Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

$K_2TeP_2O_8$: A new telluro-phosphate with a pentagonal Te−P−O layer structure

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $K_2TeP_2O_8$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
K(1)	9850(2)	8262(2)	-72(4)	24(1)
K(2)	8227(2)	5006(2)	-10(4)	32(1)
Te(1)	7342(1)	7520(1)	4630(1)	18(1)
P(1)	9939(2)	6209(2)	4894(4)	14(1)
P(2)	6238(2)	5112(2)	4926(4)	25(1)
O(1)	7875(6)	7782(6)	1681(11)	29(2)
O(2)	10150(6)	6267(5)	2272(12)	24(1)
O(3)	6656(7)	6078(6)	3365(14)	37(2)
O(4)	6256(6)	5342(6)	7553(12)	28(2)
O(5)	8819(8)	6577(9)	5823(19)	63(3)
O(6)	8178(12)	9121(7)	6032(16)	77(4)
O(7)	5809(8)	8240(10)	3537(17)	68(3)
O(8)	5000	5000	3920(20)	81(6)
O(9)	10341(9)	5023(10)	5860(20)	16(3)

Table S2. Selected bond distances (Å) and angles (deg) for $K_2TeP_2O_8$.

K(1)-O(1)	2.621(7)	O(4)#3-K(2)-O(2)#6	154.6(2)
K(1)-O(4)#1	2.769(7)	O(4)#3-K(2)-O(9)#7	97.2(3)
K(1)-O(2)	2.779(6)	O(2)#6-K(2)-O(9)#7	86.4(3)
K(1)-O(7)#2	2.888(11)	O(4)#3-K(2)-O(3)	72.4(2)
K(1)-O(3)#2	2.939(9)	O(2)#6-K(2)-O(3)	113.8(2)
K(1)-O(8)#2	3.008(9)	O(9)#7-K(2)-O(3)	153.2(3)
K(1)-O(6)#3	3.120(13)	O(4)#3-K(2)-O(6)#8	86.1(3)
K(1)-O(4)#4	3.180(7)	O(2)#6-K(2)-O(6)#8	81.8(3)
K(1)-O(5)#3	3.299(12)	O(9)#7-K(2)-O(6)#8	158.0(3)
K(1)-P(2)#2	3.727(3)	O(3)-K(2)-O(6)#8	48.1(2)
K(1)-P(2)#5	3.738(3)	O(4)#3-K(2)-O(2)	141.1(2)
K(1)-P(1)#3	3.744(3)	O(2)#6-K(2)-O(2)	64.3(2)
K(2)-O(4)#3	2.748(7)	O(9)#7-K(2)-O(2)	83.3(3)
K(2)-O(2)#6	2.787(7)	O(3)-K(2)-O(2)	89.8(2)
K(2)-O(9)#7	2.854(12)	O(6)#8-K(2)-O(2)	107.7(3)
K(2)-O(3)	2.954(9)	O(4)#3-K(2)-O(5)#3	74.8(2)
K(2)-O(6)#8	2.971(12)	O(2)#6-K(2)-O(5)#3	121.6(2)
K(2)-O(2)	3.042(7)	O(9)#7-K(2)-O(5)#3	43.2(3)
K(2)-O(5)#3	3.078(10)	O(3)-K(2)-O(5)#3	110.1(2)
K(2)-O(7)#9	3.125(13)	O(6)#8-K(2)-O(5)#3	155.5(3)
K(2)-O(1)#9	3.152(7)	O(2)-K(2)-O(5)#3	79.7(2)
K(2)-O(9)#3	3.407(11)	O(4)#3-K(2)-O(7)#9	96.5(2)
Te(1)-O(1)	1.779(6)	O(2)#6-K(2)-O(7)#9	69.0(2)
Te(1)-O(3)	2.062(7)	O(9)#7-K(2)-O(7)#9	43.2(3)
Te(1)-O(7)	2.121(8)	O(3)-K(2)-O(7)#9	159.1(2)
Te(1)-O(5)	2.210(9)	O(6)#8-K(2)-O(7)#9	114.9(2)
Te(1)-O(6)	2.325(8)	O(2)-K(2)-O(7)#9	109.1(2)
P(1)-O(2)	1.473(7)	O(5)#3-K(2)-O(7)#9	82.9(3)
P(1)-O(5)	1.504(9)	O(4)#3-K(2)-O(1)#9	67.98(19)
P(1)-O(7)#1	1.512(9)	O(2)#6-K(2)-O(1)#9	86.90(19)
P(1)-O(9)	1.615(12)	O(9)#7-K(2)-O(1)#9	90.4(3)
P(1)-O(9)#6	1.630(12)	O(3)-K(2)-O(1)#9	107.41(19)
P(2)-O(4)	1.479(7)	O(6)#8-K(2)-O(1)#9	70.6(2)
P(2)-O(6)#8	1.493(9)	O(2)-K(2)-O(1)#9	150.77(19)
P(2)-O(3)	1.543(7)	O(5)#3-K(2)-O(1)#9	114.3(3)
P(2)-O(8)	1.588(5)	O(7)#9-K(2)-O(1)#9	51.65(19)
O(1)-K(1)-O(4)#1	119.9(2)	O(4)#3-K(2)-O(9)#3	108.0(2)
O(1)-K(1)-O(2)	75.5(2)	O(2)#6-K(2)-O(9)#3	77.8(2)
O(4)#1-K(1)-O(2)	103.0(2)	O(9)#7-K(2)-O(9)#3	11.1(3)
O(1)-K(1)-O(7)#2	117.6(2)	O(3)-K(2)-O(9)#3	153.2(3)
O(4)#1-K(1)-O(7)#2	118.8(2)	O(6)#8-K(2)-O(9)#3	156.7(3)
O(2)-K(1)-O(7)#2	72.7(3)	O(2)-K(2)-O(9)#3	73.3(2)

O(1)-K(1)-O(3)#2	162.5(2)	O(5)#3-K(2)-O(9)#3	47.5(3)
O(4)#1-K(1)-O(3)#2	72.3(2)	O(7)#9-K(2)-O(9)#3	46.6(3)
O(2)-K(1)-O(3)#2	115.7(2)	O(1)#9-K(2)-O(9)#3	96.9(2)
O(7)#2-K(1)-O(3)#2	58.0(2)	O(1)-Te(1)-O(3)	89.1(3)
O(1)-K(1)-O(8)#2	118.22(16)	O(1)-Te(1)-O(7)	88.6(4)
O(4)#1-K(1)-O(8)#2	83.5(2)	O(3)-Te(1)-O(7)	84.9(4)
O(2)-K(1)-O(8)#2	159.8(2)	O(1)-Te(1)-O(5)	94.6(3)
O(7)#2-K(1)-O(8)#2	87.3(3)	O(3)-Te(1)-O(5)	88.6(4)
O(3)#2-K(1)-O(8)#2	47.54(15)	O(7)-Te(1)-O(5)	172.8(5)
O(1)-K(1)-O(6)#3	75.6(3)	O(1)-Te(1)-O(6)	90.0(3)
O(4)#1-K(1)-O(6)#3	122.1(2)	O(3)-Te(1)-O(6)	178.0(4)
O(2)-K(1)-O(6)#3	134.3(2)	O(7)-Te(1)-O(6)	96.9(5)
O(7)#2-K(1)-O(6)#3	90.6(3)	O(5)-Te(1)-O(6)	89.6(5)
O(3)#2-K(1)-O(6)#3	87.3(3)	O(2)-P(1)-O(5)	118.4(5)
O(8)#2-K(1)-O(6)#3	46.7(2)	O(2)-P(1)-O(7)#1	115.1(4)
O(1)-K(1)-O(4)#4	68.9(2)	O(5)-P(1)-O(7)#1	106.6(6)
O(4)#1-K(1)-O(4)#4	62.8(3)	O(2)-P(1)-O(9)	108.5(5)
O(2)-K(1)-O(4)#4	123.16(19)	O(5)-P(1)-O(9)	114.8(6)
O(7)#2-K(1)-O(4)#4	164.0(3)	O(7)#1-P(1)-O(9)	90.1(6)
O(3)#2-K(1)-O(4)#4	111.05(19)	O(2)-P(1)-O(9)#6	113.8(5)
O(8)#2-K(1)-O(4)#4	76.9(2)	O(5)-P(1)-O(9)#6	88.8(6)
O(6)#3-K(1)-O(4)#4	76.6(2)	O(7)#1-P(1)-O(9)#6	111.2(6)
O(1)-K(1)-O(5)#3	77.2(2)	O(9)-P(1)-O(9)#6	29.2(7)
O(4)#1-K(1)-O(5)#3	162.8(2)	O(4)-P(2)-O(6)#8	119.7(5)
O(2)-K(1)-O(5)#3	79.9(2)	O(4)-P(2)-O(3)	113.6(4)
O(7)#2-K(1)-O(5)#3	45.4(2)	O(6)#8-P(2)-O(3)	105.5(5)
O(3)#2-K(1)-O(5)#3	91.1(2)	O(4)-P(2)-O(8)	111.9(5)
O(8)#2-K(1)-O(5)#3	88.5(2)	O(6)#8-P(2)-O(8)	104.1(6)
O(6)#3-K(1)-O(5)#3	59.6(2)	O(3)-P(2)-O(8)	100.0(5)
O(4)#4-K(1)-O(5)#3	129.9(2)		

#1 x+1/2,-y+3/2,-z+1 #2 x+1/2,-y+3/2,-z
#3 x,y,z-1 #4 -x+3/2,y+1/2,-z+1 #5 -x+3/2,y+1/2,-z
#6 -x+2,-y+1,z #7 -x+2,-y+1,z-1 #8 -x+3/2,y-1/2,-z+1
#9 -x+3/2,y-1/2,-z #10 x-1/2,-y+3/2,-z
#11 x,y,z+1 #12 -x+2,-y+1,z+1 #13 x-1/2,-y+3/2,-z+1
#14 -x+1,-y+1,z

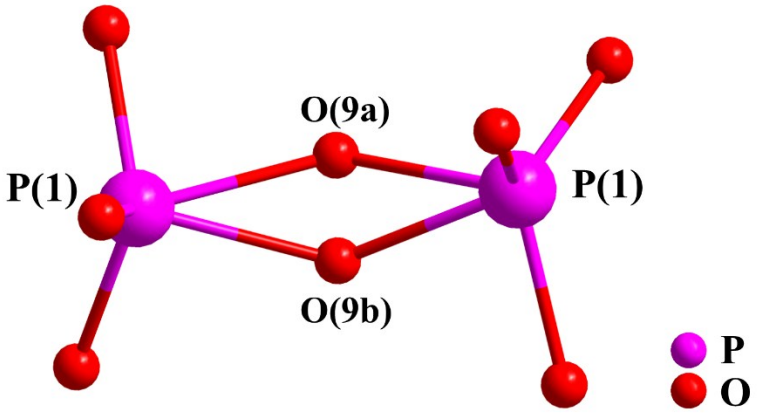

Fig. S1 The split of O(9) atom in $K_2TeP_2O_8$

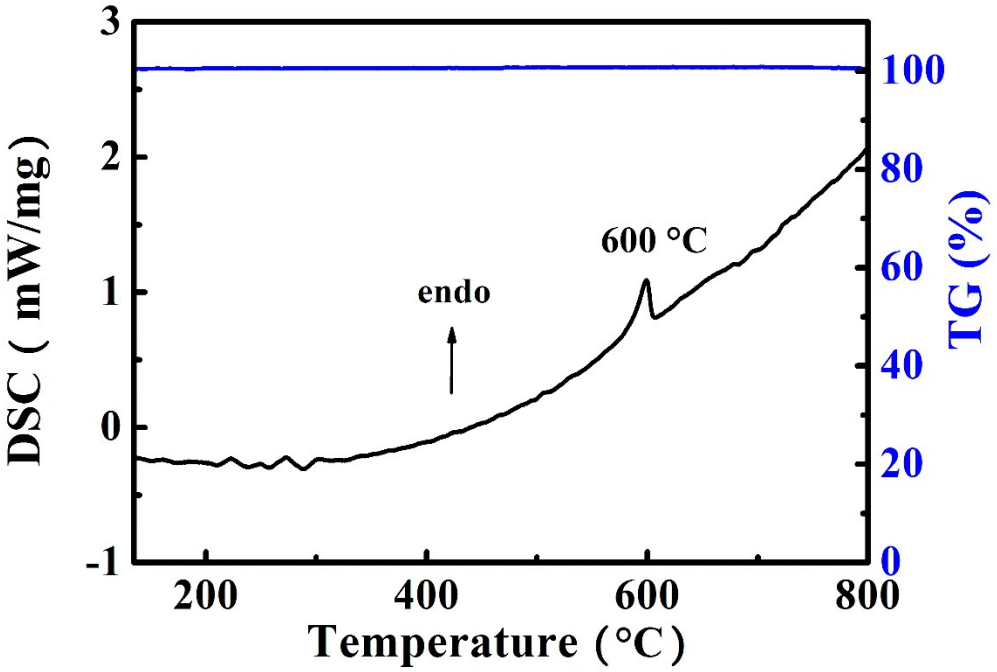

Fig. S2. TG-DSC curves of $K_2TeP_2O_8$.

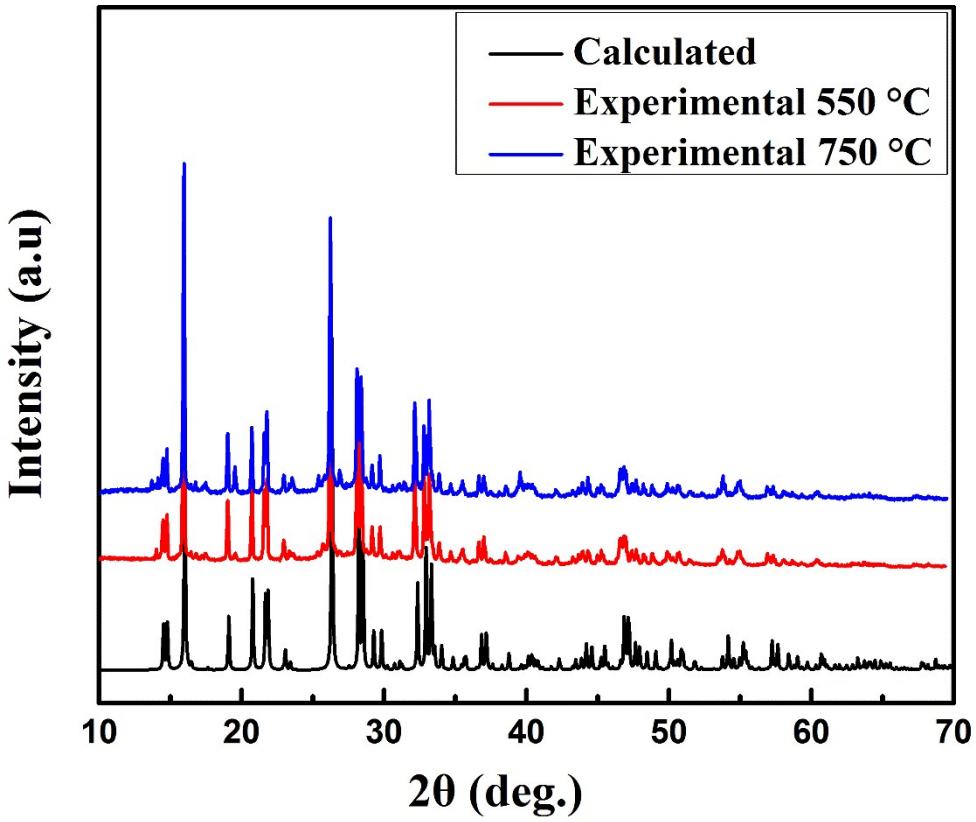

Fig. S3. Experimental and calculated XRD patterns of $K_2TeP_2O_8$.

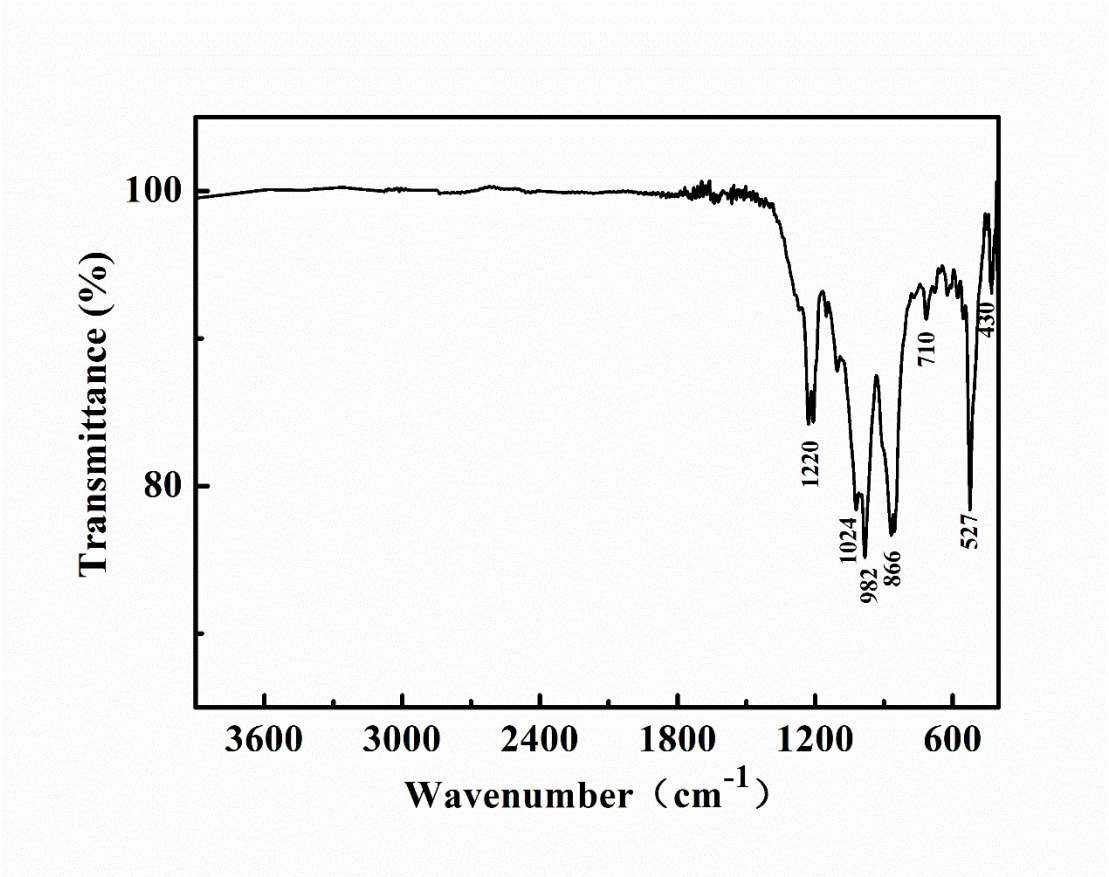

Fig. S4. IR spectrum of $K_2TeP_2O_8$.

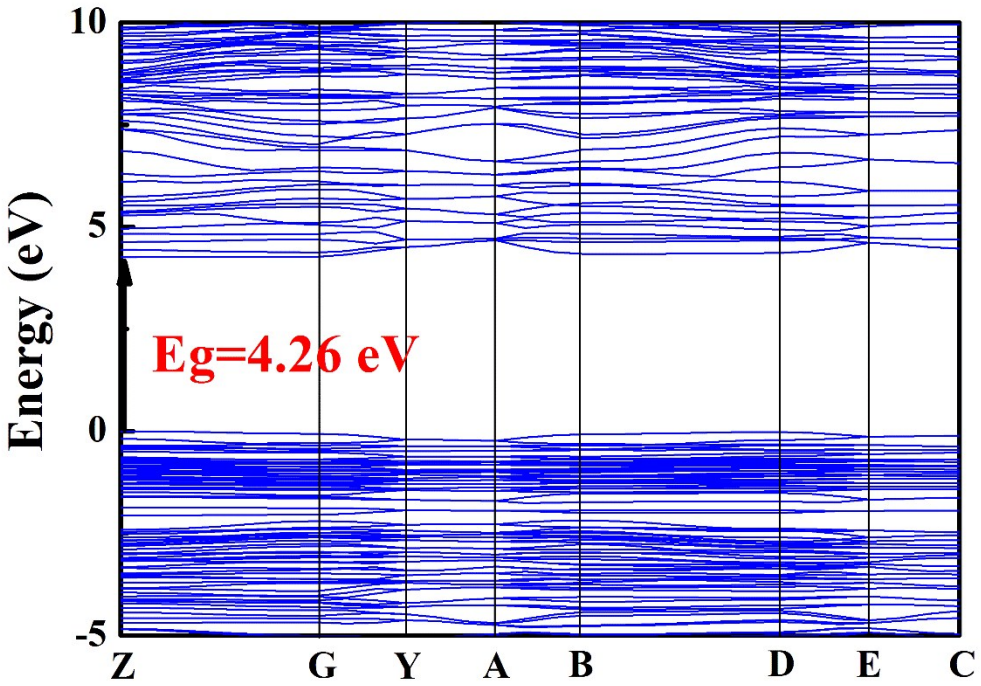

Fig. S5. Band structure of $K_2TeP_2O_8$.

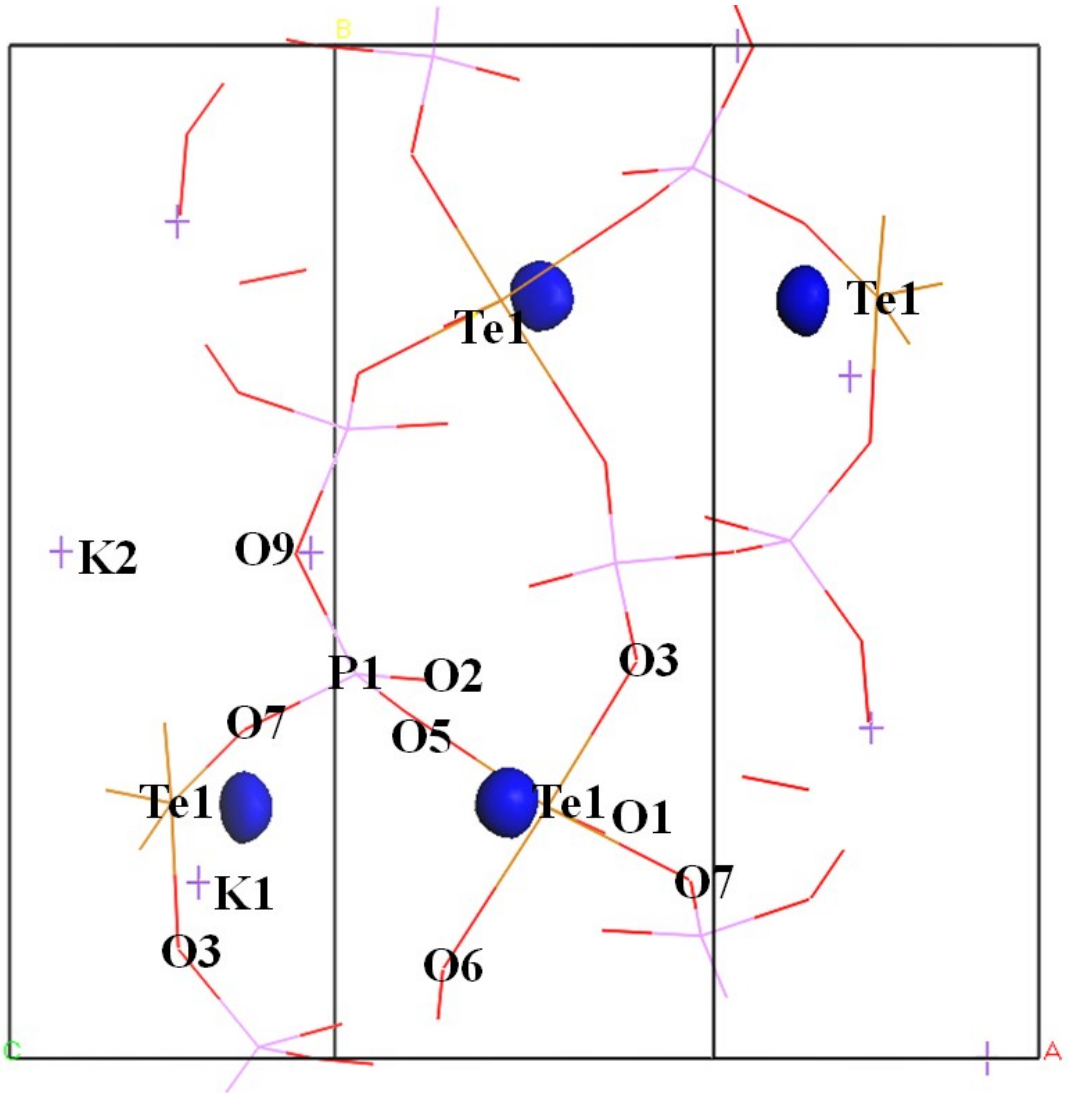

Fig. S6. The electronic local function of $K_2TeP_2O_8$.