Ionothermal synthesis, crystal structure, topology and catalytic property heterometallic coordination polymers constructed from *N*-(phosphonomethyl)iminodiacetic acid

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Supporting Information

Contents

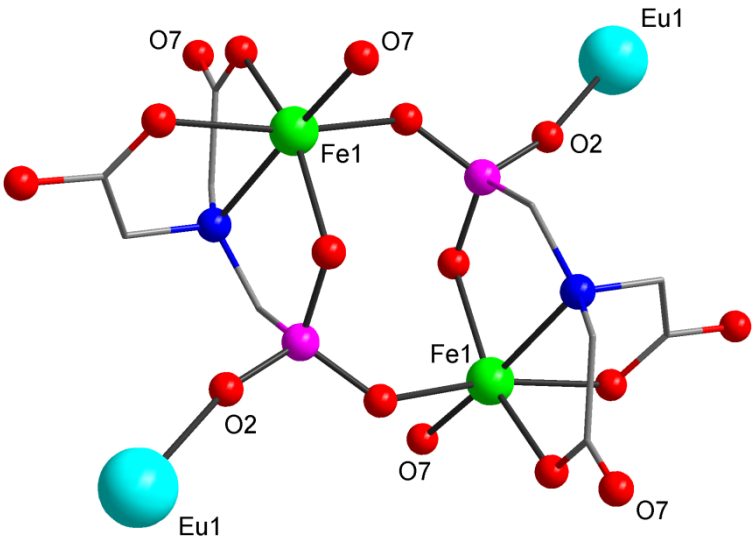

Fig. S1 The connection structure between Eu atom and $[Fe_2(Hpmida)_2]^{2-}$ in compound **1**.

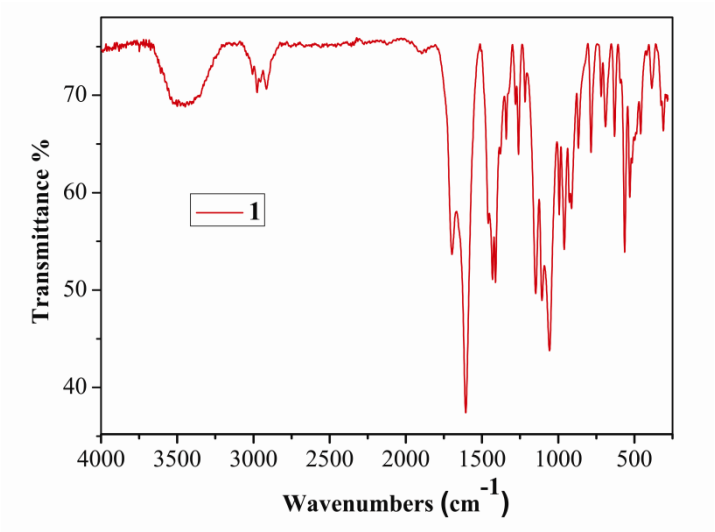

Fig. S2 IR of **1**.

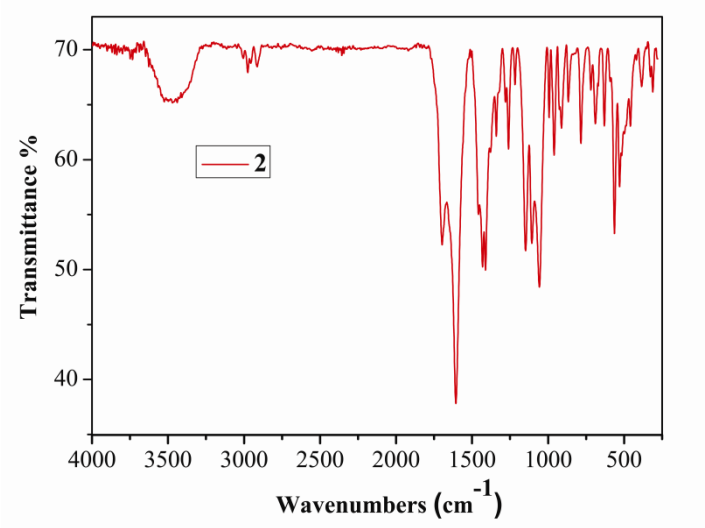

Fig. S3 IR of **2.**

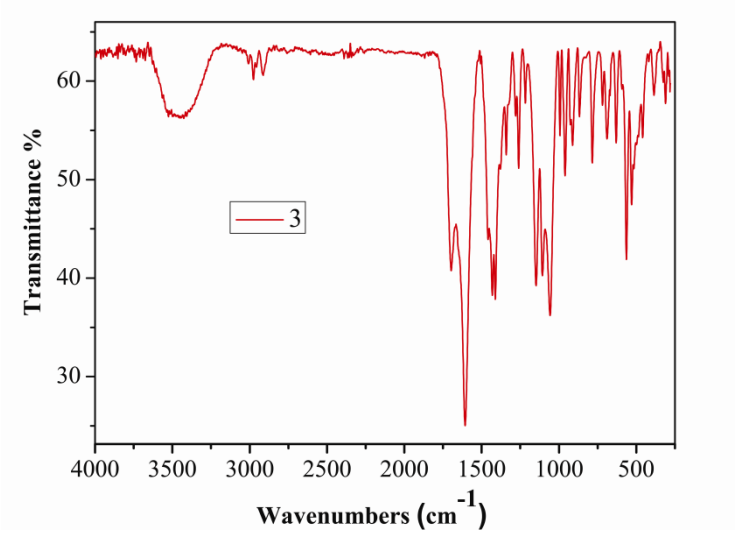

Fig. S4 IR of **3**.

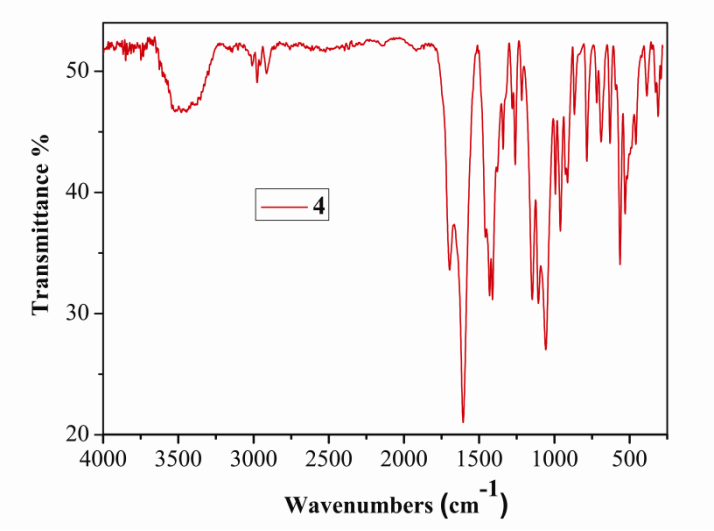

Fig. S5 IR of **4**.

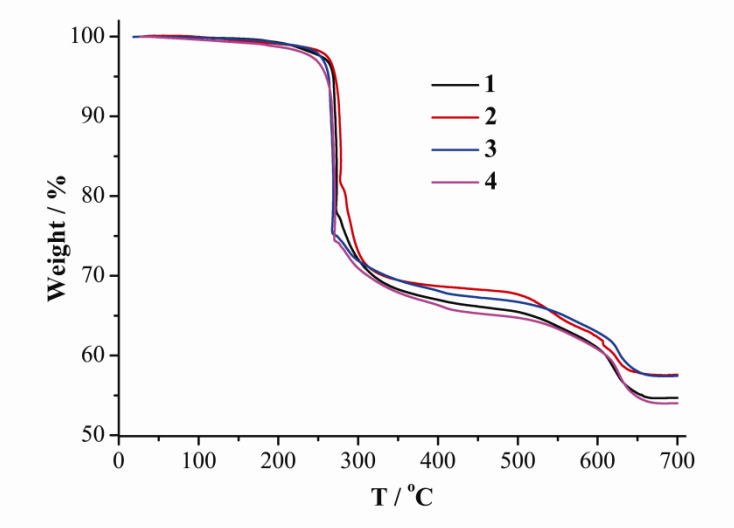

Fig. S6 TG curves of complexes **1–4** .

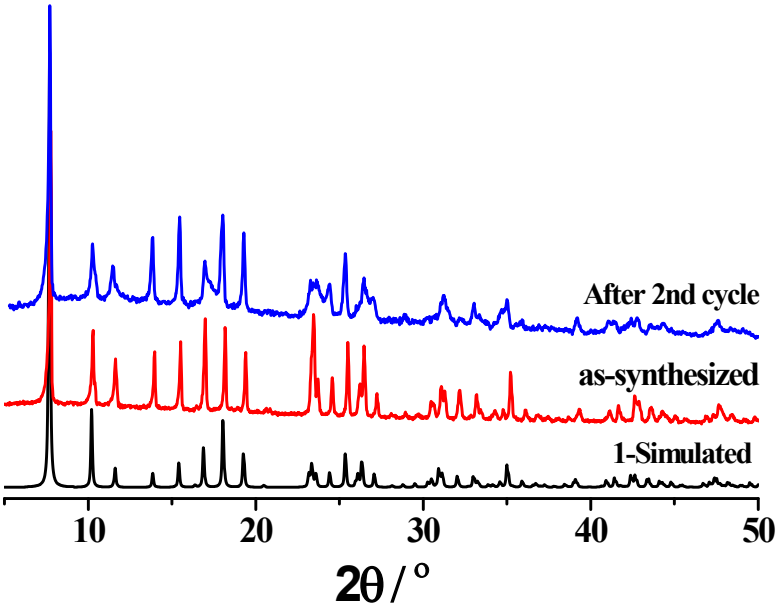

Fig. S7 The PXRD patterns of **1** in the different stages of after the 2nd cycle, as-synthesized and the simulated one from the single crystal structure.

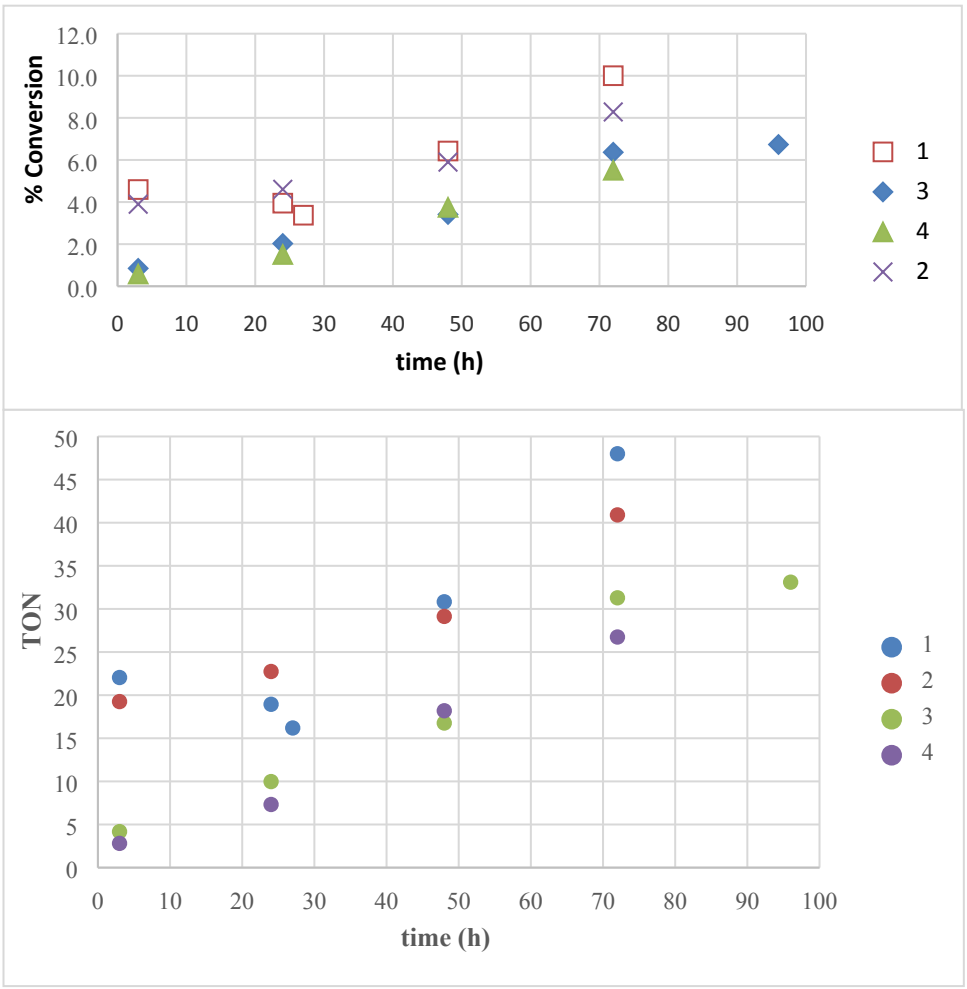

Fig. S8 Benzaldehyde conversion *vs* time and TON *vs* time for the Knoevenagel condensation with malononitrile at 60 °C using the compounds **1**–**4** in 4.0 mL of toluene performed at the same time using a Radleys carousel.

Table S1 Selected bond lengths (Å) for **1**–**4**.

	1(Eu)	**2(Dy)**	**3(Ho)**	**4(Y)**
Eu(1)-O(2A)	2.292(4)	2.254(5)	2.250(5)	2.244(4)
Eu(1)-O(2B)	2.292(4)	2.254(5)	2.250(5)	2.244(4)
Eu(1)-O(2C)	2.292(4)	2.254(5)	2.250(5)	2.244(4)
Eu(1)-O(2D)	2.292(4)	2.254(5)	2.250(4)	2.244(4)
Eu(1)-O(2E)	2.292(4)	2.254(5)	2.250(4)	2.244(4)
Eu(1)-O(2)	2.292(4)	2.254(5)	2.250(5)	2.244(4)
Fe(1)-O(1)	2.127(4)	2.120(5)	2.120(5)	2.120(4)
Fe(1)-O(6)	2.121(5)	2.123(6)	2.121(5)	2.114(4)
Fe(1)-O(7F)	2.102(5)	2.103(6)	2.101(5)	2.102(4)
Fe(1)-O(3G)	2.141(5)	2.154(5)	2.155(5)	2.143(4)
Fe(1)-O(4)	2.218(5)	2.205(6)	2.209(6)	2.206(4)
Fe(1)-N(1)	2.250(5)	2.256(6)	2.258(6)	2.251(5)
Fe(2)-O(3)	2.283(5)	2.257(6)	2.275(5)	2.267(4)
Fe(2)-O(3C)	2.283(5)	2.257(6)	2.275(5)	2.267(4)
Fe(2)-O(3D)	2.283(5)	2.257(6)	2.275(5)	2.267(4)
Fe(2)-O(6A)	2.479(5)	2.432(6)	2.406(3)	2.447(2)
Fe(2)-O(6B)	2.479(5)	2.432(6)	2.406(3)	2.447(2)
Fe(2)-O(6G)	2.479(5)	2.432(6)	2.406(3)	2.447(2)
P(1)-O(1)	1.540(4)	1.546(5)	1.545(5)	1.545(4)
P(1)-O(2)	1.505(4)	1.503(5)	1.502(5)	1.510(4)
P(1)-O(3)	1.517(5)	1.512(5)	1.517(5)	1.513(4)
P(1)-C(1)	1.817(6)	1.823(7)	1.817(7)	1.816(6)

Symmetry codes: A: x-y+1/3, x-1/3, -z+5/3; B: y+1/3, -x+y+2/3, -z+5/3; C: -x+y+1, -x+1, z; D: -y+1, x-y, z; E: -x+4/3, -y+2/3, -z+5/3; F: -y+2,x-y+1,z; G: -x+5/3,-y+4/3,-z+4/3.

Table S2 Selected bond angles [°] for **1**–**4**.

	1(Eu)	**2(Dy)**	**3(Ho)**	**4(Y)**
O(2A)-Eu(1)-O(2B)	88.57(16)	88.78(19)	88.91(19)	88.68(15)
O(2A)-Eu(1)-O(2C)	180.00(18)	180.0(2)	180.000(1)	180.000(1)
O(2B)-Eu(1)-O(2C)	91.43(16)	91.22(19)	91.09(19)	91.32(15)
O(2A)-Eu(1)-O(2D)	91.43(17)	91.22(19)	91.09(19)	91.32(15)
O(2B)-Eu(1)-O(2D)	179.998(1)	179.998(1)	180.0(2)	180.00(17)
O(2C)-Eu(1)-O(2D)	88.57(16)	88.78(19)	88.91(19)	88.68(15)
O(2A)-Eu(1)-O(2E)	88.57(17)	88.78(19)	88.91(19)	88.68(15)
O(2B)-Eu(1)-O(2E)	88.57(16)	88.78(19)	88.91(19)	88.68(15)
O(2C)-Eu(1)-O(2E)	91.43(16)	91.22(19)	91.09(19)	91.32(15)
O(2D)-Eu(1)-O(2E)	91.43(17)	91.22(19)	91.09(19)	91.32(15)
O(2A)-Eu(1)-O(2)	91.43(17)	91.22(19)	91.09(19)	91.32(15)
O(2B)-Eu(1)-O(2)	91.43(17)	91.22(19)	91.09(19)	91.32(15)
O(2C)-Eu(1)-O(2)	88.57(17)	88.78(19)	88.91(19)	88.68(15)
O(2D)-Eu(1)-O(2)	88.57(16)	88.78(19)	88.91(19)	88.68(15)
O(2E)-Eu(1)-O(2)	179.998(1)	179.998(1)	180.0(2)	180.00(17)
O(7F)-Fe(1)-O(6)	114.28(19)	114.9(2)	114.9(2)	115.00(16)
O(7F)-Fe(1)-O(1)	87.08(17)	86.2(2)	86.3(2)	86.14(15)
O(6)-Fe(1)-O(1)	158.64(18)	158.9(2)	158.8(2)	158.86(15)
O(7)F-Fe(1)-O(3G)	89.79(19)	89.8(2)	89.6(2)	89.65(16)
O(6)-Fe(1)-O(3)G	81.37(18)	80.6(2)	80.6(2)	80.79(16)
O(1)-Fe(1)-O(3G)	99.29(17)	99.9(2)	100.00(19)	100.03(15)
O(7F)-Fe(1)-O(4)	93.73(19)	93.5(2)	93.9(2)	94.10(16)
O(6)-Fe(1)-O(4)	86.00(19)	86.1(2)	86.1(2)	85.92(17)
O(1)-Fe(1)-O(4)	93.15(18)	93.5(2)	93.2(2)	93.13(15)
O(3G)-Fe(1)-O(4)	167.24(19)	166.4(2)	166.5(2)	166.54(16)
O(7)F-Fe(1)-N(1)	165.43(19)	165.0(2)	165.0(2)	165.03(17)
O(6)-Fe(1)-N(1)	77.15(18)	77.2(2)	77.3(2)	77.27(16)
O(1)-Fe(1)-N(1)	81.81(17)	82.1(2)	81.8(2)	81.90(15)
O(3G)-Fe(1)-N(1)	101.24(18)	101.5(2)	101.3(2)	101.24(17)
O(4)-Fe(1)-N(1)	77.58(18)	77.9(2)	77.9(2)	77.68(16)
O(3)C-Fe(2)-O(3)	112.35(13)	110.64(16)	109.56(15)	111.20(12)
O(3)C-Fe(2)-O(3D)	112.35(13)	110.64(16)	109.56(15)	111.20(12)
O(3)-Fe(2)-O(3D)	112.35(12)	110.64(15)	109.56(15	111.20(12)

Symmerty codes: A: x-y+1/3, x-1/3, -z+5/3; B: y+1/3, -x+y+2/3, -z+5/3; C: -x+y+1, -x+1, z; D: -y+1, x-y, z; E: -x+4/3, -y+2/3, -z+5/3; F: -y+2,x-y+1,z; G: -x+5/3,-y+4/3,-z+4/3.