Supporting Information

$(C_2H_{10}N_2)[Zn_2(HPO_4)_2Cl_2]$: Substitution-Activated New Short-Wave Ultraviolet Phosphate with Pivotal Dual-Property Enhancement

Zhi Fang[a], Yu-Ming Pan[b], Pei Han[b], Bing-Ping Yang[c] and Mei-Hong Duan*[b, d]

[a.] Chemical Synthesis and Pollution Control Key Laboratory of Sichuan Province, College of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, China

[b.] College of Physics and Astronomy, China West Normal University, Nanchong 637002, China

[c.] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

[d.] Key Laboratory of Functional Crystals and Laser Technology, TIPC, CAS, Beijing 100190, China

CONTENTS

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for EZPOC. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x/a	y/b	z/c	Ueq [$Å^2$]
Zn1	3484.6(6)	3033.7(4)	3721.5(4)	14.90(9)
Cl1	5997.5(14)	1655.2(9)	1296.2(8)	22.57(15)
P1	2147.6(13)	7346.6(8)	4178.0(8)	12.73(13)
O3	2296(4)	5614(2)	3349(2)	21.6(4)
O4	4943(4)	7383(3)	4411(2)	21.7(4)
O1	1347(4)	8826(2)	2902(2)	22.0(4)
O2	-127(4)	7801(2)	5781(2)	18.0(4)
N1	8337(5)	7281(3)	1102(3)	23.3(5)
C1	8843(6)	5326(4)	763(3)	21.9(6)
H1	960.93	9841.62	3314.4	33
H1A	7532.43	7934.09	372.73	28
H1B	9958.11	7490.16	1040.66	28
H1C	7214.21	7592.37	2098.41	28
H1D	7142.15	5132.12	634.91	26
H1E	9347.92	4632.73	1676.15	26

Table S2. Anisotropic displacement parameters, ($Å^2 \times 10^3$), for EZPOC.

Atom	U11	U22	U33	U12	U13	U23
Zn1	14.23(15)	14.26(15)	16.43(16)	-2.13(10)	-3.03(11)	-4.95(11)
Cl1	24.6(3)	20.5(3)	18.7(3)	-5.4(2)	0.4(2)	-5.1(3)
P1	12.4(3)	11.5(3)	14.5(3)	-1.1(2)	-3.7(2)	-3.4(2)
O3	28(1)	12.2(8)	25.5(10)	-2.8(7)	-9.1(8)	-5.0(8)
O4	14.0(8)	34.5(11)	19.0(9)	0.6(8)	-4.9(7)	-10.2(8)
O1	32.1(11)	15.8(9)	21.1(10)	0.9(7)	-12.1(8)	-7.3(8)
O2	15.2(8)	20.1(9)	19.2(9)	-4.2(7)	-0.6(7)	-8.6(7)
N1	22.7(12)	20.4(11)	25.7(12)	-4.3(9)	-4.1(10)	-5.8(9)
C1	23.5(14)	18.9(12)	22.8(14)	-1.3(10)	-4.3(11)	-6.5(11)

Table S3. Selected bond lengths for EZPOC.

Atom 1,2	d 1,2 [Å]
Zn1-Cl1	2.2484(7)
Zn1-O3	1.9382(18)
Zn1-O4[1]	1.9370(19)
Zn1-O2[2]	1.9705(17)
P1-O3	1.5123(19)
P1-O4	1.5196(19)
P1-O1	1.5774(19)
P1-O2	1.5270(18)
N1-C1	1.480(3)
C1-C1[3]	1.505(5)

[1]1-X,1-Y,1-Z; [2]-X,1-Y,1-Z; [3]2-X,1-Y,-Z

Table S4. Selected bond angles for EZPOC.

Atom 1,2,3	Angle 1,2 ,3[º]
O3-Zn1-Cl1	106.62(6)
O3-Zn1-O2[1]	107.37(8)
O4[2]-Zn1-Cl1	120.32(6)
O4[2]-Zn1-O3	109.81(8)
O4[2]-Zn1-O2[1]	108.42(8)
O2[1]-Zn1Cl1	103.54(5)
O3-P1-O4	113.50(11)
O3-P1-O1	102.59(11)
O3-P1-O2	112.72(11)
O4-P1-O1	107.24(11)
O4-P1-O2	110.97(11)
O2-P1-O1	109.28(11)
P1-O3-Zn1	136.73(13)
P1-O4-Zn1[2]	132.46(11)
P1-O2-Zn1[1]	123.68(11)
N1-C1-C1[3]	110.7(3)

[1]-X,1-Y,1-Z; [2]1-X,1-Y,1-Z; [3]2-X,1-Y,-Z

Table S5. Hydrogen Atom Coordinates (Å×10^4) and Isotropic displacement Parameters (Å^2×10^3) for EZPOC.

Atom	x/a	y/b	z/c	Ueq [Å^2]
H1	960.93	9841.62	3314.4	33
H1A	7532.43	7934.09	372.73	28
H1B	9958.11	7490.16	1040.66	28
H1C	7214.21	7592.37	2098.41	28
H1D	7142.15	5132.12	634.91	26
H1E	9347.92	4632.73	1676.15	26

Figure S1. Structures of EZPOC (Top) and pseudo EZPOC layer (Bottom).

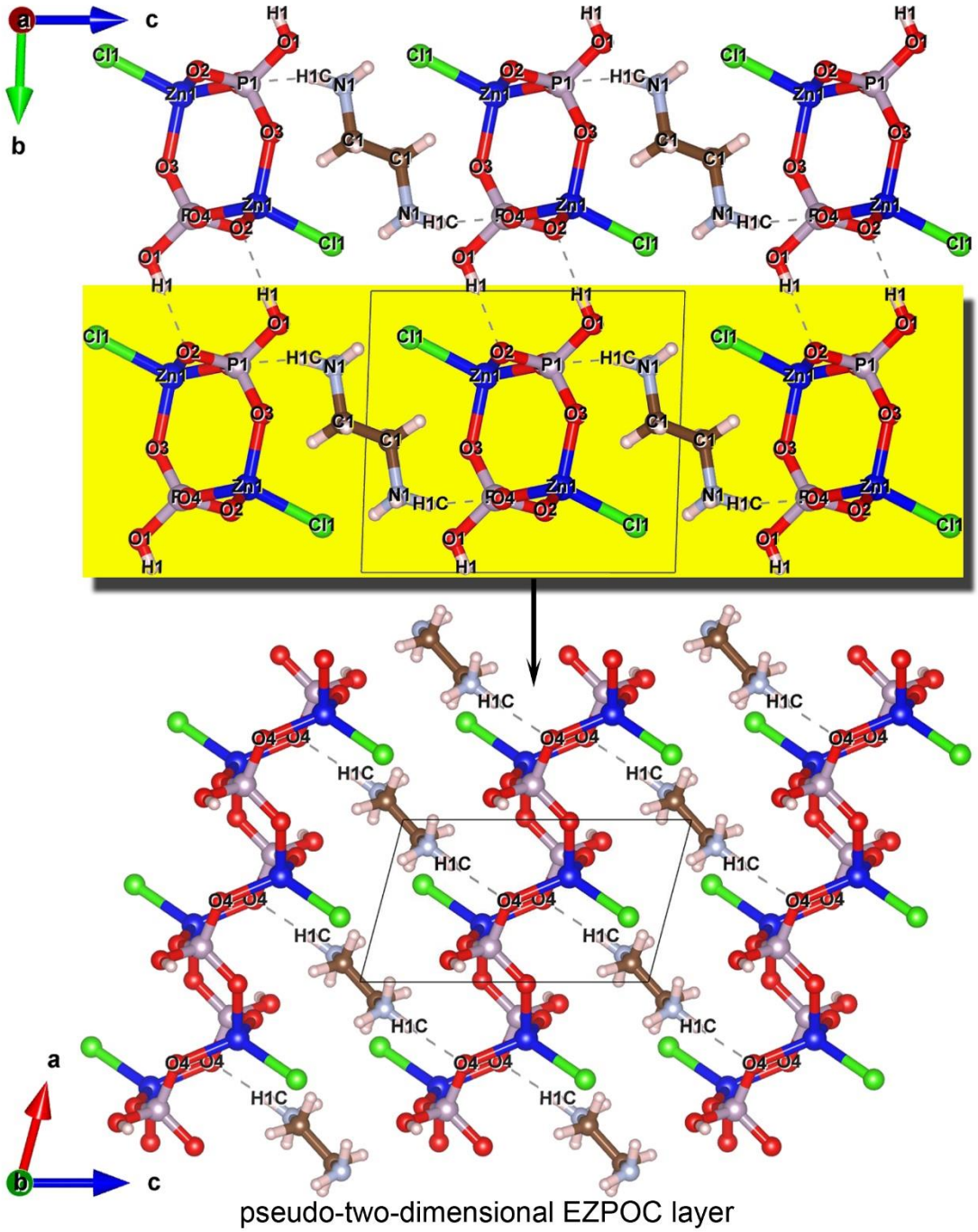


Figure S2. Measured and simulated PXRD patterns for EZPOC.

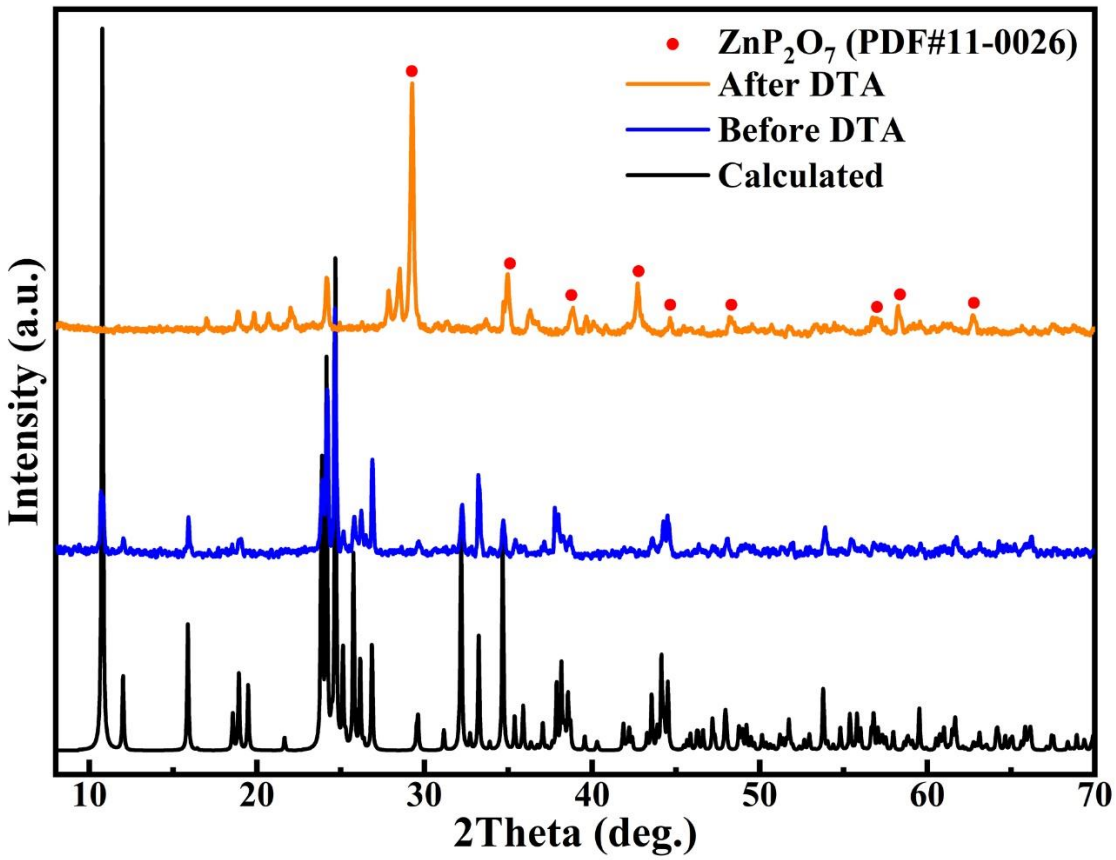
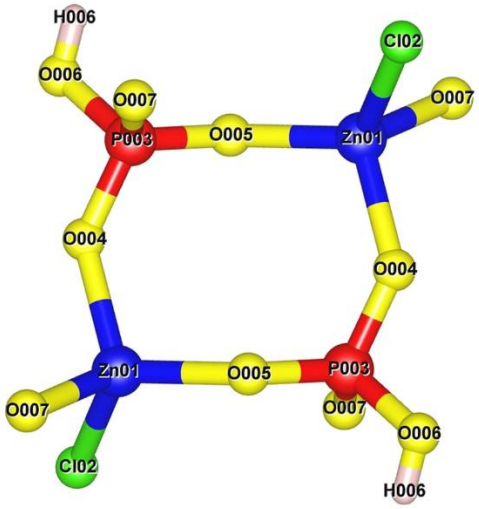
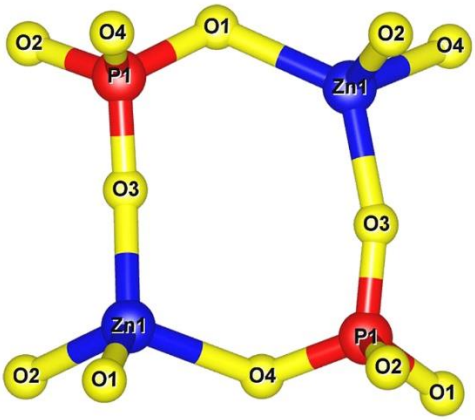


Figure S3. The $Zn_2Cl_2(HPO_4)_2O_2$ loop in EZPOC and the $Zn_2O_2(PO_4)_2O_2$ loop in KZPO.



$Zn_2Cl_2(HPO_4)_2O_2$ loop



$Zn_2O_2(PO_4)_2O_2$ loop

Figure S4. Band Structure of EZPOC.

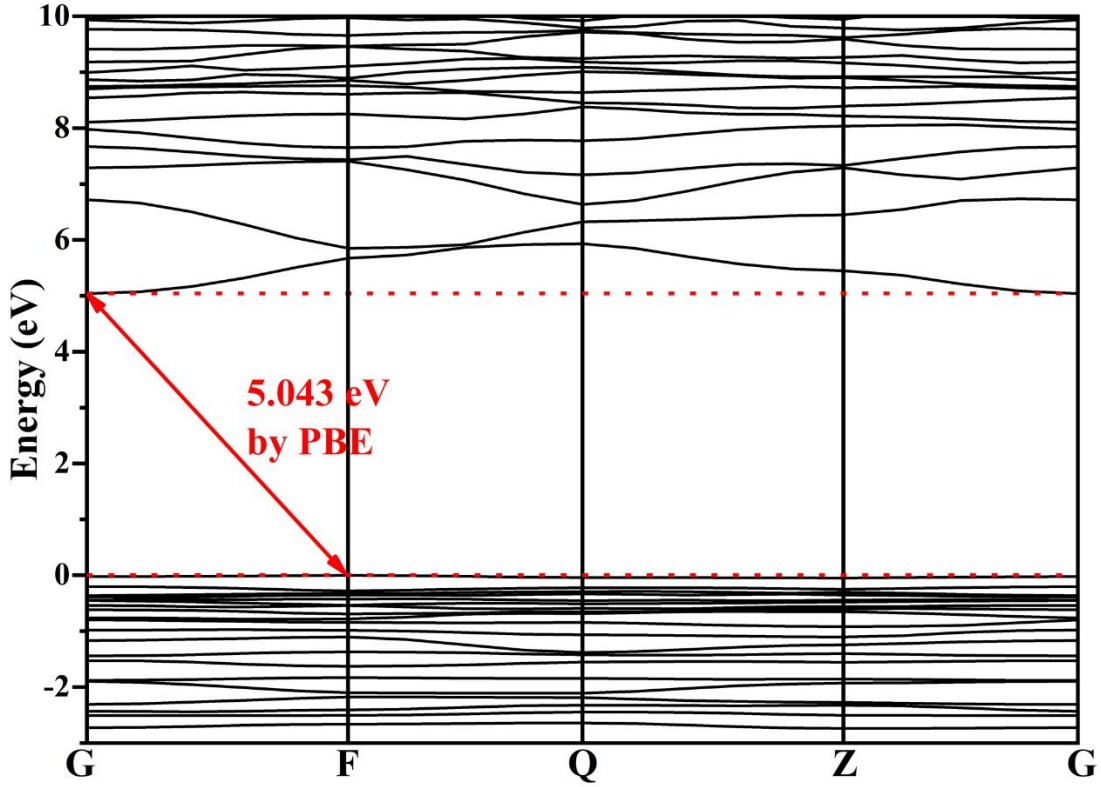


Figure S5. Band Structure of KZPO.

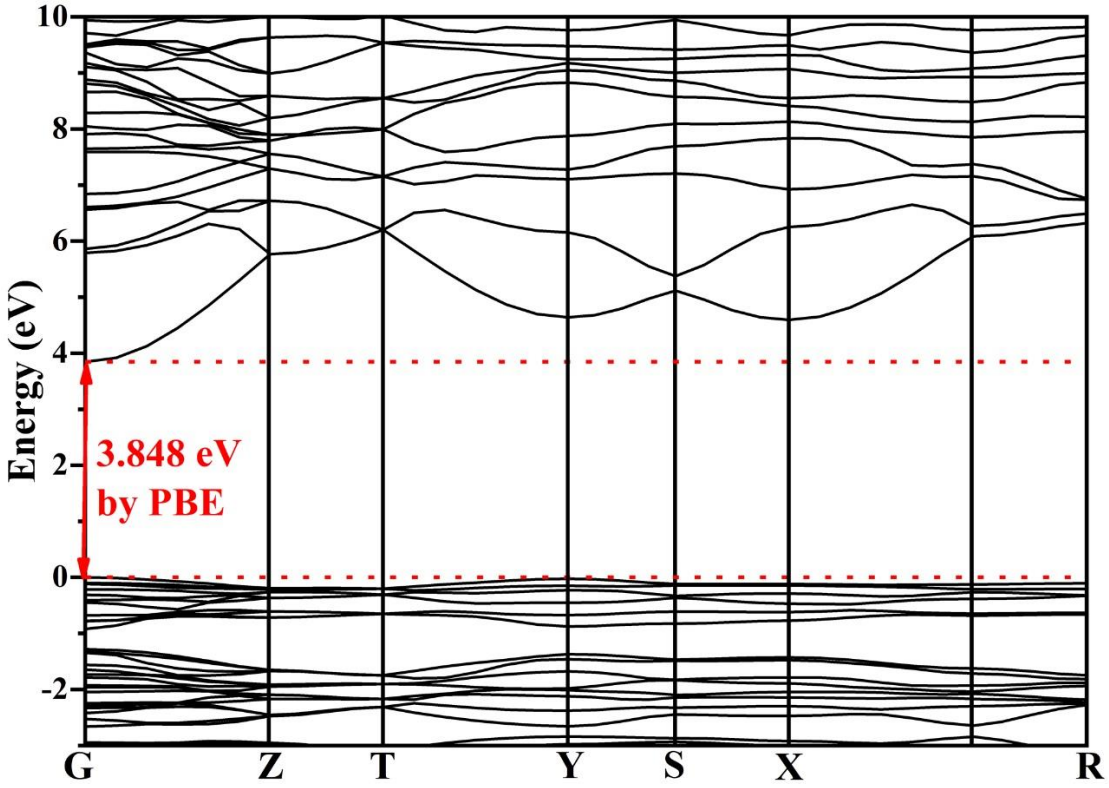


Figure S6. Calculated refractive index and birefringence for KZPO.

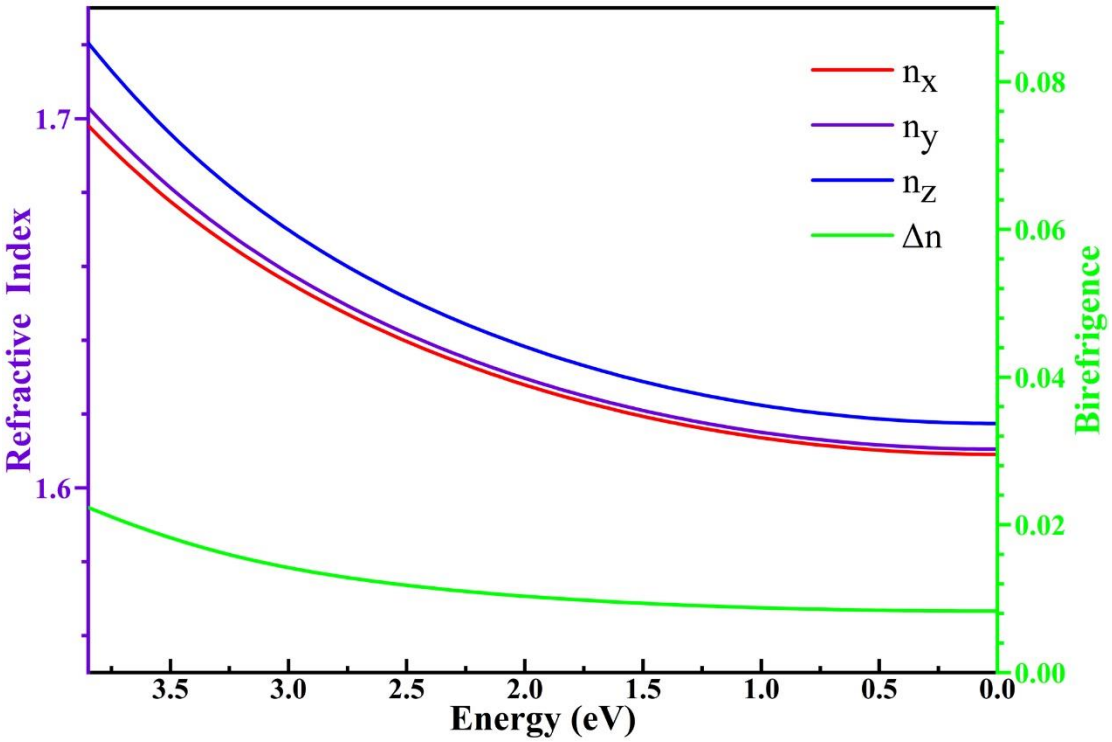


Figure S7. Comparison of birefringence between EZPOC and some commercial SUV phosphates, as well as some halogenated phosphates.