Supporting Information

Single-Crystal to Single-Crystal Transformation from a 1-D Chain-like Structure to a 2-D Coordination Polymer on Heating

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Content

Table **S1** Crystal data and structure refinement of two compounds **1**-**2**.

	1	**2**
Chemical formula	$C_9H_{16}ClErN_2O_{14}$	$C_9H_4ClErN_2O_8$
M	578.95	470.85
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a /Å	7.1312(12)	6.8722(9)
b /Å	9.5963(16)	11.948(4)
c /Å	12.431(2)	10.9592(15)
α /°	100.546(2)	101.529(2)
β /°	98.090(2)	106.681(2)
γ /°	95.025(2)	95.551(2)
V/Å^3	822.4(2)	549.87(13)
Z	2	2
T /*K*	298(2)	298(2)
F(000)	562	442
D_{calcd} / g cm^{-3}	2.338	2.844
μ /mm^{-1}	5.347	7.923
λ /Å	0.71073	0.71073
R_{int}	0.0178	0.0190
data/restraint/parm	2896 / 18 / 281	1958 / 0 / 190
GOF	1.043	1.021
R_1 [$I = 2\sigma(I)$][a]	0.0283	0.0241
wR_2 [$I = 2\sigma(I)$][b]	0.0756	0.0584
R_1 [all data][a]	0.0298	0.0259
wR_2 [all data][b]	0.0764	0.0594

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Selected atomic distances (Å) and bond angles (°) for compounds 1-2[a].

		1	
Er(1)-O(1)	2.379(4)	O(1)-Er(1)-O(10)	140.83(13)
Er(1)-O(10)	2.406(4)	O(1)-Er(1)-O(6)#1	81.63(12)
Er(1)-O(6)#1	2.441(4)	O(10)-Er(1)-O(6)#1	137.39(13)
Er(1)-O(9)	2.442(4)	O(1)-Er(1)-O(9)	76.21(13)
Er(1)-O(11)	2.459(4)	O(10)-Er(1)-O(9)	70.83(14)
Er(1)-O(4)#2	2.483(4)	O(6)#1-Er(1)-O(9)	143.78(13)
Er(1)-O(5)	2.508(4)	O(1)-Er(1)-O(11)	140.55(13)
Er(1)-O(3)#2	2.534(4)	O(10)-Er(1)-O(11)	69.63(14)
Er(1)-O(6)	2.613(4)	O(6)#1-Er(1)-O(11)	71.56(13)
O(11)-Er(1)-O(4)#2	76.30(13)	O(9)-Er(1)-O(11)	140.39(14)
O(1)-Er(1)-O(5)	79.48(13)	O(1)-Er(1)-O(4)#2	126.56(13)
O(10)-Er(1)-O(5)	77.04(14)	O(10)-Er(1)-O(4)#2	75.88(14)
O(6)#1-Er(1)-O(5)	119.00(12)	O(6)#1-Er(1)-O(4)#2	78.53(13)
O(9)-Er(1)-O(5)	84.77(13)	O(9)-Er(1)-O(4)#2	92.07(14)
O(11)-Er(1)-O(5)	88.65(14)	O(6)#1-Er(1)-O(3)#2	77.58(12)
O(4)#2-Er(1)-O(5)	152.23(13)	O(9)-Er(1)-O(3)#2	69.37(13)
O(1)-Er(1)-O(3)#2	75.43(13)	O(11)-Er(1)-O(3)#2	123.92(13)
O(10)-Er(1)-O(3)#2	110.75(14)	O(4)#2-Er(1)-O(3)#2	52.05(12)
O(3)#2-Er(1)-O(6)	132.12(12)	O(5)-Er(1)-O(3)#2	147.41(13)
O(5)-Er(1)-O(6)	54.86(11)	O(1)-Er(1)-O(6)	71.65(12)
O(4)#2-Er(1)-O(6)	136.12(12)	O(10)-Er(1)-O(6)	116.80(14)
O(11)-Er(1)-O(6)	70.79(13)	O(6)#1-Er(1)-O(6)	64.15(14)
O(9)-Er(1)-O(6)	131.69(13)		
		2	
Er(1)-O(2)#3	2.220(4)	O(2)#3-Er(1)-O(1)#4	81.19(14)
Er(1)-O(1)#4	2.281(4)	O(2)#3-Er(1)-O(5)#3	85.56(14)
Er(1)-O(5)#3	2.305(4)	O(1)#4-Er(1)-O(5)#3	142.77(14)
Er(1)-O(6)	2.315(4)	O(2)#3-Er(1)-O(6)	98.09(14)
Er(1)-O(8)#5	2.375(4)	O(1)#4-Er(1)-O(6)	75.05(14)
Er(1)-O(4)	2.404(4)	O(5)#3-Er(1)-O(6)	141.56(14)
Er(1)-O(3)#3	2.405(4)	O(2)#3-Er(1)-O(8)#5	89.18(14)
Er(1)-O(3)	2.445(4)	O(1)#4-Er(1)-O(8)#5	72.79(13)
Er(1)-Er(1)#3	3.8698(6)	O(5)#3-Er(1)-O(8)#5	72.38(13)
O(5)#3-Er(1)-O(4)	108.88(14)	O(6)-Er(1)-O(8)#5	145.47(13)
O(6)-Er(1)-O(4)	79.32(14)	O(2)#3-Er(1)-O(4)	160.07(14)
O(8)#5-Er(1)-O(4)	82.55(14)	O(1)#4-Er(1)-O(4)	79.05(14)
O(2)#3-Er(1)-O(3)#3	72.76(13)	O(1)#4-Er(1)-O(3)#3	133.48(13)

O(5)#3-Er(1)-O(3)#3	73.32(13)	O(6)-Er(1)-O(3)#3	71.42(13)
O(8)#5-Er(1)-O(3)#3	142.20(13)	O(4)-Er(1)-O(3)#3	123.81(13)
O(6)-Er(1)-O(3)	78.82(13)	O(2)#3-Er(1)-O(3)	145.90(13)
O(8)#5-Er(1)-O(3)	112.72(13)	O(1)#4-Er(1)-O(3)	129.09(13)
O(4)-Er(1)-O(3)	53.43(13)	O(5)#3-Er(1)-O(3)	77.32(13)
O(3)#3-Er(1)-O(3)	74.14(14)		

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

Table S**3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1**-**2**.

D-H···A	Distance (D-H)	Distance (H···A)	Distance(D···A)	Angle (D-H···A)
		1		
O(9)-H(9A)...O(12)#3	0.848(10)	2.04(3)	2.804(6)	150(5)
O(9)-H(9B)...O(3)	0.848(10)	2.021(17)	2.857(6)	168(6)
O(10)-H(10A)...O(2)#3	0.845(10)	1.82(2)	2.651(6)	167(7)
O(10)-H(10B)...O(8)#4	0.845(10)	1.937(14)	2.778(6)	173(7)
O(10)-H(10B)...Cl(1)#4	0.845(10)	2.98(4)	3.735(4)	150(6)
O(11)-H(11A)...O(1)#1	0.847(10)	1.876(14)	2.718(5)	173(6)
O(11)-H(11B)...O(5)#4	0.846(10)	2.21(2)	3.037(6)	164(7)
O(11)-H(11B)...O(8)#4	0.846(10)	2.65(5)	3.168(6)	121(5)
O(11)-H(11B)...Cl(1)#4	0.846(10)	2.91(3)	3.677(4)	151(5)
O(12)-H(12A)...O(4)	0.851(10)	2.029(19)	2.869(6)	169(8)
O(12)-H(12B)...O(8)#5	0.848(10)	2.40(5)	3.041(6)	132(5)
O(13)-H(13A)...O(7)#6	0.845(10)	2.37(3)	3.171(7)	159(7)
O(13)-H(13B)...O(8)#7	0.844(11)	2.06(2)	2.893(7)	168(9)
O(13)-H(13B)...Cl(1)#7	0.844(11)	2.99(6)	3.688(6)	142(7)
O(14)-H(14A)...O(7)	0.850(10)	1.93(2)	2.773(7)	168(8)
O(14)-H(14B)...O(13)#8	0.849(10)	2.04(3)	2.862(8)	164(9)
N(1)-H(1)...O(14)	0.86	1.98	2.761(7)	150.3
N(1)-H(1)...O(12)#6	0.86	2.46	2.990(7)	120.9
π...π[a]			3.569	
π...π[b]			3.835	
		2		
N(1)-H(1)...O(8)#9	0.86	2.11	2.945(6)	163.0
N(1)-H(1)...O(1)#10	0.86	2.46	2.886(6)	111.3
C(7)-H(7)...O(8)#9	0.930	2.543(5)	3.469(5)	173.6
π...π[a]			3.514 and 3.751	

*Symmetry transformation used to generate equivalent atoms: #1 -x+1,-y,-z; #2 -x+1,-y+1,-z; #3 x+1,y,z; #4 -x+2,-y,-z; #5 x-1,y+1,z; #6 -x+1,-y+1,-z+1; #7 -x+2,-y+1,-z+1; #8 x,y-1,z; #9 -x,-y+1,-z+1; #10 -x+1,-y+2,-z+1. π...π[a] denotes the centroid-to-centroid distance (Å) between the adjacent benzene ring and imidazole ring, and and π...π[b] denotes the centroid-to-centroid distance (Å) between two imidazole rings from two adjacent layers.

Figure S1

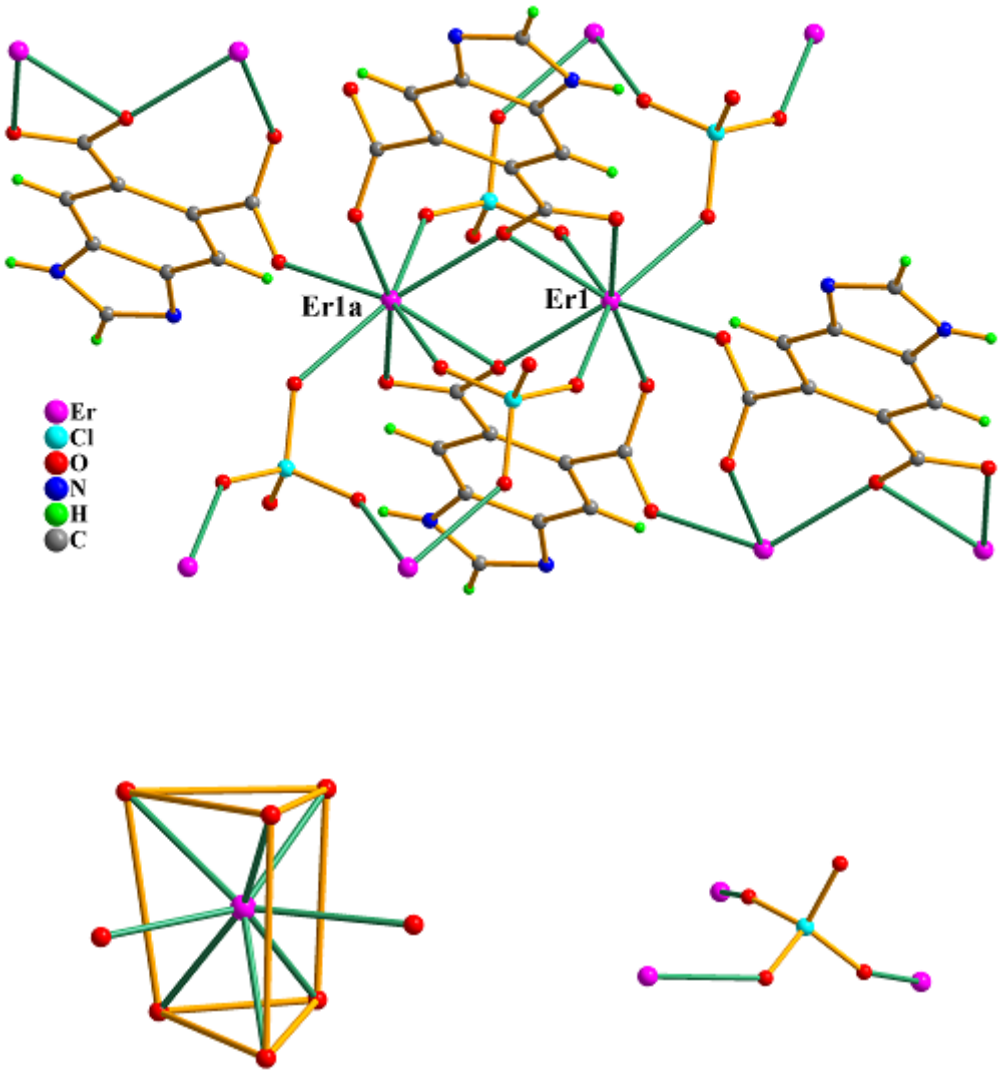


Figure S2

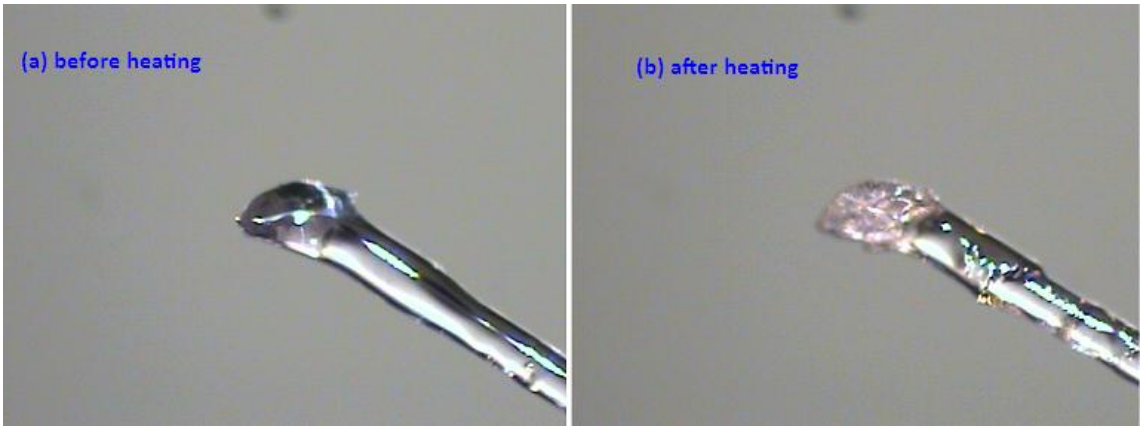
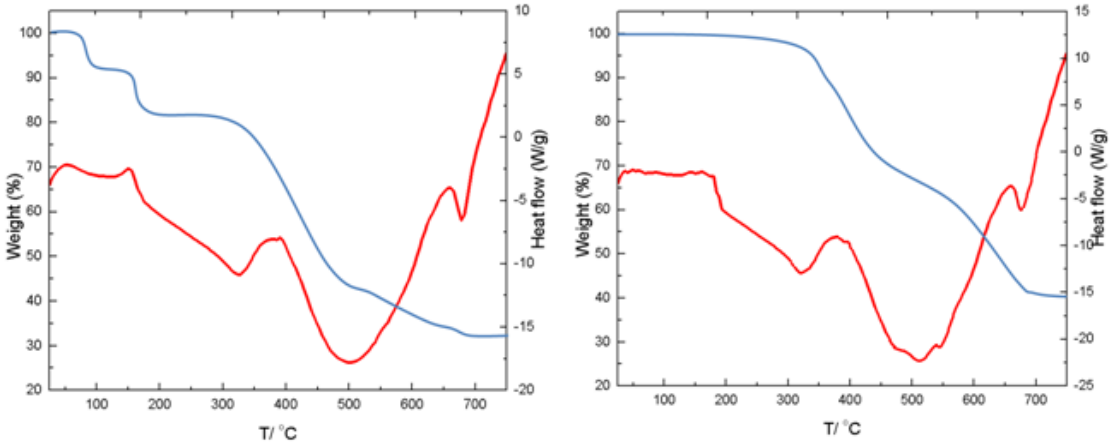
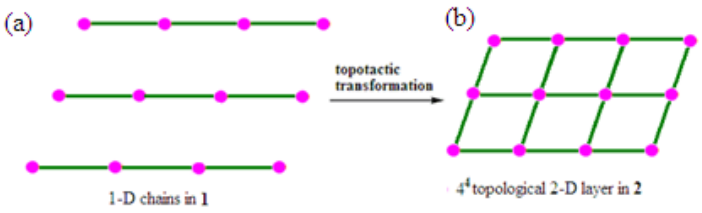


Figure S3



(a) **(b)**

Figure S4.



From above figure S4 (a, b), the topotactic behavior was happened in this system, each dinuclear Er(III) can be viewed as node in both **1** and **2**, and node-and-linker 1-D chain was formed for **1**, while (4,4) topology was simplified for **2**. With increase of the temperature, Er^{3+} ions as well as conformational changes of ligand $bidc^{2-}$ underwent upward and downward/left and right movement, and the weak interaction between 1-D chains in complex **1** was changed into coordination bonding interaction, and then adjacent chains are connected with each other to form the 2-D framework, which finally resulted in the structural transformation to coordination polymer **2**. Although both crystals **1** and **2** were crystallized in the same triclinic space group *P*-1, however, the cell volume of **2** decreased 273 $Å^3$, stemming from the departure of three coordinated and three lattice water molecules in **1**. Therefore, the single crystal transformation between **1** and **2** is maybe ascribes to hydrogen bond transform to coordination bond after increasing temperature.

checkCIF/PLATON (full publication check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: CCDC 897010(1)

Bond precision: C-C = 0.0076 A Wavelength=0.71073

Cell: a=7.1312(12) b=9.5963(16) c=12.431(2)
alpha=100.546(2) beta=98.090(2) gamma=95.025(2)

Temperature: 298 K

	Calculated	Reported
Volume	822.4(2)	822.4(2)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C9 H10 Cl Er N2 O11, 3(H2 O)	?
Sum formula	C9 H16 Cl Er N2 O14	C9 H16 Cl Er N2 O14
Mr	578.95	578.95
Dx,g cm-3	2.338	2.338
Z	2	2
Mu (mm-1)	5.347	5.347
F000	562.0	562.0
F000'	562.14	
h,k,lmax	8,11,14	8,11,14
Nref	2961	2896
Tmin,Tmax	0.304,0.526	0.373,0.566
Tmin'	0.281	

Correction method= MULTI-SCAN

Data completeness= 0.978 Theta(max)= 25.200

R(reflections)= 0.0283(2758) wR2(reflections)= 0.0764(2896)

S = 1.043 Npar= 281

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.978
PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?
PLAT213_ALERT_2_C Atom C4 has ADP max/min Ratio ..... 3.2 prola
PLAT417_ALERT_2_C Short Inter D-H..H-D H13B .. H14B .. 2.11 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10B .. CL1 .. 2.98 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H11B .. O8 .. 2.65 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H11B .. CL1 .. 2.91 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H13B .. CL1 .. 2.99 Ang.
PLAT732_ALERT_1_C Angle Calc 114(7), Rep 113(3) ..... 2.33 su-Ra
H14B -O14 -H14A 1.555 1.555 1.555 # 74
PLAT732_ALERT_1_C Angle Calc 114(7), Rep 113(3) ..... 2.33 su-Ra
H14A -O14 -H14B 1.555 1.555 1.555 # 76

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 7.48
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.00200 Deg.

checkCIF/PLATON (full publication check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: CCDC 897011 (2)

Bond precision: C-C = 0.0076 A Wavelength=0.71073

Cell: a=6.8722(9) b=7.8857(11) c=10.9592(15)
alpha=101.529(2) beta=106.681(2) gamma=95.551(2)

Temperature: 298 K

	Calculated	Reported
Volume	549.87(13)	549.87(13)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C9 H4 Cl Er N2 O8	?
Sum formula	C9 H4 Cl Er N2 O8	C9 H4 Cl Er N2 O8
Mr	470.85	470.85
Dx,g cm-3	2.844	2.844
Z	2	2
Mu (mm-1)	7.923	7.923
F000	442.0	442.0
F000'	442.04	
h,k,lmax	8,9,13	8,9,13
Nref	1994	1958
Tmin,Tmax	0.148,0.281	0.233,0.364
Tmin'	0.117	

Correction method= MULTI-SCAN

Data completeness= 0.982 Theta(max)= 25.250

R(reflections)= 0.0241(1833) wR2(reflections)= 0.0594(1958)

S = 1.021 Npar= 190

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF: ER1 -- ER1 .. 3.87 Ang.

Alert level G

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.00200 Deg.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.21 Ratio

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected