Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

From $(NH_4)_3[Zr(PO_4)_2F]$ to $(NH_4)_3[Sn_2(PO_4)_2]Cl$: Rational Design of a Tin-based Short-Wave Ultraviolet Phosphate with Large Optical Anisotropy

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $(NH_4)_3Sn_2(PO_4)_2Cl$.

Atom	x/a	y/b	z/c	Ueq [Å^2]	S.O.F.	Wyckoff
Sn1	0.61623(4)	0.34466(4)	0.37526(4)	0.02020(17)	1	4d
P1	0.34477(16)	0.36179(15)	0.53080(14)	0.0189(4)	1	4d
Cl1	0.5	0.0386(9)	0.25	0.118(3)	0.802(13)	8d
O1	0.4253(5)	0.3038(5)	0.4422(4)	0.0314(12)	1	4d
O3	0.3261(5)	0.5137(4)	0.5146(4)	0.0257(11)	1	4d
O2	0.2000(4)	0.2976(4)	0.5259(4)	0.0264(11)	1	4d
O4	0.4144(6)	0.3331(5)	0.6278(4)	0.0402(14)	1	4d
N2	0.6962(7)	0.3401(7)	0.6766(5)	0.048(2)	1	4d
H2A	0.746423	0.341314	0.62118	0.058	1	4d
H2B	0.714013	0.413514	0.71205	0.058	1	4d
H2C	0.717753	0.267654	0.71205	0.058	1	4d
H2D	0.604683	0.337914	0.66075	0.058	1	4d
N1	0	0.5	0.5	0.080(5)	1	8d
H1A	-0.01353	0.51373	0.43541	0.096	0.5	4d
H1B	-0.07918	0.47475	0.52815	0.096	0.5	4d
H1C	0.02955	0.57559	0.52815	0.096	0.5	4d
H1D	0.06458	0.43449	0.50847	0.096	0.5	4d
Cl2	0.916(5)	0.571(3)	0.694(3)	0.14(2)	0.099(6)	4d

Table S2. Anisotropic displacement parameters for $(NH_4)_3Sn_2(PO_4)_2Cl$, in $Å^2$.

Atom	U11	U22	U33	U12	U13	U23
Sn1	0.0203(2)	0.0209(3)	0.0194(3)	0.00118(17)	0.00197(18)	-0.00050(19)
P1	0.0156(7)	0.0164(7)	0.0247(10)	-0.0016(6)	0.0008(7)	0.0006(7)
Cl1	0.087(4)	0.188(8)	0.077(5)	0.00000	0.029(4)	0.00000
O1	0.018(2)	0.033(3)	0.042(3)	-0.005(2)	0.008(2)	-0.012(3)
O3	0.034(3)	0.014(2)	0.030(3)	-0.001(2)	0.001(2)	0.0009(19)
O2	0.019(2)	0.021(2)	0.039(3)	-0.0048(19)	0.003(2)	0.004(2)
O4	0.032(3)	0.056(4)	0.033(3)	0.000(3)	-0.010(2)	0.015(3)
N2	0.047(4)	0.070(5)	0.028(4)	0.023(4)	-0.007(3)	-0.001(4)
N1	0.022(5)	0.056(7)	0.161(15)	0.005(5)	0.006(7)	0.052(8)
Cl2	0.24(5)	0.052(17)	0.14(4)	0.09(2)	-0.13(4)	-0.05(2)

Table S3. Selected bond lengths for $(NH_4)_3Sn_2(PO_4)_2Cl$.

Atom 1,2	d 1,2 [Å]
Sn1-O1	2.093(5)
Sn1-O3	2.122(5)
Sn1-O2	2.106(5)
P1-O1	1.537(5)
P1-O3	1.540(4)
P1-O2	1.539(4)
P1-O4	1.497(6)

Table S4. Selected bond angles for $(NH_4)_3Sn_2(PO_4)_2Cl$.

Atom 1,2,3	Angle 1,2 ,3[º]
O1-Sn1-O3	93.41(18)
O1-Sn1-O2	86.32(19)
O2-Sn1-O3	84.52(18)
O1-P1-O3	108.6(3)
O1-P1-O2	105.7(3)
O2-P1-O3	107.2(3)
O4-P1-O1	112.2(3)
O4-P1-O3	111.4(3)
O4-P1-O2	111.5(3)
P1-O1-Sn1	135.0(3)
P1-O3-Sn1	121.6(3)
P1-O2-Sn1	127.0(3)

Table S5. Bond valence sums (BVS) for $(NH_4)_3Sn_2(PO_4)_2Cl$.

Atom	BVS
Sn1	2.15
P1	5.07
O1	-1.99
O2	-1.95
O3	-1.92

Figure S1. Measured and calculated PXRD patterns for $(NH_4)_3Sn_2(PO_4)_2Cl$.

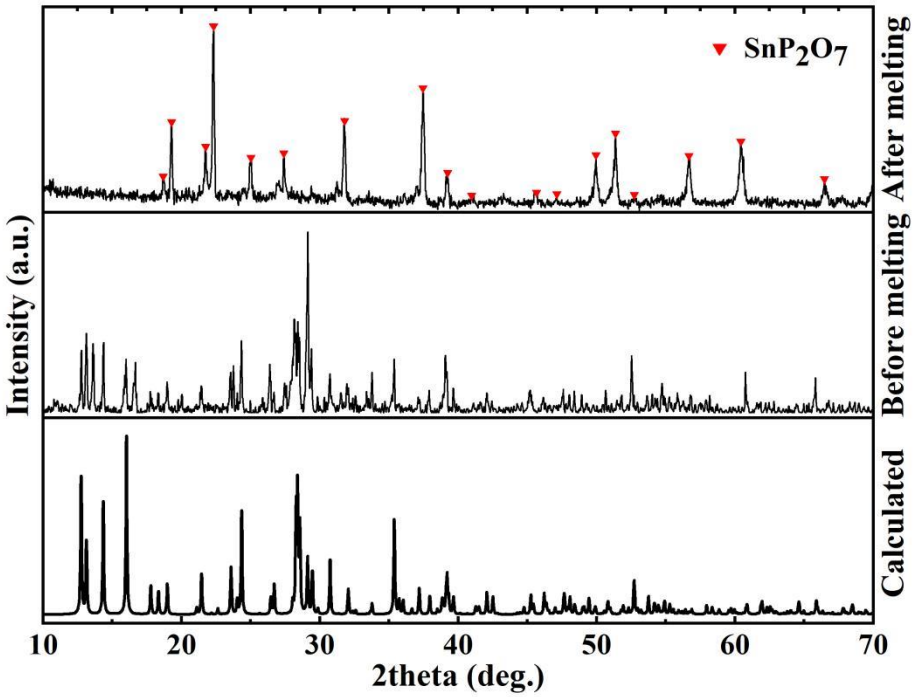

Figure S2. Measured TG curve for $(NH_4)_3Sn_2(PO_4)_2Cl$.

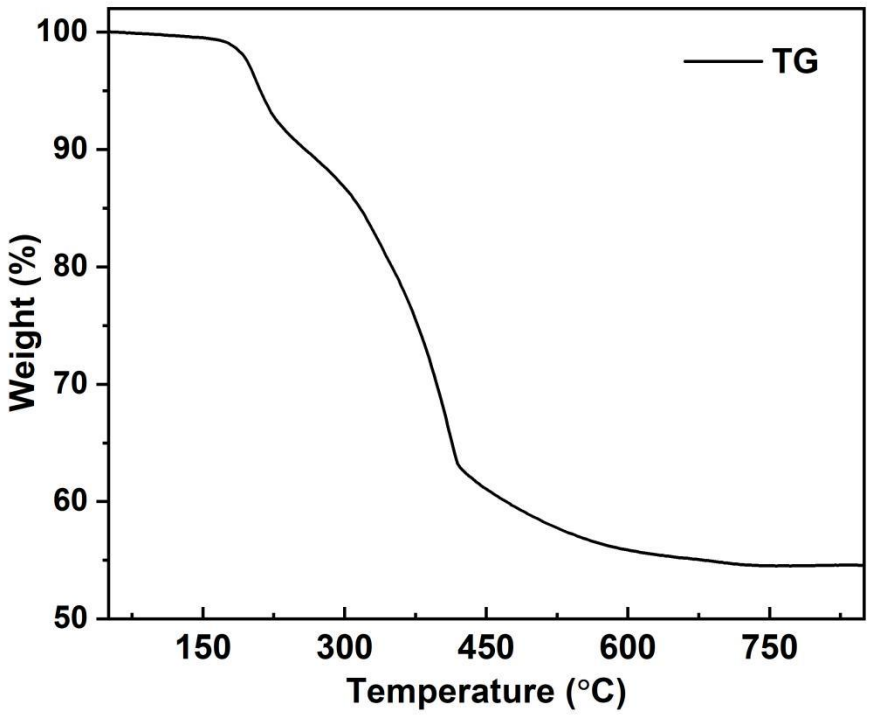

Figure S3. IR spectrum for $(NH_4)_3Sn_2(PO_4)_2Cl$.

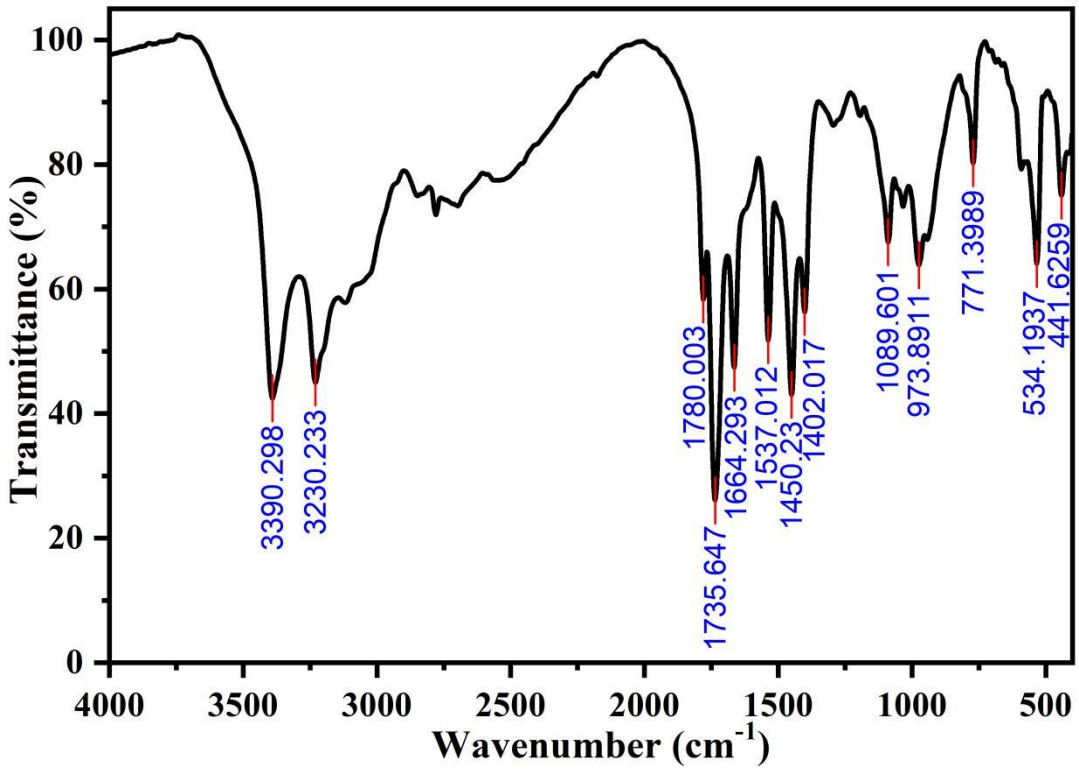

Figure S4. EDS map for $(NH_4)_3Sn_2(PO_4)_2Cl$.