Supporting Information

A Stable 3D Porous Coordination Polymer as Multi-Chemosensor to Cr(IV) anion and Fe(III) cation and Its Selective Adsorption of Malachite Green Oxalate Dye

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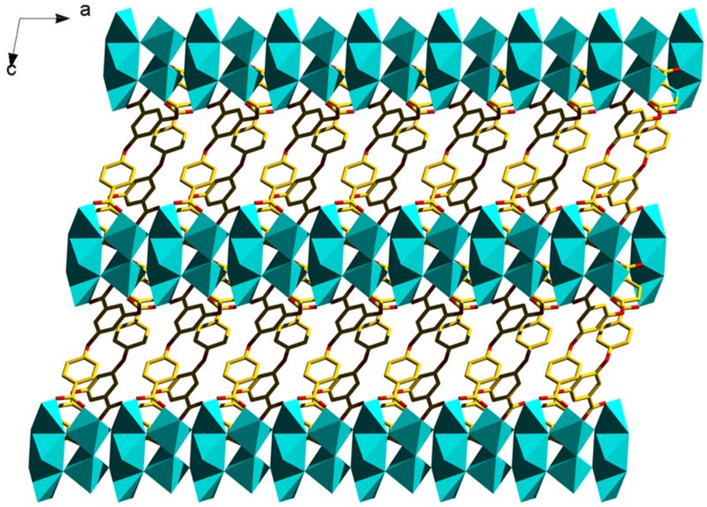
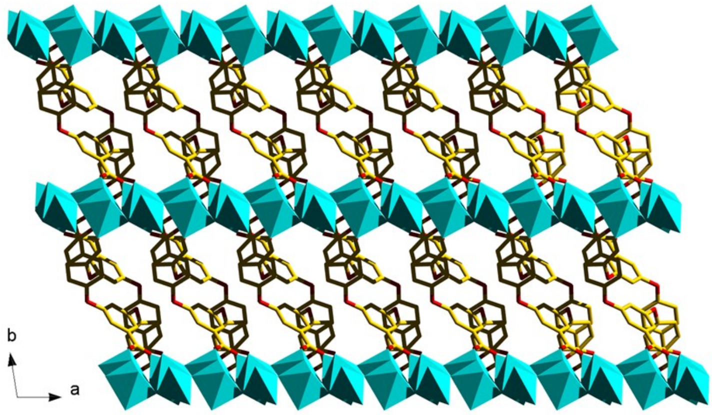


Figure S1. The 3D structure of **1** along the *b* axis.



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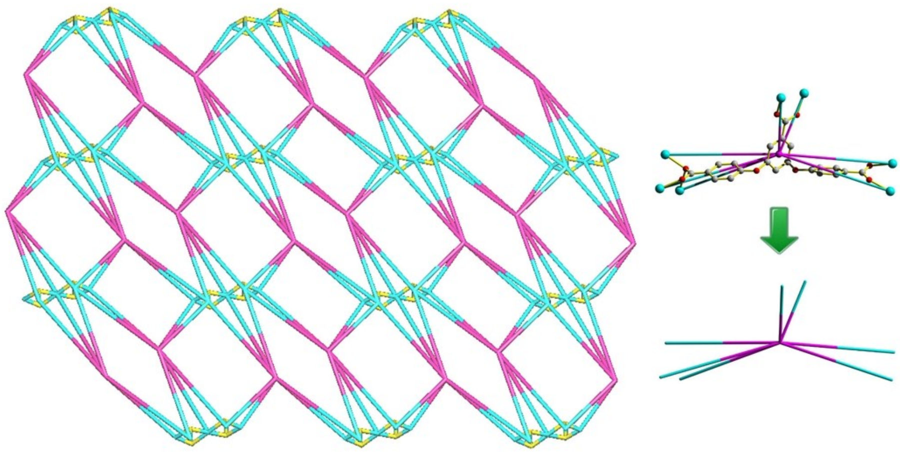

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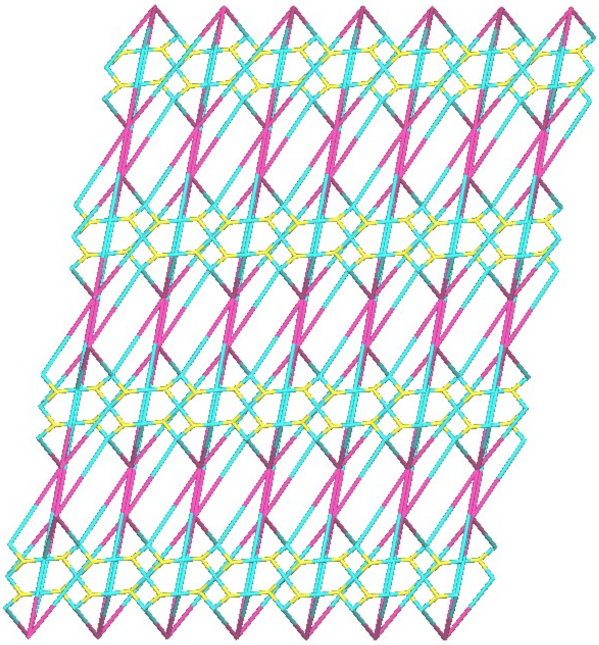

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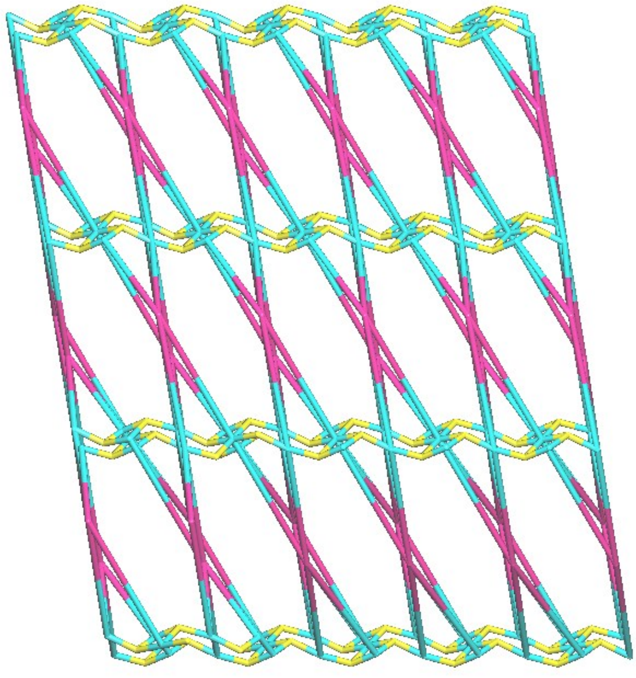

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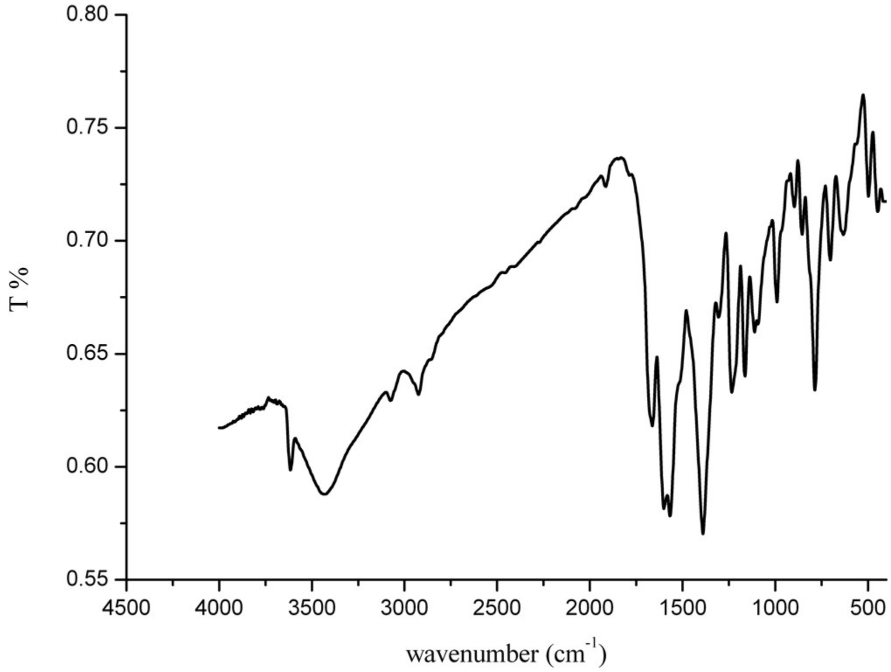
(2) IR RESULTs



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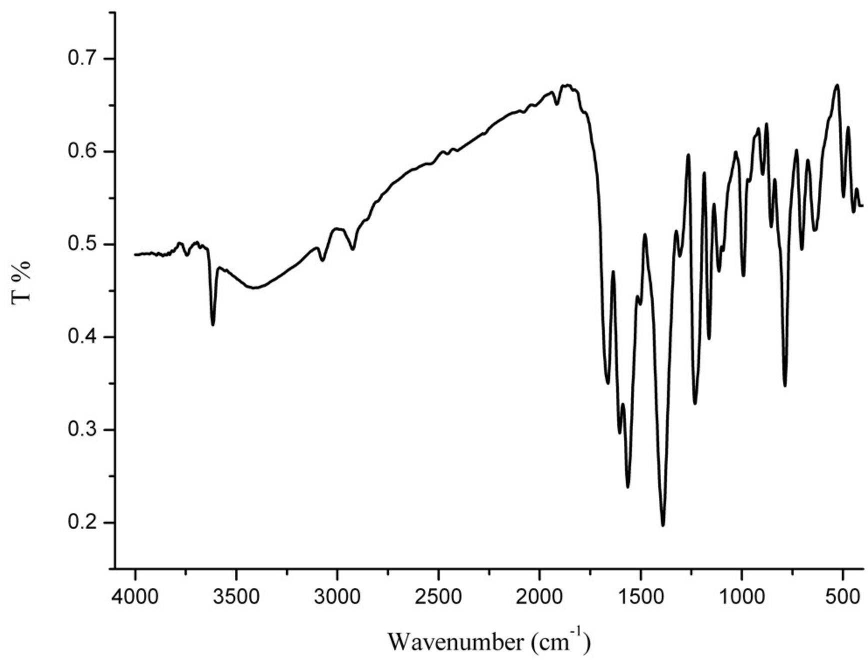

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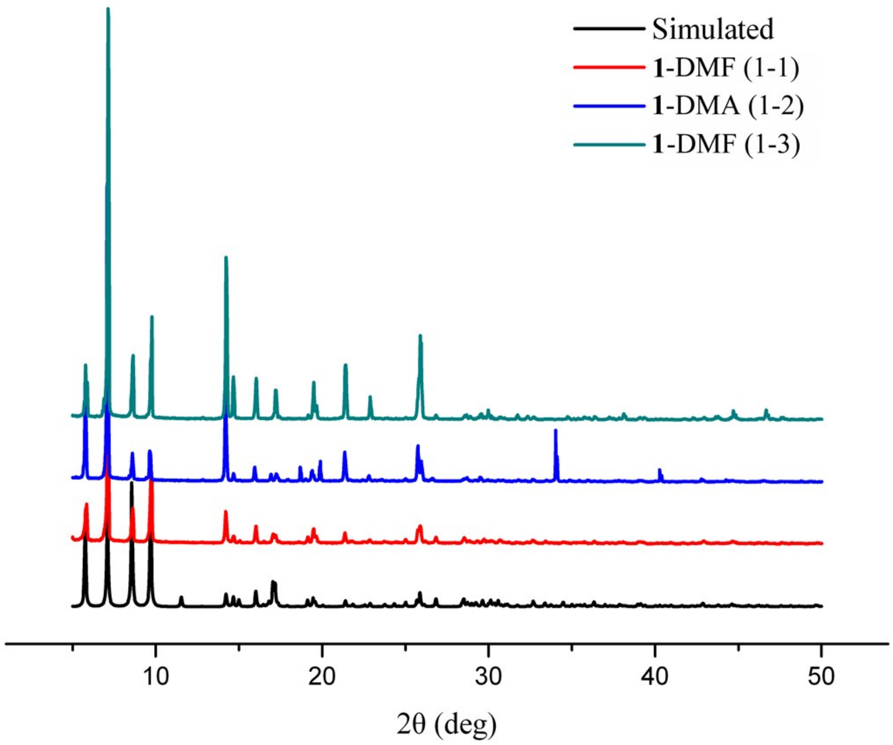

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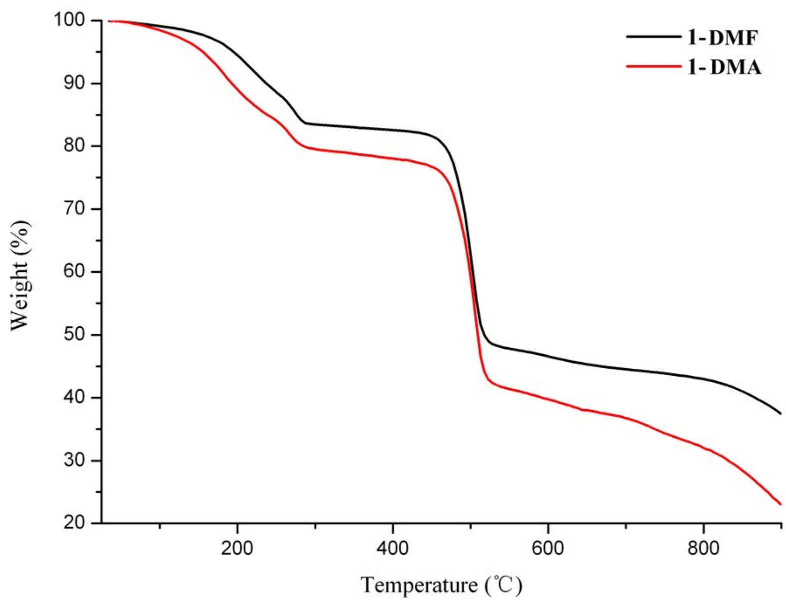

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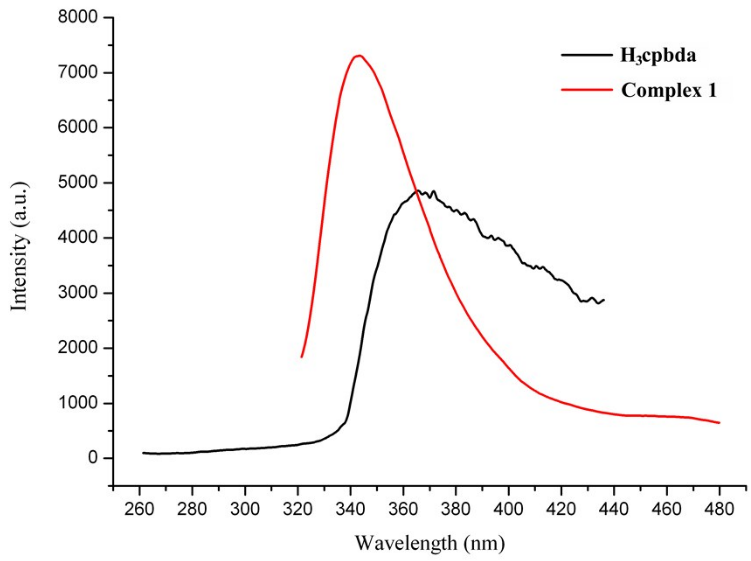

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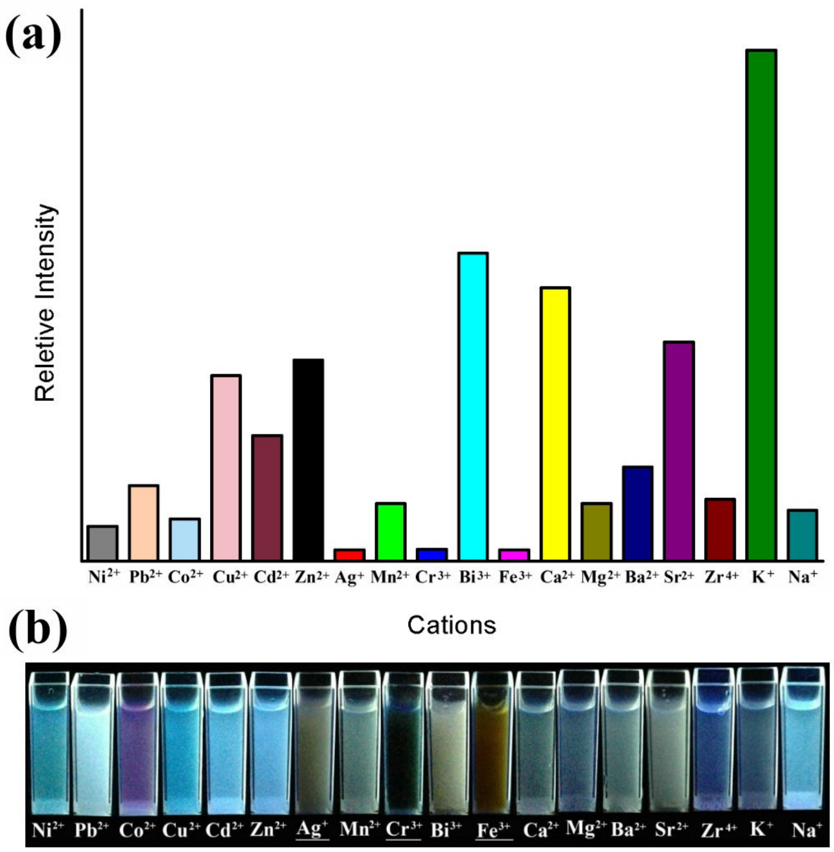

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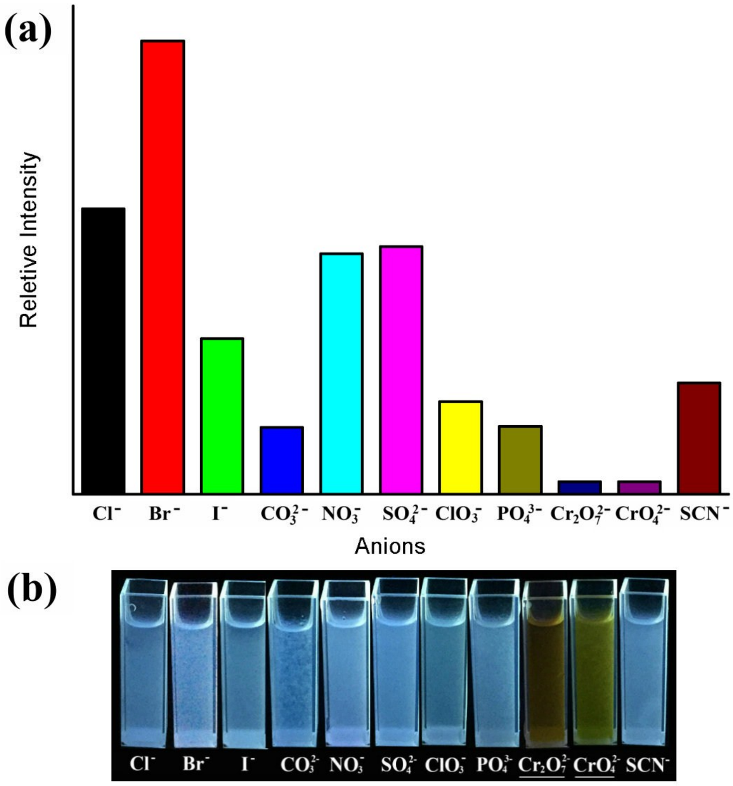

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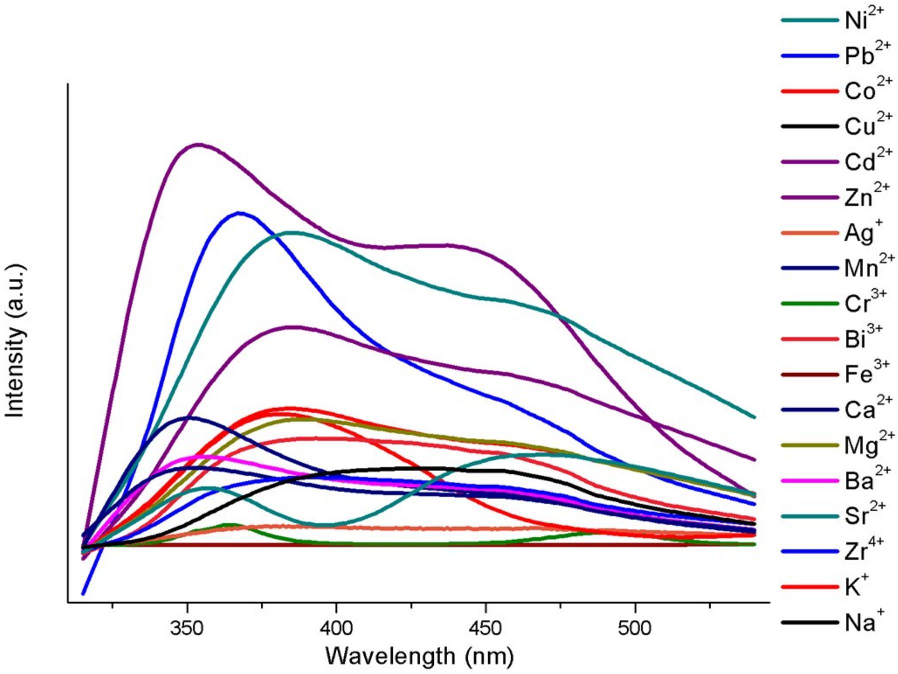

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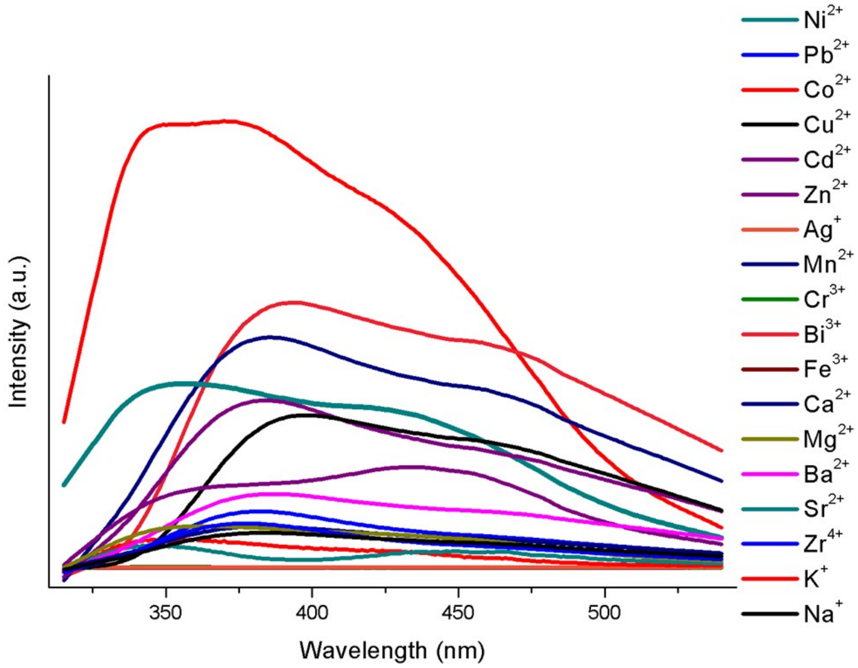

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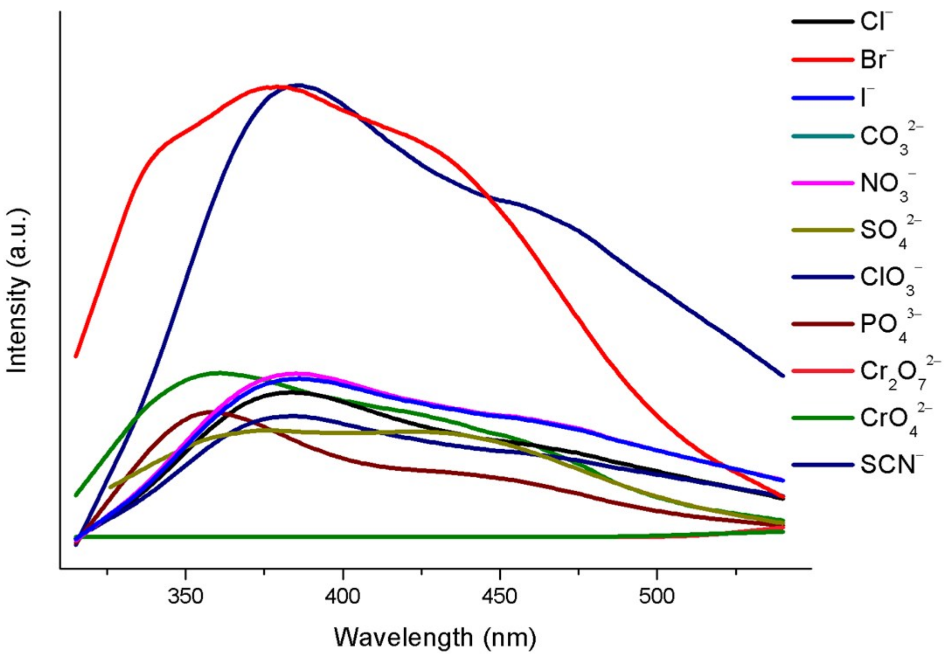

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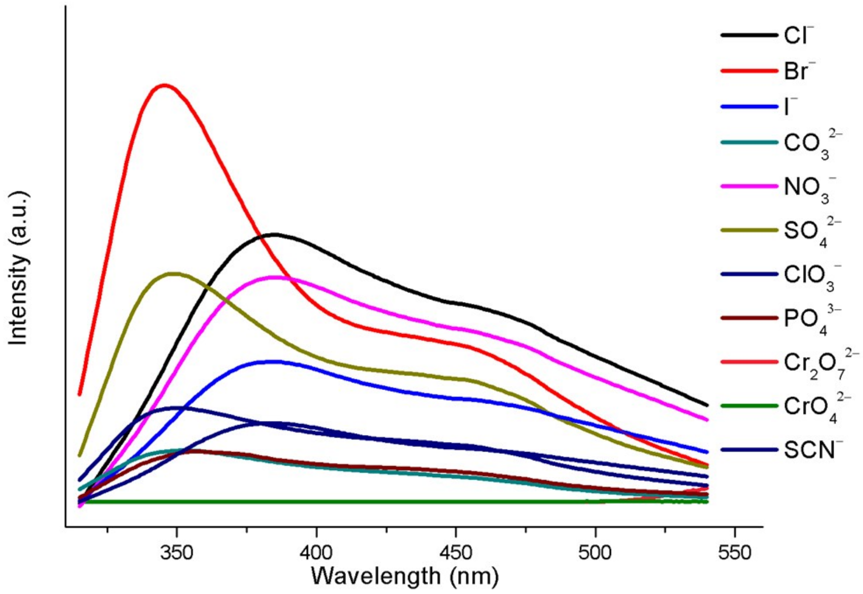

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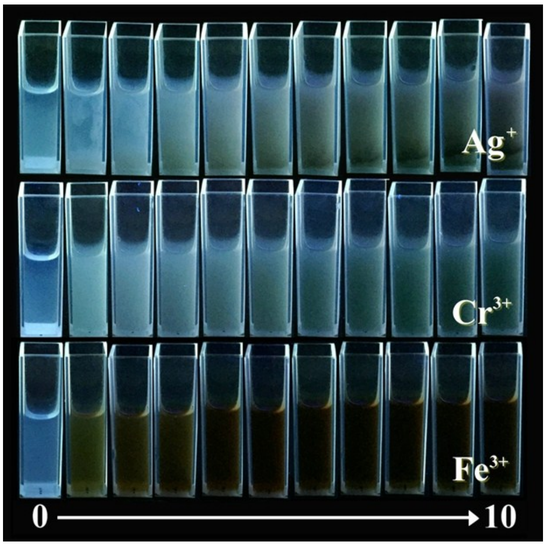

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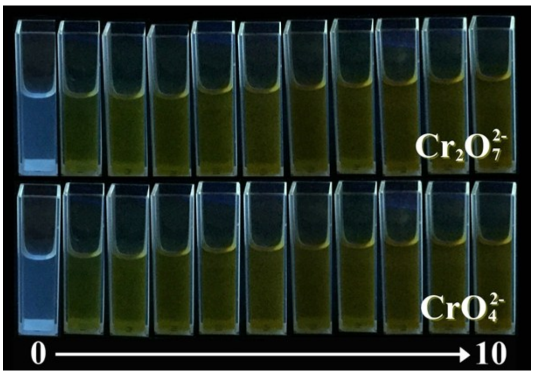

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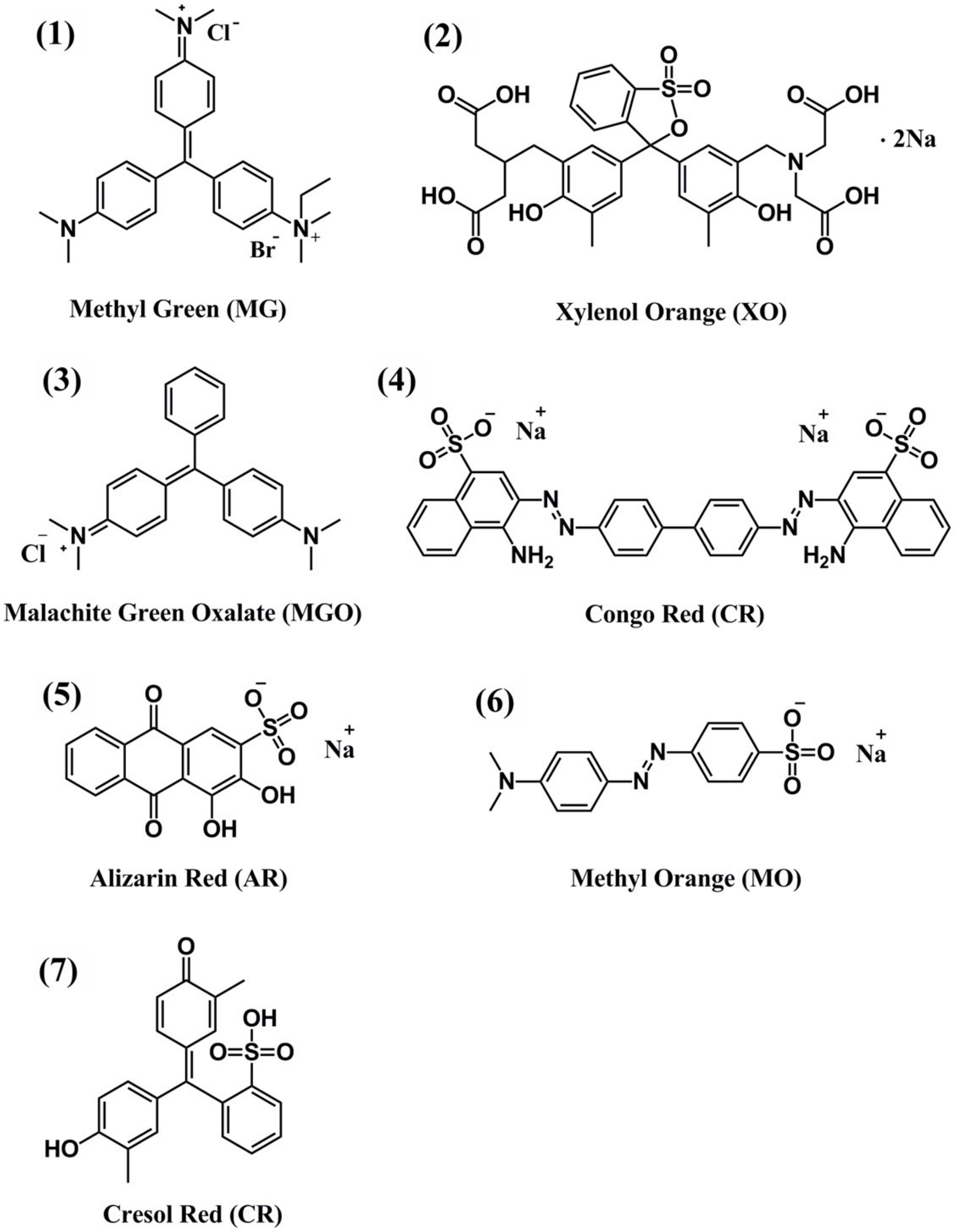
(5) MOLECULAR FORMULA OF DYES



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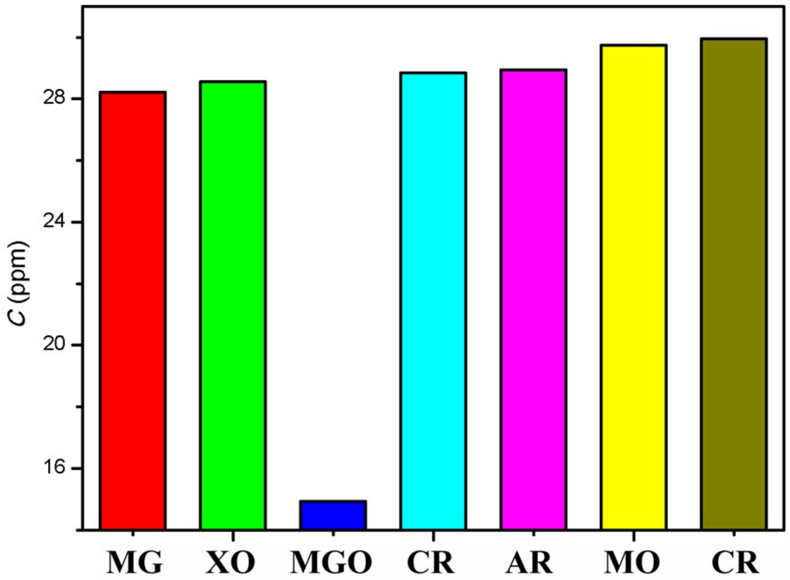

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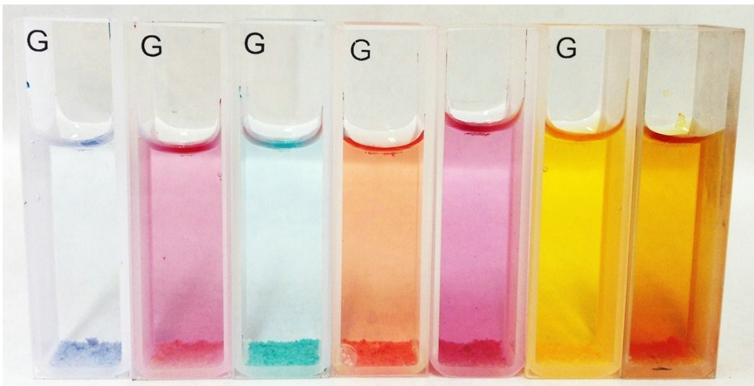

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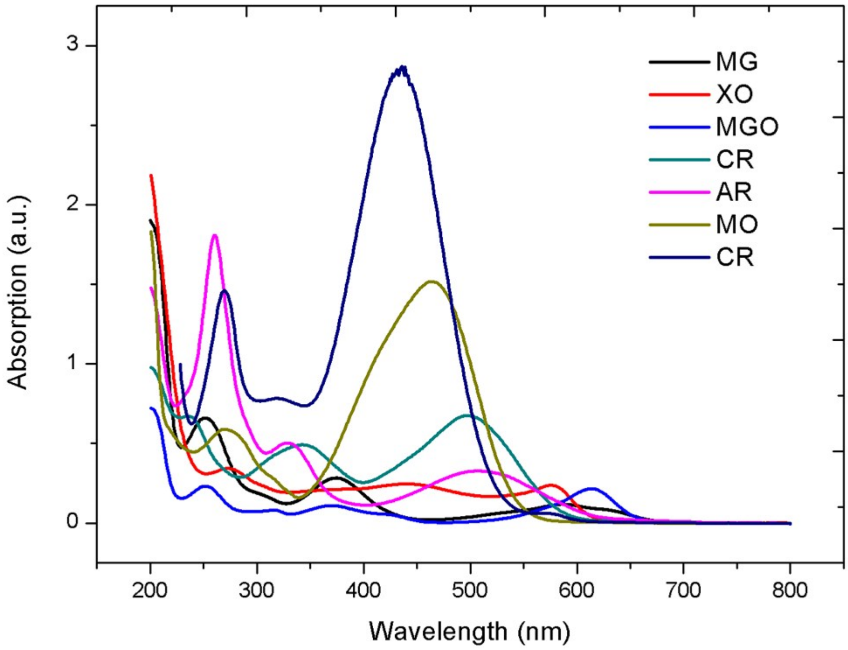

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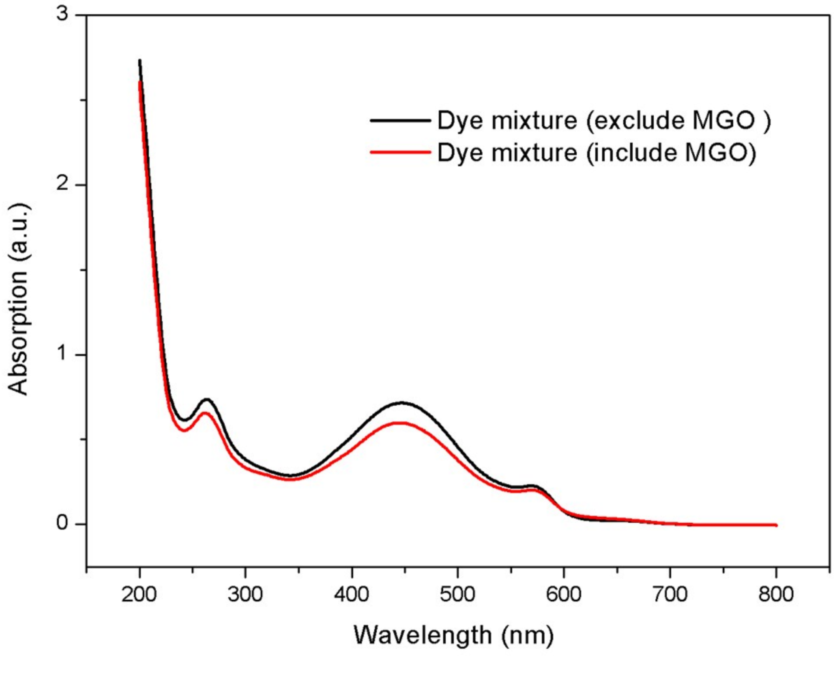

Figure S23. The UV spectrum of six dyes mixture (exclude MGO) and seven dyes mixture (include MGO)

(6) CRYSTALLOGRAPHIC DATAS TABLES

Table S1. Crystallographic data and details of diffraction experiments for complexes **1**.

Complex 1			
Formula	C42 H26 O20 Zn5	V (Å^3)	1217.3
M_r	1177.48	Z	1
Crystal system	triclinic	ρ (g cm^{-3})	1.606
Space group	$P\bar{1}$	μ (mm^{-1})	2.501
a (Å)	6.327	T (K)	296(2)
b (Å)	12.671	Goof	1.001
c (Å)	15.684	R [$I > 2\sigma(I)$]	R_1 = 0.0432
α (°)	95.69		wR_2 = 0.1390
β (°)	99.77	R (all data)	R_1 = 0.0530
γ (°)	98.01		wR_2 = 0.1454

Table S2. Selected Bond Lengths (Å) and Angles (deg) for **1**.

Complex **1**			
Zn(1)-O(2W)	2.007(3)	Zn(1)-O(8)#4	2.102(4)
Zn(1)-O(1)	2.064(4)	Zn(1)-O(4)#2	2.130(3)
Zn(1)-O(1W)	2.012(3)	Zn(1)-O(4)#7	2.435(3)
Zn(2)-O(2)	1.924(4)	Zn(2)-O(1W)	1.981(3)
Zn(2)-O(7)#5	1.924(4)	Zn(2)-O(2W)#8	1.978(3)
Zn(3)-O(1W)	2.080(3)	Zn(3)-O(2W)#8	2.200(3)
Zn(3)-O(5)#2	2.063(3)		
O(1W)-Zn(1)-O(4)#7	78.40(12)	O(4)#2-Zn(1)-O(4)#7	81.89(13)
O(1W)-Zn(1)-O(8)#4	85.14(14)	O(2W)-Zn(1)-O(4)#2	86.85(13)
O(8)#4-Zn(1)-O(4)#7	88.69(14)	O(2W)-Zn(1)-O(4)#7	90.32(12)
O(2W)-Zn(1)-O(8)#4	92.13(14)	O(1)-Zn(1)-O(8)#4	92.97(16)
O(1W)-Zn(1)-O(4)#2	93.99(13)	O(1W)-Zn(1)-O(1)	94.72(14)
O(2W)-Zn(1)-O(1)	96.64(15)	O(1)-Zn(1)-O(4)#2	96.51(14)
O(2W)-Zn(1)-O(1W)	168.44(14)	O(8)#4-Zn(1)-O(4)#2	170.51(15)
O(1)-Zn(1)-O(4)#7	172.77(12)	O(2W)#8-Zn(2)-O(1W)	91.45(13)
O(2)-Zn(2)-O(7)#5	113.48(17)	O(2)-Zn(2)-O(2W)#8	118.09(17)
O(7)#5-Zn(2)-O(2W)#8	111.92(14)	O(2)-Zn(2)-O(1W)	109.20(15)
O(7)#5-Zn(2)-O(1W)	110.39(15)	O(5)#9-Zn(3)-O(1W)	84.85(13)
O(1W)-Zn(3)-O(2W)#8	82.89(12)	O(5)#9-Zn(3)-O(2W)#8	93.94(13)
O(5)#2-Zn(3)-O(2W)#8	86.06(13)	O(5)#2-Zn(3)-O(1W)	95.15(13)
O(1W)-Zn(3)-O(2W)#11	97.11(12)	O(1W)#10-Zn(3)-O(1W)	180.0
O(5)#9-Zn(3)-O(5)#2	180.00(19)		

Symmetry transformations used to generate equivalent atoms: #1 x-1,y+1,z; #2 -x+2,-y+1,-z+1; #3 x,y+1,z; #4 -x+2,-y,-z; #5 -x+3,-y,-z; #6 x-1,y,z; #7 x,y-1,z; #8 x+1,y,z; #9 x+1,y-1,z; #10 -x+3,-y,-z+1; #11 -x+2,-y,-z+1.

REFERENCES

[1] Sheldrick G M. *SHELXL-97*, *Program for Crystal Structure Determination*, University of Göttingen, Germany, 1997.

[2] Sheldrick G M. *SHELXL-97*, P*rogram for Crystal Structure Refinement*, University of Göttingen, Germany, 1997.