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新型 Zn^{2+}基金属有机框架结构的温度依赖的导电、发光性能及理论计算

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Temperature-Dependent Conductivity, Luminescence and Theoretical Calculations of a Novel Zn(II)-Based Metal-Organic Framework

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Table S1 Crystal data and details of data collection and refinement for compound 1

Compound	1
Formula	$C_{35}H_{37}N_3O_8Zn$
M_r	693.05
Crystal system	Monoclinic
Space group	P2(1)/n
a/nm	1.40797(7)
b/nm	0.90269(3)
c/nm	2.74319(12)
α/(°)	90.00
β/(°)	91.187(5)
γ/(°)	90.00
V/nm^3	3.4857(3)
Z	4
D_c/(g cm^{-3})	1.321
μ/mm^{-1}	0.758
Data/params	6128/424
θ/(°)	2.97-25.00
Obs reflns	4096
Goof on F^2	1.062
$R_1[I>2\sigma(I)]$[a]	0.0613
wR_2(All data)[b]	0.1584

[a] $R_1 = \sum ||F_O| - |F_C|| / \sum |F_O|$; [b] $wR_2 = \{\sum [w(F_O^2 - F_C^2)^2] / \sum [w(F_O^2)^2]\}^{1/2}$

Table S2 Bond length of bond angle of compound 1

Label	Value	Label	Value
Zn(1)-O(1)	0.1946(3)	Zn(1)-O(5)#1	0.1954(3)
Zn(1)-O(4)#2	0.1960(3)	Zn(1)-O(7)	0.2032(3)
O(1)-Zn(1)-O(5)#1	111.36(15)	O(1)-Zn(1)-O(4)#2	106.29(14)
O(5)#1-Zn(1)-O(4)#2	128.78(14)	O(1)-Zn(1)-O(7)	89.38(14)
O(5)#1-Zn(1)-O(7)	108.81(13)	O(4)#2-Zn(1)-O(7)	104.96(15)
C(1)-O(1)-Zn(1)	130.6(3)	C(20)-O(4)-Zn(1)#3	112.1(3)
C(27)-O(5)-Zn(1)#4	109.9(3)	C(33)-O(7)-Zn(1)	128.5(3)

symmetric code: #1 *x*+1/2, -*y*-3/2, *z*-1/2; #2 *x*-1/2, -*y*-1/2, *z*-1/2; #3 *x*+1/2, -*y*-1/2, *z*+1/2; #4 *x*-1/2, -*y*-3/2, *z*+1/2

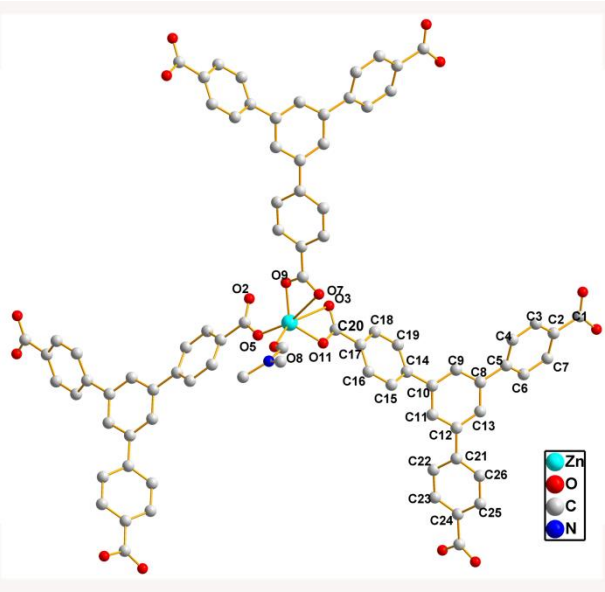

Fig.S1 Coordination environment of Zn^{2+} in 1

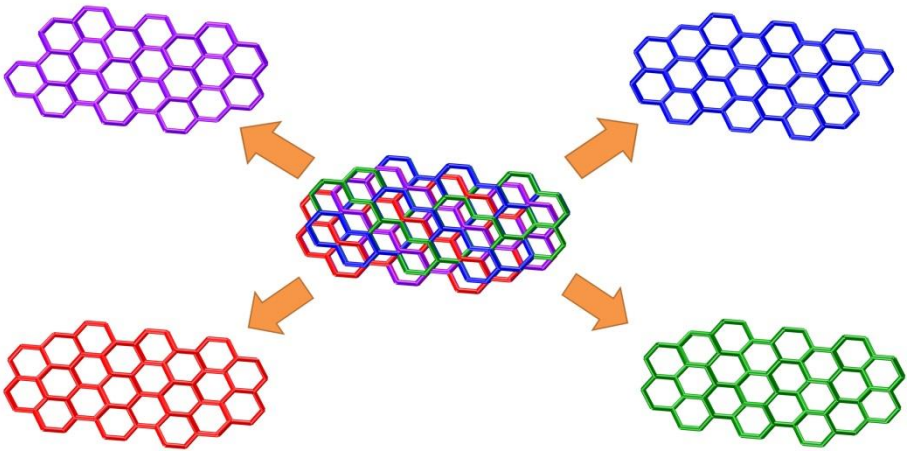

Fig.S2 Four fold interpenetrations structure of 1

Table S3 Comparison between experimental structure and optimized structure

Label	Experimental data	Optimized data
O3-Zn1	0.20309	0.1998
O9-Zn1	0.19528	0.1973
O7-Zn1	0.27506	0.2798
O11-Zn1	0.19626	0.1991
O5-Zn1	0.19456	0.2081
C20-O11	0.12652	0.1258
C20-O3	0.12198	0.1249

atomic label as shown in Fig.S1

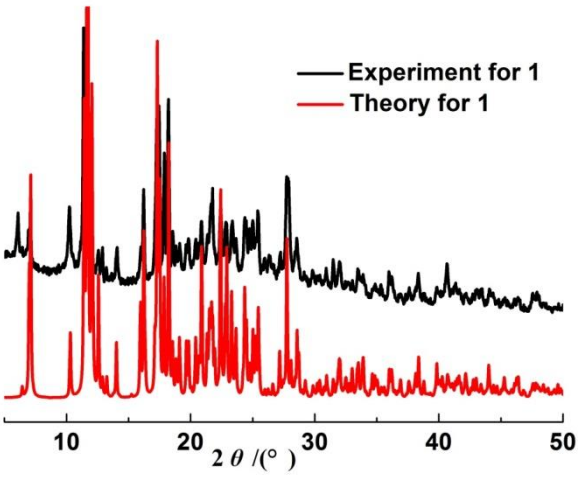

Fig.S3 Experimental and Theoretical PXRD curve of 1

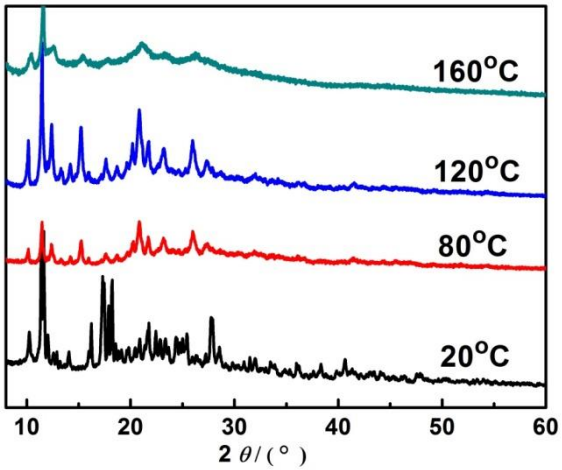

Fig.S4 Experimental PXRD curve of 1 at 20, 80, 120 and 160 °C

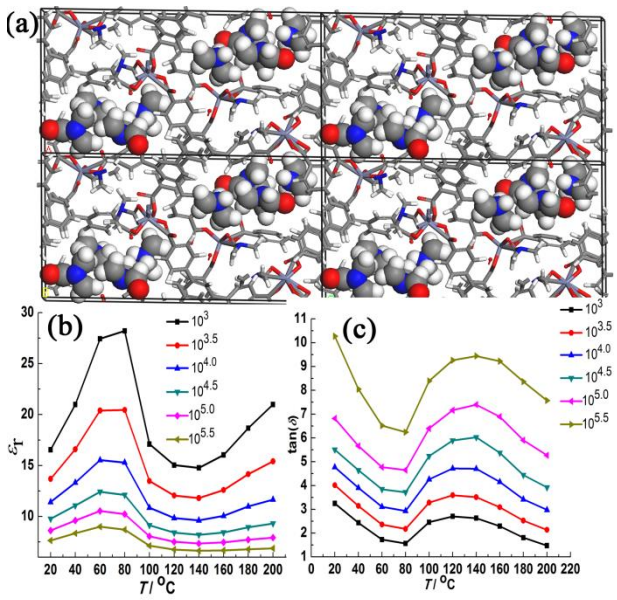

Fig.S5 (a) Relaxed structure at 443 K based on MD simulation; the dielectric constant (b) and the dielectric loss (c) for 1 measured as a function of temperature at various frequencies

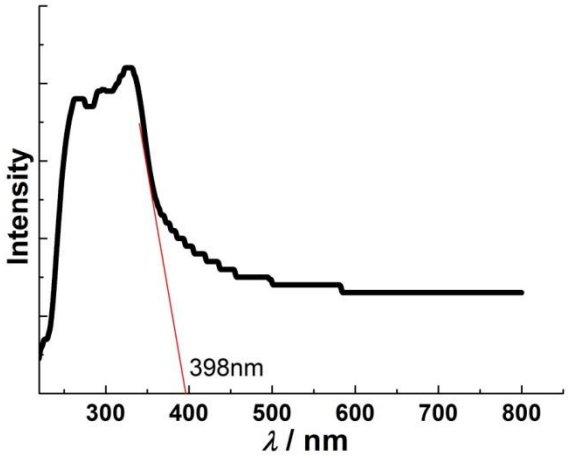

Fig.S6 UV curve of compound 1