Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Modulating the microporosity of cobalt phosphonates *via* positional isomerism of co-linkers

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Table S1 Selected bond lengths (Å) and angles (deg) of compound **1**

Co1-O7A	2.047(2)	O7A-Co1-O2	87.0(1)	O2-Co2-O1W	162.0(1)
Co1-O2	2.066(2)	O7A-Co1-O2C	93.0(1)	N4D-Co2-O1W	90.0(1)
Co1-O4	2.116(2)	O7A-Co1-O4C	89.8(1)	O2W-Co2-O1W	85.5(1)
Co2-O6B	2.058(2)	O2-Co1-O4C	81.3(1)	O6B-Co2-O4C	96.3(1)
Co2-O2	2.080(2)	O7A-Co1-O4	90.2(1)	O2-Co2-O4C	77.4(1)
Co2-N4D	2.092(2)	O2-Co1-O4	98.7(1)	N4D-Co2-O4C	174.7(1)
Co2-O2W	2.107(2)	O6B-Co2-O2	91.8(1)	O2W-Co2-O4C	89.2(1)
Co2-O1W	2.124(2)	O6B-Co2-N4D	86.2(1)	O1W-Co2-O4C	85.1(1)
Co2-O4C	2.273(2)	O2-Co2-N4D	107.3(1)	O1D-Co3-O8A	107.9(1)
Co3-O1D	1.932(2)	O6B-Co2-O2W	174.5(1)	O1D-Co3-O3	108.1(1)
Co3-O8A	1.951(2)	O2-Co2-O2W	90.0(1)	O8A-Co3-O3	112.5(1)
Co3-O3	1.956(2)	N4D-Co2-O2W	88.3(1)	O1D-Co3-N1	108.5(1)
Co3-N1	2.002(2)	O6B-Co2-O1W	94.4 (1)	O8A-Co3-N1	113.8(1)
				O3-Co3-N1	105.9(1)

Symmetric codes for **1**: A: x-1,y,z; B: -x+2,-y+2,-z+2; C: -x+1,-y+2,-z+2 ; D: -x+1,-y+1,-z+2; E: x+1,y,z.

Table S2 Selected bond lengths (Å) and angles (deg) of compound **1a**

Co1-O7A	2.033(4)	O7A-Co1-O2	92.7(1)	O2-Co2-O2W	82.6(1)
Co1-O2	2.043(3)	O7B-Co1-O2	87.3(1)	O1W-Co2-O2W	87.3(2)
Co1-O4	2.121(3)	O7A-Co1-O4	90.7(1)	N4D-Co2-O2W	84.9(2)
Co2-O6A	2.052(4)	O2-Co1-O4	100.3(1)	O6A-Co2-O4C	94.8(1)
Co2-O2	2.075(3)	O7A-Co1-O4C	89.3(1)	O2-Co2-O4C	75.3(1)
Co2-O1W	2.091(4)	O2-Co1-O4C	79.7(1)	O1W-Co2-O4C	82.7(1)
Co2-N4D	2.142(5)	O6A-Co2-O2	93.2(1)	N4D-Co2-O4C	173.2(1)
Co2-O2W	2.192(4)	O6A-Co2-O1W	100.9(2)	O2W-Co2-O4C	95.3(1)
Co2-O4C	2.286(4)	O2-Co2-O1W	154.7(1)	O3-Co3-O1D	109.9(1)
Co3-O3	1.926(4)	O6A-Co2-N4D	85.9(2)	O3-Co3-O8B	111.1(1)
Co3-O1D	1.937(3)	O2-Co2-N4D	111.5(1)	O1D-Co3-O8B	108.6(1)
Co3-O8B	1.949(3)	O1W-Co2-N4D	90.5(2)	O3-Co3-N1	117.7(1)
Co3-N1	2.023(5)	O6A-Co2-O2W	167.7(2)	O1D-Co3-N1	99.4(1)
				O8B-Co3-N1	109.2(2)

Symmetric codes for **1a**: A: -x-1,-y+1,-z+1; B: x+1,y,z; C: -x,-y+1,-z+1; D: -x,-y,-z+1; E: x-1,y,z.

Table S3 Selected bond lengths (Å) and angles (deg) of compound **2**

Co1-O7A	2.055(6)	O16B-Co1-O12	87.5(3)	O2-Co3-O11	109.2(2)
Co1-O16B	2.053(6)	O7A-Co1-O3	86.9(3)	O2-Co3-O17F	107.7(2)
Co1-O12C	2.054(7)	O16B-Co1-O3	92.7(3)	O11-Co3-O17F	110.7(2)
Co1-O3	2.057(6)	O12C-Co1-O3	179.6(3)	O2-Co3-N5	103.1(2)
Co1-O13C	2.115(6)	O7A-Co1-O13C	89.5(3)	O11-Co3-N5	114.5(3)
Co1-O4	2.111(6)	O16B-Co1-O13	89.0(2)	O17F-Co3-N5	111.1(3)

Co2-O6D	2.070(6)	O12C-Co1-O13	99.7(3)	O15G-Co4-O4W	93.7(3)
Co2-O12	2.086(6)	O3-Co1-O13C	80.6(3)	O15G-Co4-O3H	91.3(2)
Co2-O2W	2.097(7)	O7A-Co1-O4	91.0(2)	O4W-Co4-O3H	159.4(3)
Co2-N4	2.115(8)	O16B-Co1-O4	90.5(2)	O15G-Co4-O3W	171.9(3)
Co2-O1W	2.112(6)	O12C-Co1-O4	79.9(3)	O4W-Co4-O3W	91.2(3)
Co2-O4E	2.279(7)	O3-Co1-O4	99.8(3)	O3H-Co4-O3W	86.4(2)
Co3-O2	1.941(7)	O13C-Co1-O4	179.4(3)	O15G-Co4-N1	87.3(3)
Co3-O11	1.948(6)	O6D-Co2-O12	92.2(2)	O4W-Co4-N1	91.8(3)
Co3-O17F	1.962(6)	O6D-Co2-O2W	174.6(3)	O3H-Co4-N1	108.5(3)
Co3-N5	2.000(9)	O12-Co2-O2W	88.3(2)	O3W-Co4-N1	86.1(3)
Co4-O15G	2.063(6)	O6D-Co2-N4	86.4(3)	O15G-Co4-O13I	97.6(2)
Co4-O4W	2.088(7)	O12-Co2-N4	109.1(3)	O4W-Co4-O13I	82.9(3)
Co4-O3H	2.091(6)	O2W-Co2-N4	88.3(3)	O3H-Co4-O13I	76.6(2)
Co4-O3W	2.101(7)	O6D-Co2-O1W	96.6(3)	O3W-Co4-O13I	89.5(3)
Co4-N1	2.114(9)	O12-Co2-O1W	158.6(2)	N1-Co4-O13I	173.0(3)
Co4-O13I	2.257(6)	O2W-Co2-O1W	84.9(2)	O10J-Co5-O8K	109.7(3)
Co5-O10J	1.919(7)	N4-Co2-O1W	91.0(3)	O10J-Co5-O1J	109.8(2)
Co5-O8K	1.944(6)	O6D-Co2-O4E	95.2(2)	O8K-Co5-O1J	110.9(3)
Co5-O1J	1.963(6)	O12-Co2-O4E	75.5(2)	O10J-Co5-N8	102.5(3)
Co5-N8	1.989(7)	O2W-Co2-O4E	90.2(3)	O8K-Co5-N8	115.8(3)
O7A-Co1-O16	178.5(2)	N4-Co2-O4E	175.2(2)	O1J-Co5-N8	107.8(3)
O7A-Co1-O12	92.9(3)	O1W-Co2-O4E	84.3(2)		

Symmetric codes for **2**: A: x, y–1, z; B: x+1, y+1, z; C: x+1, y, z; D: x-1,y-1,z; E: x-1,y,z; F: x,y+1,z; G: x,-y-1,z-1/2; H: x-1,-y,z-1/2; I: x,-y,z-1/2; J: x,-y,z+1/2; K: x,-y+1,z+1/2.

Table S4 Selected bond lengths (Å) and angles (deg) of compound **3**

Co1-O2	2.048(3)	O2-Co1-O7B	93.0(1)	O2-Co2-N4D	104.2(1)
Co1-O7B	2.052(3)	O2-Co1-O4A	80.3(1)	O2W-Co2-N4D	94.0(1)
Co1-O4	2.118(3)	O7C-Co1-O4A	89.4(1)	O6B-Co2-O4A	97.7(1)
Co2-O6B	2.044(3)	O2-Co1-O4	99.7(1)	O1W-Co2-O4A	89.0(1)
Co2-O1W	2.078(3)	O7C-Co1-O4	90.6(1)	O2-Co2-O4A	77.0(1)
Co2-O2	2.081(3)	O6B-Co2-O1W	173.3(1)	O2W-Co2-O4A	84.8(1)
Co2-O2W	2.103(3)	O6B-Co2-O2	91.0(1)	N4D-Co2-O4A	176.2(1)
Co2-N4D	2.115(4)	O1W-Co2-O2	89.3(1)	O1E-Co3-O3	103.7(1)
Co2-O4A	2.237(3)	O6B-Co2-O2W	92.4(1)	O1E-Co3-O8C	109.9(1)
Co3-O1E	1.923(3)	O1W-Co2-O2W	89.3(1)	O3-Co3-O8C	114.9(1)
Co3-O3	1.945(3)	O2-Co2-O2W	161.7(1)	O1E-Co3-N1	105.1(1)
Co3-O8C	1.950(3)	O6B-Co2-N4D	86.0(1)	O3-Co3-N1	111.8(1)
Co3-N1	1.992(4)	O1W-Co2-N4D	87.4(1)	O8C-Co3-N1	110.9(1)

Symmetric codes for **3**: A: –x+2,–y+2,–z; B: –x+3,–y+2,–z; C: x-1, y,z; D: x+1, y, z-1; E: –x+2, –y+1,–z.

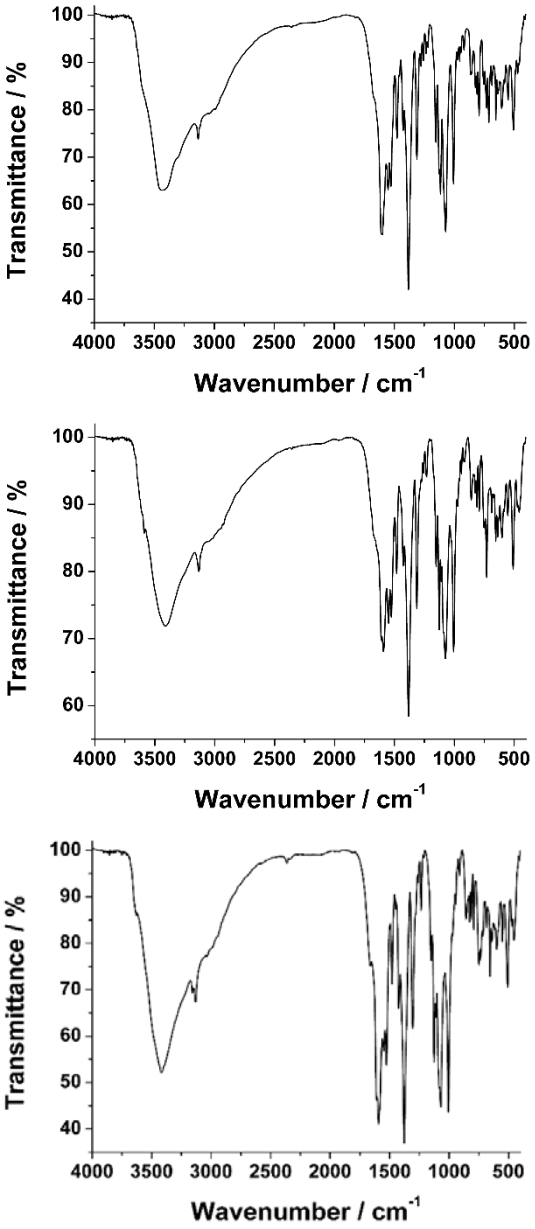

Figure S1 IR spectra of **1** (top), **2** (middle), **3** (bottom).

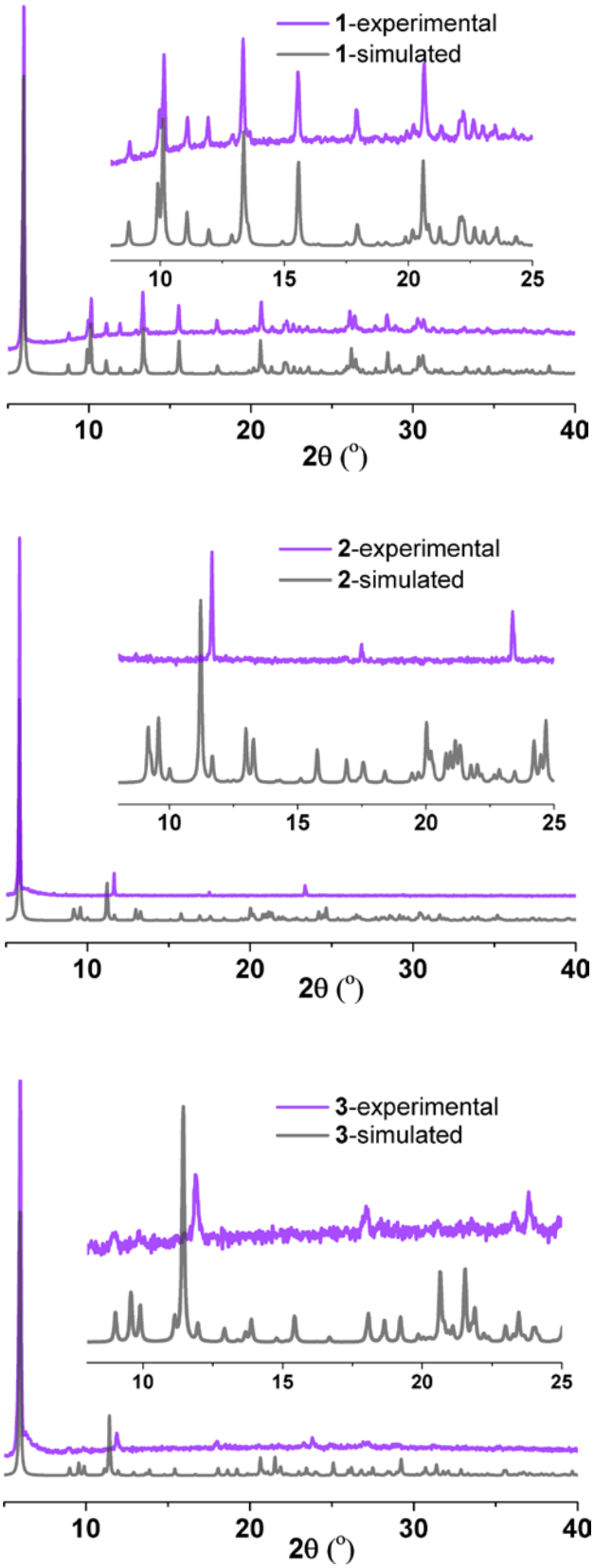

Figure S2 XRD patterns of **1** (top), **2** (middle), **3** (bottom)

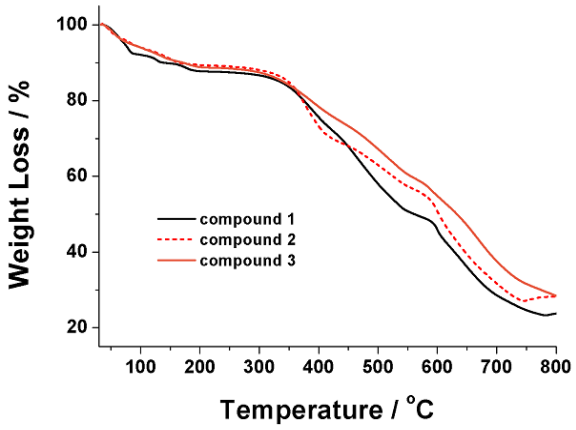

Figure S3 TGA curves of compounds **1**-**3**.

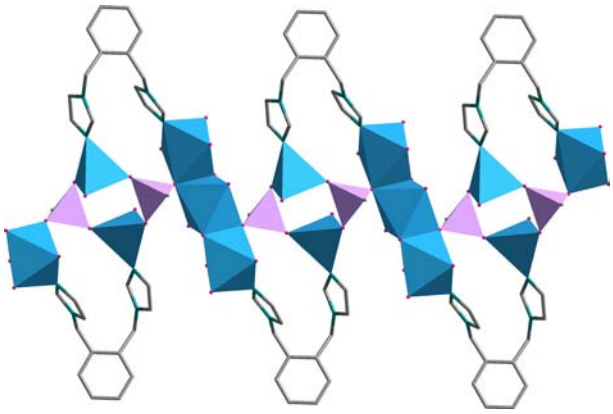

Figure S4 Bridging mode of 1,2-bix in compound **1**.

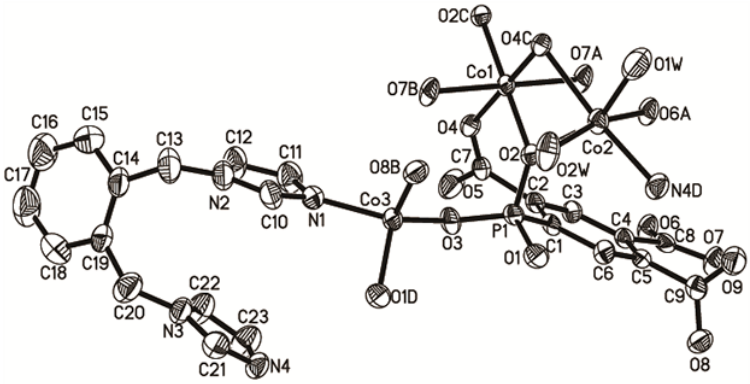

Figure S5 Building unit of compound **1a**. All hydrogen atoms and lattice water molecules are omitted for clarity.

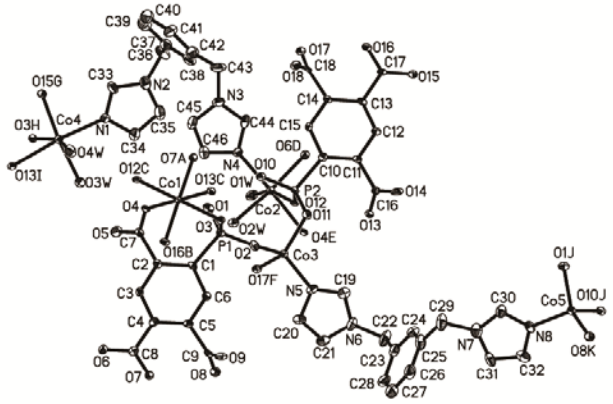

Figure S6 Building unit of compound **2**. All hydrogen atoms and lattice water molecules are omitted for clarity.

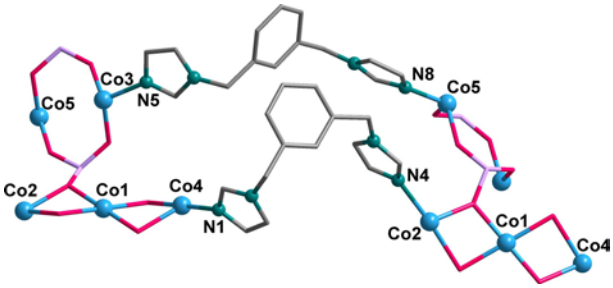

Figure S7 Bridging modes of 1,3-bix in compound **2**.

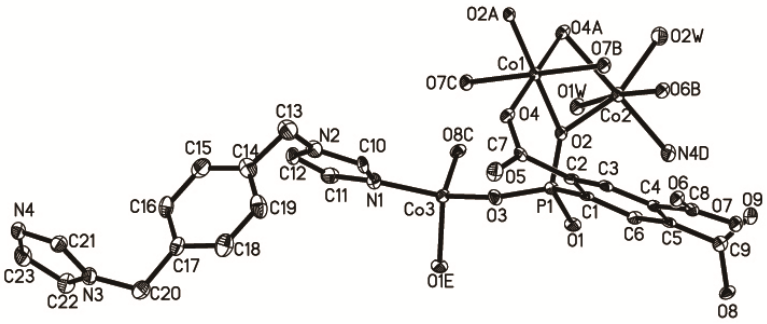

Figure S8 Building unit of compound **3**. All hydrogen atoms and lattice water molecules are omitted for clarity.