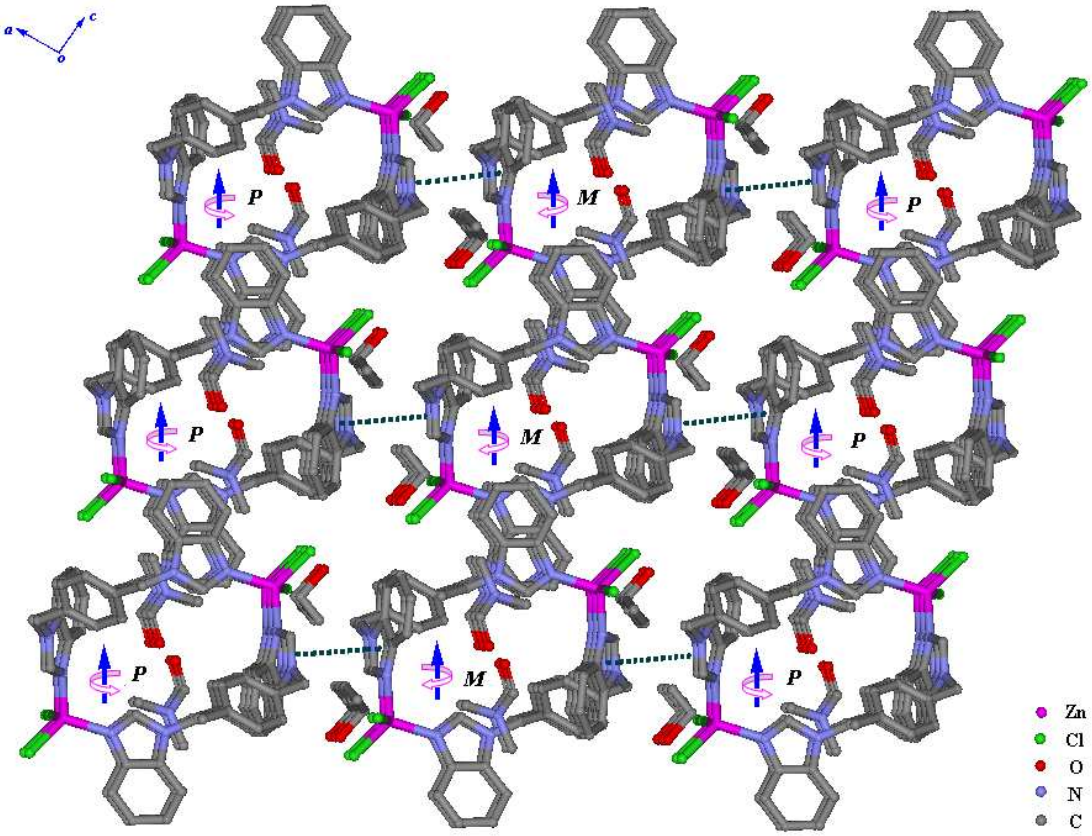
4. Fig. **S3**



5. Fig. S4

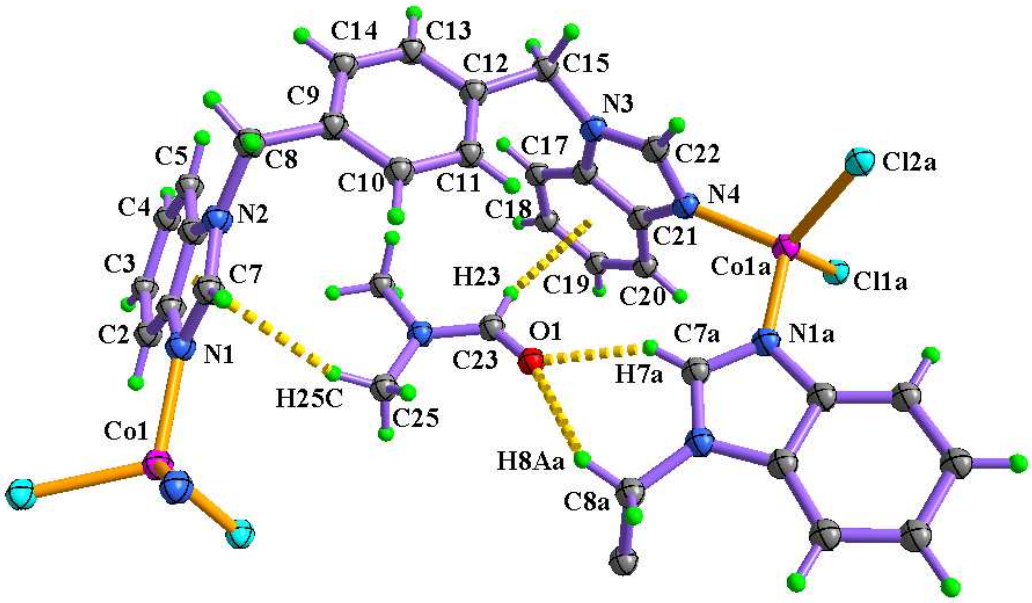


6. Fig. S5

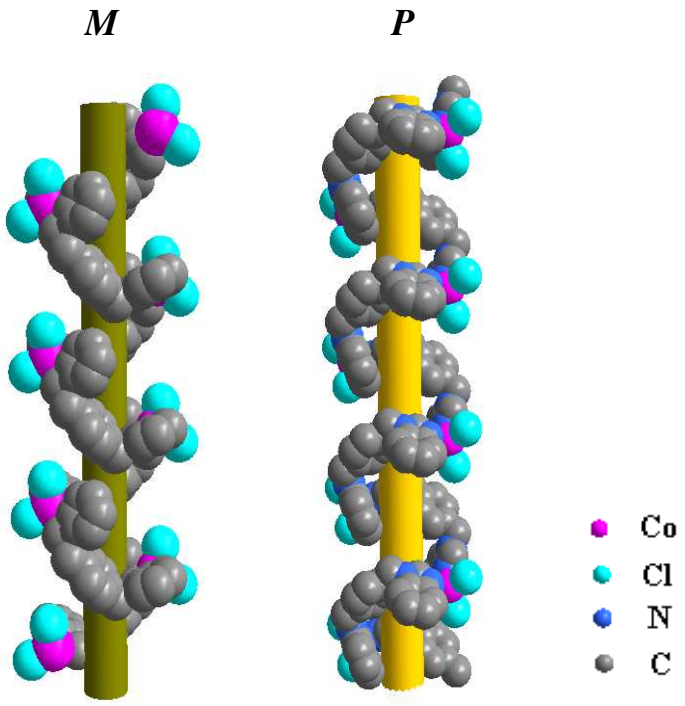


7. Fig. S6

(a)


C14
C13
C12
C15
C9
N3
C5
C8
C17
C22
Cl2a
C10
C11
N4
C4
N2
C18
C21
C3
C7
H23
C19
C20
Co1a
Cl1a
C2
N1
O1
C7a
N1a
C23
H7a
H25C
C25
Co1
H8Aa
C8a

(**b**)


M
P
Co
Cl
N
C

(**c**)