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Supporting information

Hydrous salts of 1-aminoethylidenediphosphonic acid and piperazidine: temperature induced reversible structural transformation in humid environment

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Figure S-1. The ORTEP of compound 1 with thermal ellipsoids at the 30% probability level.

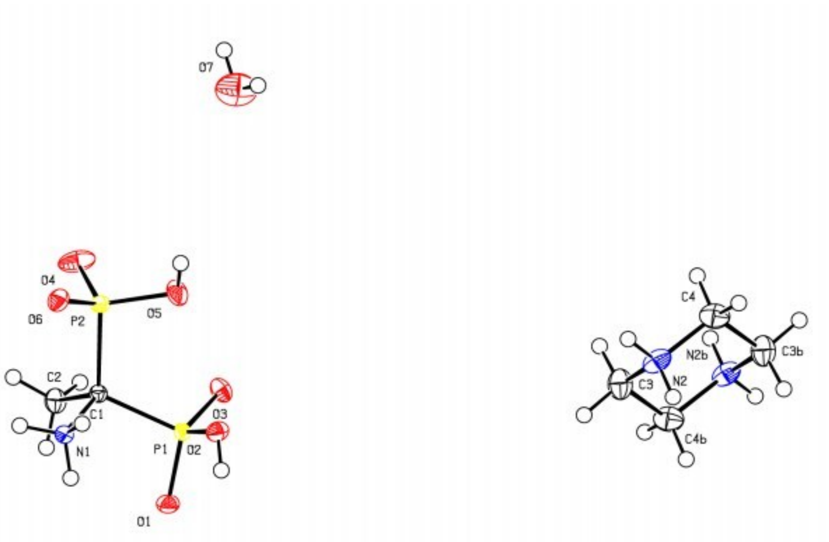

Figure S-2. The ORTEP of compound 2 with thermal ellipsoids at the 30% probability level.

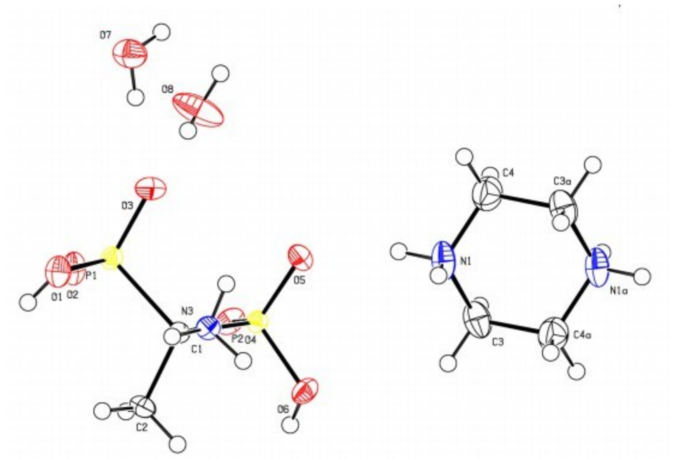

Figure S-3. The ORTEP of compound 3 with thermal ellipsoids at the 30% probability level.

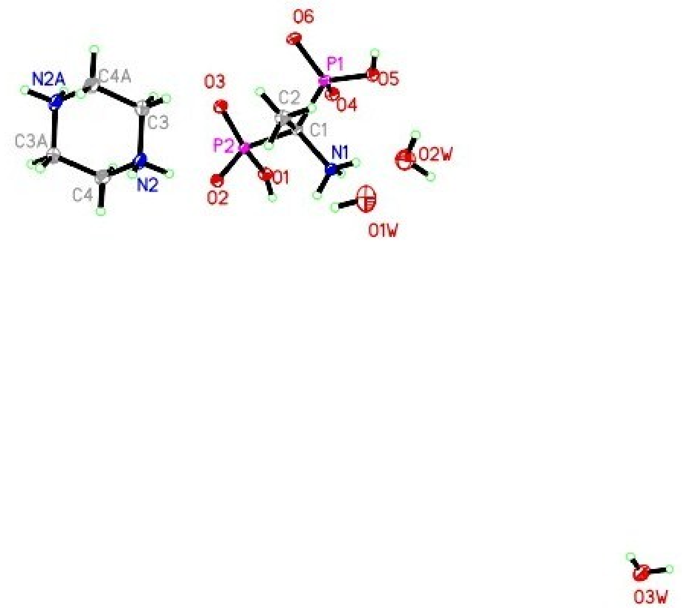

Figure S-4. IR spectra of compounds 1-3.

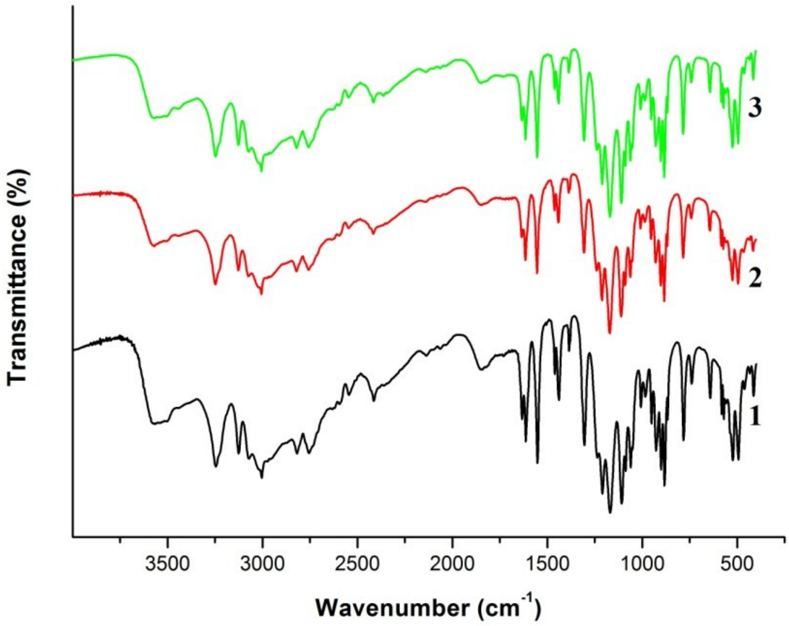

Figure S-5. TG curves of compounds 1-3 in air (black line:compound1; blue line: compound 2; red line:compound 3). Compound 1 can be stable up to 150 °C in air, then, it decomposes until 185 °C, one lattice water is lost on the first stage with the weight decreasing 3.96% (theoretical value is 3.50%). The weight loss occurring between 292℃ and 800 °C corresponds to the decomposition of the dehydration products. The final product in 800 °C is probably assumed to be P_2O_3, and the observed total weight loss (42.21%) is similar to the calculated value (42.78%). The thermo-gravimetric curves of compound 2 and 3 are similar. The first step start at 50℃ and end at 185℃, corresponding to the release of lattice water molecules. The observed weight loss (12.53%) of compound 2 is approximate to the calculated value (12.67%), the observed weight loss (18.50%) of compound 3 is also approximate to the calculated value (17.87%). The second step cover the temperature from 292℃ and 800 °C. The final product of compound 2 are probably assumed to be P_2O_3, and the observed total weight loss (38.56%) is similar to the calculated value (38.71%). The final products of compound 3 are probably assumed to be the mixture of P_2O_3 and P_2O_5, the observed total weight loss (44.25%) contains 25.87% P_2O_3 and 74.13% P_2O_5.

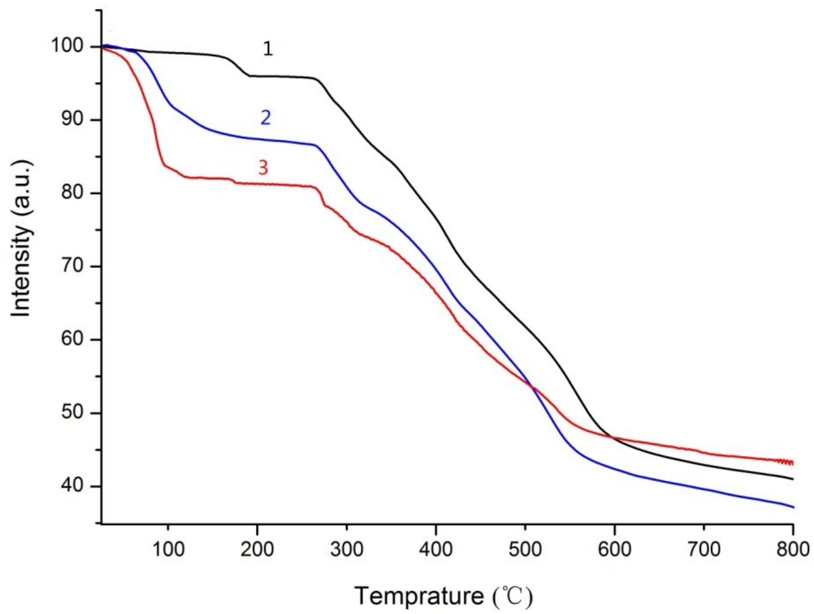

Table S-1. Hydrogen bonds of compounds 1 [Å and °].

Donor-H···Acceptor	D(Donor...Acceptor)	<(Donor-H···Acceptor)
O(5)-H(5)...O(1)#2	2.5234(15)	151.2
O(2)-H(2)...O(6)#3	2.5359(14)	169.5
N(2)-H(2B)...O(3)#4	2.7266(16)	157.3
N(2)-H(2A)...O(4)#5	2.6963(17)	161.6
N(1)-H(1C)...O(1)	3.0146(15)	114.5
N(1)-H(1C)...O(2)#3	3.0281(15)	157.2
N(1)-H(1B)...O(1)#6	2.7956(15)	166.0
N(1)-H(1A)...O(6)#7	2.7543(15)	172.8

Symmetry transformations used to generate equivalent atoms: #1 –x,-y+1,-z; #2 x,y+1,z; #3 -x+1/2,y-1/2,-z+3/2; #4 x,-y+1,z-1/2; #5 x,y,z-1; #6 -x+1/2,y+1/2,-z+3/2; #7 -x+1/2,-y+1/2,-z+2.

Table S-2. Hydrogen bonds of compounds 2 [Å and °].

Donor-H···Acceptor	D(Donor...Acceptor)	<(Donor-H···Acceptor)
O(6)-H(6)...O(4)#2	2.5614(18)	172.3
O(1)-H(7)...O(2)#3	2.5794(19)	175.3
N(3)-H(1A)...O(2)#4	2.8075(19)	149.1
N(3)-H(1B)...O(8)#4	2.738(2)	141.7
N(3)-H(1C)...O(4)#4	2.8021(18)	149.7
N(1)-H(2D)...O(5)	2.750(2)	164.3
N(1)-H(2E)...O(7)#5	2.680(2)	165.3
O(7)-H(3)...O(5)#6	2.739(2)	155(3)
O(7)-H(4)...O(3)	2.671(2)	176(3)
O(8)-H(5)...O(3)	2.830(2)	173(3)

O(8)-H(2)...O(5)#6	2.927(2)	138(3)
O(8)-H(2)...O(3)#6	3.268(2)	137(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+2,-z+1; #2 -x+1,-y+1,-z; #3 -x+1,-y,-z; #4 x+1,y,z; #5 -x+2,-y+1,-z+1; #6 -x+1,-y+1,-z+1.

Table S-3. Hydrogen bonds of compounds 3 [Å and °].

Donor-H···Acceptor	D(Donor...Acceptor)	<(Donor-H···Acceptor)
O(1)-H(1)...O(4)#2	2.5388(18)	173(4)
O(5)-H(5)...O(6)#3	2.5141(19)	172(4)
O(1W)-H(1W1)...O(5)#4	2.879(2)	152(4)
O(1W)-H(2W1)...O(2W)	2.821(3)	153(4)
O(2W)-H(1W2)...O(3W)#5	2.757(3)	171(5)
O(2W)-H(2W2)...O(1W)#6	2.797(3)	167(5)
O(3W)-H(1W3)...O(3)#7	3.007(2)	156(2)
O(3W)-H(1W3)...O(6)#7	2.982(2)	123(2)
O(3W)-H(2W3)...O(3)#8	2.854(2)	174(3)
N(1)-H(1A)...O(2W)	2.786(2)	167.2
N(1)-H(1B)...O(2)#9	2.7891(18)	160.4
N(1)-H(1C)...O(1)#2	2.951(2)	157.6
N(1)-H(1C)...O(4)#2	3.078(2)	118.2
N(2)-H(2D)...O(2)	2.781(2)	149.5
N(2)-H(2D)...O(4)#4	2.953(2)	119.6
N(2)-H(2E)...O(3)#4	2.926(2)	145.8
N(2)-H(2E)...O(6)#4	3.037(2)	129.3

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z; #2 -x+1/2,y+1/2,-z+1/2; #3 -x+1,y,-z+1/2; #4 x,y+1,z; #5 x+1/2,-y+1/2,z-1/2; #6 -x+1,-y+1,-z+1; #7 x+1/2,-y+1/2,-z+1; #8 x,y,z+1; #9 -x+1/2,y-1/2,-z+1/2.