

Supporting information

Investigation on the structure variation of metal diphosphonates with the changing of N-donor auxiliary ligands and Their Properties

Si-Fu Tang*, Liang-Jun Li, Chao Wang and Xue-Bo Zhao*

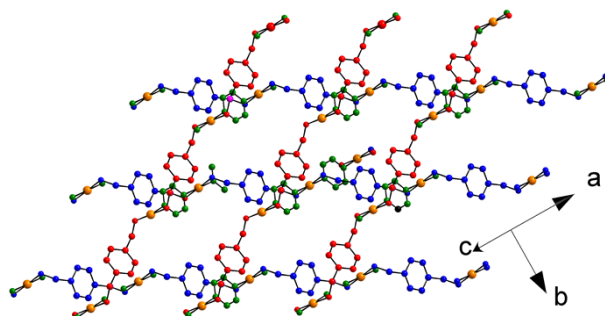


Fig. S1 Packing diagram assembled from 1D chains in two directions (red and blue) and pyrazine molecules (green) of compound **2**. The hydrogen atoms, methyl groups and uncoordinated phosphonate oxygen atoms are omitted for clarity.

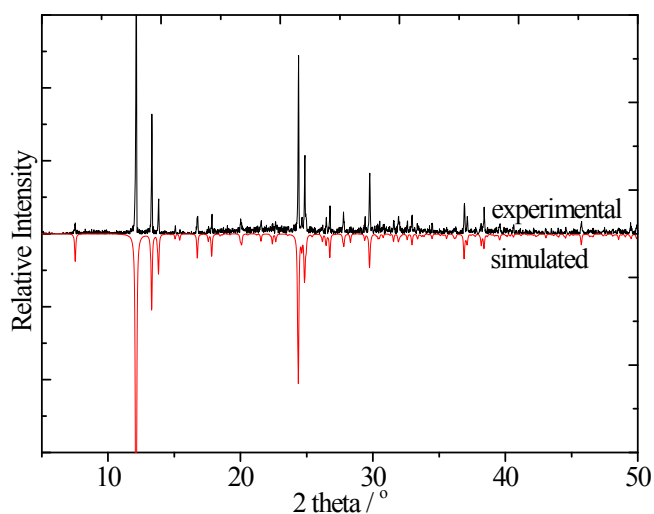


Fig. S2 XRD patterns of compound **1**.

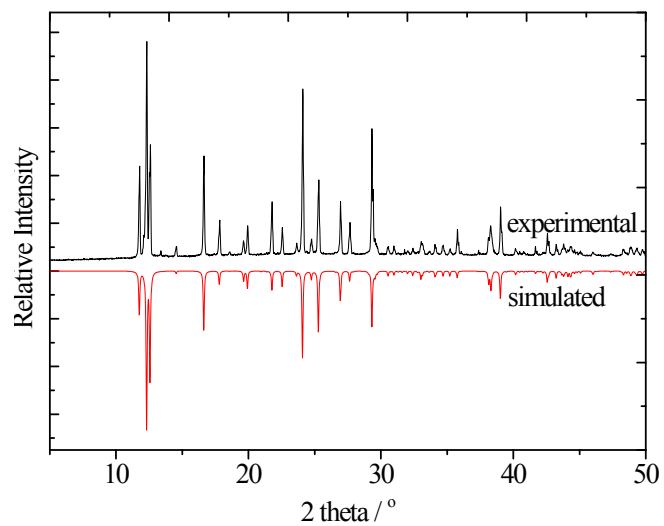


Fig. S3 XRD patterns of compound 2.

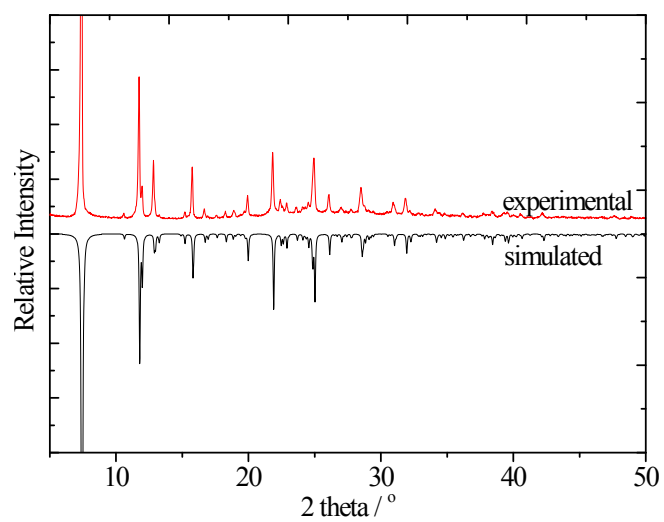


Fig. S4 XRD patterns of compound 3.

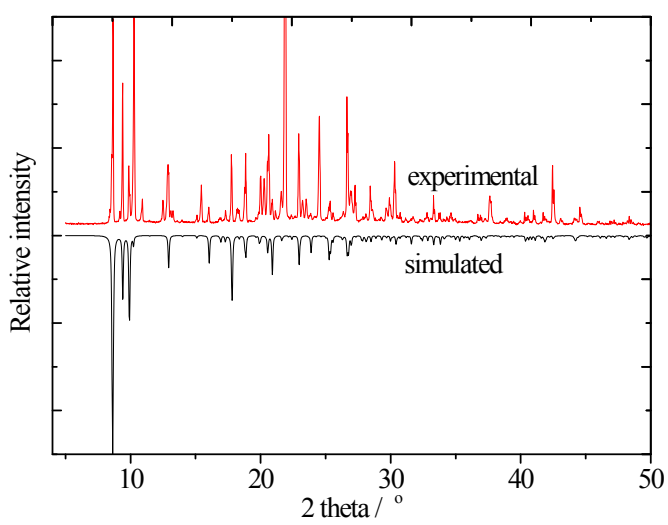


Fig. S5 XRD patterns of compound 4.

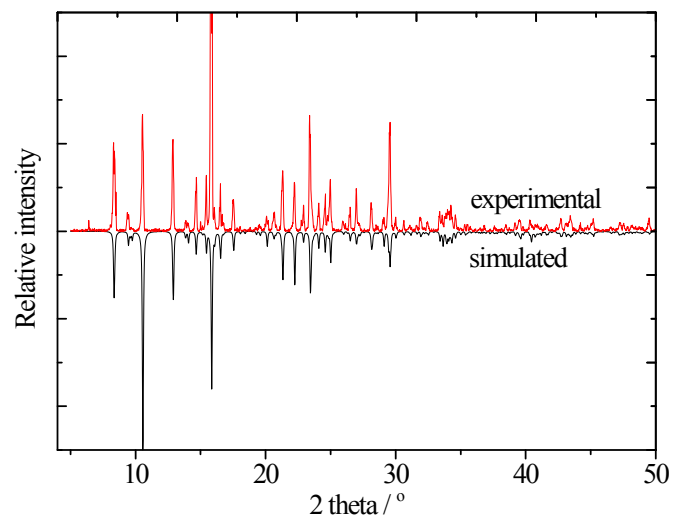


Fig. S6 XRD patterns of compound 5.

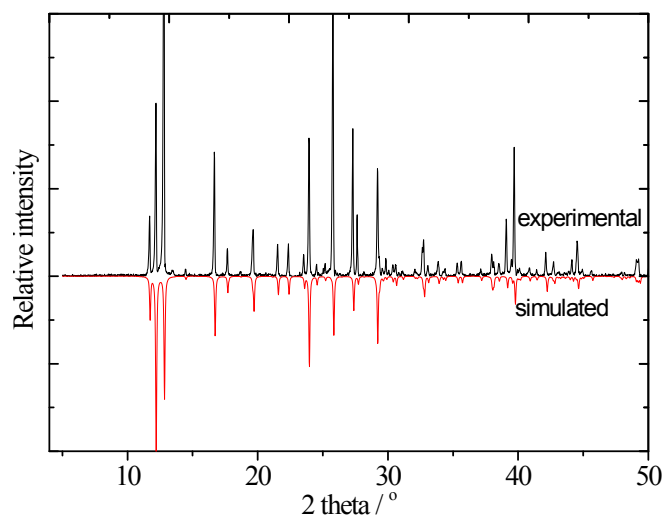


Fig. S7 XRD patterns of compound 6.

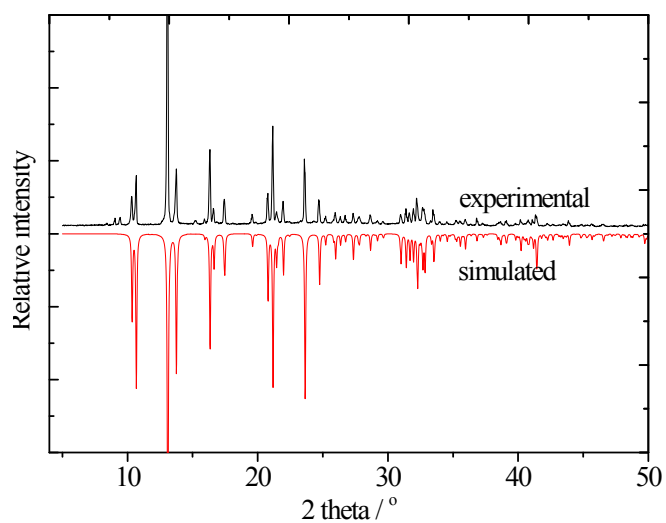


Fig. S8 XRD patterns of compound 7.

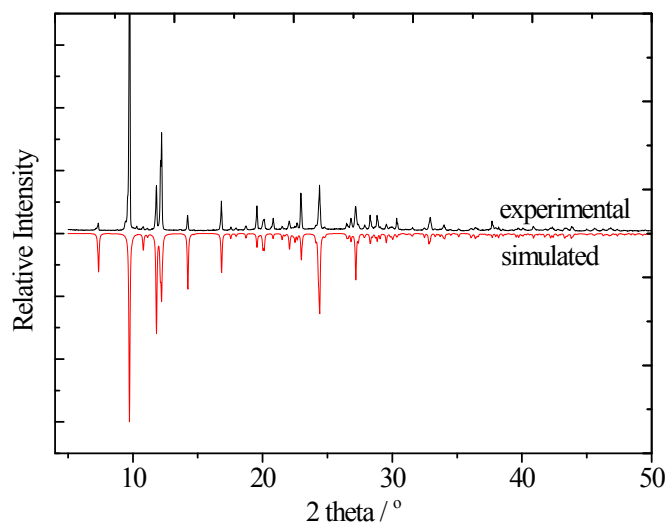


Fig. S9 XRD patterns of compound **8**.

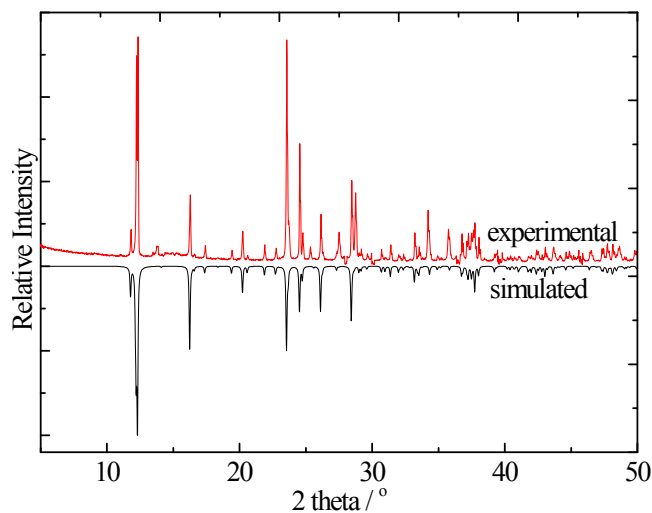


Fig. S10 XRD patterns of compound **9**.

Table S1. Specified hydrogen bonds (with esds except fixed and riding H)

D-H	H... A	D...A	<(DHA)	
1				
0.85	2.07	2.796(3)	142.4	O1W-H1W...O3_\$1
0.85	1.88	2.695(3)	160.4	O1W-H2W...O6_\$2
2				
0.85	1.82	2.663(2)	172.6	O1W-H2W...O2_\$1
0.82	1.81	2.608(2)	163.5	O3-H3A...O1_\$2
3				
0.82	1.80	2.620(8)	177.2	O5-H5A...O1_\$1

0.85	2.38	3.129(10)	147.3	O1W-H2W...O3_\$1
4				
0.85	1.99	2.792(5)	157.5	O1W-H2W...O1_\$1
0.85	2.29	2.907(5)	129.1	O1W-H1W...O3_\$1
0.85	2.04	2.781(5)	145.7	O1W-H1W...O6
0.85	2.38	2.599(6)	95.1	O2W-H4W...O1
0.85	2.02	2.770(6)	146.4	O2W-H3W...O2_\$2
0.85	2.31	2.837(9)	120.1	O3W- H6W...O2W_\$3
0.82	1.76	2.569(6)	166.4	O1-H1A...O2W
0.82	1.74	2.539(5)	164.6	O5-H5A...O2_\$4
5				
0.82	1.72	2.527(4)	168.3	O1-H1B...O4_\$1
0.82	1.77	2.580(4)	169.2	O5-H5B...O2_\$1
0.85	1.99	2.794(5)	156.4	O4W- H7W...O3W_\$2
0.85	2.17	3.013(5)	169.5	O3W-H6W...O5
0.85	2.46	3.022(5)	124.0	O3W-H6W...O6
0.85	2.12	2.944(6)	162.2	O4W-H8W...O3W
6				
0.85	1.86	2.716(4)	175.7	O1W-H2W...O2_\$1
0.82	1.95	2.745(4)	161.6	O3-H3A...O1_\$2
7				
0.82	1.73	2.549(4)	172.4	O1-H1B...O2_\$1
8				
0.82	1.68	2.469(3)	161.2	O5-H5B...O4_\$1
9				
0.87	1.82	2.677(3)	169.6	O1W-H2W...O2_\$1
0.82	1.79	2.577(3)	158.9	O3-H3A...O1_\$2

Operators

for

generating equivalent atoms: For **1**: \$1 -x+1, y+1/2, -z+1/2; \$2 -x+2, y+1/2, -z+1/2. For **2**, **6** and **9**: \$1 x, -y+1, z-1/2; \$2 -x+1/2, y+1/2, -z+1/2. For **3**: \$1 -x+y-2/3, y-1/3, z+1/6. For **4**: \$1 x+1, y, z; \$2 -x+1, -y+1, -z; \$3 x-1, y, z+1; \$4 -x+1, -y+1, -z+1. For **5**: \$1 -x-1, -y-1, -z; \$2 -x-1, -y, -z. For **7**: \$1 -x+1, -y, -z+1. For **8**: 1-x, 1-y, 1-z.