Supporting information

Four New Silver Phosphonates Constructed from Semi-rigid Phosphonate ligands: Syntheses, Structures and Properties

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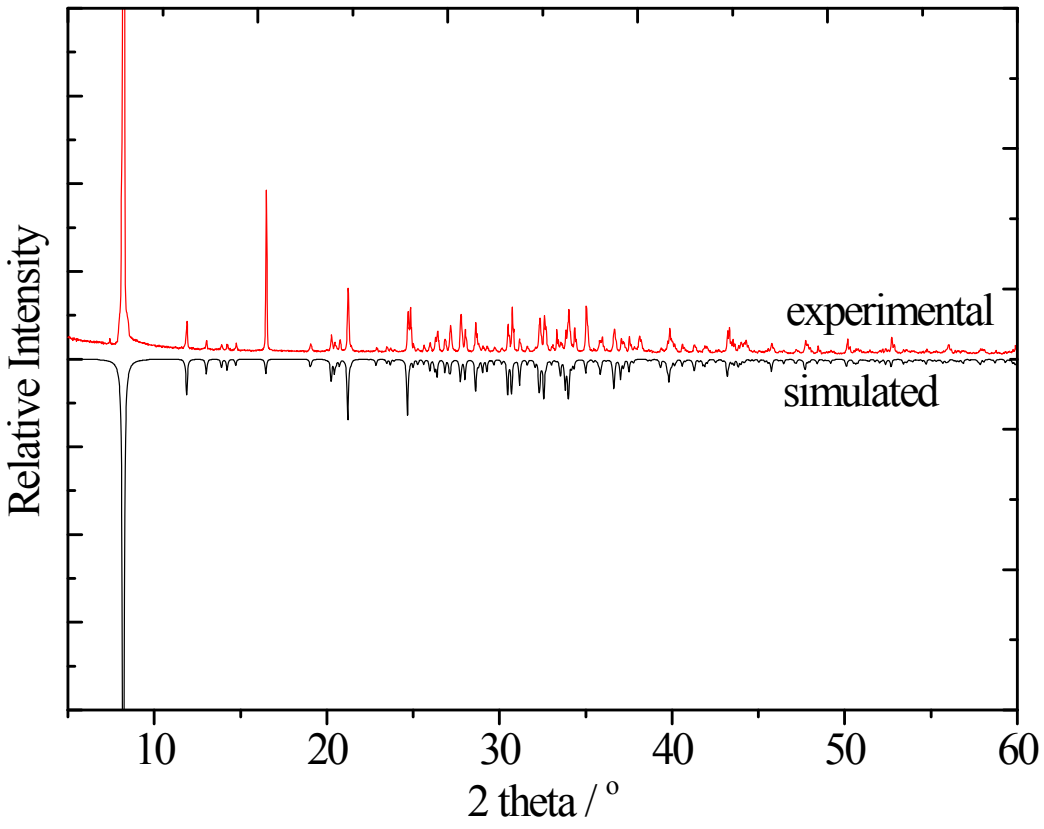

Fig. S1 Experimental and simulated powder X-ray diffraction patterns of compound **1**.

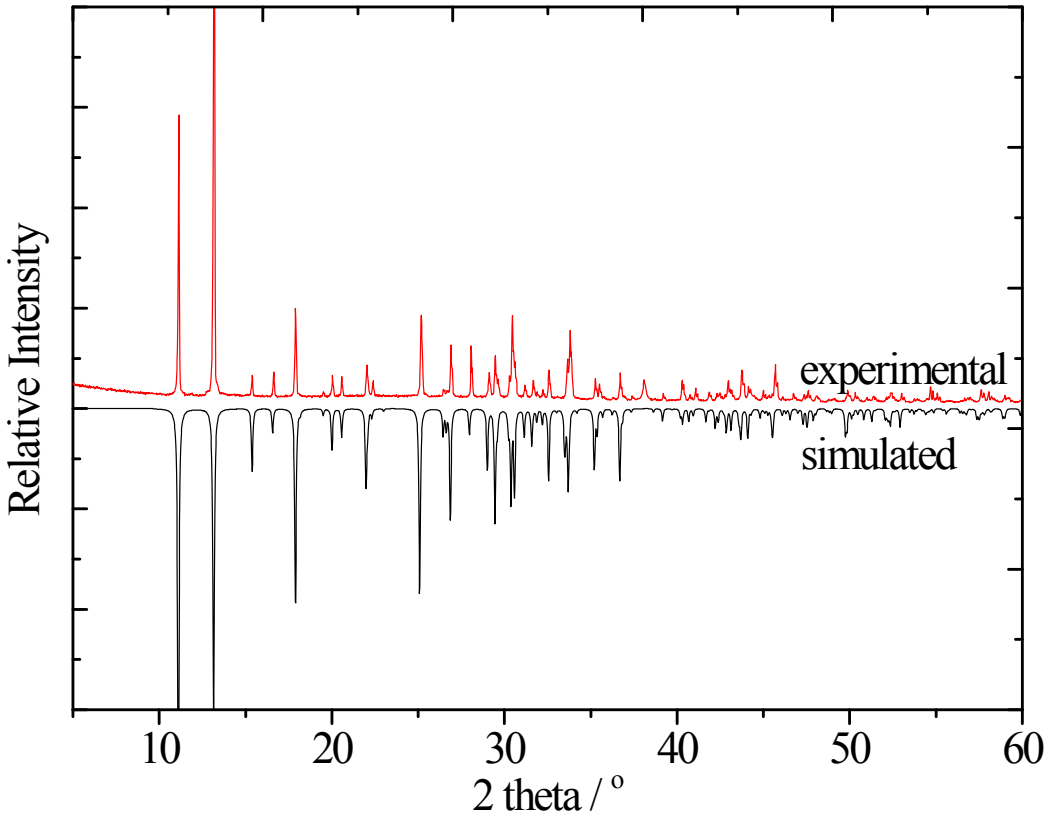

Fig. S2 Experimental and simulated powder X-ray diffraction patterns of compound **2**.

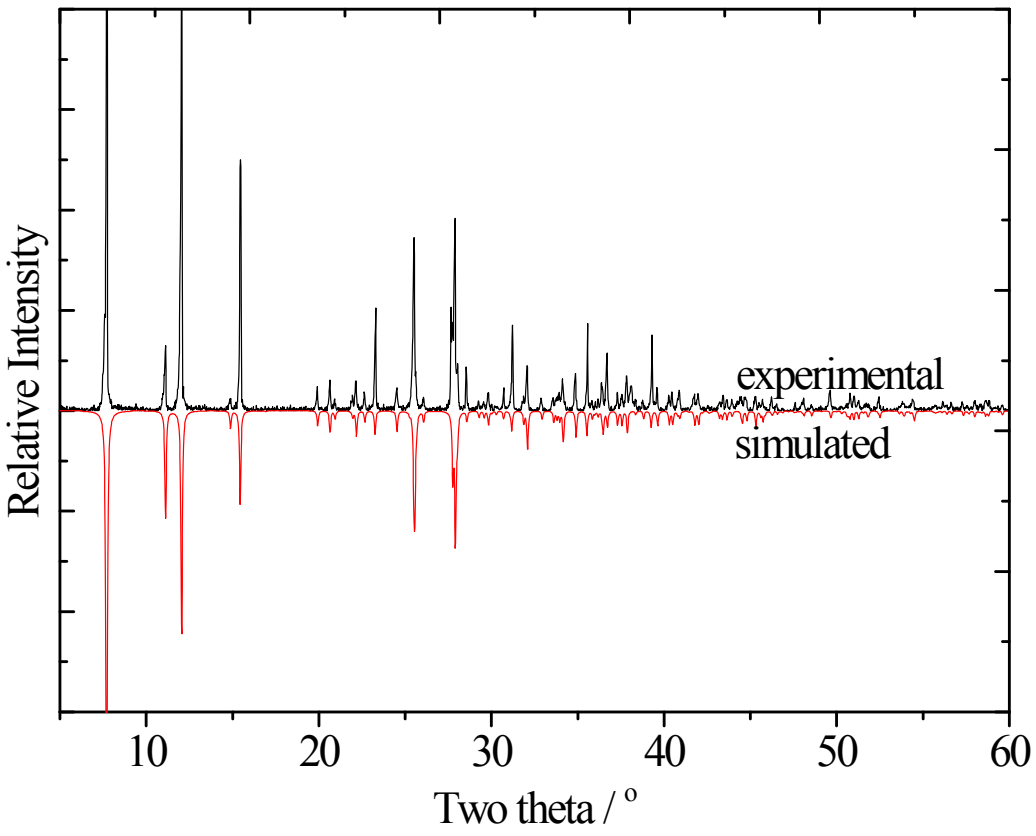

Fig. S3 Experimental and simulated powder X-ray diffraction patterns of compound **3**.

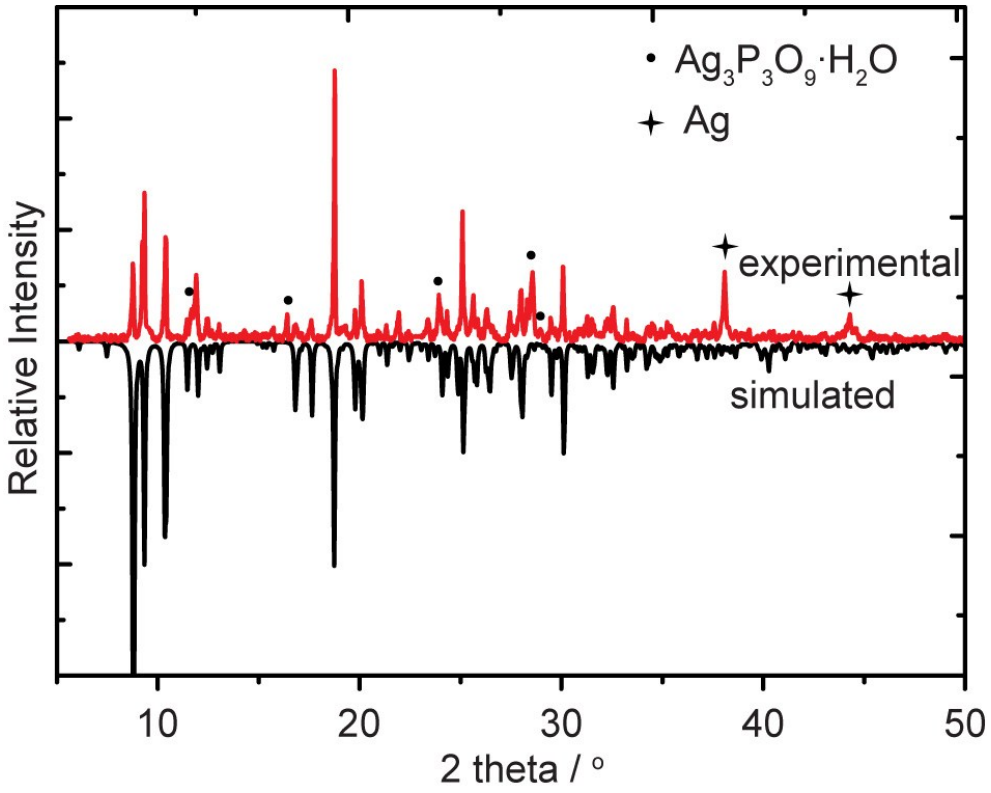

Fig. S4 Experimental and simulated powder X-ray diffraction patterns of compound **4**.

There are a few unexpected peaks (2θ = 11.89, 16.43, 23.93, 28.57, 28.99°, marked with •; and 2θ = 38.07, 44.29°, marked with ✦) on the patterns of compound **4**. With the aid of JADE, these peaks could be ascribed to Ag (PDF: 04-0783) and $Ag_3P_3O_9·H_2O$ (PDF: 26-0955).

Table S1. Selected angels (°) in compounds **1**-**4**.

Compound **1**			
O(8)#1-Ag(1)-O(1)	113.09(13)	O(9)#4-Ag(2)-O(5)	131.66(14)

O(8)#1-Ag(1)-O(6)#2	150.14(13)	O(3)#5-Ag(2)-O(5)	94.48(14)
O(1)-Ag(1)-O(6)#2	83.63(12)	O(9)#4-Ag(2)-O(4)#6	87.81(14)
O(8)#1-Ag(1)-O(6)#1	88.48(12)	O(3)#5-Ag(2)-O(4)#6	112.78(13)
O(1)-Ag(1)-O(6)#1	110.36(12)	O(5)-Ag(2)-O(4)#6	95.37(13)
O(6)#2-Ag(1)-O(6)#1	109.42(10)	O(3)#8-Ag(3)-O(6)	161.37(12)
O(8)#1-Ag(1)-O(5)#2	93.21(13)	O(3)#8-Ag(3)-O(8)	101.38(13)
O(1)-Ag(1)-O(5)#2	103.27(12)	O(6)-Ag(3)-O(8)	96.31(12)
O(6)#2-Ag(1)-O(5)#2	57.96(11)	O(3)#8-Ag(3)-O(3)#9	80.90(13)
O(6)#1-Ag(1)-O(5)#2	142.57(11)	O(6)-Ag(3)-O(3)#9	85.45(12)
O(9)#4-Ag(2)-O(3)#5	128.43(12)	O(8)-Ag(3)-O(3)#9	119.02(13)
Compound **2**			
O(3)-Ag(1)-O(1)#1	121.16(13)	O(3)-Ag(1)-C(4)#1	140.35(15)
O(3)-Ag(1)-O(1)#2	93.87(14)	O(1)#1-Ag(1)-C(4)#1	87.55(15)
O(1)#1-Ag(1)-O(1)#2	110.23(9)	O(1)#2-Ag(1)-C(4)#1	101.28(15)
Compound **3**			
O(1)-Ag(1)-O(2)#1	150.24(10)	O(2)#1-Ag(1)-N(1)	92.10(10)
O(1)-Ag(1)-N(1)	114.45(11)		
O(1)-Ag(1)-Ag(1)#2	83.03(7)	O(2)#1-Ag(1)-Ag(1)#1	79.18(7)
O(2)#1-Ag(1)-Ag(1)#2	108.97(7)	N(1)-Ag(1)-Ag(1)#1	170.32(8)
N(1)-Ag(1)-Ag(1)#2	94.97(8)	Ag(1)#2-Ag(1)-Ag(1)#1	91.870(18)
O(1)-Ag(1)-Ag(1)#1	73.17(7)		
Compound **4**			
N(1)-Ag(1)-N(3)	175.73(16)	N(4)#1-Ag(2)-N(2)#1	160.02(16)
N(1)-Ag(1)-O(2)	99.97(15)	N(4)#1-Ag(2)-O(8)	100.94(15)
N(3)-Ag(1)-O(2)	84.01(14)	N(2)#2-Ag(2)-O(8)	90.80(14)
N(1)-Ag(1)-Ag(2)	87.99(12)	N(4)#1-Ag(2)-Ag(1)	97.04(12)
N(3)-Ag(1)-Ag(2)	94.92(12)	N(2)#2-Ag(2)-Ag(1)	102.88(11)
O(2)-Ag(1)-Ag(2)	68.68(12)	O(8)-Ag(2)-Ag(1)	58.77(10)

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

Table S2. C-H···O interactions in compounds **3**-**4**.

	C-H (Å)	H···O (Å)	C···O (Å)	< C-H···O (º)
Compound **3**				

C6-H6A···O2#1	0.9300	2.5800	3.236(5)	128.00
Compound **4**				
C1-H1A···O8	0.9300	2.5700	3.072(8)	114.00
C6-H6A···O3#1	0.9300	2.5300	3.294(7)	140.00
C10-H10A···O1	0.9300	2.5000	3.209(7)	133.00
C11-H11A···O2	0.9300	2.5900	3.094(9)	114.00
C16-H16A···O9#2	0.9300	2.4200	3.282(8)	154.00
C20-H20A···O7	0.9300	2.4500	3.251(8)	145.00
C25-H25A···O6#3	0.9300	2.5800	3.443(6)	154.00
C26-H26C···O3#4	0.9600	2.5700	3.425(7)	148.00
C29-H29A···O9#5	0.9700	2.3600	3.288(8)	159.00

Symmetry transformations used to generate equivalent atoms: For **3**: #1: 1-x, -1-y, -z; For **4**: #1: 2-x, -y, 1-z; #2: 1-x, 1-y, -z; #3: 1+x, y, z; #4: -1+x, y, z; #5: m1-x, 1-y, 1-z;