Supporting information

Structural varieties in zinc telluro-phosphates: synthesis, crystal structure and characterization of $Sr_2Zn_3Te_2P_2O_{14}$, $Pb_2Zn_3Te_2P_2O_{14}$ and $Ba_2Zn_2TeP_2O_{11}$

Mingjun Xia and R. K. Li*

Beijing Center for Crystal Research and Development, Key Laboratory of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

Fig.S1. Powder X-ray diffraction patterns of 1.

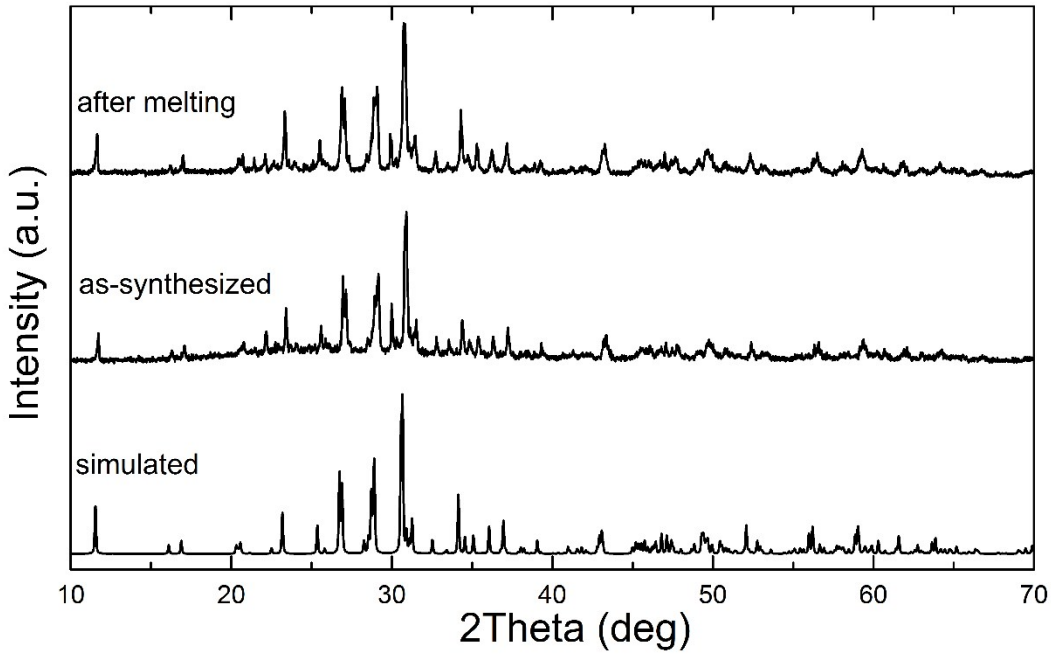

Fig.S2. Powder X-ray diffraction patterns of 2.

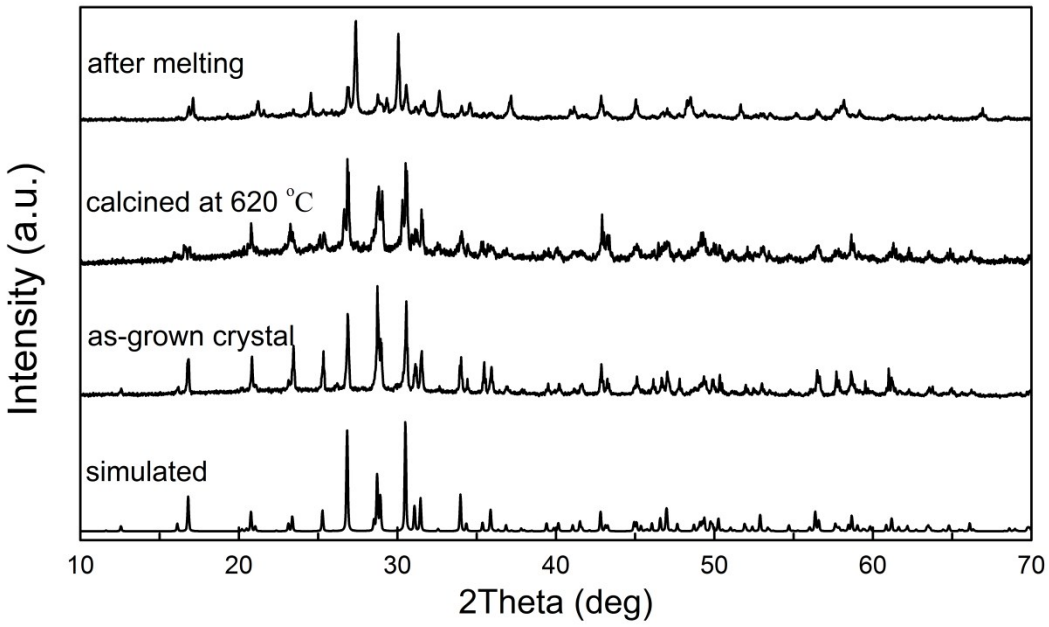

Fig.S3. Powder X-ray diffraction patterns of 3.

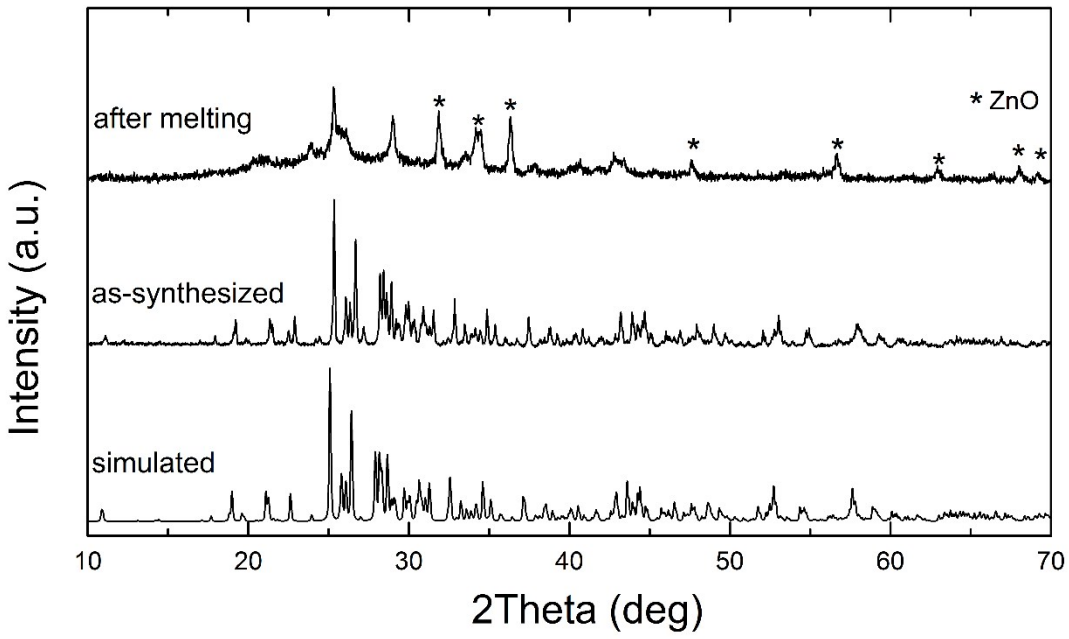

Fig. S4. DSC curves for 1.

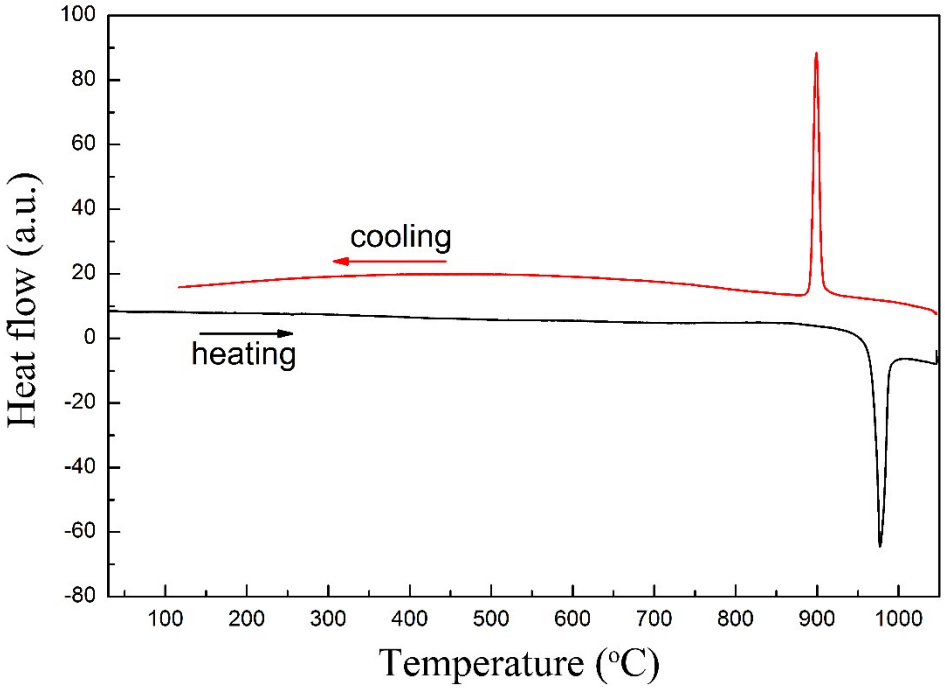

Fig. S5. DSC curves for 2.

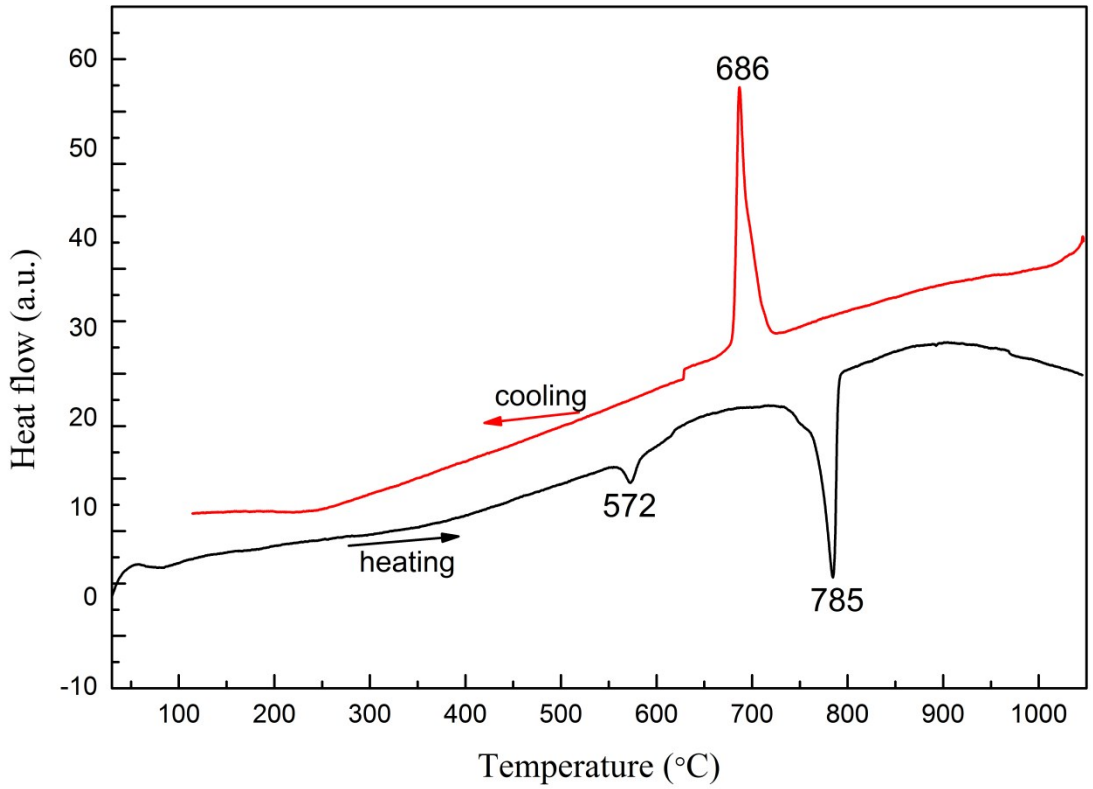

Fig. S6. DSC curves for 3.

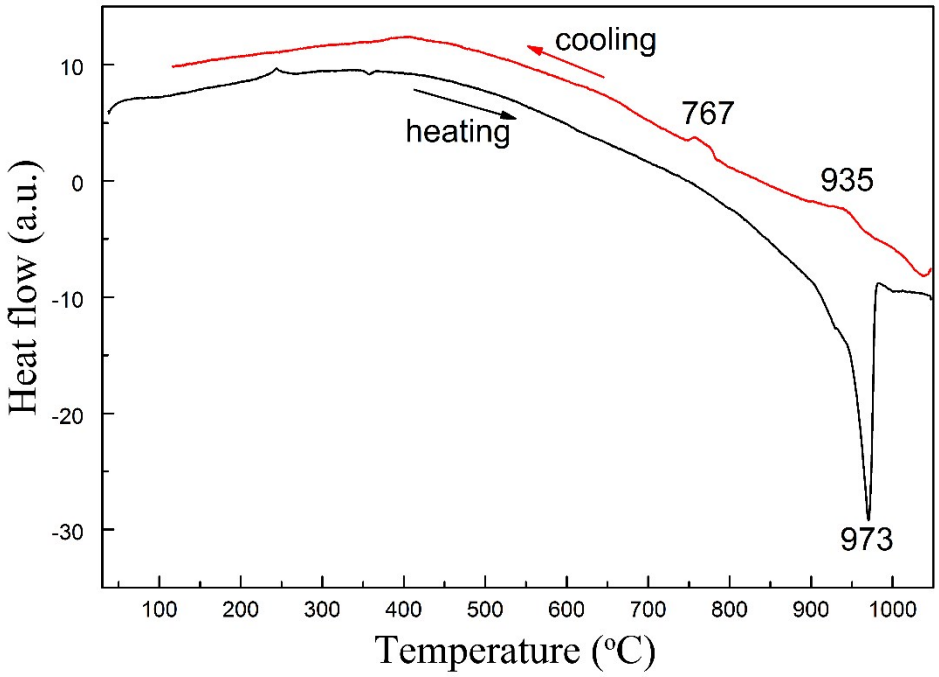

Fig. S7. XPS patterns of 2.

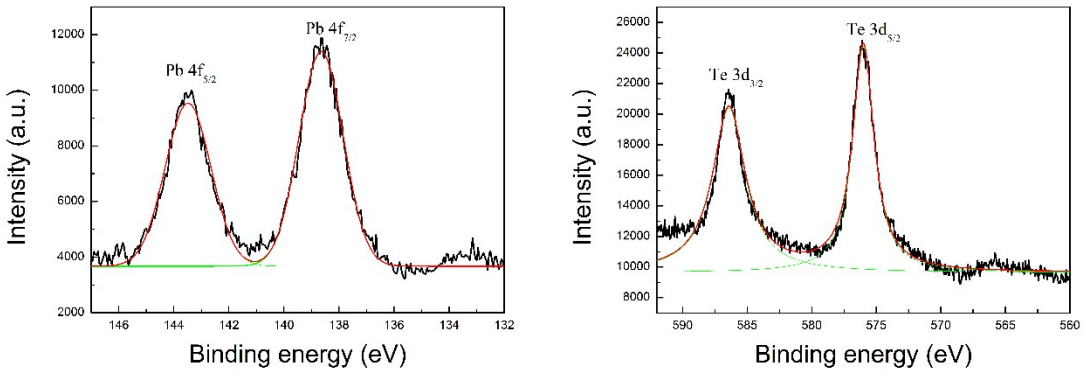

Table S1. Atomic coordinates, equivalent isotropic displacement parameters ($Å^2$) and BVS for 1. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Sr1	0.50188(12)	0.94914(9)	0.70308(5)	0.00959(18)	1.926
Te1	0.51464(8)	0.72900(6)	0.49242(3)	0.00907(15)	3.749
Zn1	0.99096(15)	0.60861(11)	0.61694(5)	0.0099(2)	1.985
Zn2	0	0	0.5	0.0317(4)	1.698
P1	0.9537(3)	0.7350(2)	0.80708(12)	0.0076(4)	4.915
O1	0.8010(9)	0.6832(7)	0.7238(3)	0.0085(10)	2.067
O2	0.2535(11)	0.7588(7)	0.5746(4)	0.0222(14)	1.987
O3	0.7044(9)	0.8983(6)	0.5536(3)	0.0107(11)	2.036
O4	0.8417(9)	0.9093(6)	0.8309(4)	0.0122(11)	1.949
O5	0.8837(10)	0.6065(7)	0.8782(4)	0.0164(12)	1.780
O6	0.2402(9)	0.7383(7)	0.7898(4)	0.0129(11)	2.057
O7	0.7112(10)	0.5492(7)	0.5391(4)	0.0173(12)	1.782

Table S2. Atomic coordinates, equivalent isotropic displacement parameters (Å^2) and BVS for 2. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Pb1	0.49629(7)	0.94022(5)	0.69846(3)	0.0125(2)	1.796
Te1	0.48318(11)	0.72243(8)	0.48834(4)	0.0079(2)	3.991
Zn1	0.0097(2)	0.60969(14)	0.61482(8)	0.0088(3)	1.999
Zn2	0	0	0.5	0.0349(6)	1.910
P1	0.0359(4)	0.7382(3)	0.8080(2)	0.0068(5)	4.977
O1	0.1856(12)	0.6969(9)	0.7221(4)	0.0114(14)	2.026
O2	-0.2476(13)	0.7482(10)	0.7893(5)	0.017(2)	1.842
O3	0.0938(14)	0.5993(10)	0.8740(5)	0.019(2)	1.789
O4	0.8513(14)	0.4059(9)	0.6600(5)	0.018(2)	1.886
O5	0.2921(14)	0.8893(10)	0.5501(5)	0.019(2)	2.056
O6	0.2947(14)	0.5479(9)	0.5400(5)	0.016(2)	2.073
O7	0.7461(16)	0.7602(10)	0.5712(7)	0.032(2)	2.035

Table S3. Atomic coordinates, equivalent isotropic displacement parameters (Å^2) and BVS for 3. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Ba1	0.25688(6)	0.40618(2)	0.53472(4)	0.01197(13)	1.992
Ba2	0.72283(6)	0.25980(2)	0.38528(4)	0.01210(13)	1.989
Te1	0.16770(6)	0.55588(2)	0.88885(5)	0.01194(14)	3.972
Zn1	0.43250(12)	0.45631(4)	0.19955(8)	0.0132(2)	2.015
Zn2	0.18539(11)	0.14390(5)	0.41805(8)	0.0126(2)	1.979
P1	0.2044(2)	0.28595(10)	0.2256(2)	0.0086(3)	4.925
P2	0.2265(2)	0.60096(10)	0.3371(2)	0.0099(3)	4.896
O1	0.2899(6)	0.2000(3)	0.2807(5)	0.0119(9)	2.036
O2	0.3806(6)	0.3471(3)	0.2744(5)	0.0142(9)	2.073
O3	0.3720(6)	0.6735(3)	0.3755(5)	0.0141(9)	1.955
O4	0.3508(7)	0.5202(3)	0.3453(5)	0.0156(10)	2.061
O5	0.1068(7)	0.5933(3)	0.4442(5)	0.0188(11)	1.931
O6	0.0394(7)	0.3114(3)	0.2897(5)	0.0163(10)	1.837
O7	0.0933(7)	0.6121(3)	0.1827(5)	0.0155(10)	1.833
O8	0.1327(7)	0.2813(3)	0.0628(5)	0.0150(10)	1.949
O9	0.2557(7)	0.4629(3)	0.0115(5)	0.0150(10)	2.241
O10	0.2847(7)	0.5177(3)	0.7493(5)	0.0193(10)	2.112
O11	0.3595(8)	0.6315(3)	0.9670(6)	0.0248(12)	1.860