Electronic Supplementary Information (ESI)

$K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$: A potential UV nonlinear optical material with large birefringence

Yan Chen, [a,b,c,d] Chunli Hu, [a] Zhi Fang,[a] Jianggao Mao*[a]

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

[b] School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China

[c] University of Chinese Academy of Sciences, Beijing 100049, China

[d] Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201210, China

Email: mjg@fjirsm.ac.cn

Table of Contents

Table S1. Bond lengths (Å) for $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$.

$K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$

K(1)-O(2)#1	2.731(5)	C(1)-N(1)	1.380(9)
K(1)-O(2)	2.731(5)	C(2)-O(2)	1.217(9)
K(1)-O(5)#1	2.705(5)	C(2)-N(2)	1.367(10)
K(1)-O(5)	2.705(5)	C(2)-N(1)	1.372(9)
K(1)-O(1W)	2.682(8)	C(3)-O(3)	1.250(9)
K(1)-O(3W)#2	2.736(8)	C(3)-N(3)	1.351(9)
K(2)-O(2)#3	2.987(5)	C(3)-N(2)	1.396(10)
K(2)-O(2)#4	2.987(5)	C(4)-O(4)	1.250(9)
K(2)-O(5)#1	2.875(6)	C(4)-N(6)	1.349(10)
K(2)-O(5)	2.875(6)	C(4)-N(4)	1.386(9)
K(2)-O(6)#5	2.952(5)	C(5)-O(5)	1.230(9)
K(2)-O(6)#6	2.952(5)	C(5)-N(5)	1.361(9)
K(2)-O(2W)#6	2.734(8)	C(5)-N(4)	1.379(9)
K(2)-O(4W)#6	2.892(9)	C(6)-O(6)	1.234(9)
Pb(1)-N(6)	2.575(6)	C(6)-N(6)	1.353(9)
Pb(1)-N(6)#7	2.576(6)	C(6)-N(5)	1.400(9)
Pb(1)-O(4)	3.060(5)	N(1)-H(1)	0.8600
Pb(1)-O(4)#7	3.060(5)	N(2)-H(2)	0.8602
Pb(1)-O(1W)#8	2.836(7)	N(4)-H(4)	0.8598
Pb(1)-O(2W)	2.583(8)	N(5)-H(5)	0.8600
Pb(1)-O(3W)	2.550(8)	O(1W)-H(1WA)	0.9139
Pb(1)-O(4W)	2.589(7)	O(2W)-H(2WA)	0.9429
C(1)-O(1)	1.264(9)	O(3W)-H(3WA)	1.0063
C(1)-N(3)	1.348(9)	O(4W)-H(4WA)	0.96(10)

Symmetry transformations used to generate equivalent atoms:

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

#5 x-1/2, -y+1/2, z #6 x-1/2, y+1/2, z #7 x, -y, z #8 x-1/2, y-1/2, z

$K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$

K(1)-O(1)#1	2.804(3)	C(2)-N(2)	1.335(4)
K(1)-O(1)#2	2.804(3)	C(2)-N(1)	1.382(4)
K(1)-O(6)	2.727(3)	C(3)-O(3)	1.239(4)
K(1)-O(6)#3	2.727(3)	C(3)-N(2)	1.337(4)
K(1)-O(3W)#4	3.261(4)	C(3)-N(3)	1.384(4)
K(1)-O(5W)	2.793(4)	C(4)-O(4)	1.238(4)
K(1)-O(6W)	2.773(4)	C(4)-N(4)	1.340(4)
K(2)-O(1)	3.053(2)	C(4)-N(6)	1.384(4)
K(2)-O(1)#5	3.053(2)	C(5)-O(5)	1.239(4)
K(2)-O(1)#6	3.306(3)	C(5)-N(4)	1.336(4)
K(2)-O(1)#7	3.306(3)	C(5)-N(5)	1.381(4)
K(2)-O(5)	2.781(2)	C(6)-O(6)	1.227(4)
K(2)-O(5)#5	2.781(2)	C(6)-N(6)	1.358(4)

K(2)-O(3W)	2.831(4)	C(6)-N(5)	1.358(4)
K(2)-O(4W)	2.809(4)	C(7)-O(7)	1.222(5)
K(2)-O(6W)#8	2.841(5)	C(7)-N(7)#11	1.361(3)
K(3)-O(3)#9	3.028(3)	C(7)-N(7)	1.361(3)
K(3)-O(3)#1	3.028(3)	C(8)-O(8)	1.239(4)
K(3)-O(6)#9	3.401(3)	C(8)-N(8)	1.340(3)
K(3)-O(6)#1	3.401(3)	C(8)-N(7)	1.383(4)
K(3)-O(7)	2.786(2)	N(1)-H(1)	0.8600
K(3)-O(7)#10	2.786(2)	N(3)-H(3)	0.8600
K(3)-O(1W)	3.002(5)	N(5)-H(5)	0.8600
K(3)-O(2W)	2.778(4)	N(6)-H(6)	0.8600
K(3)-O(5W)#9	2.848(5)	N(7)-H(7)	0.8600
Pb(1)-N(4)	2.609(3)	O(1W)-H(1WA)	1.0101
Pb(1)-N(4)#5	2.610(3)	O(2W)-H(2WA)	0.8500
Pb(1)-O(4)	2.927(2)	O(2W)-H(2WA)#5	0.8499
Pb(1)-O(4)#5	2.927(2)	O(3W)-H(3WA)	0.8501
Pb(1)-O(1W)	2.777(4)	O(3W)-H(3WA)#5	0.8500
Pb(1)-O(2W)	2.453(4)	O(4W)-H(4WA)	0.8500
Pb(1)-O(3W)	2.746(4)	O(4W)-H(4WA)#5	0.8500
Pb(1)-O(4W)	2.616(4)	O(5W)-H(5WA)	0.8499
C(1)-O(1)	1.226(4)	O(5W)-H(5WA)#3	0.8500
C(1)-N(1)	1.362(4)	O(6W)-H(6WA)	0.8500
C(1)-N(3)	1.363(4)	O(6W)-H(6WA)#3	0.8500
C(2)-O(2)	1.245(4)		

Symmetry transformations used to generate equivalent atoms:

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

#6 -x+1, -y+1, -z #7 -x+1, y, -z #8 x+1/2, y-1/2, z #9 x-1/2, y-1/2, z #10 -x, -y+1, -z+1

#11 -x, y, -z+1

Table S2. Hydrogen bonds for $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ [Å and deg.].

$K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(6)#1	0.86	1.92	2.765(8)	165.4
N(2)-H(2)...O(4)#2	0.86	1.97	2.827(8)	175.7
N(4)-H(4)...O(3)#3	0.86	1.90	2.744(8)	165.7
N(5)-H(5)...O(1)#4	0.86	1.96	2.815(8)	178.0
O(1W)-H(1WA)...O(1)#2	0.91	2.02	2.896(7)	159.2
O(2W)-H(2WA)...O(3)#5	0.94	1.77	2.692(6)	164.2
O(3W)-H(3WA)...O(1)#6	1.01	1.79	2.776(6)	166.8
O(4W)-H(4WA)...N(3)#6	0.96(10)	2.01(10)	2.926(8)	160(9)

Symmetry transformations used to generate equivalent atoms:

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

#4 x+1/2, -y+1/2, z+1 #5 x, -y, z #6 x, y, z+1

$K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(2)#1	0.86	1.93	2.781(3)	173.0
N(3)-H(3)...O(5)	0.86	1.94	2.794(3)	173.5
N(5)-H(5)...O(3)	0.86	1.90	2.754(3)	173.0
N(6)-H(6)...O(8)	0.86	1.97	2.829(3)	173.8
N(7)-H(7)...O(4)	0.86	1.95	2.812(3)	175.2
O(1W)-H(1WA)...O(6)#2	1.01	1.90	2.891(4)	166.2
O(2W)-H(2WA)...N(2)#3	0.85	1.90	2.733(3)	168.1
O(3W)-H(3WA)...O(2)#4	0.85	2.02	2.863(3)	172.3
O(4W)-H(4WA)...N(8)#5	0.85	2.03	2.880(4)	177.5
O(6W)-H(6WA)...O(8)#6	0.85	2.00	2.827(3)	165.6

Symmetry transformations used to generate equivalent atoms:

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

#4 x-1/2, -y+3/2, z #5 x+1/2, y-1/2, z #6 x, -y+2, z

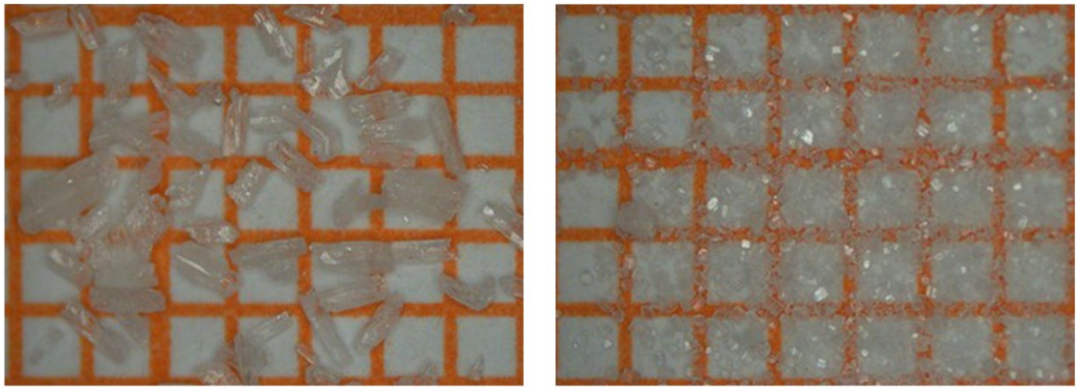

Figure S1. Crystal pictures of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

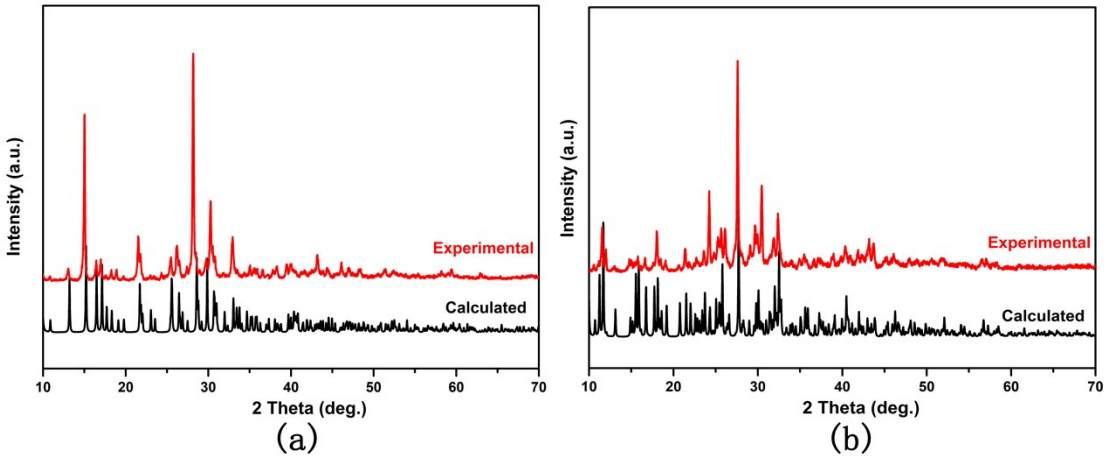

Figure S2. Powder X-ray diffractions patterns of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

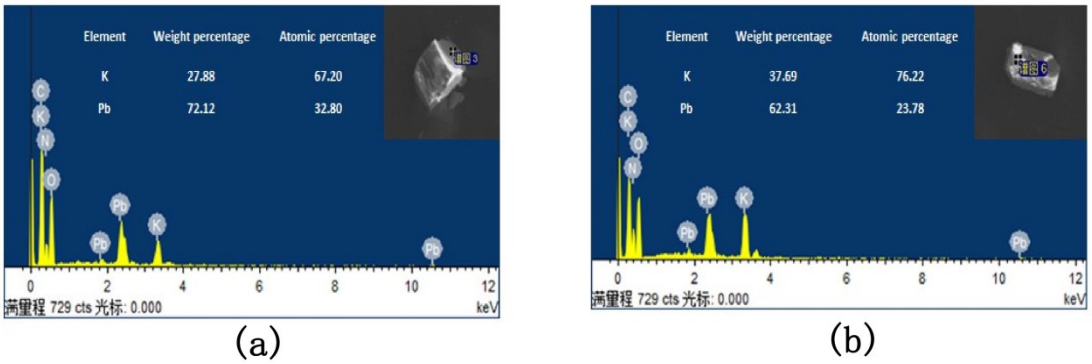

Figure S3. Energy dispersive X-ray spectroscopy analysis of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

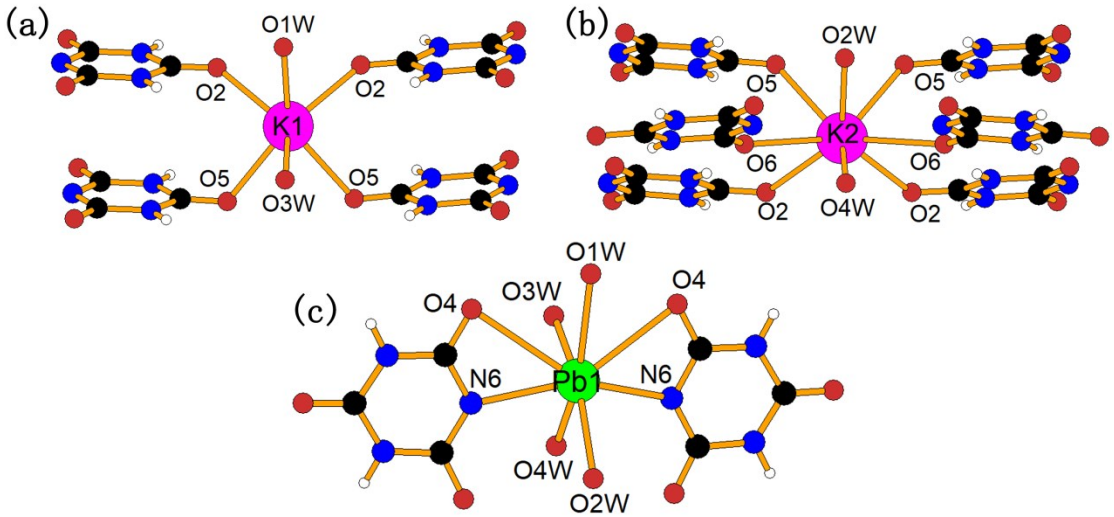

Figure S4. Coordination geometries around K(1) (a), K(2) (b) and Pb(1) (c) in compound $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$.

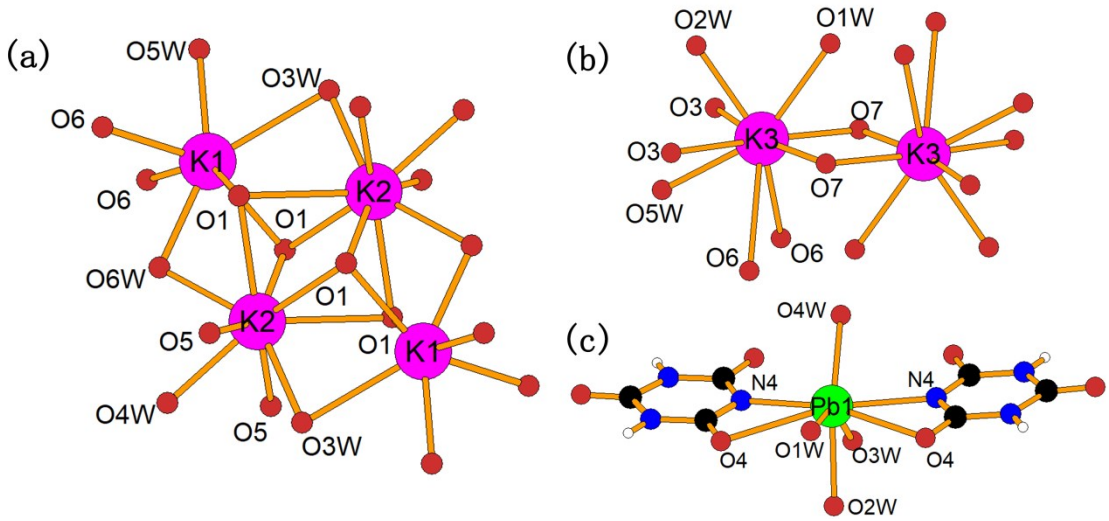

Figure S5. Coordination geometries around K(1) and K(2) (a), K(3) (b), and Pb(1) (c) in compound $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$.

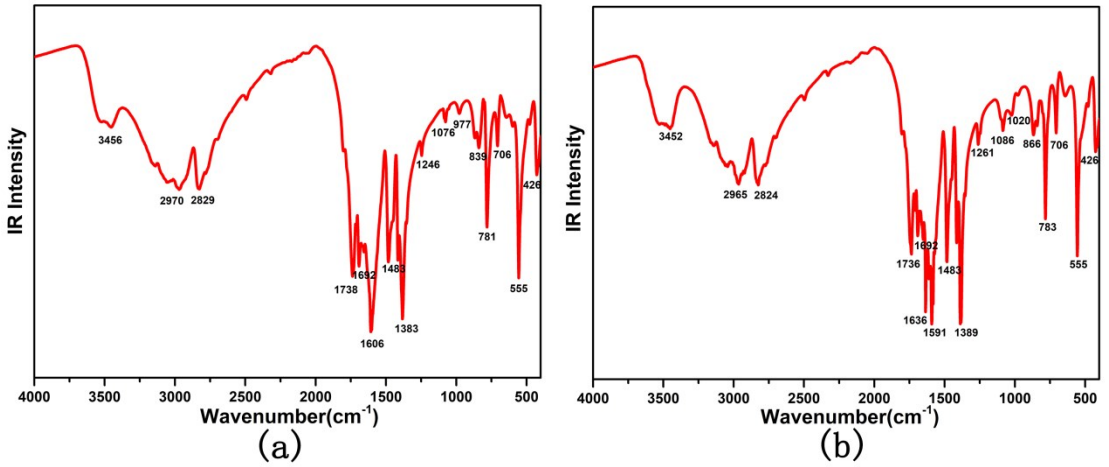

Figure S6. The experimental IR spectra of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

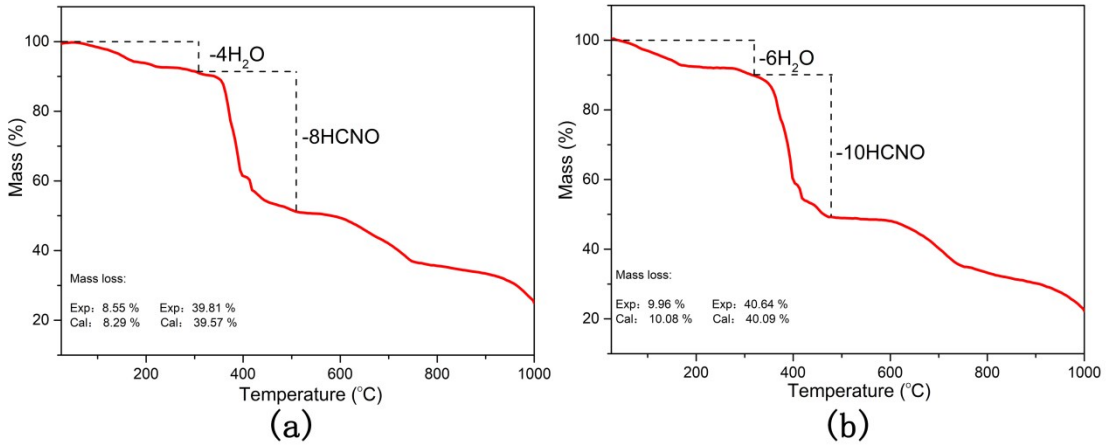

Figure S7. The thermogravimetric analyses (TGA) curves of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

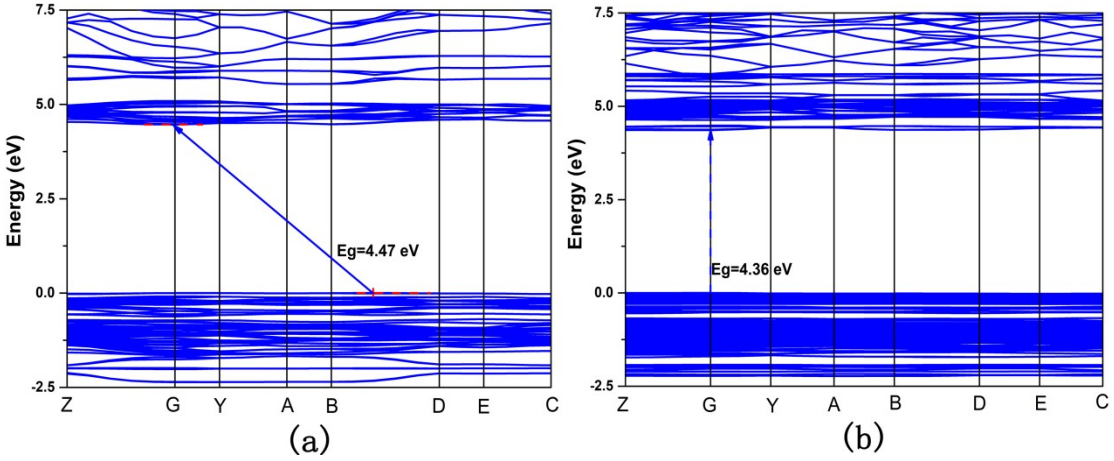

Figure S8. The band structures of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).

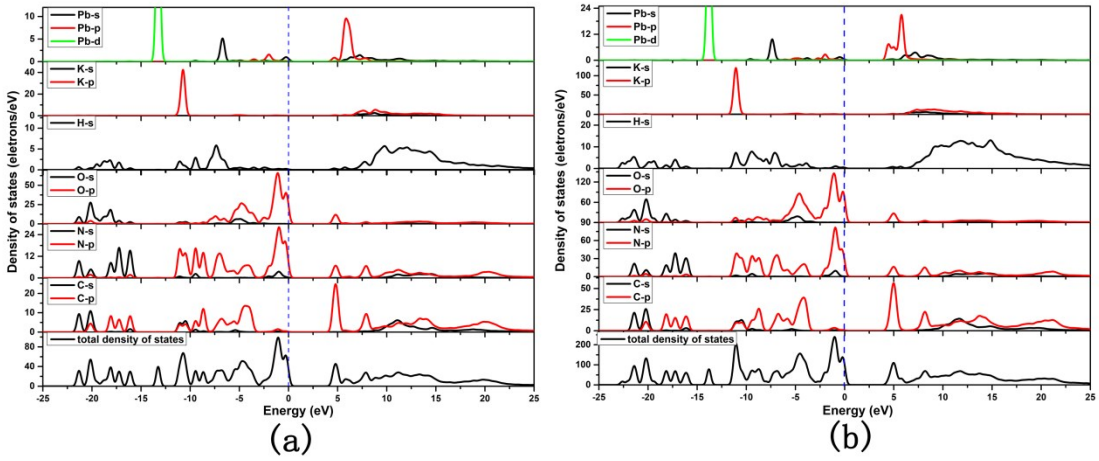

Figure S9. The total and partial densities of states of $K_2Pb(H_2C_3N_3O_3)_4(H_2O)_4$ (a) and $K_3Pb(H_2C_3N_3O_3)_5(H_2O)_6$ (b).