

## Supporting materials

### Tuning zinc(II) coordination polymers based on bis(1,2,4-triazol-1-yl)ethane and 5-substituted 1,3-benzenedicarboxylates: Syntheses, structures and properties

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**Table S1** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **1-6**

1			
Zn(1)-N(3)	2.020(5)	Zn(1)-N(6B)	2.026(5)
Zn(1)-O(1)	2.003(4)	Zn(1)-O(3A)	1.960(4)
N(3)-Zn(1)-N(6B)	113.1(2)	O(1)-Zn(1)-N(3)	107.1(2)
O(3A)-Zn(1)-N(3)	103.6(2)	O(1)-Zn(1)-N(6B)	115.6(2)
O(3A)-Zn(1)-N(6B)	115.0(2)	O(3 <sup>a</sup> )-Zn(1)-O(1)	101.20(18)
2			
Zn(1)-N(3)	2.049(4)	Zn(1)-N(6B)	2.009(4)
Zn(1)-O(1)	1.975(3)	Zn(1)-O(3A)	1.975(3)
N(6B)-Zn(1)-N(3)	108.82(14)	O(1)-Zn(1)-N(3)	114.01(13)
O(3A)-Zn(1)-N(3)	108.76(13)	O(1)-Zn(1)-N(6B)	109.87(13)
O(3A)-Zn(1)-N(6B)	112.93(13)	O(3 <sup>a</sup> )-Zn(1)-O(1)	102.43(11)
3			
Zn(1)-N(3)	2.123(4)	Zn(1)-N(6B)	2.142(4)
Zn(1)-O(1)	2.104(3)	Zn(1)-O(4A)	2.059(3)
Zn(1)-O(5)	2.104(3)		
N(3)-Zn(1)-N(6B)	93.07(15)	O(1)-Zn(1)-N(3)	134.71(13)
O(4A)-Zn(1)-N(3)	128.05(12)	O(5)-Zn(1)-N(3)	90.50(15)
O(1)-Zn(1)-N(6B)	86.81(14)	O(4A)-Zn(1)-N(6B)	91.78(14)
O(5)-Zn(1)-N(6B)	175.85(15)	O(4A)-Zn(1)-O(1)	97.20(13)
O(5)-Zn(1)-O(1)	89.17(13)	O(4A)-Zn(1)-O(5)	87.67(13)
4			
Zn(1)-N(3)	2.194(4)	Zn(1)-N(6A)	2.160(4)

Zn(1)-N(9)	2.171(4)	Zn(1)-N(12A)	2.193(4)
Zn(1)-O(1)	2.089(4)	Zn(1)-O(2)	2.156(4)
N(6A)-Zn(1)-N(3)	90.54(14)	N(9)-Zn(1)-N(3)	87.68(15)
N(12A)-Zn(1)-N(3)	178.49(14)	N(6A)-Zn(1)-N(9)	176.84(15)
N(6A)-Zn(1)-N(12A)	90.11(14)	N(9)-Zn(1)-N(12A)	91.60(15)
O(1)-Zn(1)-N(3)	88.25(15)	O(2)-Zn(1)-N(3)	90.73(14)
O(1)-Zn(1)-N(6A)	88.50(15)	N(6A)-Zn(1)-O(2)	86.53(15)
O(1)-Zn(1)-N(9)	88.84(15)	O(2)-Zn(1)-N(9)	96.10(16)
O(1)-Zn(1)-N(12A)	90.41(15)	O(2)-Zn(1)-N(12A)	90.66(14)
O(1)-Zn(1)-O(2)	174.91(15)		
<b>5</b>			
Zn(1)-N(3)	2.004(3)	Zn(1)-N(6B)	2.029(3)
Zn(1)-O(1)	1.974(3)	Zn(1)-O(3A)	1.963(3)
N(3)-Zn(1)-N(6B)	110.99(13)	O(1)-Zn(1)-N(3)	117.09(13)
O(3A)-Zn(1)-N(3)	111.61(13)	O(1)-Zn(1)-N(6B)	110.01(13)
O(3A)-Zn(1)-N(6B)	97.47(13)	O(3A)-Zn(1)-O(1)	107.88(12)
<b>6</b>			
Zn(1)-N(3)	2.058(5)	Zn(1)-N(3C)	2.058(5)
Zn(1)-O(6A)	1.990(4)	Zn(1)-O(6B)	1.990(4)
Zn(2)-N(6)	1.998(4)	Zn(2)-O(1)	1.973(4)
Zn(2)-O(4D)	1.946(4)	Zn(2)-O(7)	2.028(4)
N(3C)-Zn(1)-N(3)	93.1(3)	O(6B)-Zn(1)-N(3)	95.42(18)
O(6A)-Zn(1)-N(3)	117.71(18)	O(6A)-Zn(1)-N(3C)	95.42(18)
O(6B)-Zn(1)-N(3C)	117.71(18)	O(6A)-Zn(1)-O(6B)	132.0(2)
O(1)-Zn(2)-N(6)	119.69(17)	O(4D)-Zn(2)-N(6)	119.04(18)
N(6)-Zn(2)-O(7)	106.06(17)	O(4D)-Zn(2)-O(1)	100.32(16)
O(1)-Zn(2)-O(7)	106.69(16)	O(4D)-Zn(2)-O(7)	103.47(17)

Symmetry transformations used to generate equivalent atoms: A x, y, z-1; B -x+1, -y, -z+1 for **1**; A x+1, y-1, z; B -x+1, -y, -z for **2**; A x, y+1, z; B -x, -y+1, -z+1 for **3**; A x, -y+1/2, z+1/2 for **4**; A x+1/2, -y+1/2, z+1/2; B -x+1/2, y-1/2, -z+3/2 for **5**; A x-1/2, -y+3/2, z+1/2; B -x+3/2, -y+3/2, -z+1; C -x+1, y, -z+3/2; D x-1/2, y+1/2, z for **6**.

**Table S2** Hydrogen bondings for **3** (Å and °)

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
O(5)-H(1W)···O(6) <sup>i</sup>	0.886(19)	1.89(2)	2.751(5)	163(5)
O(5)-H(2W)···O(2) <sup>i</sup>	0.889(19)	1.783(19)	2.681(5)	178(4)
O(6)-H(3W)···O(3)	0.87(2)	1.92(3)	2.746(5)	159(5)
O(6)-H(4W)···N(5) <sup>ii</sup>	0.90(2)	2.46(5)	3.223(6)	143(6)

Symmetry transformations used to generate equivalent atoms: i -x+1/2, -y+1/2, -z+1; ii x, y-1, z.

**Table S3** Hydrogen bondings for **4** ( $\text{\AA}$  and  $^\circ$ )

D-H $\cdots$ A	d(D-H)	d(H $\cdots$ A)	D(D $\cdots$ A)	$\angle$ (DHA)
O(1)-H(1W) $\cdots$ O(10)	0.80(5)	1.96(5)	2.742(6)	166(6)
O(1)-H(2W) $\cdots$ O(12)	0.76(6)	1.92(6)	2.681(6)	171(6)
O(2)-H(3W) $\cdots$ O(10) <sup>i</sup>	0.84(6)	2.08(6)	2.913(6)	174(6)
O(2)-H(4W) $\cdots$ O(8)	0.88(6)	1.85(6)	2.721(6)	167(5)
O(5)-HWA $\cdots$ O(4) <sup>ii</sup>	0.88(2)	1.67(2)	2.534(5)	166(5)
O(10)-H(5W) $\cdots$ O(7) <sup>iii</sup>	0.74(6)	2.25(6)	2.916(6)	152(7)
O(10)-H(6W) $\cdots$ O(11)	0.78(6)	2.03(6)	2.734(6)	149(6)
O(11)-H(7W) $\cdots$ O(3) <sup>iv</sup>	0.92(7)	1.96(7)	2.802(5)	152(6)
O(11)-H(8W) $\cdots$ O(13)	0.91(6)	1.99(7)	2.893(6)	174(6)
O(12)-H(9W) $\cdots$ O(8) <sup>iii</sup>	0.95(6)	1.93(7)	2.835(7)	159(6)
O(12)-H(10W) $\cdots$ O(7) <sup>v</sup>	0.82(4)	2.38(5)	3.142(7)	154(6)
O(13)-H(11W) $\cdots$ N(11) <sup>vi</sup>	0.87(2)	2.16(2)	3.030(6)	174(5)
O(13)-H(12W) $\cdots$ O(4) <sup>ii</sup>	0.90(2)	2.14(2)	3.021(5)	169(6)

Symmetry transformations used to generate equivalent atoms: i -x+1, y-1/2, -z+3/2; ii -x, y+1/2, -z+3/2; iii x, -y+1/2, z+1/2; iv x, y+1, z; v -x+1, y+1/2, -z+3/2; vi -x, -y+1, -z+1.

**Table S4** Hydrogen bondings for **5** ( $\text{\AA}$  and  $^\circ$ )

D-H $\cdots$ A	d(D-H)	d(H $\cdots$ A)	D(D $\cdots$ A)	$\angle$ (DHA)
O(6)-H(1W) $\cdots$ O(5) <sup>i</sup>	0.894(19)	1.73(2)	2.624(4)	175(4)
O(7)-H(2W) $\cdots$ O(8) <sup>ii</sup>	0.908(19)	2.06(4)	2.818(8)	140(4)
O(7)-H(3W) $\cdots$ O(9) <sup>ii</sup>	0.900(19)	1.83(3)	2.749(8)	162(5)

Symmetry transformations used to generate equivalent atoms: i -x+3, -y, -z+1; ii x+1, y, z.

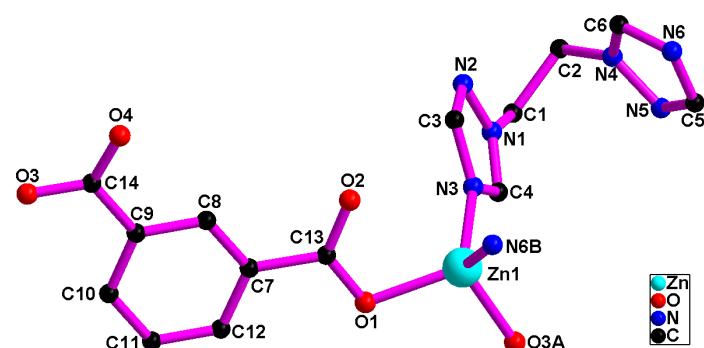
**Table S5** Hydrogen bondings for **6** ( $\text{\AA}$  and  $^\circ$ )

D-H $\cdots$ A	d(D-H)	d(H $\cdots$ A)	D(D $\cdots$ A)	$\angle$ (DHA)
O(7)-H(1W) $\cdots$ O(2) <sup>i</sup>	0.84(2)	1.88(2)	2.704(6)	168(6)
O(7)-H(2W) $\cdots$ O(8) <sup>ii</sup>	0.83(2)	1.86(2)	2.684(6)	169(6)
O(8)-H(3W) $\cdots$ O(8) <sup>iii</sup>	0.85(2)	1.99(3)	2.772(6)	152(5)
O(8)-H(4W) $\cdots$ O(9) <sup>iv</sup>	0.847(19)	1.91(3)	2.736(6)	166(5)

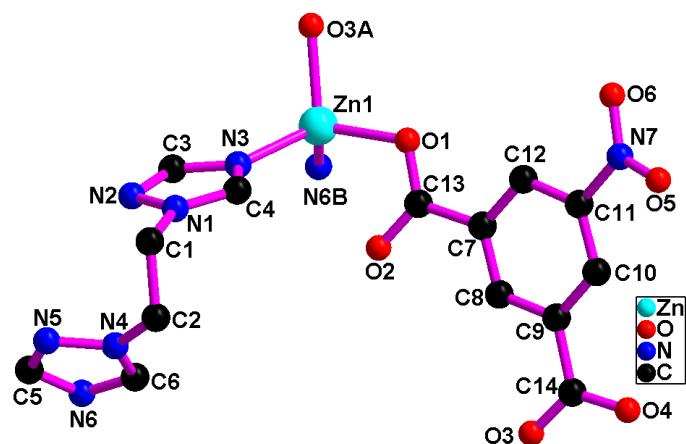
Symmetry transformations used to generate equivalent atoms: i -x+3/2, -y+1/2, -z+1; ii -x+1, -y+1, -z+1; iii -x+3/2, -y+3/2, -z+1; iv x-1/2, y+1/2, z.

**Table S6** The dihedral angle between the two triazol rings, and the torsion angle  $N_{\text{triazole}}-(\text{C}-\text{C})_{\text{ethane}}-\text{N}_{\text{triazole}}$  and  $\text{Zn}\cdots\text{Zn}$  distances bridged by bte in **1-6**

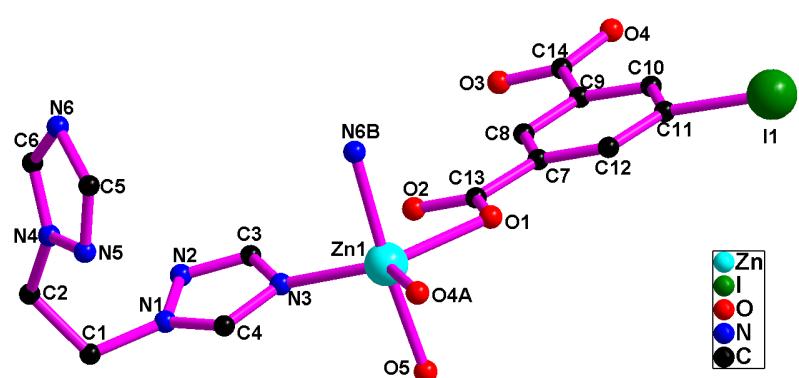
compound	dihedral angle (°)	torsion angle (°)	$\text{Zn}\cdots\text{Zn}$ distance (Å)
1	53.0(2)	47.4(8)	6.540(2)
2	51.8(2)	-62.7(5)	7.711(3)
3	67.2(2)	-49.6(6)	7.9020(10)
4	53.28(4), 59.62(2)	65.5(5), 64.6(5)	8.327(2)
5	40.71(2)	179.0(4)	9.392(2)
6	41.20(2)	71.5(7)	8.1715(11)



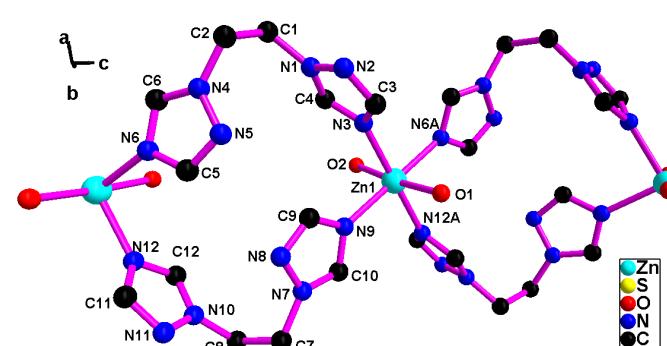
**Fig. S1** The coordination environment of The Zn(II) atom in **1**.



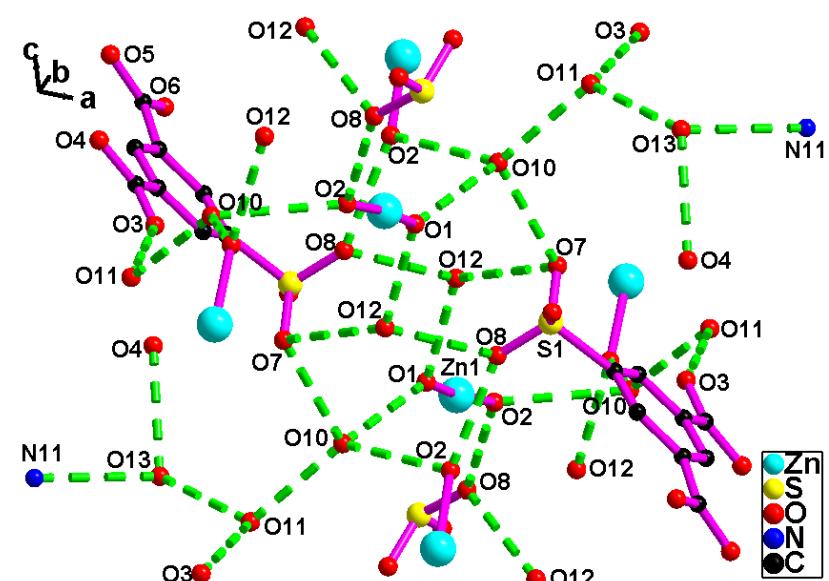
**Fig. S2** The coordination environment of The Zn(II) atom in **2**.



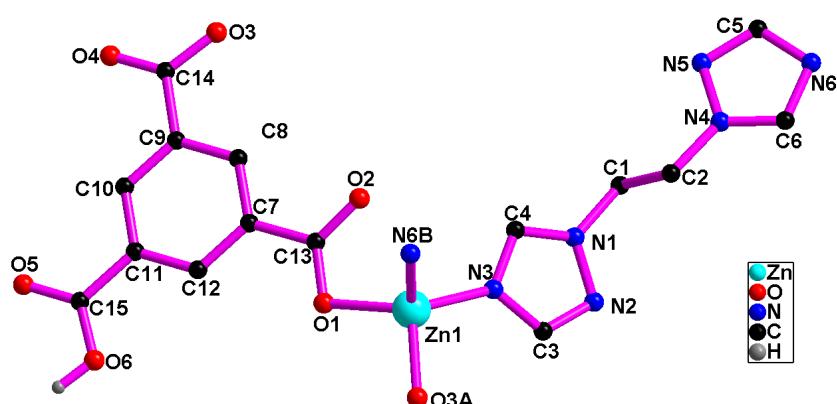
**Fig. S3** The coordination environment of The Zn(II) atom in 3.



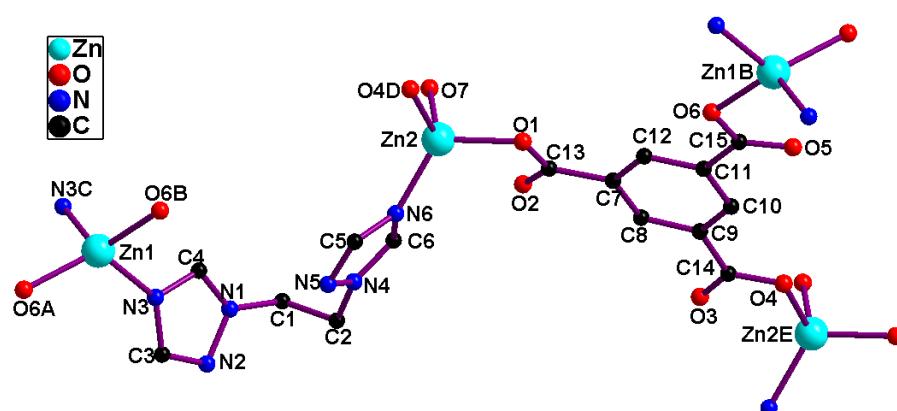
**Fig. S4** The coordination environment of The Zn(II) atom in 4.



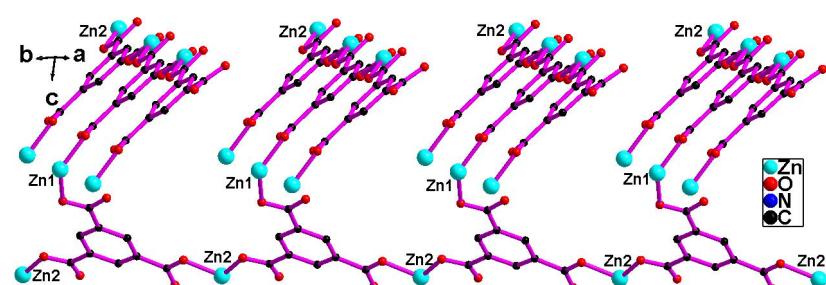
**Fig. S5** The hydrogen bond interactions in 4.



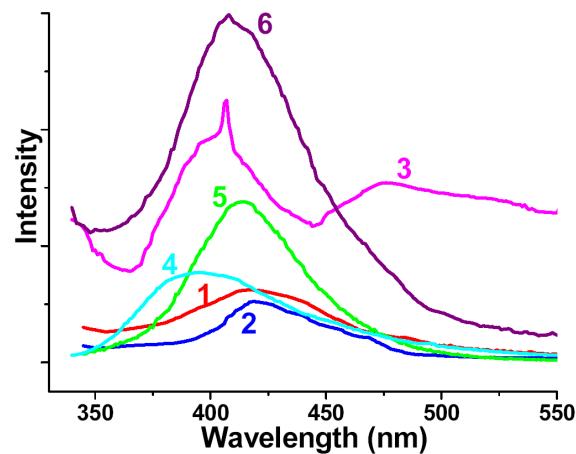
**Fig. S6** The coordination environment of The Zn(II) atom in **5**.



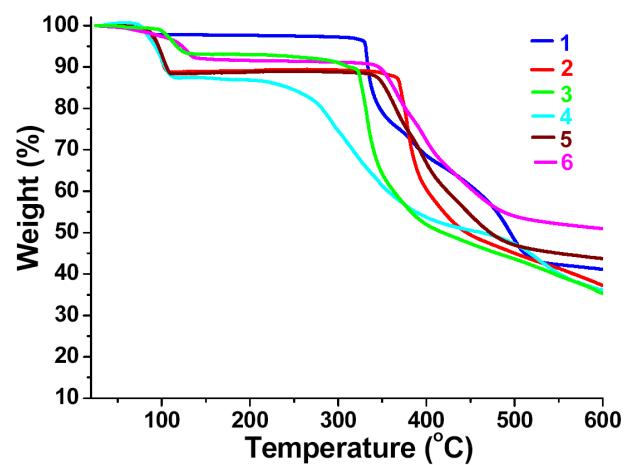
**Fig. S7** The coordination environment of the Zn(II) atoms in **6**.



**Fig. S8** Each Zn1 atom connects two  $[Zn(btc)]_n$  chain based on Zn2 atoms and btc ligands in **6**.



**Fig. S9** Solid state emissions of compounds **1**, **2**, **3**, **4**, **5** and **6**.



**Fig. S10** The TG curves of compounds **1**, **2**, **3**, **4**, **5** and **6**.