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三氮唑取代杯[4]芳烃配位聚合物的合成与荧光性能

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Syntheses and Luminescent Properties of Coordination Polymers Based on 1,2,4-Triazole Substituted Resorcin[4]arene

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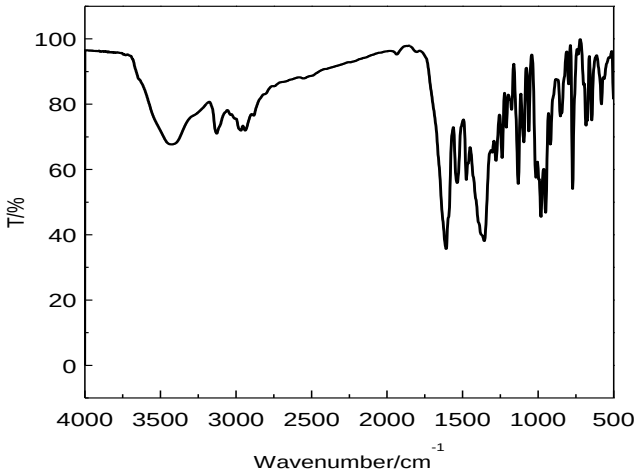

图 S1　化合物 1 的红外光谱

Fig. S1　IR spectrum of compound 1.

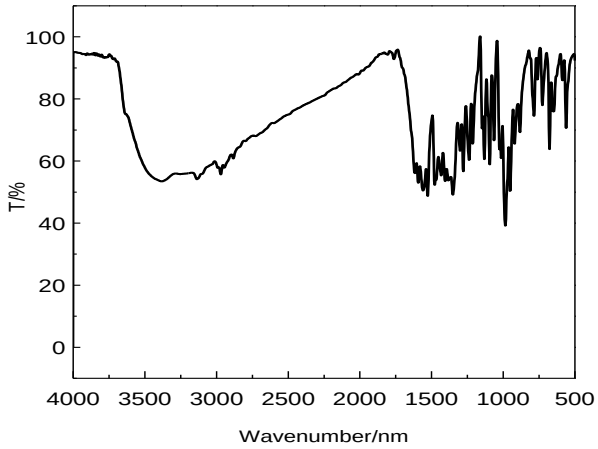

图 S2　化合物 2 红外光谱

Fig. S2　IR spectrum of compound 2.

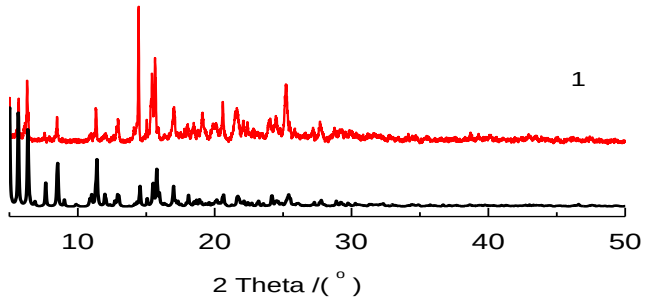

图 S3　化合物 1 模拟(黑线)和测定(红线)的 PXRD

Fig. S3　Simulated (black) and experimental (red) PXRD patterns for compound 1.

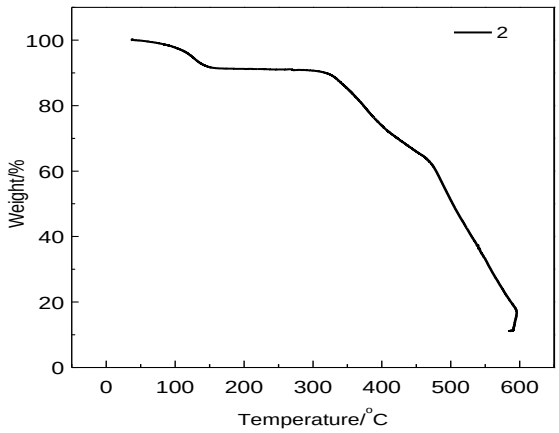

图 S4　化合物 2 的热重图

Fig. S4　TGA of compound 2.

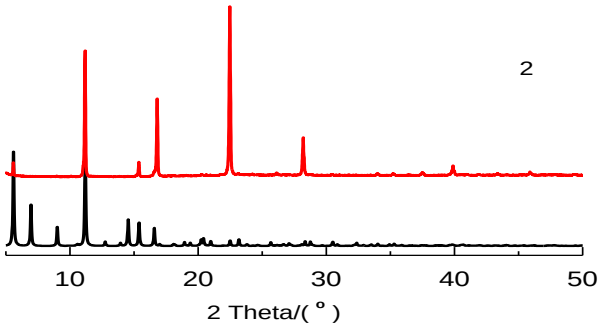

图 S5　化合物 2 模拟(黑线)和测定(红线)的 PXRD

Fig. S5　Simulated (black) and experimental (red) PXRD patterns for compound 2.

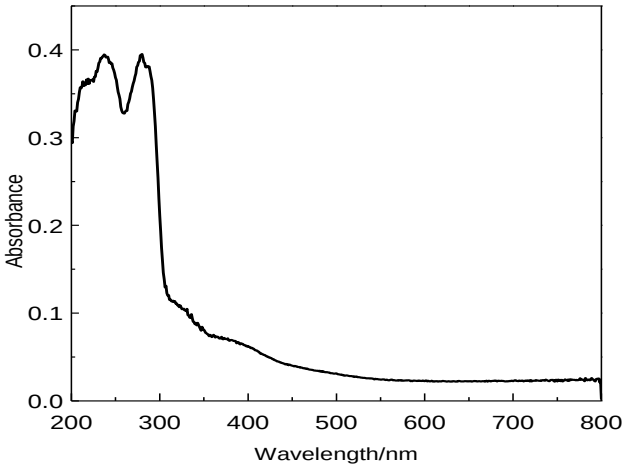

图 S6　室温下，化合物 1 在固态时的紫外吸收光谱

Fig. S6　UV-Vis spectrum of compound 1 in the solid state at room temperature.

表 S1　化合物 1 的键长(nm)和键角(°)

Table S1　Selected bond distances (nm) and angles (°) for compound 1.

Item	Value	Item	Value
Zn(1)－O(13)	0.1901(3)	Zn(1)－O(11)	0.1986(3)
Zn(1)－N(9)	0.2019(3)	Zn(1)－N(12)	0.2063(3)
Zn(2)－O(10)	0.2034(5)	Zn(2)－N(3)	0.2046(4)
Zn(2)－N(6)	0.2060(3)	Zn(2)－O(15)$^{\#1}$	0.2087(4)
Zn(2)－O(16)$^{\#1}$	0.2297(4)	Zn(2)－C(61)$^{\#1}$	0.2546(5)
O(13)－Zn(1)－O(11)	111.69(13)	O(13)－Zn(1)－N(9)	123.68(13)
O(11)－Zn(1)－N(9)	109.74(13)	O(13)－Zn(1)－N(12)	117.42(13)
O(11)－Zn(1)－N(12)	94.62(14)	N(9)－Zn(1)－N(12)	95.07(13)
O(10)－Zn(2)－N(3)	136.4(3)	O(10)－Zn(2)－N(6)	97.84(18)
N(3)－Zn(2)－N(6)	93.82(14)	O(10)－Zn(2)－O(15)$^{\#1}$	91.99(18)
N(3)－Zn(2)－O(15)$^{\#1}$	102.96(17)	N(6)－Zn(2)－O(15)$^{\#1}$	143.48(18)
O(10)－Zn(2)－O(16)$^{\#1}$	127.8(3)	N(3)－Zn(2)－O(16)$^{\#1}$	93.93(16)
N(6)－Zn(2)－O(16)$^{\#1}$	89.61(14)	O(15)$^{\#1}$－Zn(2)－O(16)$^{\#1}$	57.43(17)

表 S2　化合物 2 的键长(nm)和键角(°)

Table S2　Selected bond distances (nm) and angles (°) for compound 2.

Item	Value	Item	Value
Co(1)－Cl(2)	0.2110(7)	Co(1)－N(2)$^{\#1}$	0.2134(3)
Co(1)－N(2)	0.2134(3)	Co(1)－N(2)$^{\#2}$	0.2134(3)
Co(1)－N(2)$^{\#3}$	0.2134(3)	Co(1)－Cl(1)	0.2459(3)
Cl(2)－Co(1)－N(2)$^{\#1}$	89.42(10)	Cl(2)－Co(1)－N(2)	89.42(10)
N(2)$^{\#1}$－Co(1)－N(2)	178.85(19)	Cl(2)－Co(1)－N(2)$^{\#2}$	89.42(10)
N(2)$^{\#1}$－Co(1)－N(2)$^{\#2}$	89.994(3)	N(2)－Co(1)－N(2)$^{\#2}$	89.994(2)
Cl(2)－Co(1)－N(2)$^{\#3}$	89.42(10)	N(2)$^{\#1}$－Co(1)－N(2)$^{\#3}$	89.994(2)
N(2)－Co(1)－N(2)$^{\#3}$	89.994(3)	N(2)$^{\#2}$－Co(1)－N(2)$^{\#3}$	178.85(19)
Cl(2)－Co(1)－Cl(1)	180.000(1)	N(2)$^{\#1}$－Co(1)－Cl(1)	90.58(10)
N(2)－Co(1)－Cl(1)	90.58(10)	N(2)$^{\#2}$－Co(1)－Cl(1)	90.58(10)
N(2)$^{\#3}$－Co(1)－Cl(1)	90.58(10)		