Electronic Supplementary Information (ESI)

Solvent-controlled Three Families of Zn(II) Coordination Compounds: Synthesis, Crystal structure, Solvent-Induced Structural Transformation, Supramolecular Isomerism and Photoluminescence

Lu-Lu Han,[a,⊥] Tuo-Ping Hu,[b,⊥] Kai Mei,[a] Zhi-Min Guo,[a] Chen Yin,[a] Ya-Xin Wang,[a] Jun Zheng,[c] Xing-Po Wang[a] and Di Sun,*[,a]

[a]*Key Lab for Colloid and Interface Chemistry of Education Ministry, School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, People's Republic of China. E-mail: dsun@sdu.edu.cn*; *Fax: 86-531-88364218.*

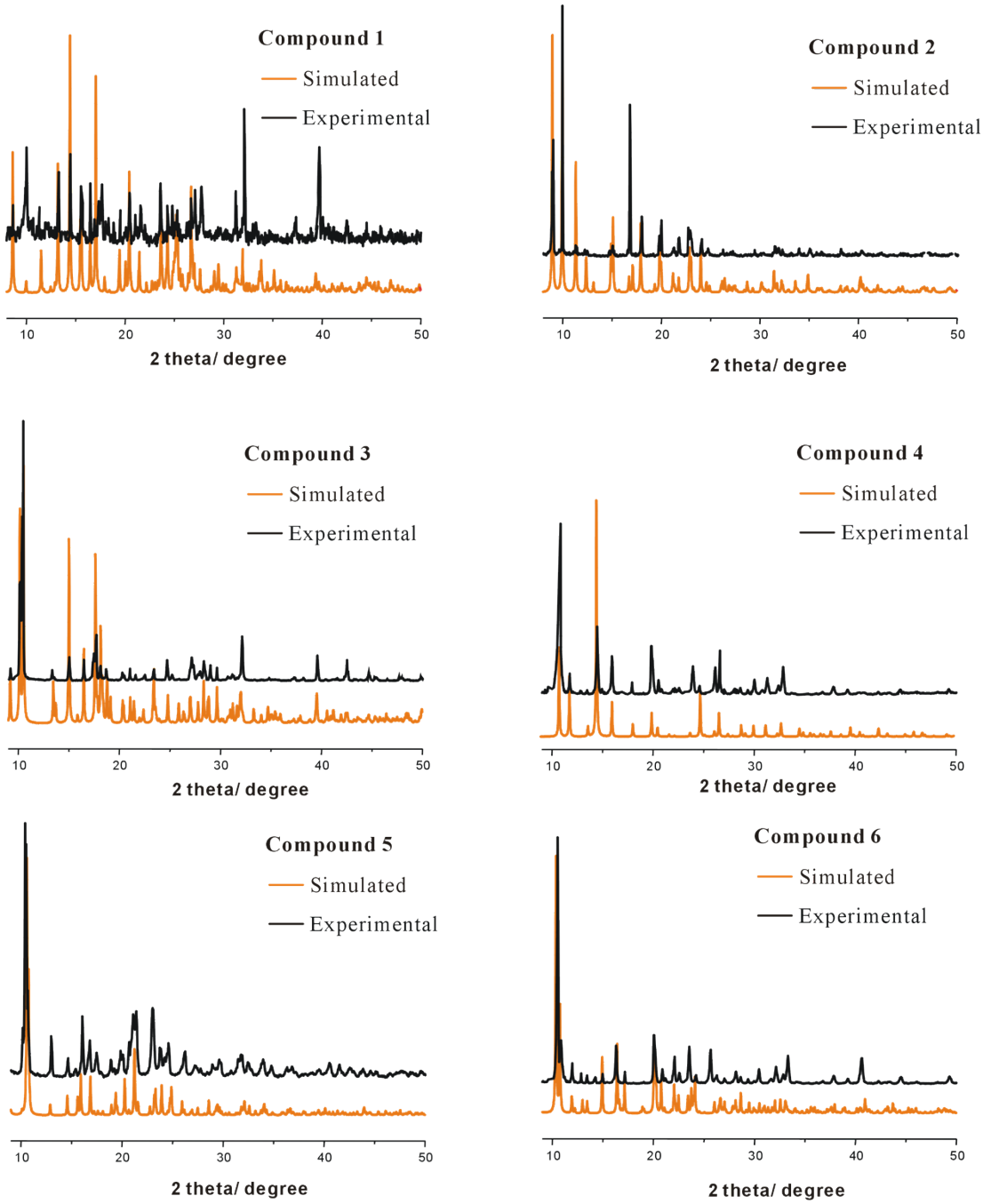
[b]*Department of Chemistry, North University of China, Taiyuan, Shanxi 030051, People's Republic of China.*

[c]*Center of Modern Experimental Technology, Anhui University, Hefei 230039, People's Republic of China.*

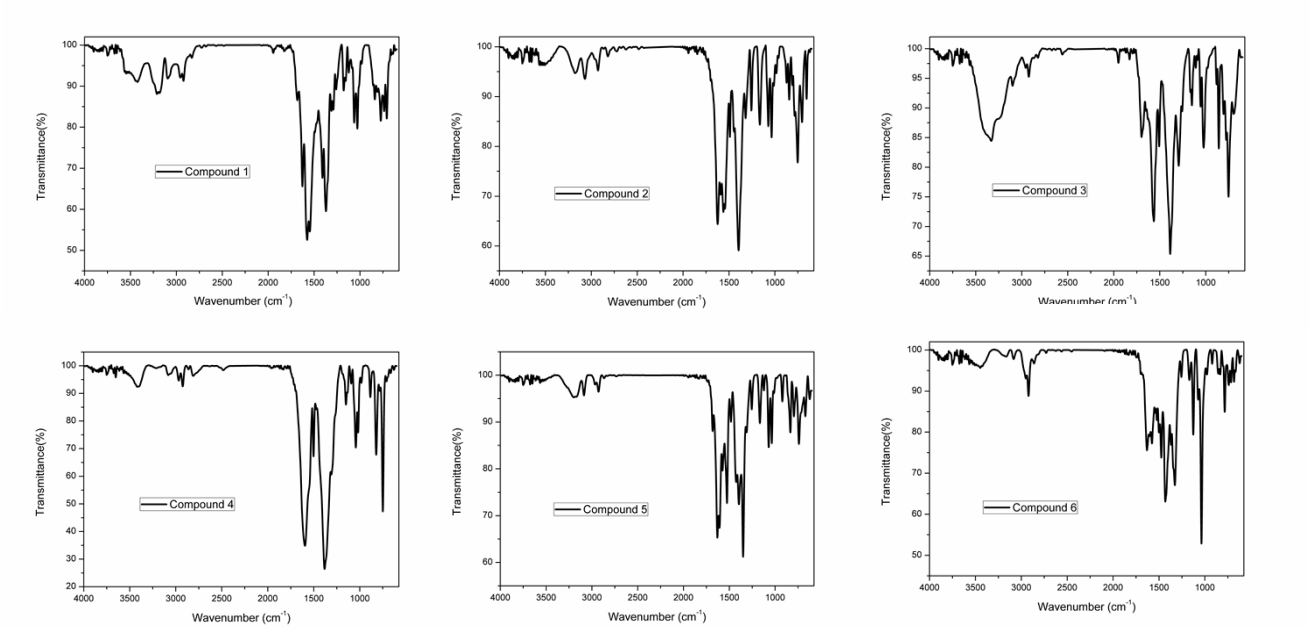
[⊥]*These authors contributed equally.*

Content

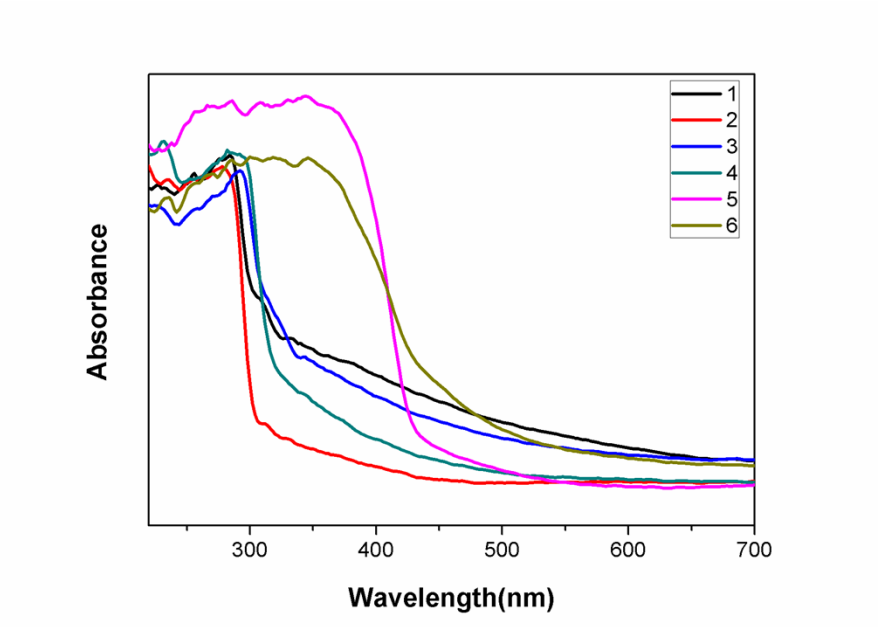
(1) Fig. S1: XRD spectra of 1-6.



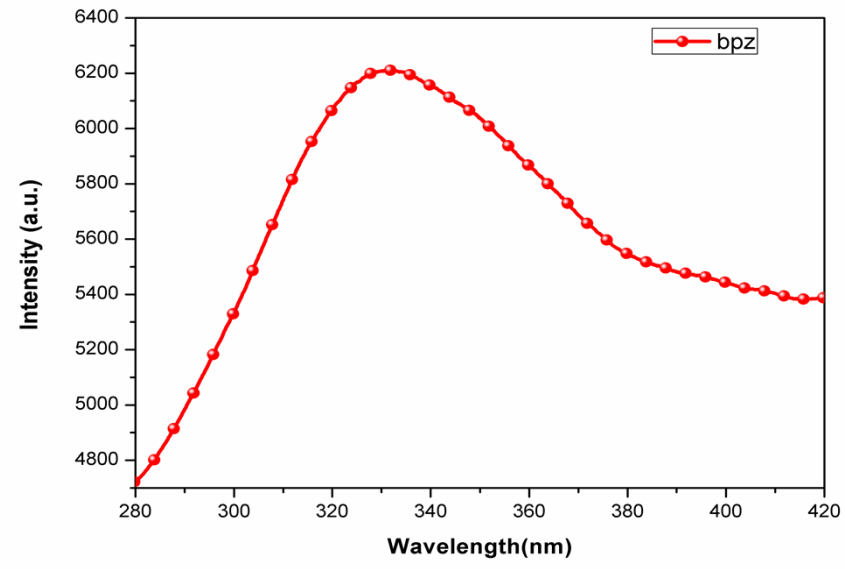
(2) Fig. S2: IR of 1-6.



(3) Fig. S3: UV-Vis spectra for 1-6.



(4) Fig. S4: Luminescence spectra of bpz.



(5) Table S1: Selected bond lengths and angles of Compounds 1-6.

Compound 1					
Zn1—O1W	2.021 (2)	Zn1—O2W	2.2007 (14)	Zn1—N1	2.0481 (15)
O1W—Zn1—N1	115.89 (5)	O1W—Zn1—O2W	86.80 (4)	N1—Zn1—N1^{i}	128.23 (9)
N1—Zn1—O2W	93.27 (6)	N1—Zn1—O2W^{i}	89.53 (6)	O2W^{i}—Zn1—O2W	173.59 (8)
Symmetry code: (i) −x+1, y, −z+1/2.					
Compound 2					
Zn1—O1	2.026 (5)	Zn1—O4^{i}	1.944 (5)	Zn1—N1	2.037 (5)
Zn1—N4^{ii}	2.053 (5)				
N1—Zn1—N4^{ii}	113.0 (2)	O1—Zn1—N1	93.3 (2)	O1—Zn1—N4^{ii}	98.2 (2)
O4^{i}—Zn1—N1	111.5 (2)	O4^{i}—Zn1—O1	141.9 (2)	O4^{i}—Zn1—N4^{ii}	97.8 (2)
Symmetry codes: (i) −x+1, −y, z+1/2; (ii) x−1/2, −y+1/2, z.					
Compound 3					
Zn1—O1W	2.038 (2)	Zn1—N1	2.159 (3)	Zn1—N3^{i}	2.197 (3)
Zn1—O1	2.253 (2)	Zn1—O2	2.129 (2)	Zn1—O3	2.057 (2)
O1W—Zn1—O1	92.07 (9)	O1W—Zn1—O2	152.11 (9)	O1W—Zn1—O3	99.27 (9)
O1W—Zn1—N1	90.27 (10)	O1W—Zn1—N3^{i}	90.81 (10)	O2—Zn1—O1	60.04 (8)
O2—Zn1—N1	90.96 (10)	O2—Zn1—N3^{i}	89.23 (10)	O3—Zn1—O1	168.63 (9)
O3—Zn1—O2	108.61 (9)	O3—Zn1—N1	89.17 (10)	O3—Zn1—N3^{i}	88.24 (10)
N1—Zn1—O1	91.50 (9)	N1—Zn1—N3^{i}	177.32 (10)	N3^{i}—Zn1—O1	90.91 (9)
Symmetry code: (i) x+1/2, −y+1/2, z−1/2.					
Compound 4					
Zn1—O2	1.941 (6)	Zn1—N2	2.007 (7)		
O2—Zn1—N2	107.5 (3)	O2—Zn1—N2i	114.3 (3)	O2i—Zn1—O2	102.3 (5)
N2i—Zn1—N2	110.8 (4)				
Symmetry code: (i) −x+y+1, y, −z+2/3.					
Compound 5					
Zn1—O1	1.981 (5)	Zn1—O4^{i}	1.961 (5)	Zn1—N2	2.017 (7)
Zn1—N3	1.999 (8)				
O1—Zn1—N2	99.6 (3)	O1—Zn1—N3	97.1 (3)	O4^{i}—Zn1—O1	135.9 (2)
O4^{i}—Zn1—N2	101.5 (3)	O4^{i}—Zn1—N3	111.0 (3)	N3—Zn1—N2	110.3 (3)
Symmetry code: (i) −x+3/2, y−1/2, −z+2.					
Compound 6					
Zn1—O1	1.982 (7)	Zn1—O4^{i}	1.923 (7)	Zn1—N1	2.030 (8)
Zn1—N3^{ii}	1.988 (9)				
O1—Zn1—N1	101.3 (3)	O1—Zn1—N3^{ii}	98.7 (3)	O4^{i}—Zn1—O1	134.0 (3)
O4^{i}—Zn1—N1	97.3 (3)	O4^{i}—Zn1—N3^{ii}	111.8 (3)	N3^{ii}—Zn1—N1	113.2 (3)
Symmetry codes: (i) −x+2, −y+1, z−1/2; (ii) x+1/2, −y+3/2, z.					

(6) Table S2: Hydrogen bond parameters of Compound 1-6.

Compound 1				
D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O4^{ii}	0.89	1.96	2.686 (2)	136.9
O1W—H1WB···O4^{iii}	0.90	1.92	2.686 (2)	142.2
O2W—H2WA···O3^{ii}	0.87	2.11	2.917 (2)	152.9
O2W—H2WB···N3^{iv}	0.88	1.96	2.792 (2)	158.1
N2—H2···O3^{iii}	0.86	2.12	2.975 (2)	174.9
N4—H4···O1^{v}	0.86	2.05	2.903 (2)	175.2
O2—H2A···O3	0.82	1.64	2.457 (3)	175.9
Symmetry codes: (ii) x, −y+1, z−1/2; (iii) −x+1, −y+1, −z+1; (iv) −x+3/2, y−1/2, −z+1/2; (v) x+1/2, y+1/2, z.				
Compound 2				
D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{iii}	0.86	1.86	2.713 (8)	173.2
N3—H3···O3^{iv}	0.86	1.86	2.684 (7)	159.3
N3—H3···O1^{iv}	0.86	2.64	3.120 (7)	116.9
Symmetry codes: (iii) −x+1, −y, z−1/2; (iv) x+1/2, −y+1/2, z.				
Compound 3				
D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4	0.86	2.06	2.886 (4)	160.2
N4—H4···O4^{ii}	0.86	2.26	3.099 (4)	166.1
O1W—H1WA···O2^{iii}	0.87	1.88	2.607 (3)	140.4
O1W—H1WB···O4^{iii}	0.87	1.94	2.726 (3)	149.4
O1W—H1WB···N4^{i}	0.87	2.57	3.144 (4)	124.7
Symmetry codes: (i) x+1/2, −y+1/2, z−1/2; (ii) x, y, z+1; (iii) x+1/2, −y+1/2, z+1/2.				
Compound 4				
D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	1.87	2.663 (10)	152.5
Symmetry code: (i) −x+y+1, y, −z+2/3.				
Compound 5				
D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2^{ii}	0.90	1.80	2.69 (2)	169.5
Symmetry code: (ii) −x+3/2, y+1/2, −z+2.				
Compound 6				
D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3	0.88	1.85	2.699 (12)	162.8
N4—H4···O2^{iii}	0.88	1.81	2.691 (12)	178.1
Symmetry code: (iii) −x+3/2, y+1/2, z+1/2.				