

Supporting information

Fabrication of New Metal Phosphonates from Tritopic Trisphosphonic Acid Containing Methyl Groups and Auxiliary Ligands: Syntheses, Structures and Gas Adsorption Properties

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Table S1. Specified hydrogen bonds for **1-8** (with esds except fixed and riding H).

D-H	H···A	D···A	<(DHA)	
1				
0.85	2.03	2.745(9)	141.8	O1W-H1W···O3W
0.85	1.99	2.778(12)	154.4	O3W-H6W···O6W
0.96	1.83	2.778(8)	168.4	N1-H0A···O11
0.96	1.78	2.702(9)	159.2	N2-H0B···O1
0.85	1.91	2.723(7)	158.4	O1W-H2W···O5_\$1
0.85	1.98	2.716(8)	143.8	O2W-H3W···O4W_\$2

0.85	1.96	2.775(8)	160.8	O2W-H4W···O14_\$3
0.82	1.64	2.449(8)	170.8	O2-H2B···O7_\$4
0.82	1.83	2.596(7)	155.8	O4-H4B···O11_\$5
0.85	2.36	2.884(11)	120.8	O6W-H11W···O2_\$6
0.82	1.73	2.545(7)	174.6	O8-H8C···O5_\$7
0.82	1.69	2.499(8)	168.9	O10-H10A···O16_\$8
0.82	1.71	2.520(8)	170.6	O13-H13B···O1_\$4
0.82	1.73	2.540(8)	170.1	O17-H17C···O14_\$2
2				
0.85	1.88	2.654(5)	150.4	O2W-H3W···O3W
0.85	2.21	2.937(4)	143.0	O1W-H1W···O2_\$1
0.82	1.80	2.615(4)	178.8	O2-H2A···O1_\$1
0.82	1.90	2.663(4)	155.3	O5-H5A···O1_\$1
3				
0.80(4)	2.05(4)	2.810(3)	159(3)	O2W-H3W···O9
0.82	1.81	2.618(3)	170.7	O2-H2A···O1_\$3
0.82	1.73	2.547(3)	173.9	O4-H4A···O1_\$3
0.82	2.01	2.774(3)	154.2	O8-H8D···O2_\$3
0.85	1.96	2.810(3)	174.4	O1W-H1W···O7_\$1
0.85	2.19	2.960(3)	150.9	O1W-H2W···O7_\$2
0.84(4)	1.88(4)	2.698(3)	165(3)	O2W-H4W···O9_\$1
0.82	1.76	2.562(3)	164.5	O5-H5A···O7_\$2
4				
0.85	1.93	2.770(3)	167.8	O1W-H1W···O6_\$1
0.85	2.01	2.802(3)	154.4	O2W-H3W···O5
0.85	1.83	2.681(3)	175.9	O2W-H4W···O5_\$1
0.82	1.77	2.574(3)	168.4	O2-H2A···O1_\$2

0.82	1.72	2.524(3)	167.4	O7-H7C···O6_\$3
0.82	1.74	2.558(3)	173.5	O8-H8D···O1_\$2
0.85	2.16	3.003(3)	169.0	O1W-H2W···O6_\$3
5				
0.82	1.82	2.628(4)	169.6	O1-H1A···O3_\$1
0.82	1.62	2.395(4)	155.6	O4-H4A···O7_\$2
0.82	1.79	2.559(4)	156.0	O5-H5A···O3_\$1
6				
0.82	1.76	2.551(2)	160.6	O1-H1A···O6_\$1
0.82	1.71	2.525(2)	170.0	O3-H3A···O9_\$2
0.82	1.75	2.549(2)	165.2	O5-H5A···O9_\$3
0.82	1.92	2.723(3)	166.9	O8-H8D···O6_\$4
7				
0.82	1.746	2.539	162.31	O3-H3A···O1_\$1
0.82	1.810	2.628	174.99	O4-H4A···O9_\$2
0.82	1.665	2.455	160.89	O7-H7C···O2_\$1
0.82	1.817	2.623	167.30	O8-H8D···O1_\$1
8				
0.85	1.84	2.48(2)	131.0	O1W-H2W···O4W
0.85	1.92	2.747(4)	163.6	O1W-H2W···O3W
0.85	2.64	3.363(4)	143.3	O3W-H6W···O2
0.85	2.14	2.929(3)	153.6	O2W-H3W···O7_\$1
0.82	1.91	2.687(3)	157.6	O2-H2A···O8_\$1
0.85	2.39	3.129(4)	146.4	O3W-H6W···O5_\$2
0.82	1.78	2.597(3)	178.7	O7-H7C···O8_\$1

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

-y+1, -z; for 4: \$1 -x+1, -y+1, -z; \$2 -x+1, -y+1, -z+1; \$3 x, y-1, z; for 5: \$1 -x, -y, -z+1; \$2 x-1, y+1, z; for 6: \$1 x-1/2, -y+3/2, z-1/2; \$2 x+1/2, -y+3/2, z-1/2; \$3 -x+5/2, y+1/2, -z+1/2; \$4 -x+5/2, y-1/2, -z+1/2; for 7: \$1 -x, -y+1, -z; x+1, y-1, z; for 8: \$1 -x+2, -y+1, -z; \$2 x, y-1, z.

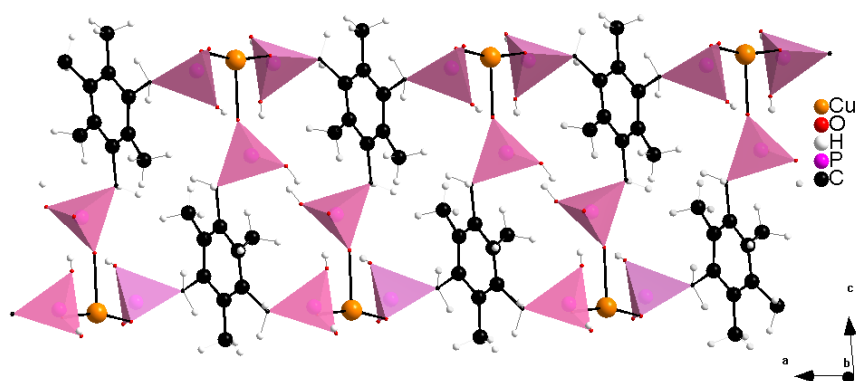


Figure S1. One dimensional infinite corrugated tape found in compound **5**.

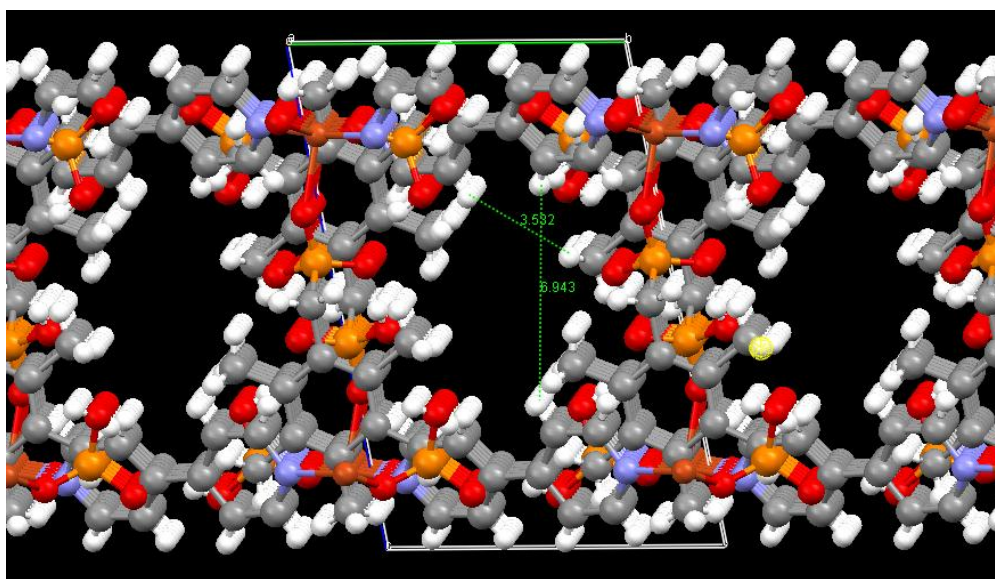


Figure S2. Ball-stick diagram of compound **5** with window size labeled.

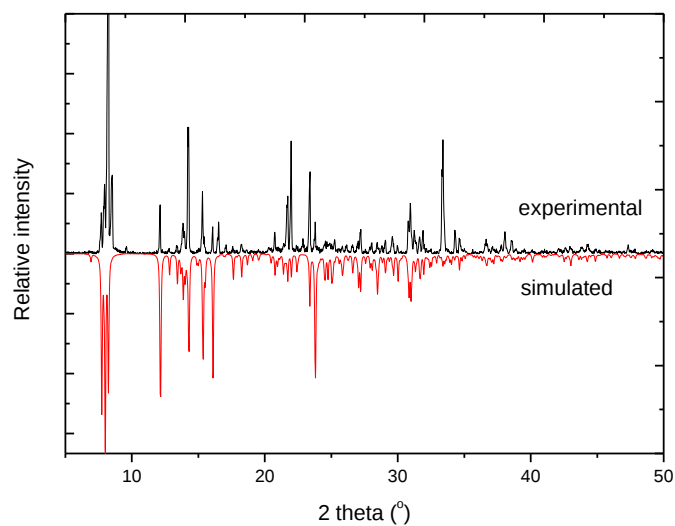


Figure S3. Comparison of the simulated and experimental PXRD patterns of compound 1.

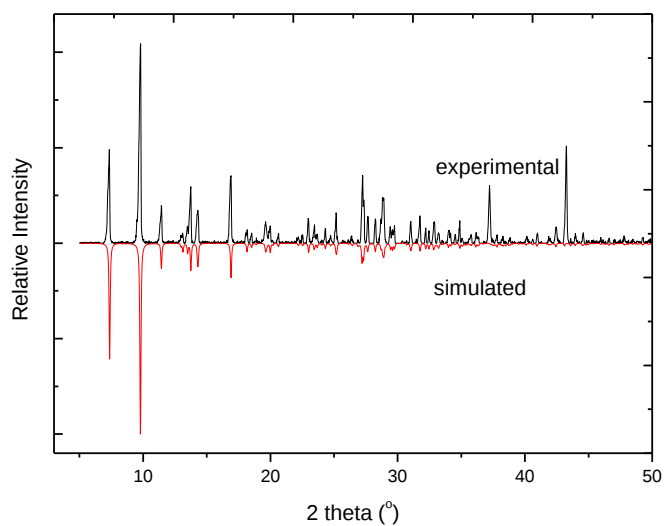


Figure S4. Comparison of the simulated and experimental PXRD patterns of compound 2.

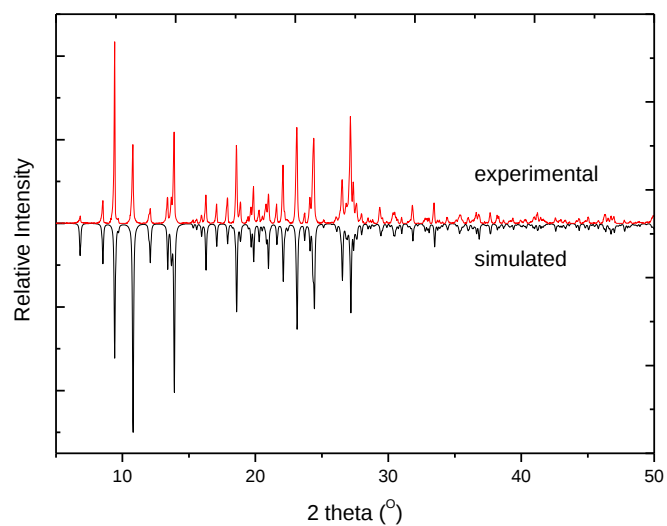


Figure S5. Comparison of the simulated and experimental PXRD patterns of compound **3**.

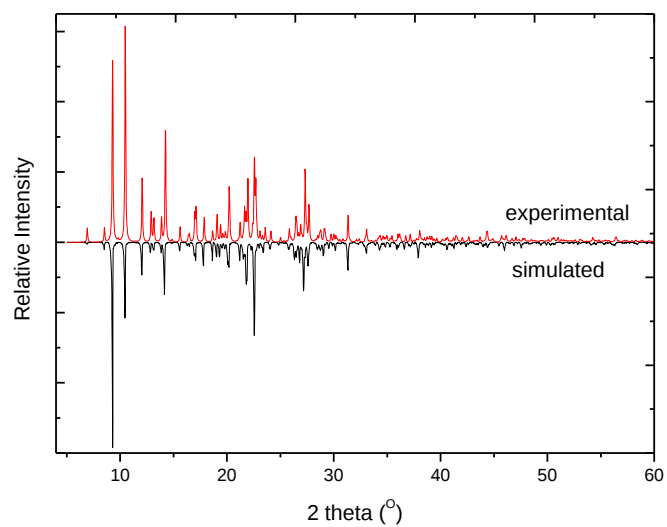


Figure S6. Comparison of the simulated and experimental PXRD patterns of compound **4**.

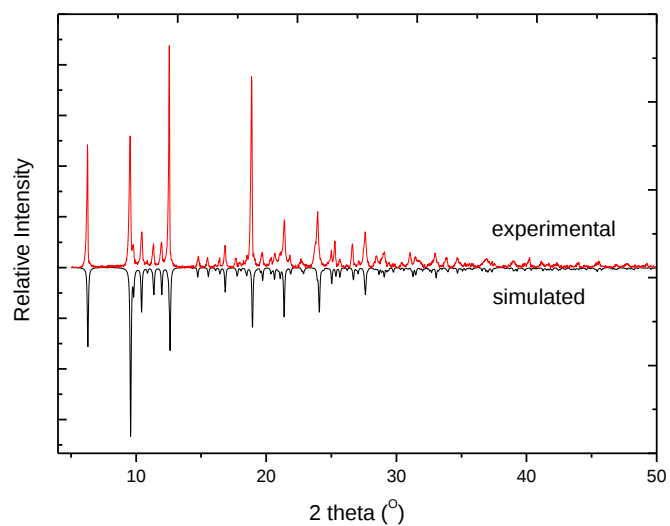


Figure S7. Comparison of the simulated and experimental PXRD patterns of compound **5**.

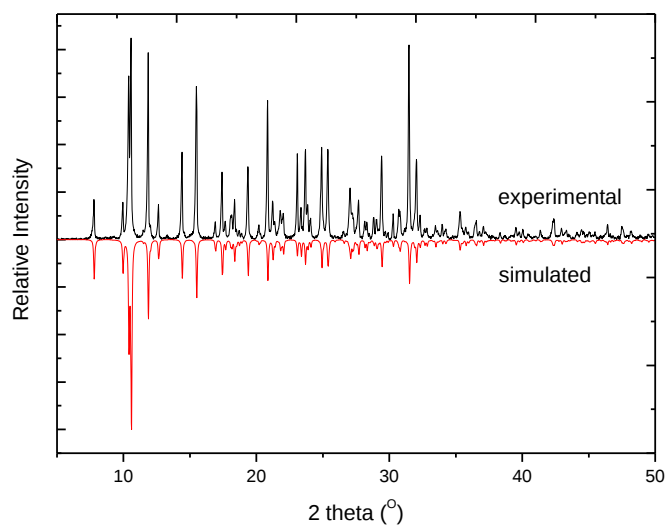


Figure S8. Comparison of the simulated and experimental PXRD patterns of compound **6**.

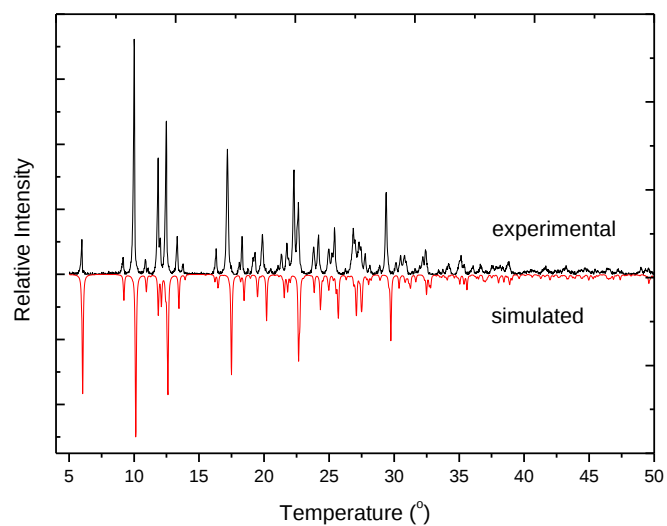


Figure S9. Comparison of the simulated and experimental PXRD patterns of compound 7.

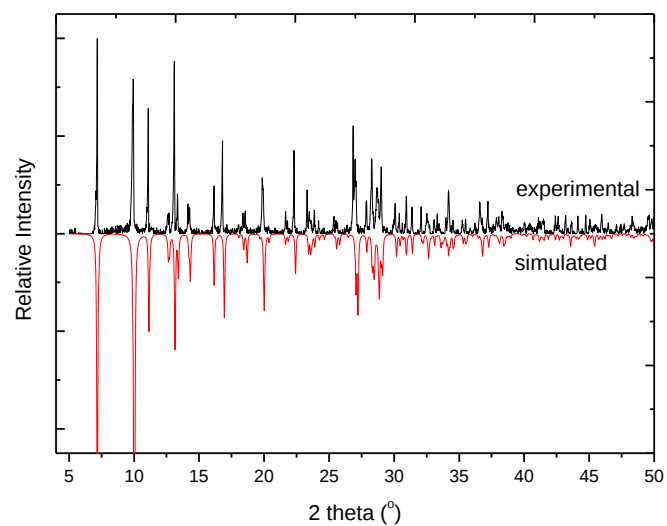


Figure S10. Comparison of the simulated and experimental PXRD patterns of compound 8.

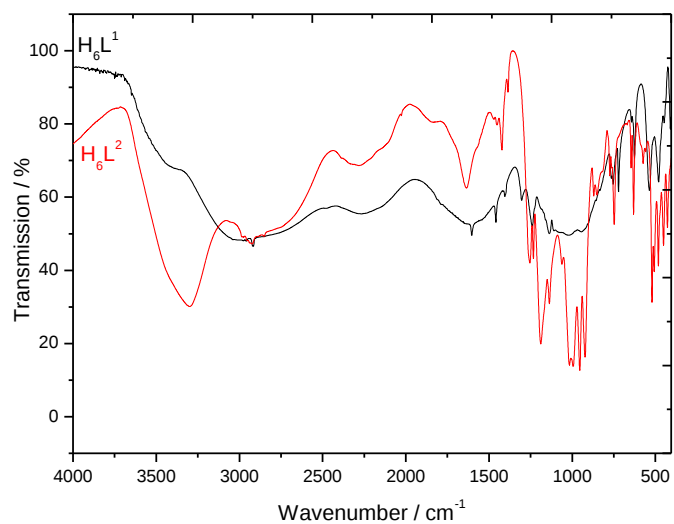


Figure S11. IR spectra of ligands H_6L^1 and H_6L^2 .

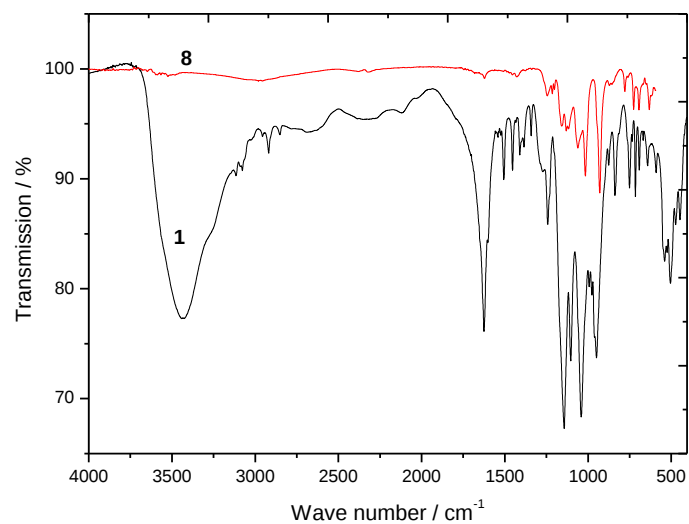


Figure S12. IR spectra of compounds **1** and **8**.

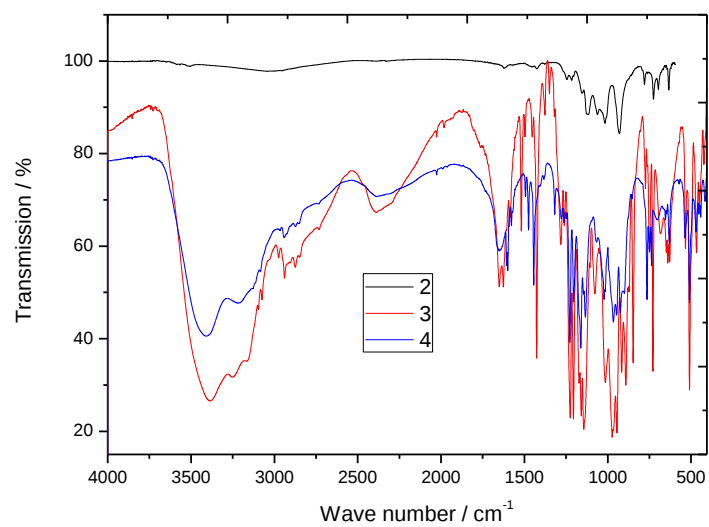


Figure S13. IR spectra of compounds **2-4**.

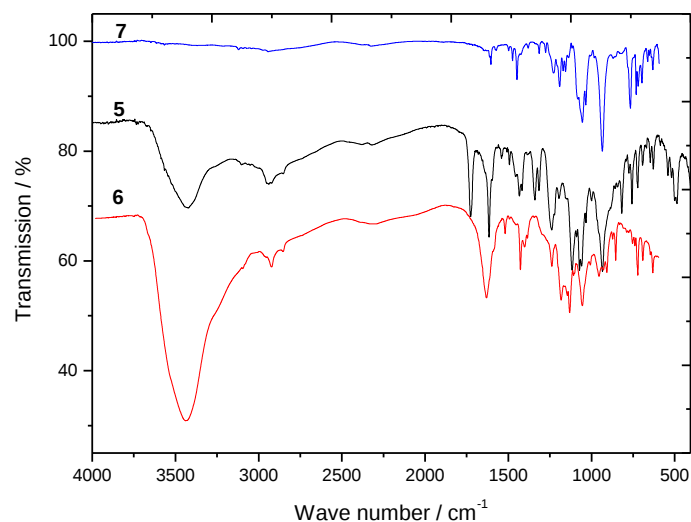


Figure S14. IR spectra of compounds **5-7**.

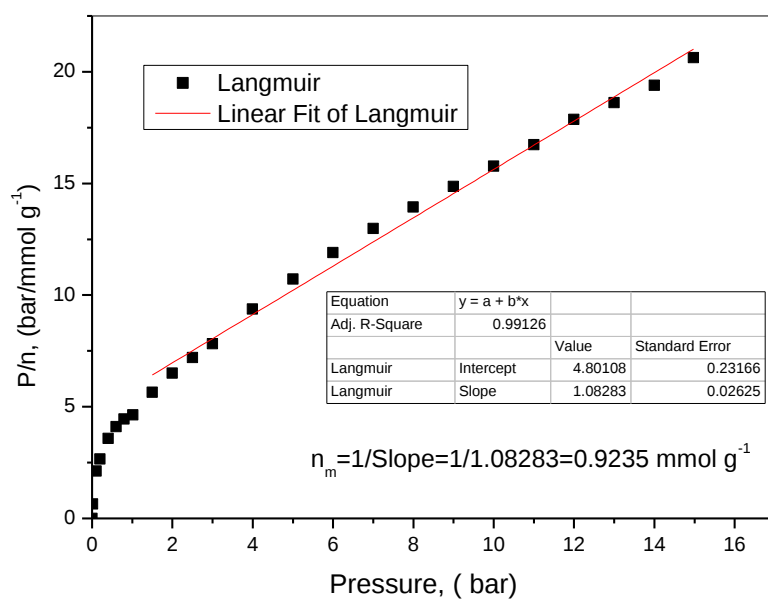


Figure S15. Langmuir graph for CO₂ adsorption on compound **5** at 273 K.