

Supporting information

Speciation of Metal Phosphonates with the assistance of weak interactions

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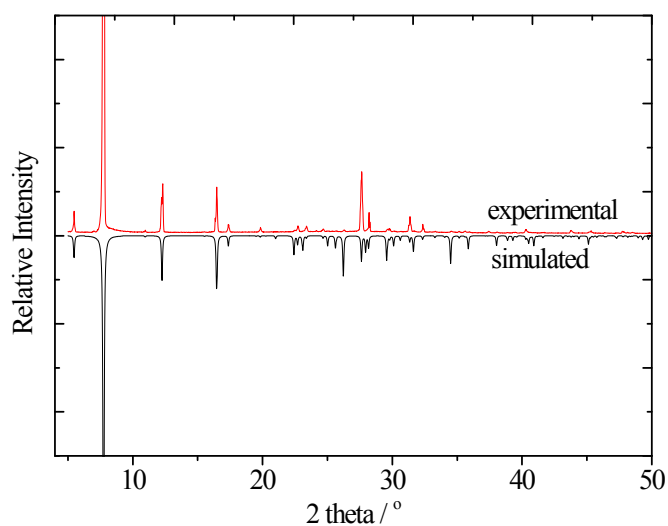


Figure S1. XRD pattern of compound 1.

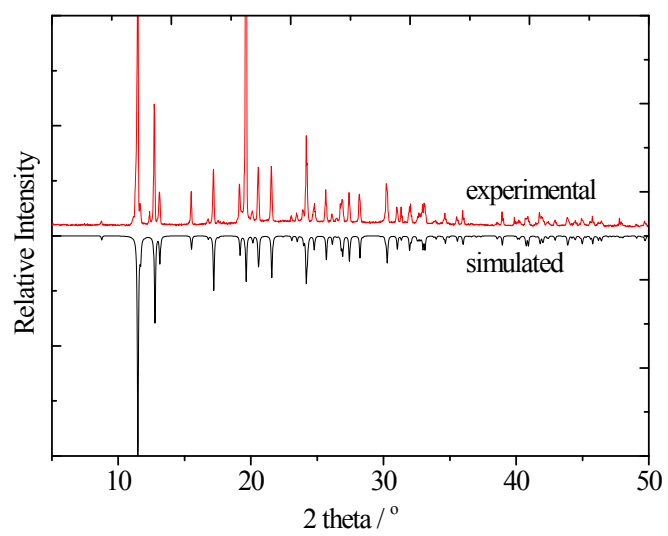


Figure S2. XRD pattern of compound **2**.

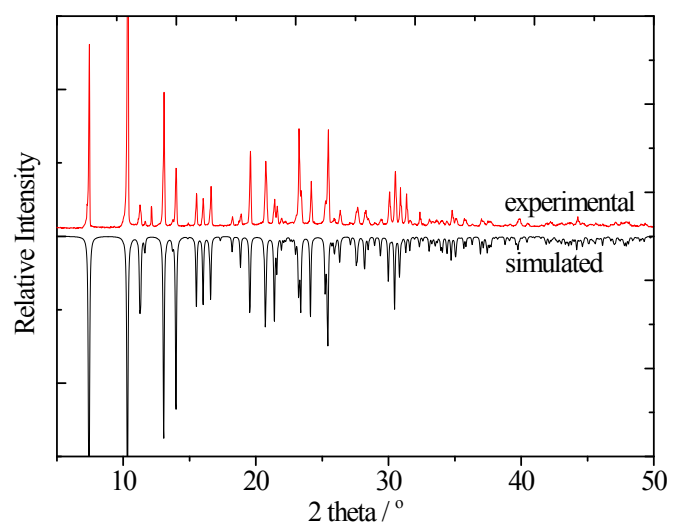


Figure S3. XRD pattern of compound **3**.

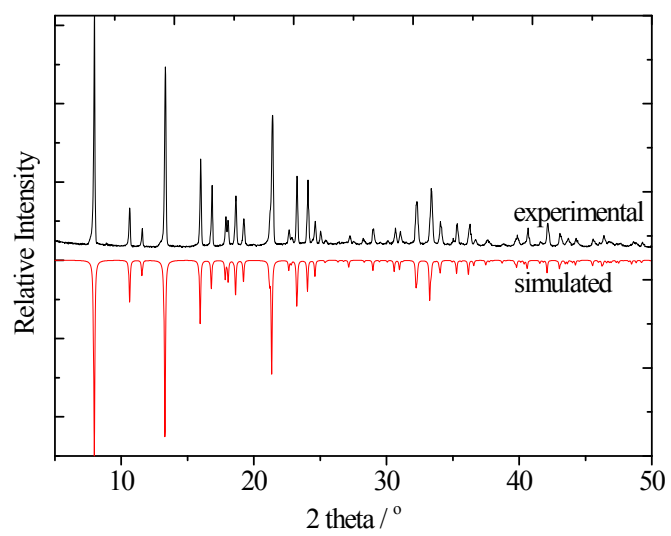


Figure S4. XRD pattern of compound 4.

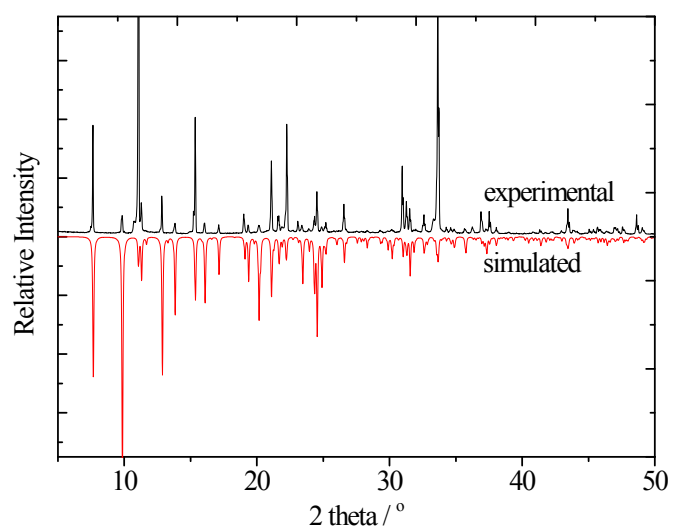


Figure S5. XRD pattern of compound 5.

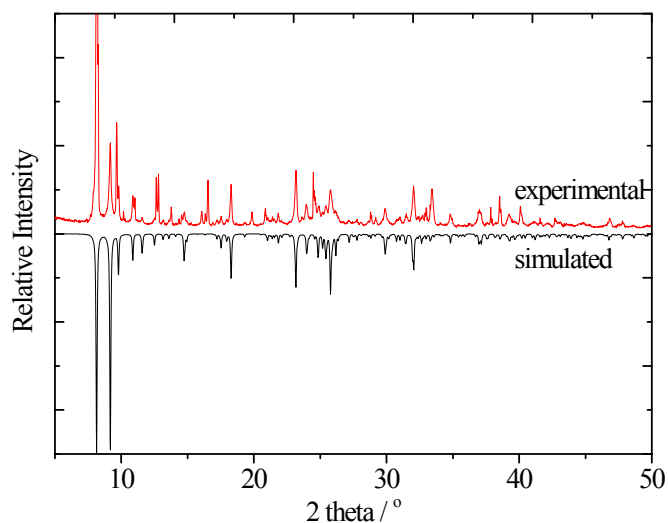


Figure S6. XRD pattern of compound **6**.

Table S1. Specified C-H $\cdots$ O interactions in compounds **1-6**.

D-H (Å)	H $\cdots$ A (Å)	D $\cdots$ A (Å)	<(DHA) (°)	
<b>1</b>				
0.93	2.93	3.31(3)	105.6	C2-H2A $\cdots$ O2W_\$4
0.93	2.58	2.96(3)	104.7	C2-H2A $\cdots$ O3
0.93	3.57	3.703(19)	90.9	C2-H2A $\cdots$ O4_a
0.93	3.57	3.703(19)	90.9	C2-H2A $\cdots$ O1W_\$4
0.93	2.14	2.84(3)	131.6	C2-H2A $\cdots$ O1W_\$5
0.93	2.67	3.25(3)	121.7	C4-H4A $\cdots$ O1_\$3
0.93	2.63	3.32(3)	131.3	C4-H4A $\cdots$ O5_a
0.93	3.12	3.27(3)	90.8	C4-H4A $\cdots$ O6_\$1a
0.93	2.95	3.19(3)	96.7	C4-H4A $\cdots$ O6_a
0.93	2.93	3.31(3)	105.6	C6-H6A $\cdots$ O1_\$1
0.93	2.58	2.96(3)	104.7	C6-H6A $\cdots$ O1
0.93	3.57	3.703(19)	90.9	C6-H6A $\cdots$ O2
0.96	3.60	4.21(3)	124.1	C7-H7A $\cdots$ O1_\$1
0.96	3.37	4.19(3)	145.0	C7-H7B $\cdots$ O1_\$2
0.96	3.40	3.92(3)	116.2	C7-H7C $\cdots$ O1_\$3
<b>2</b>				
0.93	2.62	3.010(3)	106.1	C1-H1A $\cdots$ O1
0.93	2.62	3.010(3)	106.1	C1-H1A $\cdots$ O1_\$5
0.93	3.37	3.927(5)	120.4	C1-H1A $\cdots$ O2W
0.93	3.37	3.927(5)	120.4	C1-H1A $\cdots$ O2W_\$5
0.93	2.66	3.475(4)	146.7	C3-H3A $\cdots$ O1_\$6
0.93	3.44	3.878(4)	111.3	C3-H3A $\cdots$ O1W

0.93	3.18	3.333(4)	91.3	C3-H3A...O2
0.93	2.94	3.180(4)	96.2	C3-H3A...O3
0.93	3.10	3.847(4)	139.0	C3-H3A...O3_\$6
0.96	3.34	4.234(4)	155.1	C5-H5A...O1W_\$7
0.96	3.56	4.234(4)	129.6	C5-H5C...O1W_\$8
0.96	2.92	3.628(4)	131.4	C5-H5B...O3_\$6
0.96	2.76	3.628(4)	149.9	C5-H5A...O3_\$9
0.93	2.36	3.033(4)	128.8	C6-H6A...O1W
0.93	3.23	3.463(5)	96.5	C7-H7A...O1W
0.93	2.50	2.960(4)	110.8	C7-H7A...O2_\$10
<b>3</b>				
0.93	2.44	2.965(4)	115.8	C1-H1A...O4_\$3
0.93	3.38	3.661(4)	100.0	C2-H2A...O2_\$4
0.93	2.44	3.175(4)	136.4	C3-H3A...O2_\$4
0.93	3.56	3.853(5)	101.4	C3-H3A...O3_\$4
0.93	2.94	3.624(4)	131.9	C7-H7A...O5_\$4
0.93	3.28	3.783(5)	115.9	C7-H7A...O6_\$4
0.93	3.25	3.782(5)	118.4	C8-H8A...O5_\$4
0.93	3.42	4.089(4)	131.2	C9-H9A...O3_\$5
0.93	3.00	3.388(4)	106.9	C9-H9A...O4
0.93	2.74	3.670(4)	177.5	C9-H9A...O5_\$6
0.93	3.29	3.692(5)	108.6	C9-H9A...O6
0.93	3.47	4.127(4)	129.8	C10-H10A...O3_\$5
0.93	3.43	3.765(4)	104.0	C10-H10A...O6
0.93	2.50	2.990(4)	112.8	C10-H10A...O6_\$5
0.96	2.42	3.350(4)	163.1	C11-H11C...O1_\$7
0.96	3.44	4.008(4)	119.8	C11-H11C...O2_\$2
0.93	2.58	3.441(4)	154.2	C13-H13A...O2_\$2
0.93	3.42	4.108(4)	132.2	C13-H13A...O3_\$2
0.93	2.63	3.011(4)	105.0	C13-H13A...O5
0.93	2.67	3.030(4)	103.8	C15-H15A...O3
0.93	2.75	3.058(4)	100.5	C15-H15A...O6
0.93	3.43	3.481(4)	85.7	C17-H17A...O1
0.93	3.43	4.221(4)	144.5	C17-H17A...O1_\$1
0.93	2.76	3.080(4)	101.1	C17-H17A...O2
<b>4</b>				
0.96	3.44	3.995(8)	118.7	C1-H1B...O1_\$4
0.96	2.97	3.583(9)	122.6	C1-H1D...O1W_\$5
0.96	3.49	4.190(9)	131.9	C1-H1C...O1W_\$6
0.96	3.17	3.360(5)	93.1	C3-H3A...O1
0.96	3.00	3.128(5)	88.6	C3-H3A...O3
0.93	3.13	3.861(5)	136.3	C5-H5A...O1_\$2
0.93	3.13	3.861(5)	136.3	C5-H5A...O1_\$8

0.93	2.58	2.994(4)	107.3	C5-H5A...O2
0.93	2.58	2.994(4)	107.3	C5-H5A...O2_\$7
0.93	3.02	3.339(8)	101.6	C6-H6A...O1W_\$1
0.93	2.46	2.908(7)	109.8	C6-H6A...O3_\$1
0.93	3.39	4.247(8)	154.6	C7-H7A...O1W_\$9
0.93	3.20	3.535(5)	103.6	C10-H10A...O1W_\$5
0.93	2.62	3.399(4)	141.3	C10-H10A...O3_\$5
0.93	2.67	3.304(5)	125.9	C11-H11A...O1W_\$10
0.93	2.81	3.615(5)	145.2	C11-H11A...O2_\$5
0.93	3.09	3.284(5)	93.7	C11-H11A...O3_\$10
0.93	3.20	3.697(4)	115.3	C11-H11A...O3_\$5
<b>5</b>				
0.93	2.42	3.001(4)	120.3	C1-H1A...O4_\$3
0.93	2.39	3.200(4)	145.4	C3-H3A...O2_\$4
0.93	3.47	3.855(4)	107.5	C3-H3A...O3_\$4
0.93	2.95	3.593(4)	127.9	C7-H7A...O5_\$4
0.93	3.03	3.670(4)	127.3	C7-H7A...O6_\$4
0.93	3.01	3.626(4)	125.4	C8-H8A...O5_\$4
0.93	3.48	4.054(4)	122.3	C9-H9A...O3_\$5
0.93	3.11	3.550(4)	111.1	C9-H9A...O4
0.93	2.77	3.688(4)	171.4	C9-H9A...O5_\$6
0.93	3.26	3.960(4)	133.8	C10-H10A...O3_\$5
0.93	3.21	3.782(4)	121.4	C10-H10A...O6
0.93	2.87	3.213(4)	103.1	C10-H10A...O6_\$5
0.96	2.39	3.306(4)	158.4	C11-H11C...O1_\$7
0.93	2.63	3.482(4)	151.9	C13-H13A...O2_\$2
0.93	2.68	3.044(4)	104.1	C13-H13A...O5
0.93	2.64	3.012(3)	104.4	C15-H15A...O3
0.93	2.69	3.005(3)	100.5	C15-H15A...O6
0.93	3.59	4.360(4)	141.9	C17-H17A...O1_\$1
0.93	2.77	3.083(4)	100.9	C17-H17A...O2
<b>6</b>				
0.96	3.14	3.806(8)	128.2	C1-H1D...O1W_\$6
0.96	3.48	4.078(9)	122.5	C1-H1C...O2W_\$6
0.96	3.25	4.114(9)	151.2	C1-H1B...O4W_\$7
0.96	2.73	3.618(9)	154.3	C1-H1B...O5W_\$8
0.96	3.15	3.721(8)	119.6	C1-H1C...O6W_\$9
0.96	3.14	4.017(9)	153.2	C1-H1C...O7W_\$9
0.93	2.55	3.443(7)	159.9	C3-H3A...O1W_\$6
0.93	3.20	3.310(7)	88.7	C3-H3A...O1
0.93	2.74	3.066(7)	101.5	C3-H3A...O3
0.93	3.04	3.740(7)	133.3	C3-H3A...O6_\$6
0.93	2.79	3.132(7)	103.2	C5-H5B...O2

0.93	2.73	3.091(7)	104.4	C5-H5B···O4
0.93	3.43	4.280(7)	153.0	C5-H5B···O6W
0.93	3.26	4.133(8)	156.4	C5-H5B···O7W
0.93	2.96	3.778(7)	147.1	C7-H7A···O1_\$8
0.93	3.05	3.239(8)	93.2	C7-H7A···O5
0.93	3.30	4.091(8)	143.8	C7-H7A···O5W_\$8
0.93	2.83	3.106(7)	98.2	C7-H7A···O6
0.93	2.98	3.505(8)	117.6	C8-H8A···O1W_\$10
0.93	3.42	4.048(8)	127.0	C8-H8A···O1_\$8
0.93	2.73	3.363(8)	126.5	C8-H8A···O3_\$8
0.93	3.03	3.814(8)	143.5	C8-H8A···O3W_\$8
0.93	3.58	3.923(8)	105.0	C8-H8A···O6W_\$9
0.93	2.66	3.448(9)	143.0	C9-H9A···O6W_\$9
0.93	2.81	3.533(9)	135.2	C9-H9A···O7W_\$9
0.93	3.58	4.296(9)	135.8	C10-H10A···O2W_\$6
0.93	2.69	3.497(9)	145.7	C10-H10A···O4W_\$6
0.93	2.85	3.492(9)	127.3	C10-H10A···O5_\$6
0.93	3.28	3.763(9)	114.5	C10-H10A···O7W_\$9
0.93	2.99	3.652(8)	129.2	C11-H11A···O1
0.93	2.92	3.531(8)	124.4	C11-H11A···O5_\$6
0.93	3.52	4.188(9)	130.6	C11-H11A···O5_\$1
0.93	2.90	3.538(9)	126.5	C14-H14A···O1
0.93	3.27	3.800(9)	118.5	C14-H14A···O4W_\$1
0.93	3.56	4.054(9)	115.8	C14-H14A···O5W
0.93	3.35	4.050(9)	134.3	C15-H15A···O2W_\$4
0.93	3.28	4.061(9)	143.0	C15-H15A···O3W_\$11
0.93	3.04	3.690(10)	128.0	C15-H15A···O4W_\$1
0.93	3.26	3.906(10)	128.9	C15-H15A···O5W
0.93	3.51	3.725(10)	96.2	C16-H16A···O7W_\$1
0.93	2.83	3.446(9)	125.0	C17-H17A···O1W
0.93	3.19	3.317(9)	89.3	C17-H17A···O2_\$1
0.93	3.48	4.187(9)	134.9	C17-H17A···O2W
0.93	3.04	3.801(9)	139.9	C17-H17A···O3W_\$1
0.93	3.49	3.597(9)	89.2	C17-H17A···O4
0.93	3.54	4.237(9)	134.1	C17-H17A···O5W_\$2

Operators for generating equivalent atoms: For **1**: \$1 x, y, z-1; \$2 -y, x, -z+3; \$3 -y, x, -z+4; \$4 y+1, -x, -z+3; \$5 y+1, -x, -z+3. For **2**: \$1 -x+1/2, y+1/2, -z+1/2; \$2 x-1/2, -y+1/2, -z+1/2; \$3 -x+1, -y, z; \$4 x, y, -z; \$5 x, y, -z; \$6 -x+1/2, y+1/2, -z+1/2; \$7 -x, -y+1, -z; \$8 -x, -y+1, z; \$9 -x+1/2, y+1/2, z-1/2; \$10 -x, -y, z; \$11 x, y, -z+1. For **3**: \$1 -x+1, -y+1, -z+1; \$2 x+1, y, z; \$3 x-1, y, z; \$4 x, y+1, z; \$5 -x+2, -y+1, -z+2; \$6 -x+3, -y+1, -z+2; \$7 -x+2, -y+1, -z+1. For **4**: \$1 -x+2, y, -z+5/2; \$2 -x+1, -y, -z+2; \$3 -x+2, -y, -z+2; \$4 x, -y+1, z-1/2; \$5 -x+2, -y+1, -z+2; \$6 x-1, -y+1, z-1/2; \$7 -x+1, y, -

$z+3/2$ ; \$8  $x, -y, z-1/2$ ; \$9  $x, -y+1, z+1/2$ ; \$10  $x, y+1, z$ . For **5**: \$1  $-x+1, -y+1, -z+1$ ; \$2  $x+1, y, z$ ; \$3  $x-1, y, z$ ; \$4  $x, y+1, z$ ; \$5  $-x+2, -y+1, -z+2$ ; \$6  $-x+3, -y+1, -z+2$ ; \$7  $-x+2, -y+1, -z+1$ . For **6**: \$1  $x-1/2, y, -z+1/2$ ; \$2  $x, -y+1/2, z-1/2$ ; \$3  $x+1/2, y, -z+1/2$ ; \$4  $x, -y+1/2, z+1/2$ ; \$5  $-x+3/2, -y, z+1/2$ ; \$6  $-x+3/2, -y, z+1/2$ ; \$7  $-x+2, -y, -z$ ; \$8  $-x+3/2, -y, z-1/2$ ; \$9  $-x+3/2, y-1/2, z$ ; \$10  $-x+1, -y, -z$ ; \$11  $x-1/2, -y+1/2, -z+1$ .