Supplementary Materials

One-Dimensional Fluorene-Based Co(II) Phosphonate $Co(H_2O)_2PO_3C–C_{12}H_9·H_2O$: Structure and Magnetism

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Summary

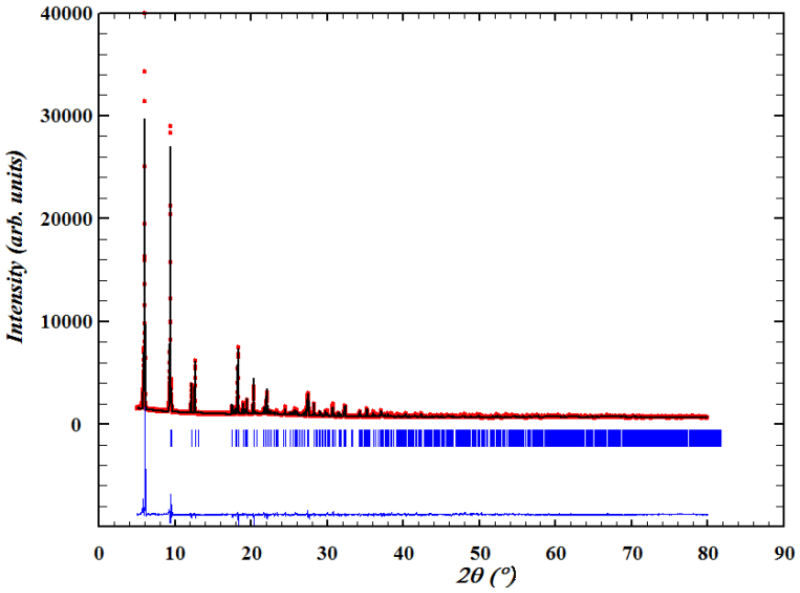
Figure S1: X-ray diffraction data recorded on powder from $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$. The vertical dashes correspond to the calculated position of the peaks, the bottom line to the difference between experimental and calculated pattern.

Figure S2: (a) Hirshfeld Surface represented on the fluorene moiety of $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$ with a shape index mapping. (b) Representation of the corresponding two-dimensional fingerprint plot showing the contribution of each contact-type in percentage. "di" and "de" data points represent the distance from the surface to the nearest atom in the molecule itself or to another molecule, respectively.

Figure S3: Representation of the AC susceptibility of $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$ showing (a) no changes in the real part of the susceptibility (m) and (b) no losses (m'') in the temperature range from 2K to 6 K, under 0.05 T with wave frequencies varying from 0.1 Hz to 1KHz.

Figure S4: X-ray diffraction data recorded on the TGA residu of $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$. The latter is compatible with the cobalt pyrophosphate $Co_2P_2O_7$ which crystallizes in the monoclinic $P2_1/c$ space group. [Ref code: 00-049-1091 from Lazoryak,B., X-ray Powder Diffraction Laboratory of Chemistry Technology, Moscow State Univ., Russia, ICDD Grant-in-Aid (1997)]

Table S1: Atomic coordinates of $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$.
Table S2: Thermal parameters of $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$.
Table S3: Bond angles for $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$
Table S4: Interatomic distances (Å) for $Co(H_2O)_2PO_3C$-$C_{12}H_9.H_2O$.



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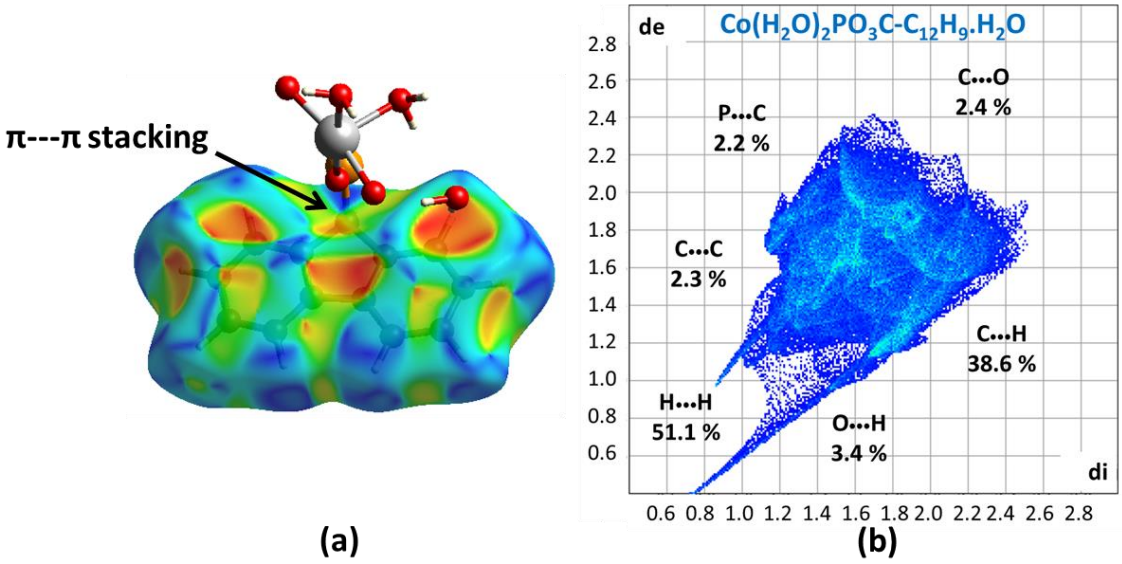

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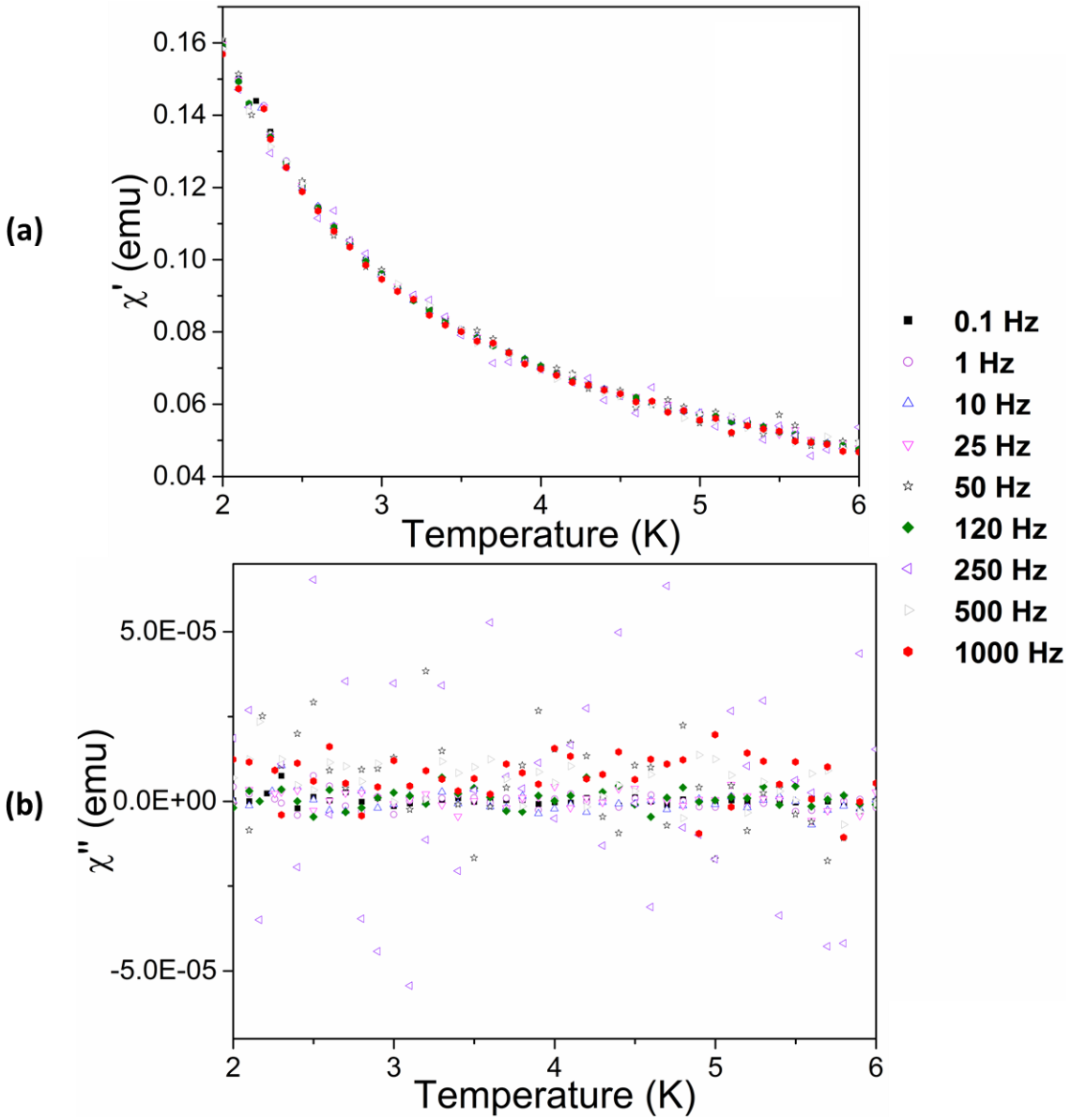

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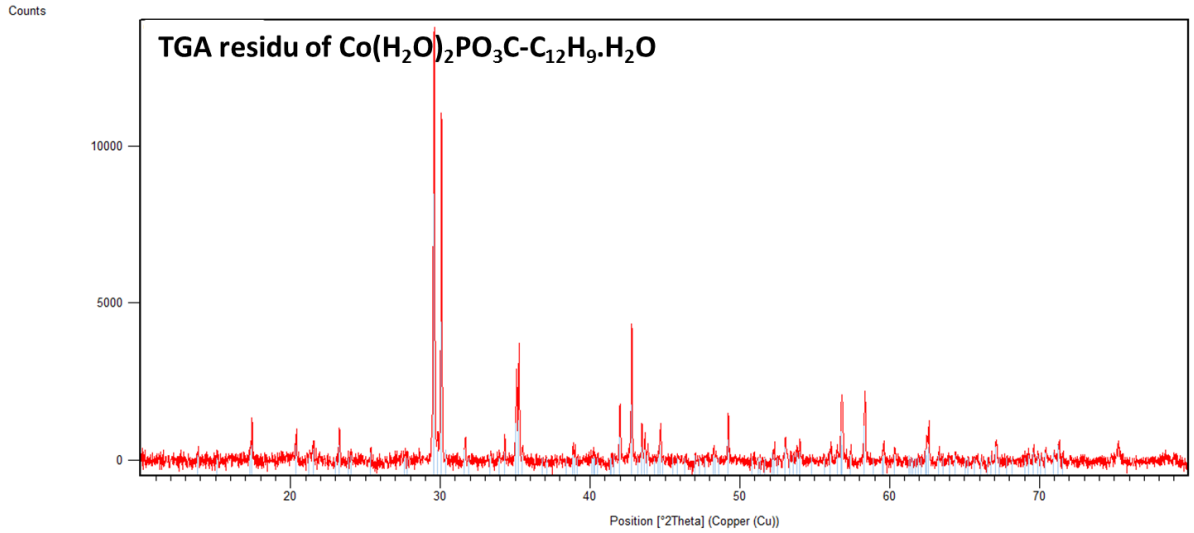

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Table S1: Atomic coordinates of $Co(H_2O)_2PO_3C\text{-}C_{12}H_9.H_2O$.

		x/a	y/b	z/c
Co1	Co	0.00571(3)	0.97164(8)	0.82215(2)
P1	P	-0.11568(5)	0.40478(14)	0.79390(4)
O1	O	-0.10822(13)	0.7178(4)	0.79278(13)
O2	O	0.07398(13)	0.7647(4)	0.76087(11)
O3	O	-0.06758(14)	1.2704(4)	0.86596(12)
C1	C	-0.23792(18)	0.3165(6)	0.77052(17)
C2	C	-0.29261(19)	0.4159(6)	0.69727(18)
C3	C	-0.2881(2)	0.3394(8)	0.63096(19)
C4	C	-0.3470(3)	0.4604(8)	0.5704(2)
C5	C	-0.4092(2)	0.6644(9)	0.5769(2)
C6	C	-0.4155(2)	0.7413(8)	0.6431(2)
C7	C	-0.3573(2)	0.6155(7)	0.70355(19)
C8	C	-0.3521(2)	0.6426(7)	0.77868(20)
C9	C	-0.4042(2)	0.8020(8)	0.8119(2)
C10	C	-0.3879(2)	0.7789(9)	0.8851(2)
C11	C	-0.3201(3)	0.6019(9)	0.9252(2)
C12	C	-0.2676(2)	0.4429(7)	0.8922(2)
C13	C	-0.2838(2)	0.4628(6)	0.81881(19)
O4	O	-0.1057(2)	0.9248(7)	0.96715(16)
H1o4	H	-0.145(3)	0.770(6)	0.9495(18)
H2o4	H	-0.107(3)	1.030(7)	0.9252(11)
O5	O	0.11970(15)	0.2480(5)	0.85676(14)
H1o5	H	0.129(3)	0.298(7)	0.812(1)
H2o5	H	0.104(3)	0.419(4)	0.8754(18)
O6	O	0.06033(17)	0.7353(5)	0.91682(13)
H1o6	H	0.083(2)	0.852(7)	0.9579(13)
H2o6	H	0.0038(15)	0.661(8)	0.9212(18)
H1c1	H	-0.23803	0.11811	0.77402
H1c3	H	-0.24430	0.20266	0.62646
H1c4	H	-0.34509	0.40379	0.52391
H1c5	H	-0.44798	0.75211	0.53472
H1c6	H	-0.45919	0.87864	0.64745
H1c9	H	-0.45057	0.92588	0.78442
H1c10	H	-0.42382	0.88633	0.90830
H1c11	H	-0.30933	0.58889	0.97590
H1c12	H	-0.22083	0.32091	0.91998

Table S2: Thermal parameters of $Co(H_2O)_2PO_3C\text{-}C_{12}H_9.H_2O$.

		U_{iso}	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co1	Co		0.01746(19)	0.00905(16)	0.0169(2)	0.00143(12)	0.00703(14)	-0.00046(14)
P1	P		0.0141(3)	0.0080(3)	0.0173(4)	0.0000(2)	0.0068(2)	0.0001(3)
O1	O		0.0193(9)	0.0067(8)	0.0309(12)	-0.0019(7)	0.0098(8)	-0.0010(8)
O2	O		0.0174(9)	0.0113(8)	0.0208(11)	0.0001(6)	0.0108(8)	0.0000(8)
O3	O		0.0222(10)	0.0156(9)	0.0193(11)	0.0033(7)	0.0073(8)	0.0024(9)
C1	C		0.0155(11)	0.0149(11)	0.0226(15)	-0.0022(9)	0.0088(10)	-0.0016(11)
C2	C		0.0147(12)	0.0190(12)	0.0241(16)	-0.0045(9)	0.0053(10)	-0.0009(12)
C3	C		0.0254(15)	0.0303(16)	0.0277(18)	-0.0010(13)	0.0083(13)	-0.0034(15)
C4	C		0.0365(19)	0.043(2)	0.0230(18)	-0.0037(16)	0.0078(15)	0.0003(17)
C5	C		0.0293(17)	0.043(2)	0.033(2)	-0.0009(15)	-0.0007(15)	0.0090(19)
C6	C		0.0231(15)	0.0337(18)	0.039(2)	0.0036(13)	0.0059(14)	0.0058(17)
C7	C		0.0163(12)	0.0244(14)	0.0273(17)	-0.0028(11)	0.0069(11)	-0.0012(13)
C8	C		0.0164(12)	0.0224(14)	0.0302(18)	-0.0002(10)	0.0086(11)	-0.0005(13)
C9	C		0.0234(15)	0.0327(17)	0.038(2)	0.0071(13)	0.0116(14)	-0.0045(17)
C10	C		0.0273(17)	0.042(2)	0.046(2)	0.0065(15)	0.0185(16)	-0.009(2)
C11	C		0.0364(19)	0.042(2)	0.031(2)	-0.0004(16)	0.0193(16)	-0.0060(18)
C12	C		0.0284(16)	0.0311(17)	0.0296(19)	0.0017(13)	0.0143(14)	-0.0001(15)
C13	C		0.0173(12)	0.0184(12)	0.0266(17)	-0.0027(10)	0.0101(11)	-0.0002(12)
O4	O		0.0512(17)	0.0435(17)	0.0273(15)	-0.0100(13)	0.0126(13)	0.0021(14)
H1o4	H	0.0486						
H2o4	H	0.0486						
O5	O		0.0232(10)	0.0222(11)	0.0318(14)	-0.0025(8)	0.0084(9)	-0.0055(10)
H1o5	H	0.0308						
H2o5	H	0.0308						
O6	O		0.0303(11)	0.0251(11)	0.0232(12)	0.0012(9)	0.0073(9)	0.0026(10)
H1o6	H	0.0316						
H2o6	H	0.0316						
H1c1	H	0.0203						
H1c3	H	0.0333						
H1c4	H	0.0413						
H1c5	H	0.0447						
H1c6	H	0.0391						
H1c9	H	0.0370						
H1c10	H	0.0441						
H1c11	H	0.0413						
H1c12	H	0.0342						

Table S3: Bond angles for $Co(H_2O)_2PO_3C\text{-}C_{12}H_9.H_2O$

Atom – Atom – Atom	Angle (°)	Atom – Atom – Atom	Angle (°)
Co1 ^{i} -Co1-Co1 ^{ii}	81.923(18)	Co1-P1-C13	113.20(7)
Co1 ^{i} -Co1-P1	54.738(19)	Co1-P1-H1c1	160.27
Co1 ^{i} -Co1-P1 ^{iii}	118.00(2)	Co1 ^{i} -P1-O1	80.37(10)
Co1 ^{i} -Co1-P1 ^{ii}	46.148(16)	Co1 ^{i} -P1-O2 ^{i}	31.85(8)
Co1 ^{i} -Co1-O1	63.30(7)	Co1 ^{i} -P1-O3 ^{iv}	119.24(10)
Co1 ^{i} -Co1-O2	32.16(5)	Co1 ^{i} -P1-C1	123.34(11)
Co1 ^{i} -Co1-O2 ^{ii}	87.92(6)	Co1 ^{i} -P1-C2	96.74(8)
Co1 ^{i} -Co1-O3	146.45(5)	Co1 ^{i} -P1-C13	145.05(7)
Co1 ^{i} -Co1-O5 ^{iii}	120.24(8)	Co1 ^{i} -P1-H1c1	120.96
Co1 ^{i} -Co1-H1o5 ^{iii}	102.6(6)	O1-P1-O2 ^{i}	112.10(13)
Co1 ^{i} -Co1-O6	103.63(7)	O1-P1-O3 ^{iv}	114.75(12)
Co1 ^{i} -Co1-H2o6	101.4(9)	O1-P1-C1	107.68(12)
Co1 ^{ii} -Co1-P1	121.64(2)	O1-P1-C2	91.85(10)
Co1 ^{ii} -Co1-P1 ^{iii}	57.83(2)	O1-P1-C13	88.77(11)
Co1 ^{ii} -Co1-P1 ^{ii}	55.871(17)	O1-P1-H1c1	132.03
Co1 ^{ii} -Co1-O1	109.27(6)	O2 ^{i} -P1-O3 ^{iv}	105.73(12)
Co1 ^{ii} -Co1-O2	77.78(6)	O2 ^{i} -P1-C1	108.54(13)
Co1 ^{ii} -Co1-O2 ^{ii}	29.56(6)	O2 ^{i} -P1-C2	92.79(10)
Co1 ^{ii} -Co1-O3	87.37(6)	O2 i -P1-C13	139.13(10)
Co1 ^{ii} -Co1-O5 ^{iii}	71.57(7)	O2 ^{i} -P1-H1c1	95.63
Co1 ^{ii} -Co1-H1o5 ^{iii}	52.6(5)	O3 ^{iv} -P1-C1	107.84(14)
Co1 ^{ii} -Co1-O6	159.89(7)	O3 ^{iv} -P1-C2	137.35(12)
Co1 ^{ii} -Co1-H2o6	175.3(7)	O3 ^{iv} -P1-C13	95.51(12)
P1-Co1-P1 ^{iii}	107.01(3)	O3 ^{iv} -P1-H1c1	92.57
P1-Co1-P1 ^{ii}	100.55(2)	C1-P1-C2	29.66(12)
P1-Co1-O1	20.75(5)	C1-P1-C13	30.69(12)
P1-Co1-O2	81.48(6)	C1-P1-H1c1	24.38
P1-Co1-O2 ^{ii}	104.52(5)	C2-P1-C13	50.19(10)
P1-Co1-O3	107.25(6)	C2-P1-H1c1	46.82
P1-Co1-O5 ^{iii}	161.18(6)	C13-P1-H1c1	48.11
P1-Co1-H1o5 ^{iii}	156.5(7)	Co1-O1-P1	130.46(12)
P1-Co1-O6	75.73(6)	Co1-O2-Co1 ^{i}	118.28(9)
P1-Co1-H2o6	58.9(7)	Co1-O2-P1 ^{ii}	124.74(11)
P1 ^{iii} -Co1-P1 ^{ii}	113.28(3)	Co1 ^{i} -O2-P1 ^{ii}	91.01(10)
P1 ^{iii} -Co1-O1	86.32(6)	Co1-O3-P1 ^{iii}	94.55(12)
P1 ^{iii} -Co1-O2	132.70(6)	P1-C1-C2	113.5(2)
P1 ^{iii} -Co1-O2 ^{ii}	34.58(6)	P1-C1-C13	111.02(19)
P1 ^{iii} -Co1-O3	33.87(6)	P1-C1-H1c1	103.75
P1 ^{iii} -Co1-O5 ^{iii}	91.34(7)	C2-C1-C13	102.7(2)
P1 ^{iii} -Co1-H1o5 ^{iii}	88.8(8)	C2-C1-H1c1	111.91
P1 ^{iii} -Co1-O6	130.78(8)	C13-C1-H1c1	114.33
P1 ^{iii} -Co1-H2o6	117.5(7)	P1-C2-C1	36.87(13)
P1 ^{ii} -Co1-O1	108.27(7)	P1-C2-C3	109.2(2)
P1 ^{ii} -Co1-O2	23.41(6)	P1-C2-C7	120.8(2)
P1 ^{ii} -Co1-O2 ^{ii}	80.33(6)	C1-C2-C3	130.3(3)
P1 ^{ii} -Co1-O3	142.15(6)	C1-C2-C7	109.8(3)
P1 ^{ii} -Co1-O5 ^{iii}	75.14(8)	C3-C2-C7	119.9(3)
P1 ^{ii} -Co1-H1o5 ^{iii}	56.5(7)	C2-C3-C4	119.7(3)
P1 ^{ii} -Co1-O6	114.34(8)	C2-C3-H1c3	120.15
P1 ^{ii} -Co1-H2o6	128.8(8)	C4-C3-H1c3	120.15
O1-Co1-O2	94.37(9)	C3-C4-C5	120.3(4)
O1-Co1-O2 ^{ii}	86.67(8)	C3-C4-H1c4	119.86

O1-Co1-O3	91.01(9)	C5-C4-H1c4	119.86
O1-Co1-O5 iii	176.43(10)	C4-C5-C6	120.8(4)
O1-Co1-H1o5 iii	160.2(4)	C4-C5-H1c5	119.62
O1-Co1-O6	90.26(9)	C6-C5-H1c5	119.62
O1-Co1-H2o6	69.7(6)	C5-C6-C7	118.6(4)
O2-Co1-O2 ii	98.16(8)	C5-C6-H1c6	120.7
O2-Co1-O3	165.15(9)	C7-C6-H1c6	120.7
O2-Co1-O5 iii	89.20(9)	C2-C7-C6	120.7(4)
O2-Co1-H1o5 iii	75.0(7)	C2-C7-C8	108.6(3)
O2-Co1-O6	96.52(9)	C6-C7-C8	130.6(3)
O2-Co1-H2o6	106.8(8)	C7-C8-C9	130.7(3)
O2 ii -Co1-O3	68.31(8)	C7-C8-C13	108.7(3)
O2 ii -Co1-O5 iii	92.93(8)	C9-C8-C13	120.6(3)
O2 ii -Co1-H1o5 iii	78.5(7)	C8-C9-C10	119.1(3)
O2 ii -Co1-O6	165.19(10)	C8-C9-H1c9	120.47
O2 ii -Co1-H2o6	146.5(6)	C10-C9-H1c9	120.47
O3-Co1-O5 iii	85.55(9)	C9-C10-C11	120.7(4)
O3-Co1-H1o5 iii	95.6(8)	C9-C10-H1c10	119.65
O3-Co1-O6	97.29(10)	C11-C10-H1c10	119.65
O3-Co1-H2o6	88.1(8)	C10-C11-C12	120.4(4)
O5 iii -Co1-H1o5 iii	22.1(5)	C10-C11-H1c11	119.79
O5 iii -Co1-O6	89.22(9)	C12-C11-H1c11	119.79
O5 iii -Co1-H2o6	109.2(6)	C11-C12-C13	119.4(3)
H1o5 iii -Co1-O6	107.3(6)	C11-C12-H1c12	120.32
H1o5 iii -Co1-H2o6	129.1(7)	C13-C12-H1c12	120.32
O6-Co1-H2o6	22.7(5)	P1-C13-C1	38.29(12)
Co1 iv -P1-Co1	107.01(3)	P1-C13-C8	122.4(3)
Co1 iv -P1-Co1 i	76.02(2)	P1-C13-C12	106.6(2)
Co1 iv -P1-O1	135.70(8)	C1-C13-C8	110.0(3)
Co1 iv -P1-O2 i	54.41(7)	C1-C13-C12	130.1(3)
Co1 iv -P1-O3 iv	51.58(9)	C8-C13-C12	119.9(3)
Co1 iv -P1-C1	116.63(9)	H1o4-O4-H2o4	104(3)
Co1 iv -P1-C2	127.52(7)	Co1 iv -O5-H1o5	101(2)
Co1 iv -P1-C13	130.41(7)	Co1 iv -O5-H2o5	113(2)
Co1 iv -P1-H1c1	92.26	H1o5-O5-H2o5	104(3)
Co1-P1-Co1 i	69.39(2)	Co1 iv -H1o5-O5	56.8(19)
Co1-P1-O1	28.79(7)	Co1-O6-H1o6	111.6(19)
Co1-P1-O2 i	98.99(8)	Co1-O6-H2o6	98.6(19)
Co1-P1-O3 iv	96.12(8)	H1o6-O6-H2o6	104(3)
Co1-P1-C1	136.23(9)	Co1-H2o6-O6	58.7(18)
Co1-P1-C2	118.89(7)	P1-H1c1-C1	51.88
Co1 i -Co1-Co1 ii	81.923(18)	Co1-P1-C13	113.20(7)

Symmetry codes: (i) -x,y-1/2,-z+3/2 ; (ii) -x,y+1/2,-z+3/2 ; (iii) x,y+1,z ; (iv) x,y-1,z.

Table S4: Interatomic distances (Å) for $Co(H_2O)_2PO_3C\text{-}C_{12}H_9.H_2O$.

Atom – Atom	Length (Å)	Atom – Atom	Length (Å)
Co1-Co1^{i}	3.6821(11)	C3-H1c3	0.96
Co1-Co1 ^{ii}	3.6821(11)	C4-C5	1.396(6)
Co1-P1	3.2563(11)	C4-H1c4	0.96
Co1-P1 ^{iii}	2.7363(10)	C5-C6	1.381(6)
Co1-P1 ^{ii}	3.2121(12)	C5-H1c5	0.96
Co1-O1	2.061(2)	C6-C7	1.391(5)
Co1-O2	2.063(2)	C6-H1c6	0.96
Co1-O2 ^{ii}	2.226(2)	C7-C8	1.457(5)
Co1-O3	2.151(2)	C8-C9	1.395(6)
Co1-O5 ^{iii}	2.134(2)	C8-C13	1.404(4)
Co1-H1o5 ^{iii}	2.50(4)	C9-C10	1.385(6)
Co1-O6	2.127(2)	C9-H1c9	0.96
Co1-H2o6	2.46(4)	C10-C11	1.391(5)
P1-O1	1.516(2)	C10-H1c10	0.96
P1-O2 ^{i}	1.553(2)	C11-C12	1.396(6)
P1-O3 ^{iv}	1.530(2)	C11-H1c11	0.96
P1-C1	1.830(3)	C12-C13	1.389(6)
P1-C2	2.798(3)	C12-H1c12	0.96
P1-C13	2.757(4)	O4-H1o4	0.96(3)
P1-H1c1	2.2594	O4-H2o4	0.96(3)
C1-C2	1.509(4)	O5-H1o5	0.96(3)
C1-C13	1.507(5)	O5-H2o5	0.96(3)
C1-H1c1	0.96	O6-H1o6	0.96(3)
C2-C3	1.372(5)	O6-H2o6	0.96(3)
C2-C7	1.408(5)	Co1-Co1 ^{i}	3.6821(11)
C3-C4	1.388(5)	C4-C5	1.396(6)

Symmetry codes: (i) -x,y-1/2,-z+3/2 ; (ii) -x,y+1/2,-z+3/2 ; (iii) x,y+1,z ; (iv) x,y-1,z.