ELECTRONIC SUPPLEMENTARY INFORMATION

The methylene spacer matters: the structural and luminescent effects of positional isomerism of n-methylpyridyltriazole car-boxylate semi-rigid ligands in the structure of Zn(II) based co-ordination polymers

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Table S1. Zn(II) ion Bond Distances (Å) of compound **1** and **2**.

1			**2**		
Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O2	2.044(2)	Zn1	O2[1]	2.151(2)
Zn1	O2[1]	2.044(2)	Zn1	O2[2]	2.151(2)
Zn1	N1[2]	2.297(3)	Zn1	N1	2.142(3)
Zn1	N1[3]	2.297(3)	Zn1	N1[3]	2.142(3)
Zn1	N4[1]	2.151(3)	Zn1	N4[1]	2.166(3)
Zn1	N4	2.151(3)	Zn1	N4[2]	2.166(3)

[1]1/2-X,3/2-Y,-Z; [2]-1/2+X,3/2-Y,-1/2+Z; [3]1-X,+Y,1/2-Z.

Table S2. Zn(II) ion coordination sphere bond angles (º) of compounds **1** and **2**.

1				**2**			
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	O2[1]	180.00(11)	O2[1]	Zn1	O2[2]	174.64(12)
O2	Zn1	N1[2]	92.14(9)	O2[1]	Zn1	N4[2]	99.77(11)
O2	Zn1	N1[3]	87.86(9)	O2[1]	Zn1	N4[1]	76.32(10)
O2[1]	Zn1	N1[3]	92.14(9)	O2[2]	Zn1	N4[1]	76.32(10)
O2[1]	Zn1	N1[2]	87.86(9)	O2[2]	Zn1	N4[1]	99.77(11)
O2	Zn1	N4[1]	100.02(9)	N1[3]	Zn1	O2[1]	87.65(11)
O2[1]	Zn1	N4	100.02(9)	N1[3]	Zn1	O2[2]	96.16(11)
O2	Zn1	N4	79.98(9)	N1	Zn1	O2[2]	87.65(11)
O2[1]	Zn1	N4[1]	79.98(9)	N1	Zn1	O2[1]	96.16(11)
N1[2]	Zn1	N1[3]	180.0	N1[3]	Zn1	N1	89.57(17)
N4[1]	Zn1	N1[3]	83.00(9)	N1[3]	Zn1	N4[2]	93.10(12)
N4	Zn1	N1[2]	83.00(9)	N1[3]	Zn1	N4[1]	163.94(12)
N4[1]	Zn1	N1[2]	97.00(9)	N1	Zn1	N4[2]	163.94(11)
N4	Zn1	N1[3]	97.00(9)	N1	Zn1	N4[1]	93.10(12)
N4[1]	Zn1	N4	180.0	N4[1]	Zn1	N4[2]	88.70(16)

[1]+X,1+Y,+Z; [2]1-X,1+Y,1/2-Z; [3]1-X,+Y,1/2-Z; [4]+X,-1+Y,+Z.

Table S3. Hydrogen bonds interactions of compound **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C3	H3	O2[1]	0.93	2.45	3.047(4)	122.4
C4	H4	O1[2]	0.93	2.48	3.163(4)	130.0
C6	H6A	O2[3]	0.97	2.67	3.391(4)	131.5
C10	H10A	N4[4]	0.96	2.78	3.424(4)	124.8
C10	H10B	O1	0.96	2.6	3.241(4)	124.5
C10	H10C	O1[5]	0.96	2.72	3.450(5)	132.9

[1]1/2+X,3/2-Y,1/2+Z; [2]1-X,1+Y,1/2-Z; [3]1/2+X,1/2+Y,+Z; [4]1-X,1-Y,-Z; [5]1-X,+Y,1/2-Z

Table S4. Hydrogen bonds interactions of compound **2**.

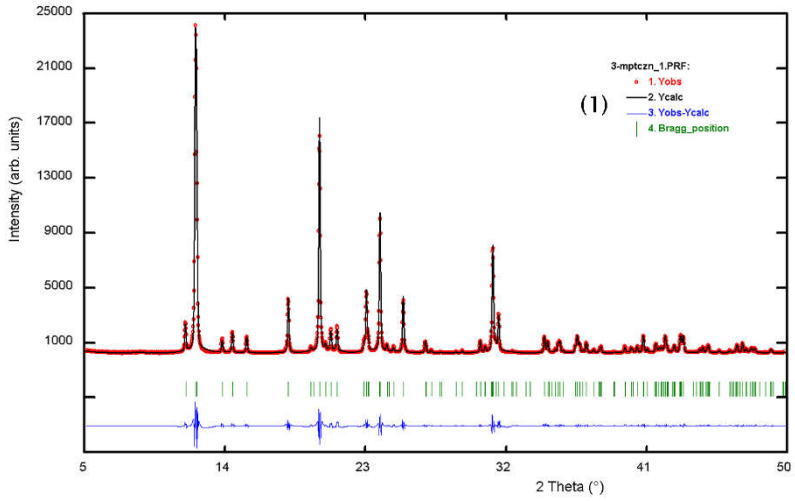
D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C4	H4	O2S[1]	0.93	2.87	3.463(7)	122.7
C5	H5	O1S[2]	0.93	2.84	3.455(6)	125.0
C6	H6A	N3[3]	0.97	2.43	3.343(5)	156.1
C10	H10B	O1	0.96	2.62	3.241(5)	122.9
O1S	H1SA	O1[4]	0.85	1.95	2.792(4)	173.2
O1S	H1SB	O1[5]	0.85	2.66	3.249(4)	127.9
O1S	H1SB	O2[5]	0.85	2.22	3.067(4)	171.5
O2S	H2SA	O1S	0.85	2.17	3.020(6)	173.7
O2S	H2SB	O1S[6]	0.85	2.13	2.979(6)	177.7

[1]1+X,1+Y,+Z; [2]3/2-X,3/2-Y,-Z; [3]1-X,1-Y,-Z; [4]+X,1-Y,-1/2+Z; [5]3/2-X,1/2+Y,1/2-Z; [6]3/2-X,1/2-Y,-Z

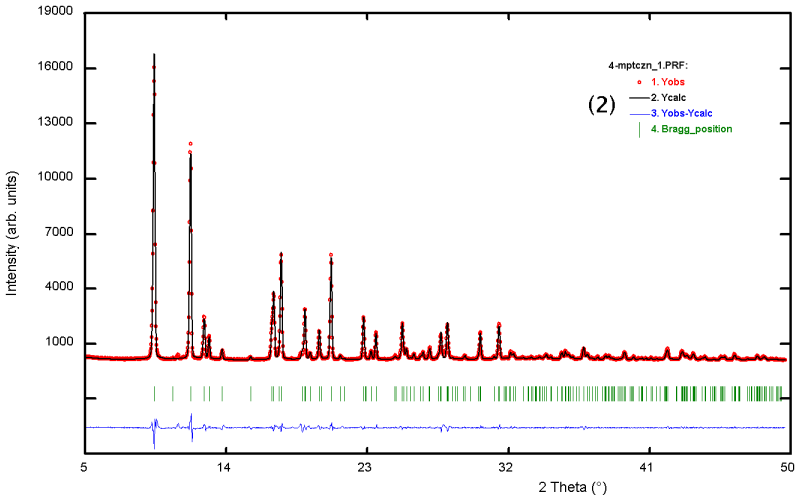
Table S5. Summary of the hydrogen bond distances (Å) and angles (°) for **2**.

D—H ···A	D – H	H···A	D – A	D – H ···A
O1S–H1SA···O1[i]	0.85	1.95	2.792(4)	173.2
O1S–H1SB···O1[ii]	0.85	2.66	3.249(4)	127.9
O1S–H1SB···O2[ii]	0.85	2.22	3.067(4)	171.9
O1S–H1SA···O1S	0.85	2.17	3.020(4)	173.7
O1S–H1SA···O1S[iii]	0.85	2.13	2.979(4)	177.7

(i) -x,-y+1,z-1/2, (ii) -x+3/2, y+1/2, -z+1/2, (iii) -x+3/2, -y+1/2, -z.



Rp= 6.6, Rwp= 8.7



Rp= 5.9, Rwp= 7.8

Figure S1. X-ray powder diffraction patterns (**1**, **2**) and Rietveld refinement plots.

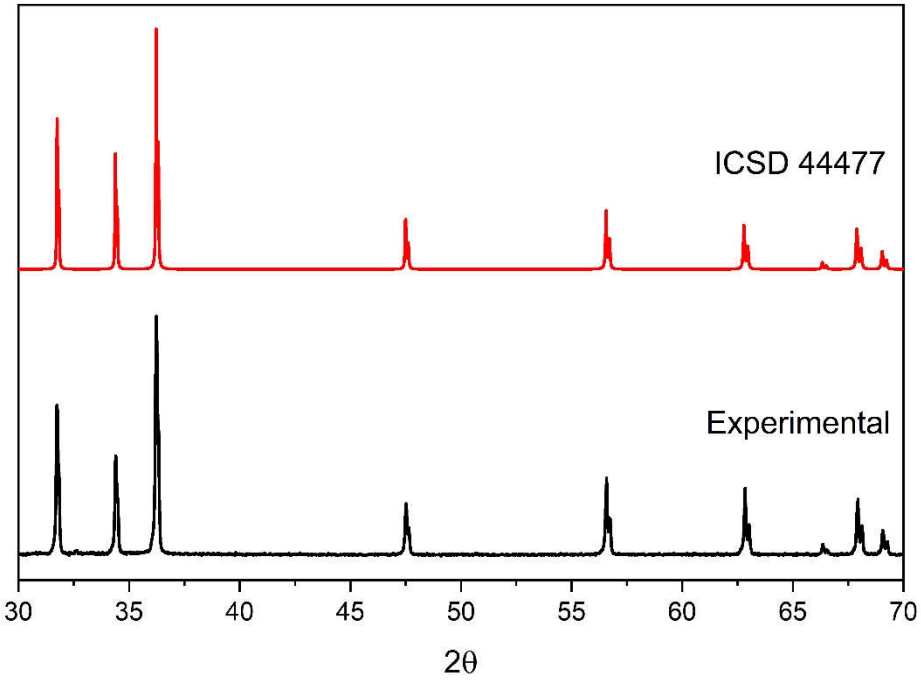


Figure S2. Experimental Powder diffractogram of compound **1** residue from TG experiment.