Supporting Information

Conversions between dimeric and polymeric ketopiperazinediacetato complexes constructed by water-layers

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Table S1 ^{13}C NMR spectral data (in ppm) of ketopiperazinediacetic acid and its zinc complexes

Table S2 Selected bond distance (Å) and angles (^{o}) for $[M_2(kpda)_2(H_2O)_4]_n \cdot 6nH_2O$ [M = Co **1**, Ni **2**, Zn **3**] and $[M_2(kpda)_2(H_2O)_6] \cdot H_2O$ [M = Co **4**, Ni **5**, Zn **6**]

Table S3. Selected bond distances and angles within the water layer in **1**.

Table S4. Selected bond distances and angles in **4**.

Figure S1

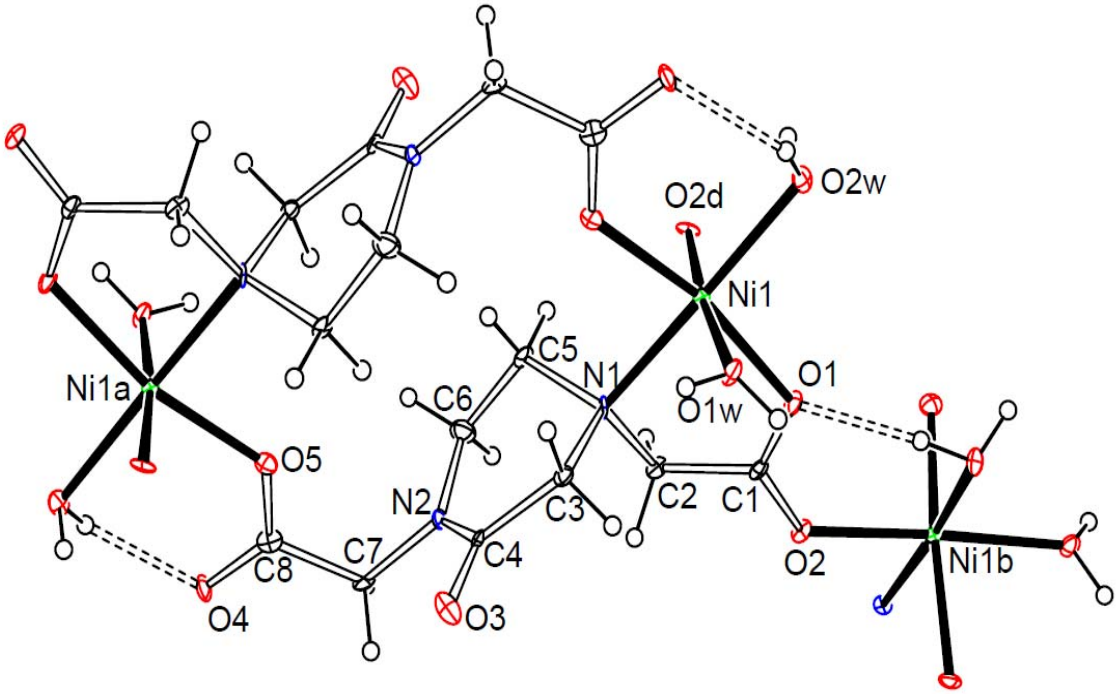

Figure S2

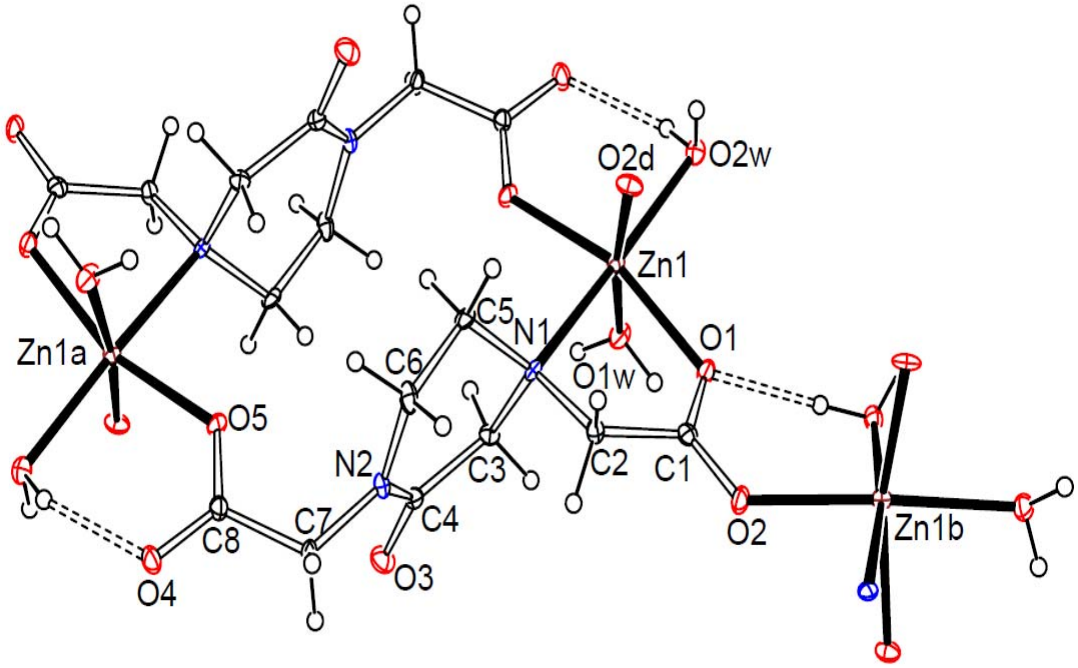

Figure S3

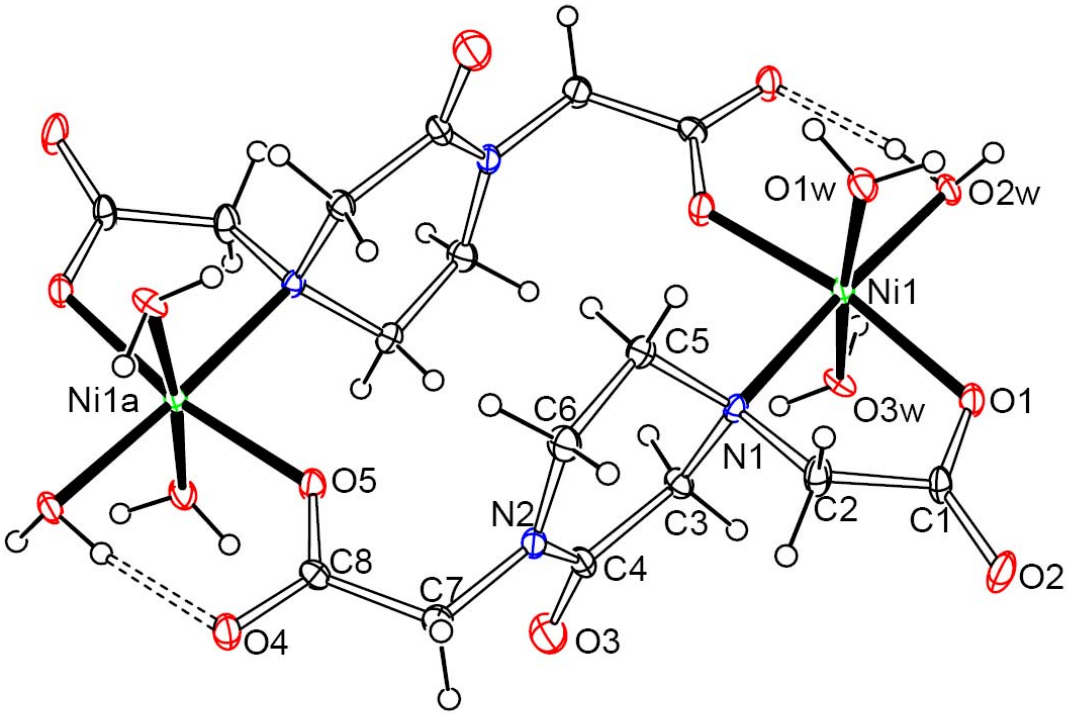

Figure S4

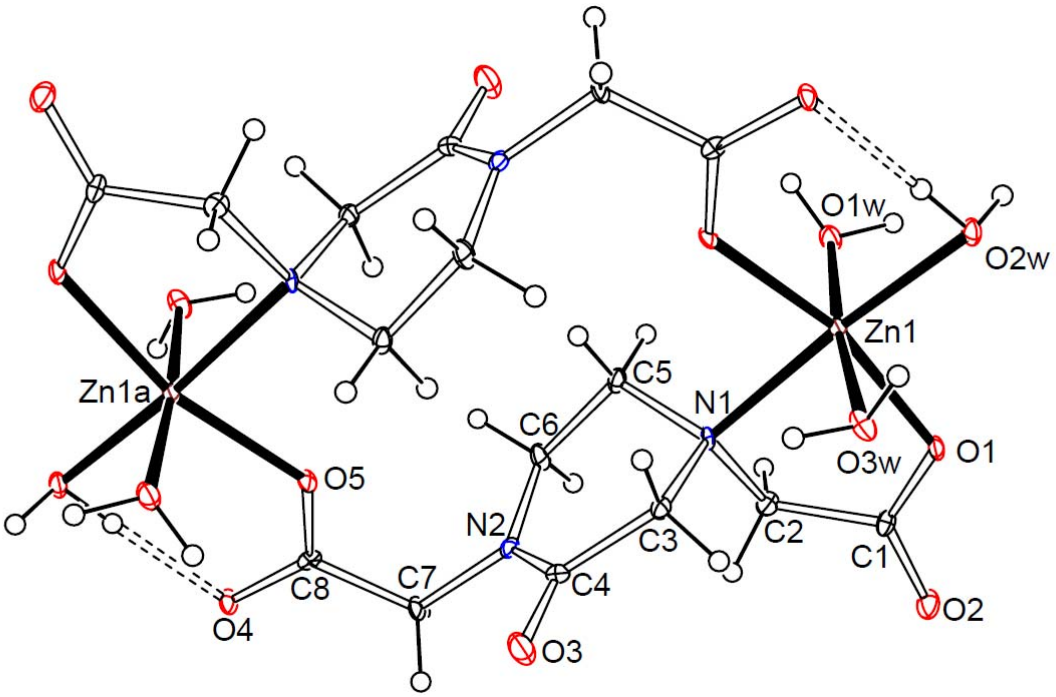

Figure S5

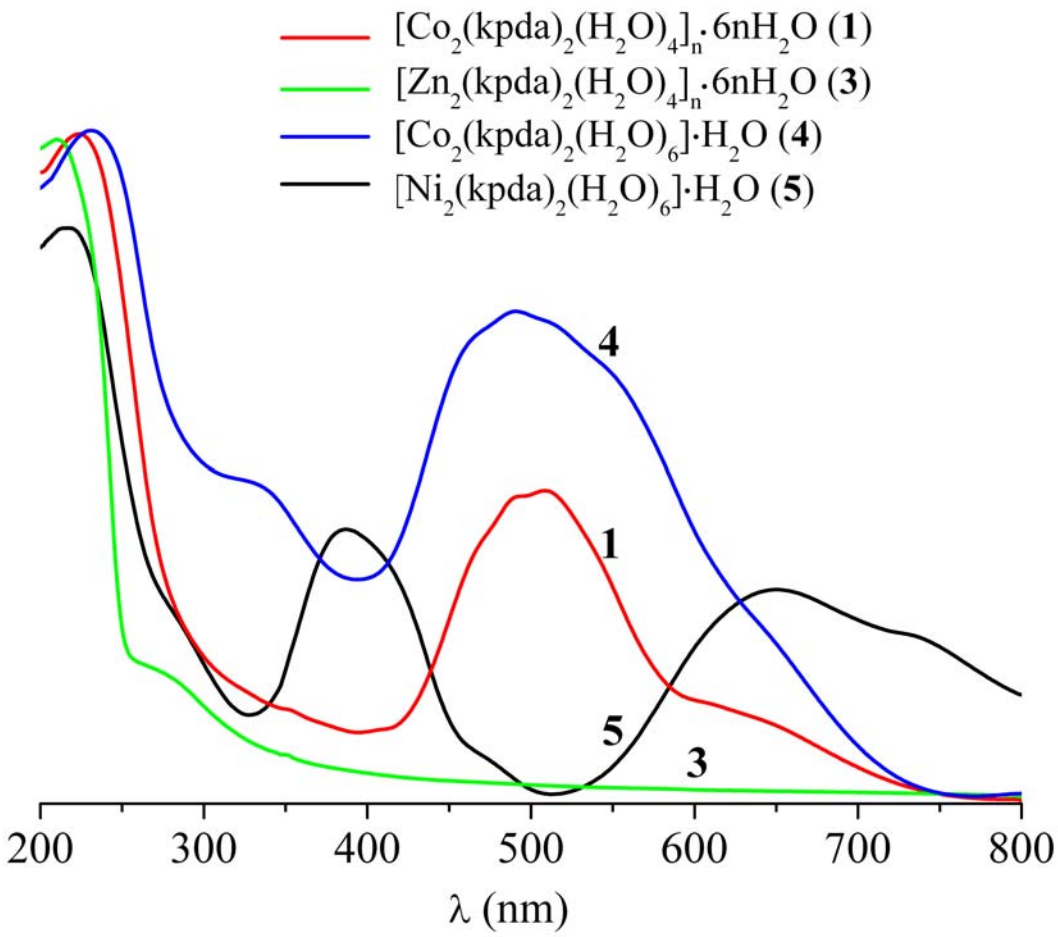

Figure S6

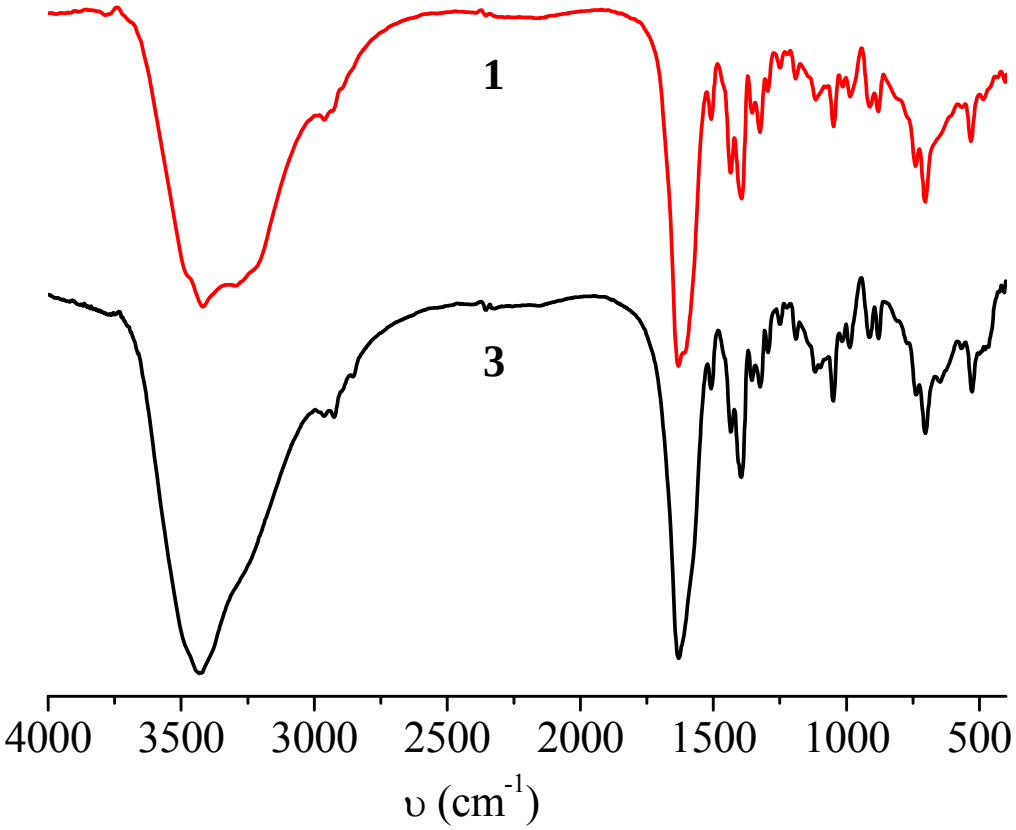

Figure S7

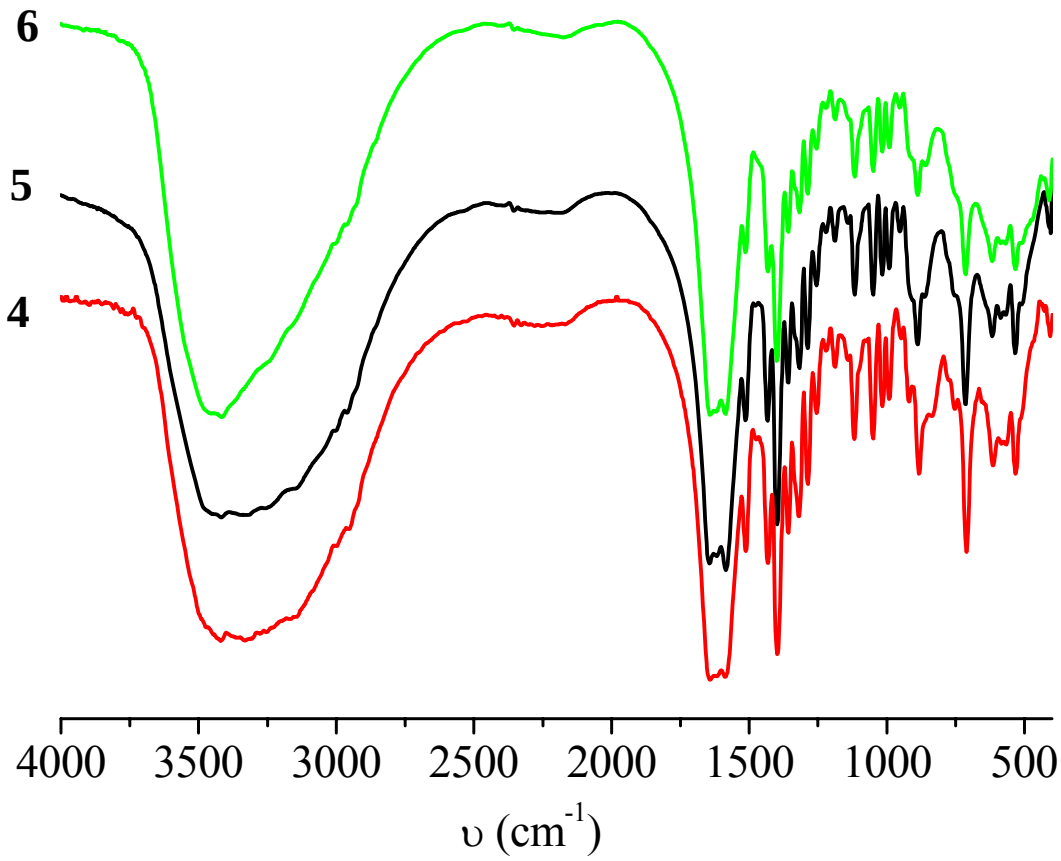

Figure S8

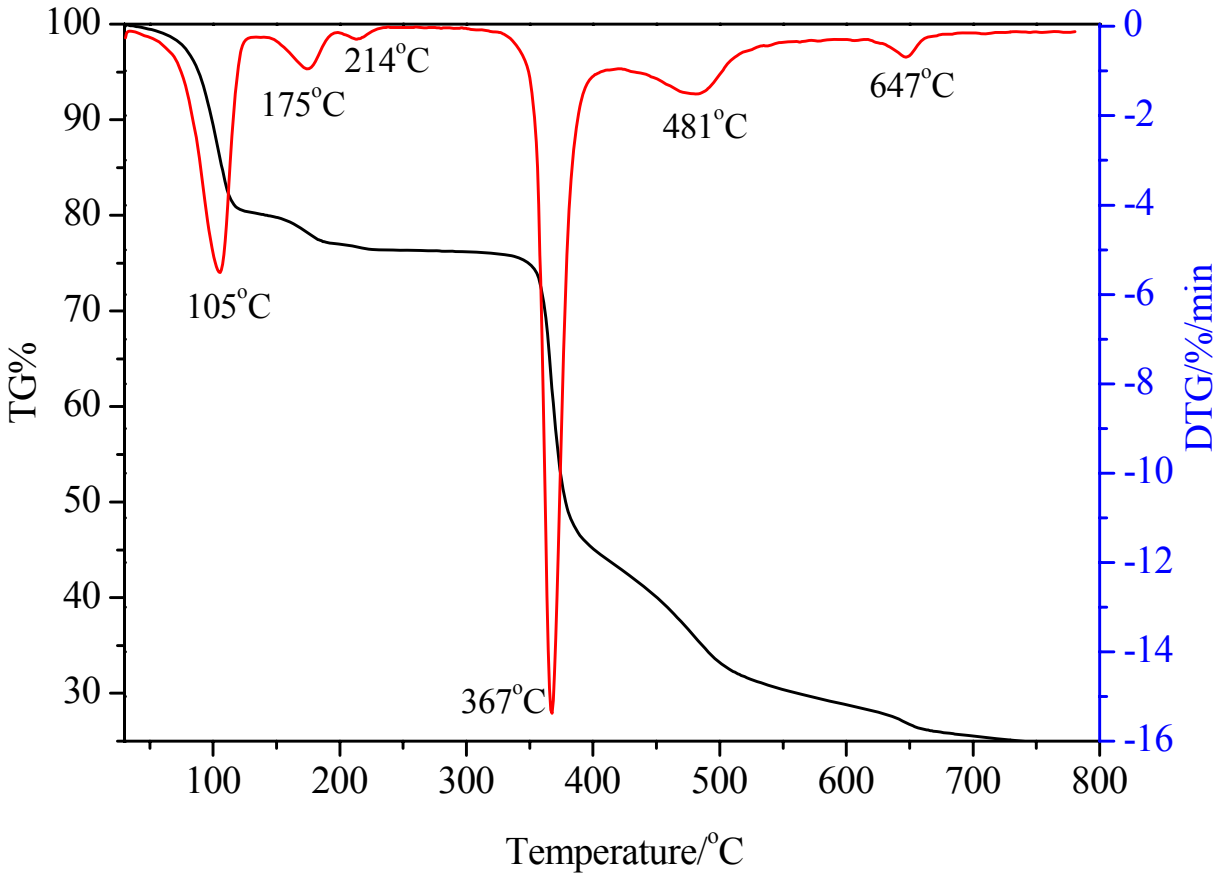

Figure S9

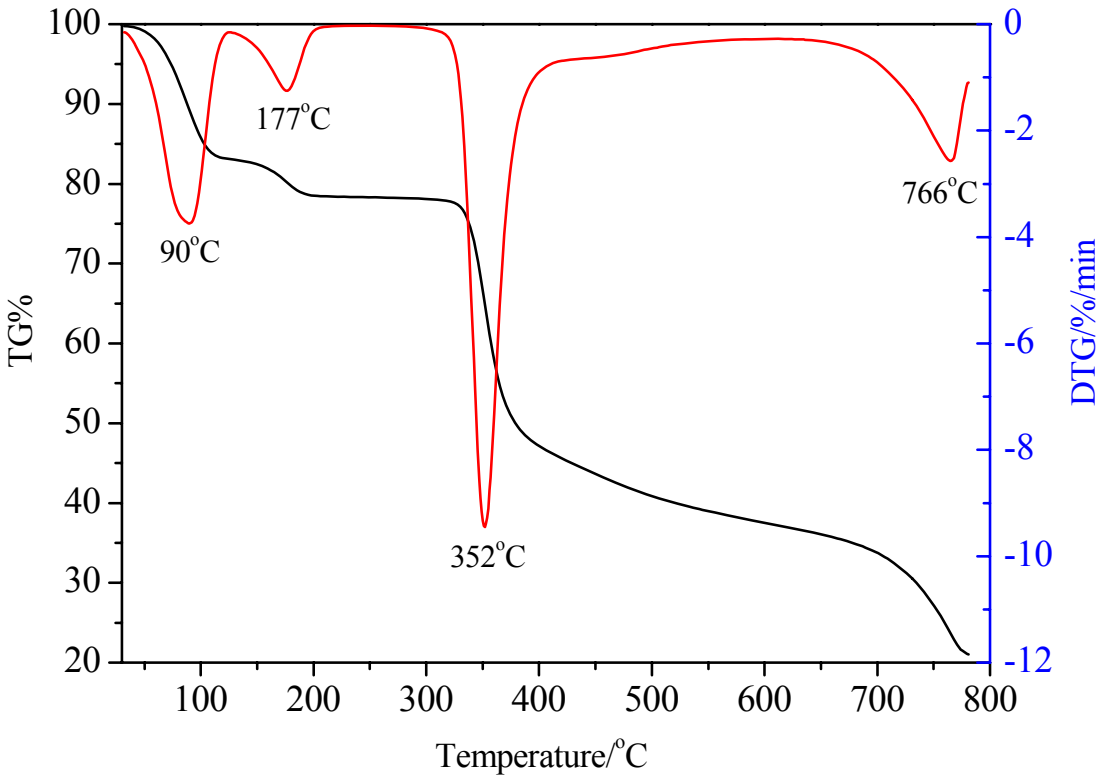

Figure S10

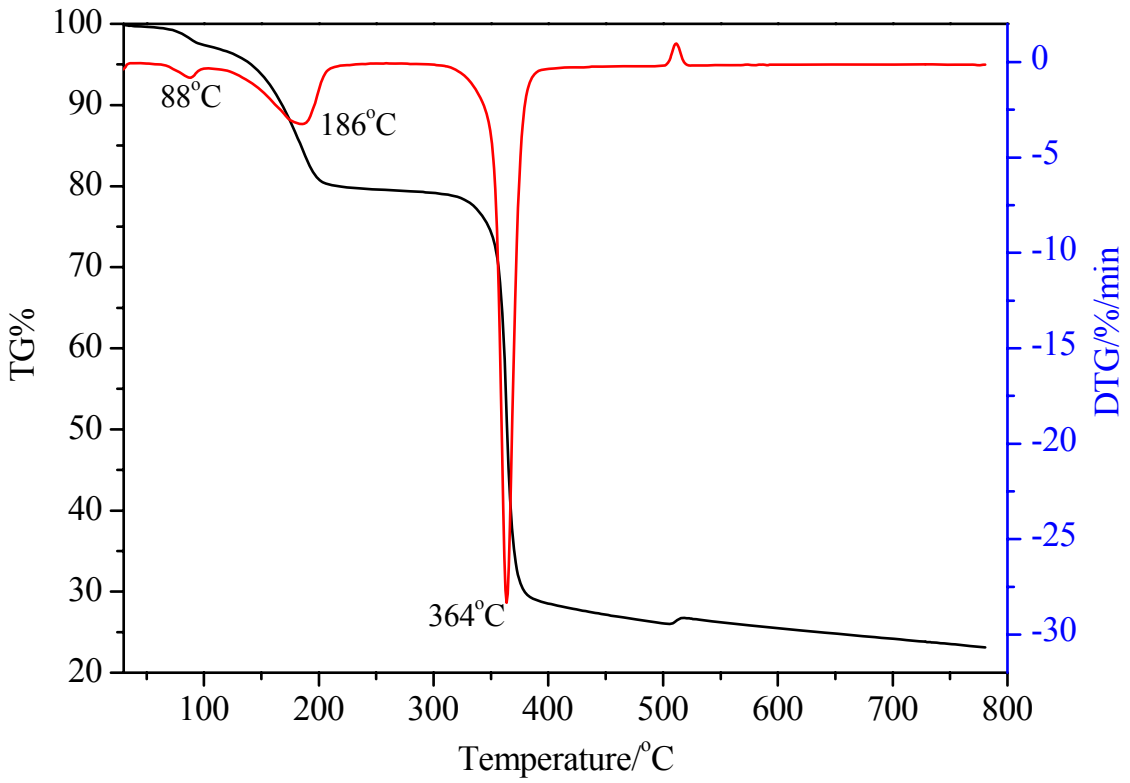

Table S1. ^{13}C NMR spectral data (in ppm) of ketopiperazinediacetic acid and its zinc complexes

Compounds	α-**C**O_2	β-**C**O_2	C=O	α-CH_2CO_2	β-CH_2CO_2	-CH_2C=O	-CH_2NC=O	-CH_2N
$kpda_{aq}$	174.9	171.6	166.3	60.2	55.4	51.4	51.3	46.8
$[Zn_2(kpda)_2(H_2O)_4]_n \cdot 6nH_2O$ (**3**)$_{solid}$	178.0(3.1)	176.2(4.6)	167.4(1.1)	55.5(-4.7)	54.4(-1.0)	49.5(-1.9)	48.8(-2.5)	44.1(-2.7)
$[Zn_2(kpda)_2(H_2O)_4]_n \cdot 6nH_2O$ (**3**)$_{aq}$		178.1(6.5)	170.5(4.2)	63.1(2.9)	58.0(2.6)	53.0(1.6)	52.3(1.0)	48.4(1.6)
$[Zn(kpda)(H_2O)_2]_n \cdot nH_2O$ (**7**)$_{aq}$[3]	179.5(4.6)	178.2(6.6)	170.6(4.3)	63.1(2.9)	58.1(2.7)	53.0(1.6)	52.4(1.1)	48.3(1.5)

Table S2. Selected bond distance (Å) and angles (°) for $[M_2(kpda)_2(H_2O)_4]_n \cdot 6nH_2O$ [M = Co **1**, Ni **2**, Zn **3**] and $[M_2(kpda)_2(H_2O)_6] \cdot H_2O$ [M = Co **4**, Ni **5**, Zn **6**]

Bond distances							
	1	**2**	**3**		**4**	**5**	**6**
M–O1	2.088(3)	2.022(4)	2.054(3)	M–O1	2.052(3)	2.041(3)	2.053(3)
M–N1	2.205(4)	2.136(6)	2.210(4)	M–N1	2.199(4)	2.140(4)	2.215(4)
M–O2d	2.049(3)	2.058(5)	2.118(3)	M–O5a	2.025 (3)	2.011(3)	2.023(4)
M–O5a	2.040(3)	2.027(5)	2.046(3)	M–O1w	2.141(3)	2.107(3)	2.142(4)
M–O1w	2.147(3)	2.078(5)	2.141(3)	M–O2w	2.084(3)	2.052(3)	2.058(4)
M–O2w	2.123(3)	2.103(5)	2.119(3)	M–O3w	2.214(3)	2.162(3)	2.273(4)

Bond angles							
	1	**2**	**3**		**4**	**5**	**6**
O5a–M–O1	161.9(1)	167.0(2)	161.8(1)	O5a–M–O1	167.2(1)	169.8(1)	166.1(1)
O5a–M–O2d	99.0(1)	96.7(2)	99.6(1)	O5a–M-O2w	96.0(1)	95.2(1)	97.2(1)
O1–M–O2d	93.0(1)	91.6(2)	92.6(1)	O1–M–O2w	96.2(1)	94.4(1)	95.5 (1)

O5a–M–O2w	93.5(1)	93.4(2)	94.1(1)	O5a–M–O1w	91.6(1)	91.2(1)	92.1(1)
O1–M–O2w	100.1(1)	96.7(2)	99.7(1)	O1–M–O1w	92.0(1)	91.8(1)	93.0(1)
O2d–M–O2w	89.9(1)	89.5(2)	88.4(1)	O2w–M–O1w	92.4(1)	91.6(1)	93.0(1)
O5a–M–O1w	86.9(1)	88.4(2)	86.6(1)	O5a–M–N1	87.2(1)	87.9(1)	86.4(1)
O1–M–O1w	82.2(1)	83.9(2)	82.4(1)	O1–M–N1	80.6(1)	82.5(1)	80.8(1)
O2d–M–O1w	172.9(1)	174.0(2)	172.6(1)	O2w–M–N1	176.7(1)	176.8(1)	175.8(2)
O2w–M–O1w	85.8(1)	87.1(2)	87.2(1)	O1w–M–N1	88.3(1)	89.3(1)	89.2(2)
O5a–M–N1	88.1(1)	88.4(2)	87.8(1)	O5a –M–O3w	90.3(1)	91.0(1)	89.7(1)
O1–M–N1	79.9(1)	82.4(2)	80.3(1)	O1–M–O3w	87.3(1)	86.9(1)	86.4(1)
O2d–M–N1	83.2(1)	84.6(2)	82.9(1)	O2w–M–O3w	82.2(1)	82.6(1)	81.6 (1)
O2w–M–N1	173.0(1)	174.0(2)	171.3(1)	O1w–M–O3w	174.5(1)	173.9(1)	174.5(1)
O1w–M–N1	101.0(1)	98.7(2)	101.4(1)	N1–M–O3w	97.0(1)	96.4(1)	96.1(1)

Symmetric transformations: for **1**, (a) $-x + 1, -y, -z + 1$; (d) $x, -y + {}^{1}/_{2}, z + {}^{1}/_{2}$; for **2**, (a) $-x - 1, -y+1, -z -1$; (d) $x, -y + {}^{1}/_{2}, z - {}^{1}/_{2}$; for **3**, (a) $-x + 1, -y, -z + 1$; (d) $x, -y + {}^{1}/_{2}, z + {}^{1}/_{2}$; for **4**, (a) $-x + 1, -y + 1, -z + 2$; for **5**, (a) $-x, -y, -z + 1$; for **6**, (a) $-x + 1, -y, -z + 1$;

Table S3. Selected bond distances and angles within the water layer in **1**

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A(°)
O1w–H···O4w	0.85(2)	1.93(2)	2.756(5)	165(4)
O1w–H···O4wa	0.84(2)	1.98(2)	2.811(5)	170(3)
O3w–H···O2w	0.85(3)	1.93(3)	2.772(5)	168(3)
O3w–H···O5wb	0.86(4)	2.01(4)	2.839(6)	162(4)
O4w–H···O5w	0.85(4)	1.95(4)	2.790(6)	172(3)
O5w–H···O3w	0.85(4)	1.85(4)	2.702(5)	175(5)

Symmetry transformations: (a) $-x, -y, -z$; (b) $x, {}^{1}/_{2} - y, {}^{1}/_{2} + z$;

Table S4. Selected bond distances and angles in **4**

D–H···A	D–H (Å)	H···A(Å)	D···A (Å)	D–H···A (°)
O1w–H···O1a	0.84(3)	1.95(3)	2.798(5)	179(3)
O1w–H···O3wb	0.85(3)	2.14(3)	2.990(5)	178(3)
O2w–H···O2c	0.85(4)	1.85(4)	2.695(5)	169(3)
O3w–H···O3d	0.86(3)	1.92(3)	2.766(5)	169(3)
O3w–H···O4e	0.85(3)	1.90(3)	2.677(5)	152(4)
O4w-H···O2	0.84(4)	2.50(5)	2.844(5)	106(3)

Symmetry transformations: (a) $x - {}^{1}/_{2}, {}^{1}/_{2} - y, z - {}^{1}/_{2}$; (b) $x, y - 1, z$; (c) $x - {}^{1}/_{2}, {}^{1}/_{2} - y, z - {}^{1}/_{2}$; (d) $x, y + 1, z$; (e) $-x + {}^{1}/_{2}, {}^{3}/_{2} - y, -z + 2$