Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supporting Information

A New Methylviologen-templated Zinc Gallophosphate Zeolite With Photo-/Thermochromism, Fluorescent and Photoelectric Properties

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Table S1 Crystal data and structure refinement for JU104[a].

Empirical formula	$Ga_{7.10}\ Zn_{2.90}\ O_{40}\ P_{10}$
Formula weight	1634.28
Temperature	296(2) K
Wavelength(Å)	0.71073
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	
a (Å)	9.8360(14)
b (Å)	12.4488(17)
c (Å)	12.6145(18)
α(deg)	63.243(2)
β(deg)	74.343(2)
γ (deg)	76.077(2)
Volume(Å^3)	1315.2(3)
Z, calculated density(mg m^{-3})	1, 2.063
Absorption coefficient(mm^{-1})	5.266
F(000)	777
Crystal size(mm^3)	0.20 x 0.18 x 0.17
θ range(°) for data collection	1.84–28.33
Limiting indices	$-12 \le h \le 13, -16 \le k \le 15, -16 \le l \le 16$
Reflections collected/unique	9796 / 6498 [*R*(int) = 0.0417]
Completeness to θ (%)	28.33, 98.9
Absorption correction	semi-empirical from equivalents
Max. and min. transmission	0.4680 and 0.4190
Refinement method	full-matrix least-squares on F^2
Data/restraints/parameters	6498 / 40 / 280
Goodness-of-fit on F^2	0.912
Final *R* indices [$I > 2\ \sigma\ (I)$]	$R_1 = 0.0456$, w$R_2 = 0.0970$
R indices (all data)	$R_1 = 0.0754$, w$R_2 = 0.1050$
Largest diff. peak and hole (eÅ^{-3})	1.553 and -1.079

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w=1/[\sigma^2(F_o^2)+(0.0595P)^2+2.8937P]$ where $P=(F_o^2+2F_c^2)/3$

Table S2 Bond lengths [Å] and angles [deg] for JU104.

Ga(1)-O(2)	1.853(4)	P(5)-O(11)	1.514(4)
Ga(1)-O(1)	1.854(4)	P(5)-O(14)	1.518(4)
Ga(1)-O(4)	1.856(4)	P(5)-O(20)#6	1.528(4)
Ga(1)-O(3)	1.872(4)	P(5)-O(17)	1.536(4)
Ga(2)-O(8)	1.809(4)	O(1)-P(2)#4	1.527(4)
Ga(2)-O(7)	1.823(4)	O(3)-P(4)#1	1.496(4)
Ga(2)-O(6)	1.824(4)	O(7)-P(4)#1	1.534(4)
Ga(2)-O(5)	1.827(4)	O(10)-P(1)#1	1.534(4)
Ga(3)-O(9)	1.832(4)	O(12)-P(3)#5	1.497(4)
Ga(3)-O(10)	1.837(4)	O(13)-P(1)#1	1.500(5)
Ga(3)-O(12)	1.835(4)	O(15)-P(1)#7	1.518(4)
Ga(3)-O(11)	1.853(4)	O(16)-P(3)#8	1.524(4)
Ga(4)-Ga(4')	0.527(6)	O(18)-P(2)#8	1.515(4)
Ga(4)-O(14)	1.801(4)	O(20)-P(5)#6	1.528(4)
Ga(4)-O(16)	1.811(4)	O(2)-Ga(1)-O(1)	114.80(18)
Ga(4)-O(13)	1.829(5)	O(2)-Ga(1)-O(4)	105.60(18)
Ga(4)-O(15)	1.863(4)	O(1)-Ga(1)-O(4	106.41(19)
Ga(4')-O(13)	1.474(11)	O(2)-Ga(1)-O(3)	107.38(18)
Ga(4')-O(15)	1.807(12)	O(1)-Ga(1)-O(3)	115.16(18)
Ga(4')-O(16)	2.064(10)	O(4)-Ga(1)-O(3)	106.79(18)
Ga(4')-O(14)	2.204(9)	O(8)-Ga(2)-O(7)	102.52(18)
Ga(5)-O(18)	1.829(4)	O(8)-Ga(2)-O(6)	110.03(19)
Ga(5)-O(19)	1.833(3)	O(7)-Ga(2)-O(6)	111.39(18)
Ga(5)-O(20)	1.841(4)	O(8)-Ga(2)-O(5)	112.12(19)
Ga(5)-O(17)	1.840(4)	O(7)-Ga(2)-O(5)	117.85(17)
P(1)-O(13)#1	1.500(5)	O(6)-Ga(2)-O(5)	103.04(18)
P(1)-O(15)#2	1.518(4)	O(9)-Ga(3)-O(10)	112.15(19)
P(1)-O(10)#1	1.534(4)	O(9)-Ga(3)-O(12)	108.3(2)
P(1)-O(2)	1.538(4)	O(10)-Ga(3)-O(12)	109.2(2)
P(1)-Zn(4')#2	2.858(10)	O(9)-Ga(3)-O(11)	105.93(19)
P(1)-Zn(4')#1	2.887(9)	O(10)-Ga(3)-O(11)	116.37(19)
P(2)-O(18)#3	1.515(4)	O(12)-Ga(3)-O(11)	104.39(18)
P(2)-O(1)#4	1.527(4)	Ga(4')-Ga(4)-O(14)	134.8(13)
P(2)-O(5)	1.527(4)	Ga(4')-Ga(4)-O(16)	111.7(13)
P(2)-O(4)	1.543(4)	O(14)-Ga(4)-O(16)	110.42(19)
P(3)-O(12)#5	1.497(4)	Ga(4')-Ga(4)-O(13)	41.2(13)
P(3)-O(9)	1.513(4)	O(14)-Ga(4)-O(13)	109.1(2)
P(3)-O(8)	1.522(4)	O(16)-Ga(4)-O(13)	108.1(2)
P(3)-O(16)#3	1.524(4)	Ga(4')-Ga(4)-O(15)	75.8(14)
P(4)-O(3)#1	1.496(4)	O(14)-Ga(4)-O(15)	105.4(2)
P(4)-O(6)	1.520(4)	O(16)-Ga(4)-O(15)	108.7(2)
P(4)-O(19)	1.535(4)	O(13)-Ga(4)-O(15)	115.1(2)
P(4)-O(7)#1	1.534(4)	Ga(4)-Ga(4')-O(13)	125.1(16)

Ga(4)-Ga(4')-O(15)	87.8(14)	O(6)-P(4)-O(19)	107.4(2)
O(13)-Ga(4')-O(15)	143.1(6)	O(3)#1-P(4)-O(7)#1	110.3(2)
Ga(4)-Ga(4')-O(16)	54.6(11)	O(6)-P(4)-O(7)#1	109.4(2)
O(13)-Ga(4')-O(16)	111.7(6)	O(19)-P(4)-O(7)#1	107.8(2)
O(15)-Ga(4')-O(16)	100.7(5)	O(11)-P(5)-O(14)	111.6(2)
Ga(4)-Ga(4')-O(14)	35.4(11)	O(11)-P(5)-O(20)#6	106.4(2)
O(13)-Ga(4')-O(14)	105.3(6)	O(14)-P(5)-O(20)#6	108.3(3)
O(15)-Ga(4')-O(14)	92.7(4)	O(11)-P(5)-O(17)	110.0(2)
O(16)-Ga(4')-O(14)	88.0(3)	O(14)-P(5)-O(17)	110.2(2)
O(18)-Ga(5)-O(19)	111.59(18)	O(20)#6-P(5)-O(17)	110.2(2)
O(18)-Ga(5)-O(20)	105.6(2)	P(2)#4-O(1)-Ga(1)	140.9(3)
O(19)-Ga(5)-O(20)	102.34(18)	P(1)-O(2)-Ga(1)	124.1(2)
O(18)-Ga(5)-O(17)	114.57(19)	P(4)#1-O(3)-Ga(1)	147.4(3)
O(19)-Ga(5)-O(17)	111.74(17)	P(2)-O(4)-Ga(1)	123.6(2)
O(20)-Ga(5)-O(17)	110.06(18)	P(2)-O(5)-Ga(2)	127.7(2)
O(13)#1-P(1)-O(15)#2	111.7(3)	P(4)-O(6)-Ga(2)	134.9(2)
O(13)#1-P(1)-O(10)#1	110.4(3)	P(4)#1-O(7)-Ga(2)	135.8(3)
O(15)#2-P(1)-O(10)#1	109.9(3)	P(3)-O(8)-Ga(2)	138.4(3)
O(13)#1-P(1)-O(2)	110.0(3)	P(3)-O(9)-Ga(3)	137.8(3)
O(15)#2-P(1)-O(2)	106.5(2)	P(1)#1-O(10)-Ga(3)	129.6(3)
O(10)#1-P(1)-O(2)	108.1(2)	P(5)-O(11)-Ga(3)	139.7(3)
O(13)#1-P(1)-Zn(4')#2	85.7(3)	P(3)#5-O(12)-Ga(3)	146.1(3)
O(15)#2-P(1)-Zn(4')#2	33.9(2)	Ga(4')-O(13)-P(1)#1	152.2(5)
O(10)#1-P(1)-Zn(4')#2	101.3(3)	Ga(4')-O(13)-Ga(4)	13.6(3)
O(2)-P(1)-Zn(4')#2	138.2(2)	P(1)#1-O(13)-Ga(4)	162.2(4)
O(13)#1-P(1)-Zn(4')#1	13.8(3)	P(5)-O(14)-Ga(4)	131.1(3)
O(15)#2-P(1)-Zn(4')#1	101.3(3)	P(5)-O(14)-Ga(4')	121.3(3)
O(10)#1-P(1)-Zn(4')#1	107.5(3)	Ga(4)-O(14)-Ga(4')	9.8(3)
O(2)-P(1)-Zn(4')#1	122.9(3)	P(1)#7-O(15)-Ga(4')	118.2(3)
Zn(4')#2-P(1)-Zn(4')#1	72.9(2)	P(1)#7-O(15)-Ga(4)	133.6(3)
O(18)#3-P(2)-O(1)#4	113.5(3)	Ga(4')-O(15)-Ga(4)	16.43(19)
O(18)#3-P(2)-O(5)	107.4(2)	P(3)#8-O(16)-Ga(4)	134.0(3)
O(1)#4-P(2)-O(5)	107.2(2)	P(3)#8-O(16)-Ga(4')	120.4(3)
O(18)#3-P(2)-O(4)	108.3(2)	Ga(4)-O(16)-Ga(4')	13.7(2)
O(1)#4-P(2)-O(4)	110.8(2)	P(5)-O(17)-Ga(5)	135.7(2)
O(5)-P(2)-O(4)	109.5(2)	P(2)#8-O(18)-Ga(5)	131.2(3)
O(12)#5-P(3)-O(9)	112.6(3)	P(4)-O(19)-Ga(5)	133.5(2)
O(12)#5-P(3)-O(8)	105.0(2)	P(5)#6-O(20)-Ga(5)	135.0(3)
O(9)-P(3)-O(8)	109.9(3)		
O(12)#5-P(3)-O(16)#3	112.3(3)		
O(9)-P(3)-O(16)#3	106.1(2)		
O(8)-P(3)-O(16)#3	111.0(2)		
O(3)#1-P(4)-O(6)	108.9(2)		
O(3)#1-P(4)-O(19)	113.1(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z #2 x+1,y+1,z-1 #3 x+1,y,z

#4 -x+3,-y+2,-z #5 -x+2,-y+1,-z+1

#6 -x+1,-y+2,-z+1 #7 x-1,y-1,z+1

#8 x-1,y,z

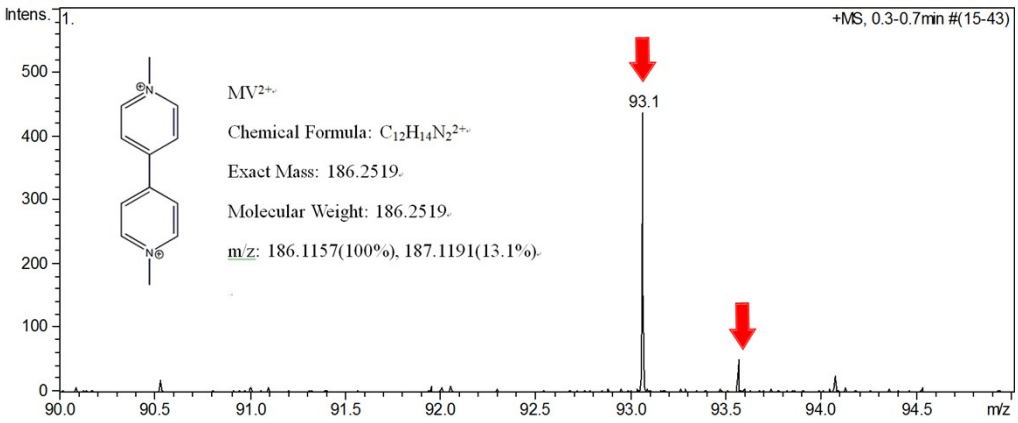


Figure S1 High resolution liquid chromatography-mass spectrum (LC-HRMS) of JU104.

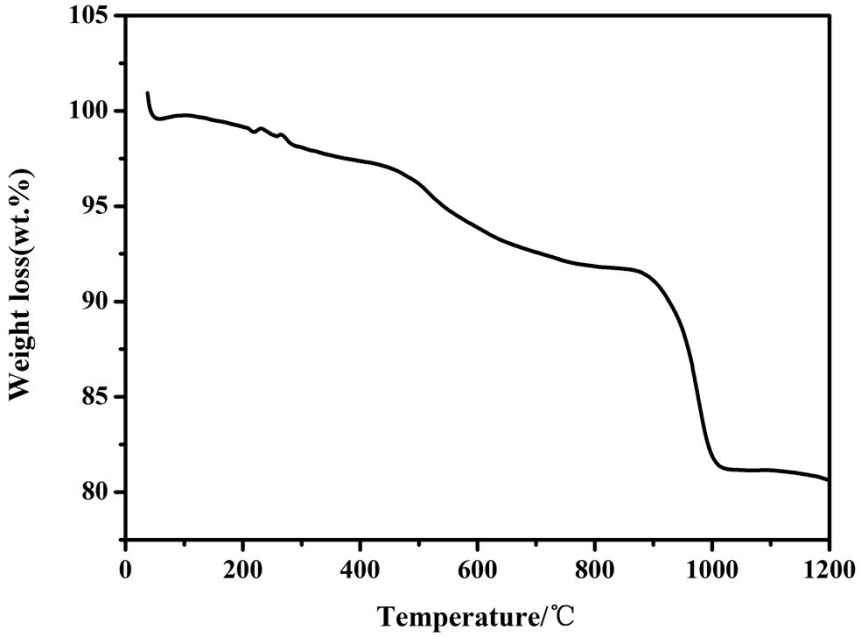


Figure S2 TG analysis of JU104 (totally weight loss: 19.68 wt% from RT to 1200 °C).

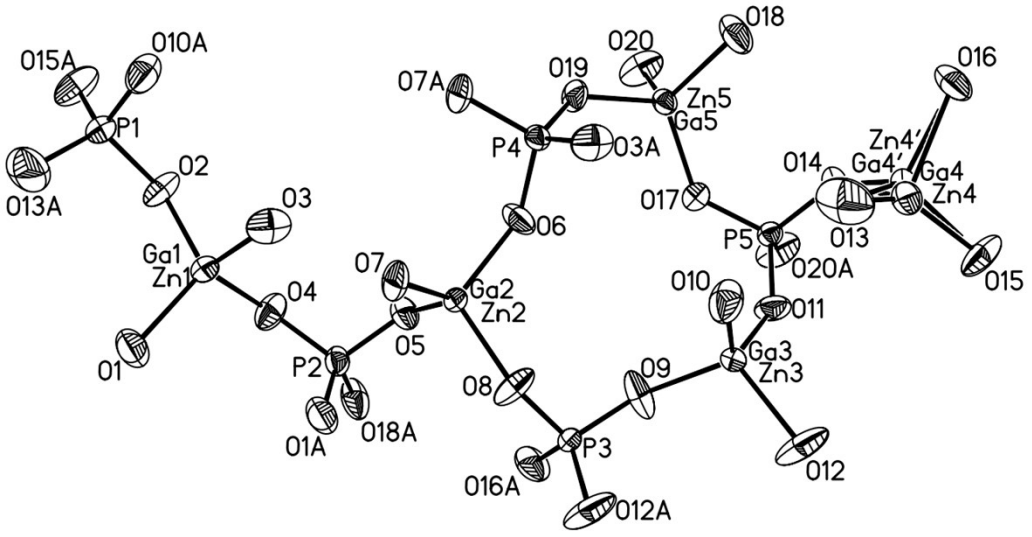


Figure S3 Thermal ellipsoids of JU104 given at 50% probability, showing the atomic labelling scheme.

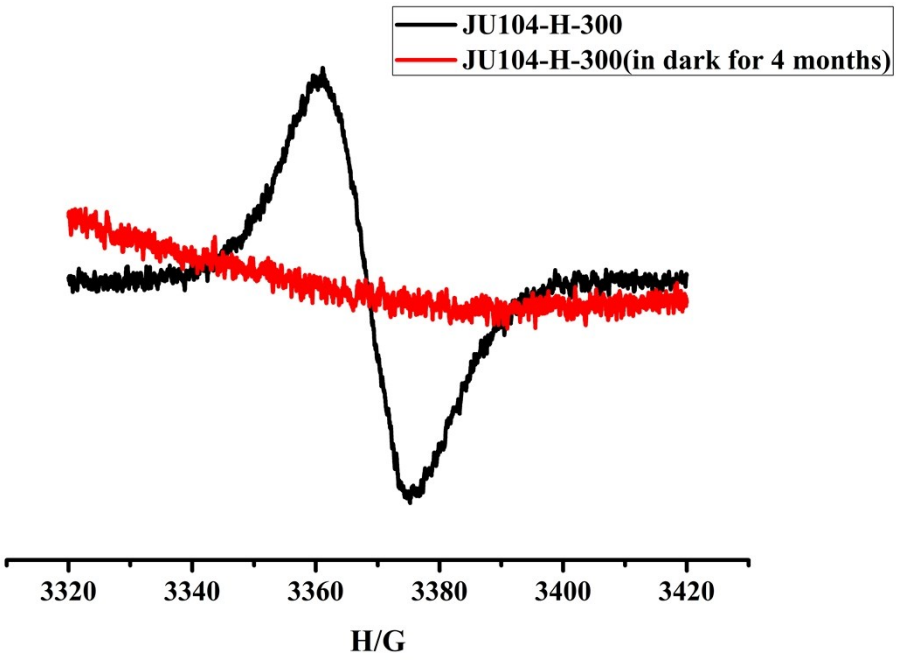
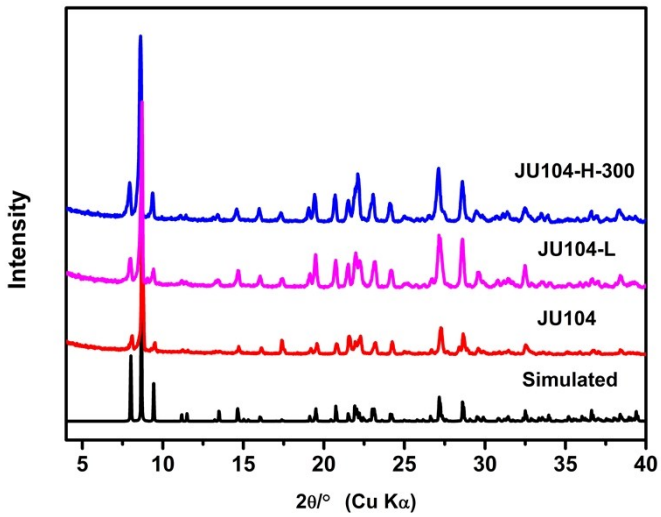
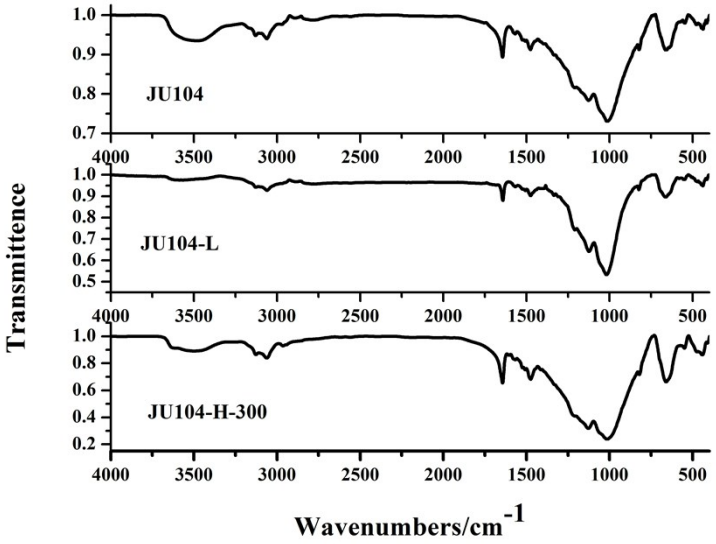


Figure S4 EPR signals of JU104-H-300 and JU104-H-300 in dark for 4months.



(a)



(b)

Figure S5 (a) Experimental and simulated PXRD patterns of JU104, UV irradiated JU104-L and heating treated JU104-H-300. (b) IR spectra of JU104, JU104-L and JU104-H-300.

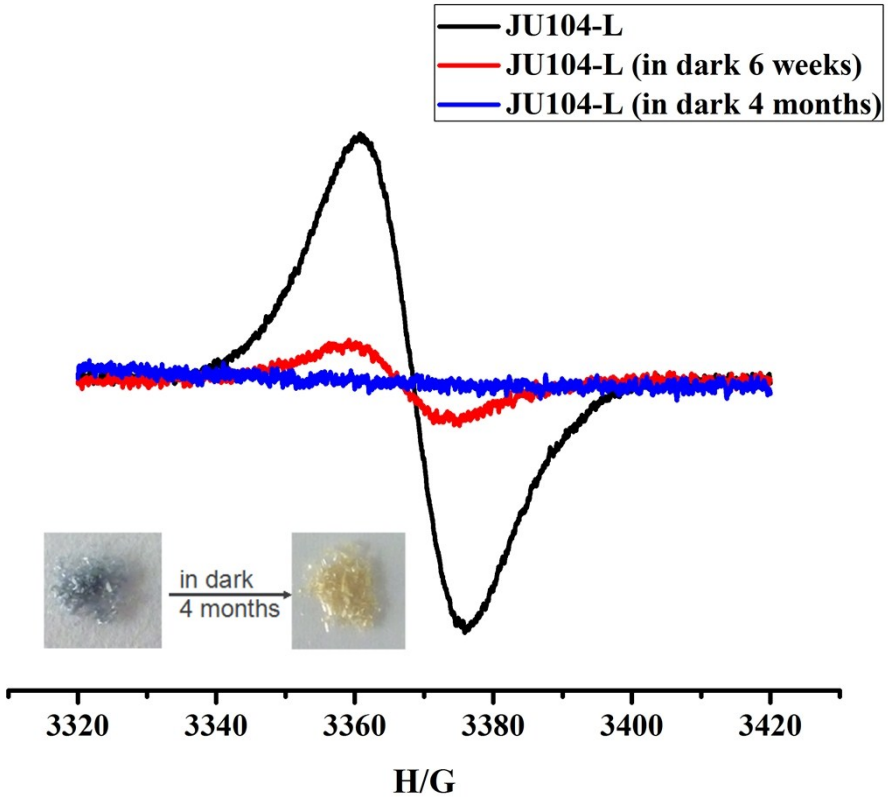


Figure S6 EPR signals of JU104-L, JU104-L in dark for 6 weeks and 4 months. Inset: color change of JU104-L kept in dark for 4 months.