Supplementary Material

Chirality and Magnetism of an Open-framework Cobalt Phosphite Containing Helical Channels from Achiral Materials†

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Synthesis: Typically, $CoCl_2 \cdot 6H_2O$ (0.178g) was first dissolved in DMF (20mL) and then 4-diazabicyclo [2, 2, 2]octane (DABCO, 1.10g) was added with stirring. Finally, H_3PO_3 (0.6mL, 50wt %) was added to the above reaction mixture. A dark-blue gel was formed after stirring for 0.5h. The gel was sealed in a Teflon-lined stainless steel autoclave and heated under autogenous pressure at 60°C for 3 days. The resulting blue block crystals were isolated by filtration, washed with ethanol and dried in air. Inductively coupled plasma (ICP) analysis (Perkin–Elmer Optima 3300 DV ICP instrument) for **1** yielded Co 17.65, P 18.03% (calcd: Co 17.71, P 18.61%). Elemental analysis (%; Perkin–Elmer 2400 elemental analyzer) calcd: C 21.62, H 4.80, N 8.41; found: C 21.65, H 4.89, N 8.33).

Structure determination: Structural analysis of a single crystal (0.21×0.18×0.16 mm^3) was performed on a Siemens SMART CCD diffractometer using graphite-monochromated MoKa radiation (λ = 0.71073 Å). Data processing was accomplished with the SAINT processing program. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares using SHELXTL97. All Co, P, and O atoms were determined directly. The hydrogen atoms of the HPO_3 groups, C, and N atoms were subsequently found in the difference Fourier map. The hydrogen atoms in the DABCO molecules were placed geometrically. All non-hydrogen atoms

of the inorganic framework were refined anisotropically. Crystal data and details of the structure determination are given in Table S1.

Crystal data: $C_6N_2H_{16}O_6P_2Co$, *M*r = 333.08, orthorhombic, space group $P2_12_12_1$ (No. 19), a = 10.1040(4), b = 10.8100(5), c = 10.9930(5) Å, V = 1200.70(9) Å^3, $Z = 4$, μ = 1.713 mm^{-1}, ρ_{calcd} = 1.843 gcm^{-3}, 6673 reflections measured, 2368 unique (R_{int} = 0.0180). The final *wR* (F^2) (all data) was 0.0608 and *R* (*F*) (I > 2σ(I)) was 0.0209. The flack parameter was 0.034(14). CCDC-723093 contains the supplementary crystallographic data for **1**.

A crystal of the enantiomorph of **1** was selected for a second structure determination. The flack parameter was 0.031(15). In all other respects, the structures of the two enatiomorphs are identical, as expected. CCDC-723094 contains the supplementary crystallographic data for the enantiomorph of **1**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray powder diffraction (XRD) data was collected on a Siemens D5005 diffractometer with CuKa radiation (λ = 1.5418 Å).

TG analysis was performed on Perkin-Elmer TGA 7 thermogravimetric analyzer in the air with a heating rate of 10 ºCmin^{-1}. TG analysis (Supporting Information Figure S9) of **1** shows a total weight loss of ca. 33.98 % between 180 and 750ºC , which is attributed to the decomposition of the organic template molecules (calc. 34.23 %). XRD analysis of the residue left after heating to 750ºC shows that the material had transformed into a dense $Co_2P_2O_7$ phase (JCPDS card No. 34-1378).

Infrared (IR) spectrum was recorded within the 400–4000 cm^{-1} region on a Nicolet Impact 410 FTIR spectrometer using KBr pellets.

Diffuse reflectance spectra were collected on Perkin-Elmer Lambda20 within the range 300–800 nm.

The circular dichroism (CD) spectra were recorded on a JASCO J-810 spectropolarimeter with KBr pellets.

The magnetic measurements were carried out on crystalline samples with a MPMS-5 SQUID magnetometer.

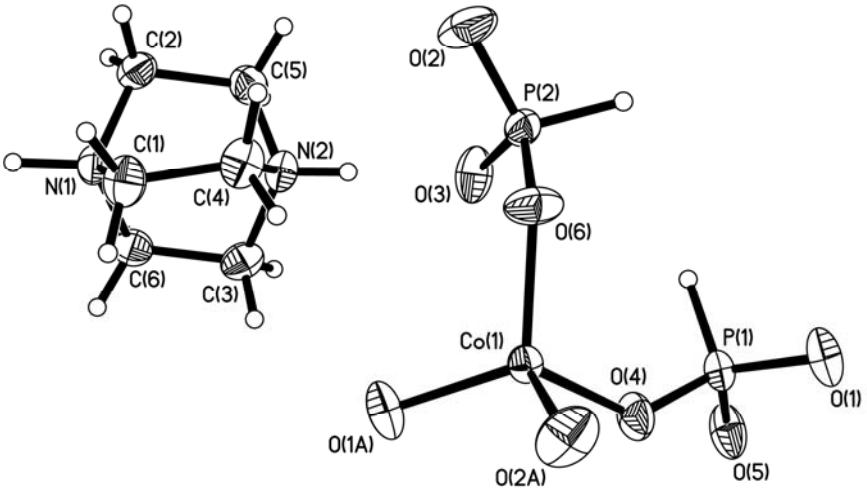

Fig. S1

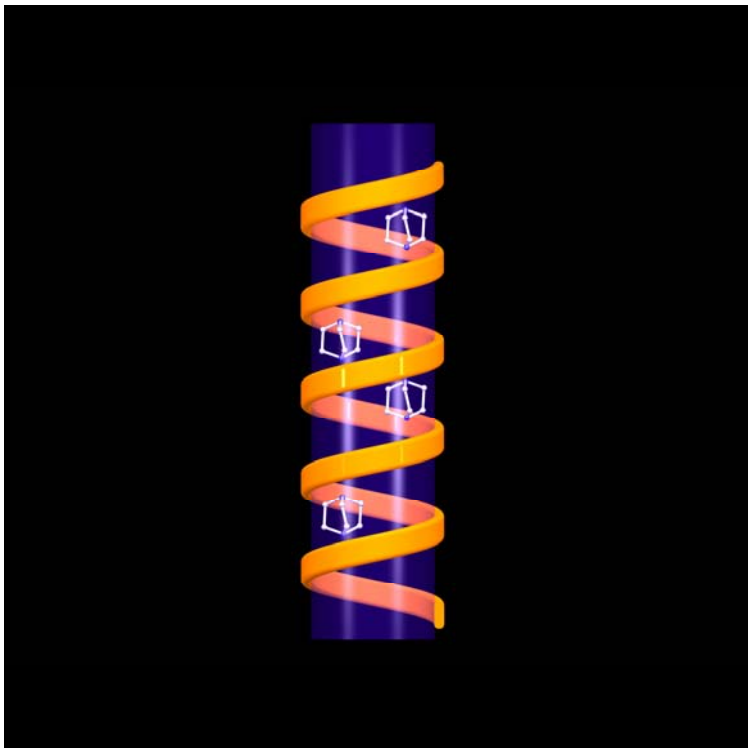

Fig. S2

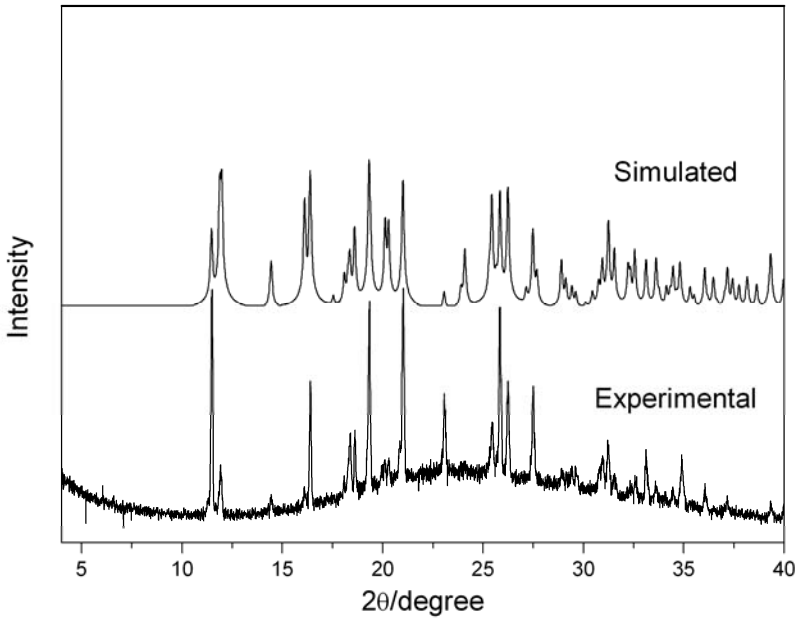
Simulated
Experimental
Intensity
5
10
15
20
25
30
35
40
2θ/degree

Fig. S3

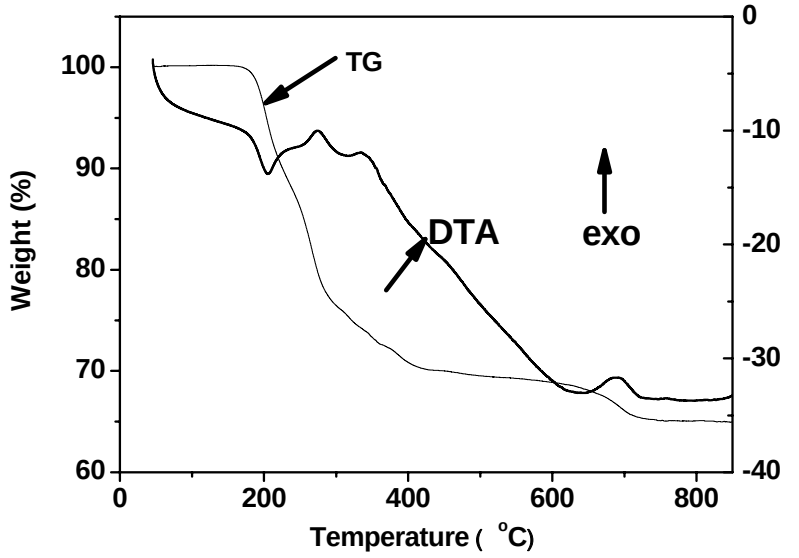
TG
DTA
exo
Weight (%)
100
90
80
70
60
0
-10
-20
-30
-40
0
200
400
600
800
Temperature (°C)

Fig. S4

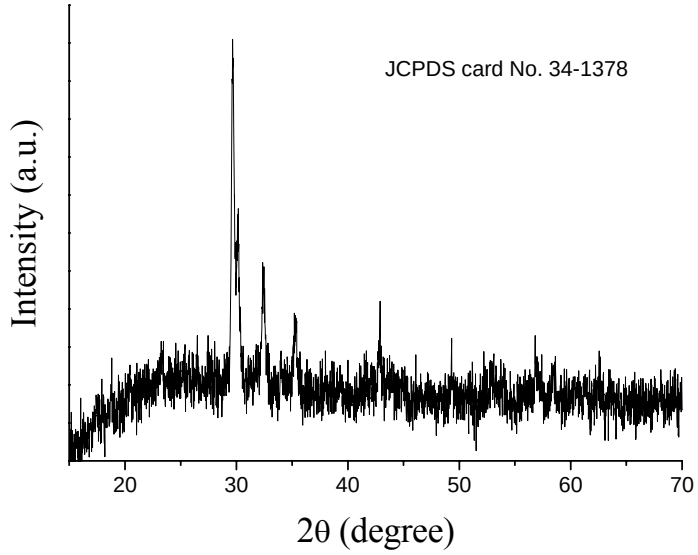
JCPDS card No. 34-1378
Intensity (a.u.)
20
30
40
50
60
70
2θ (degree)

Fig. S5

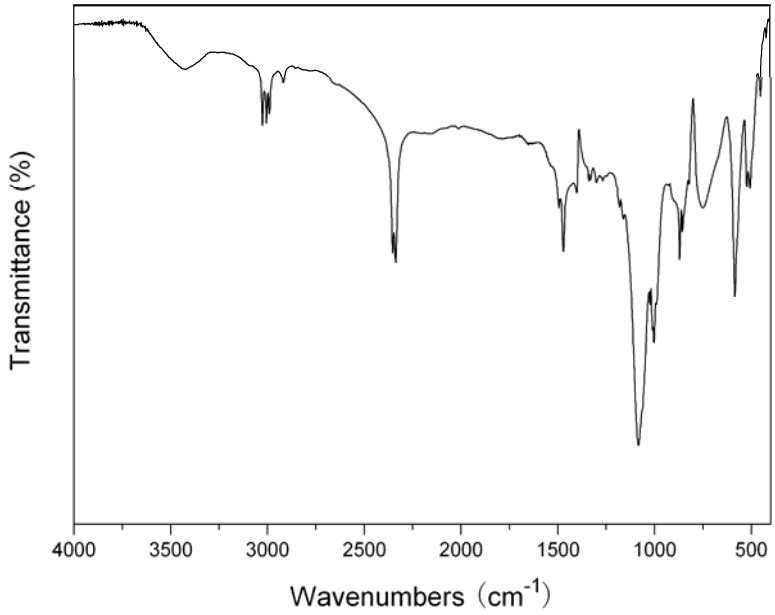
Transmittance (%)
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

Fig. S6

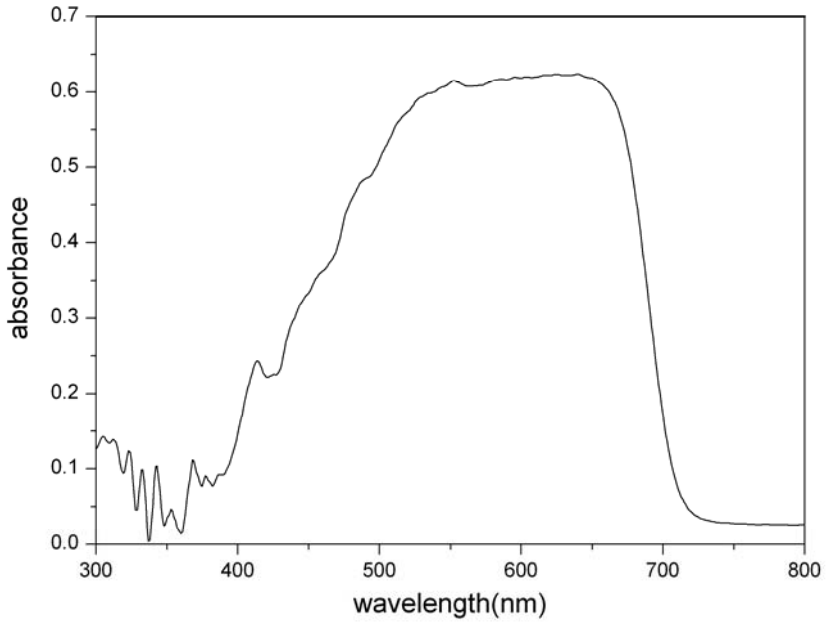
absorbance
wavelength(nm)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
300
400
500
600
700
800

Fig. S7

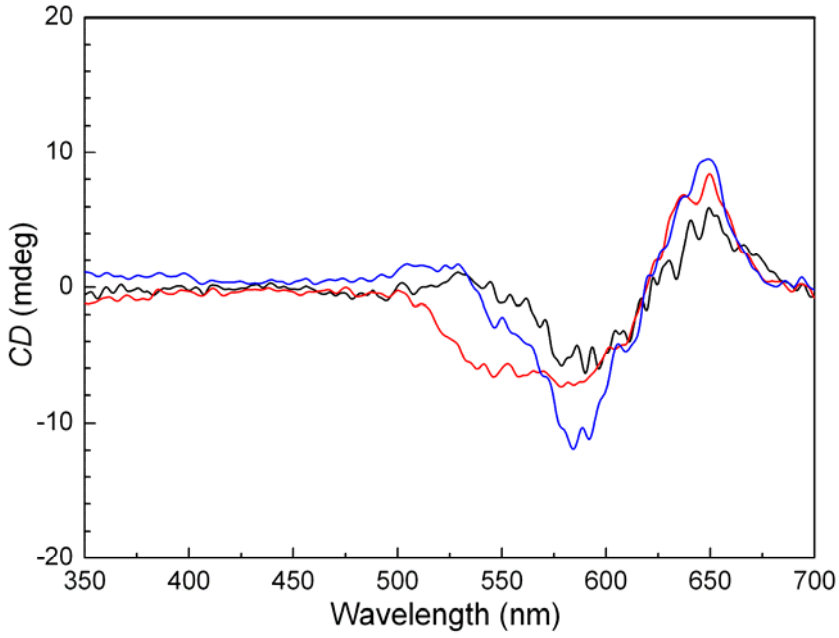
CD (mdeg)
Wavelength (nm)
20
10
0
-10
-20
350
400
450
500
550
600
650
700

Fig. S8

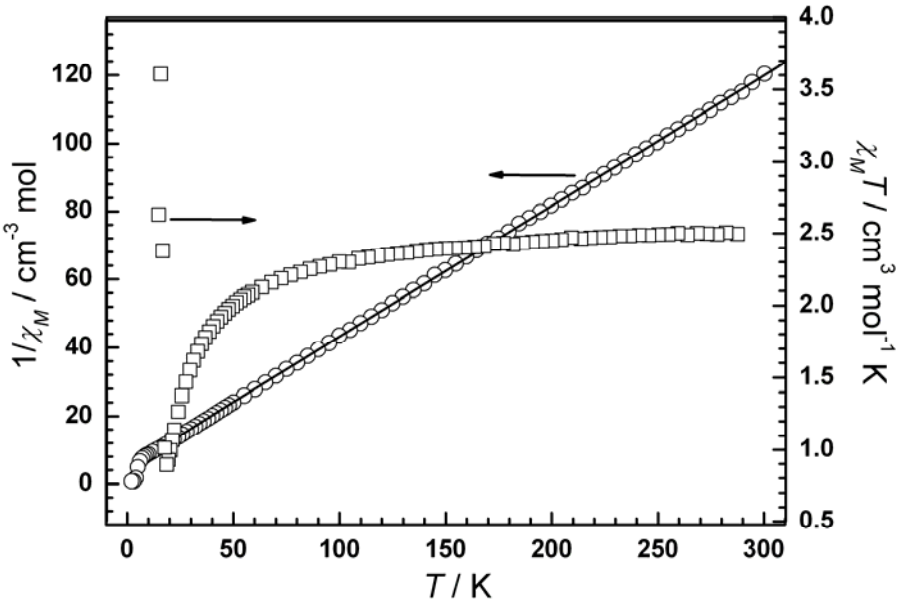

Fig. S9

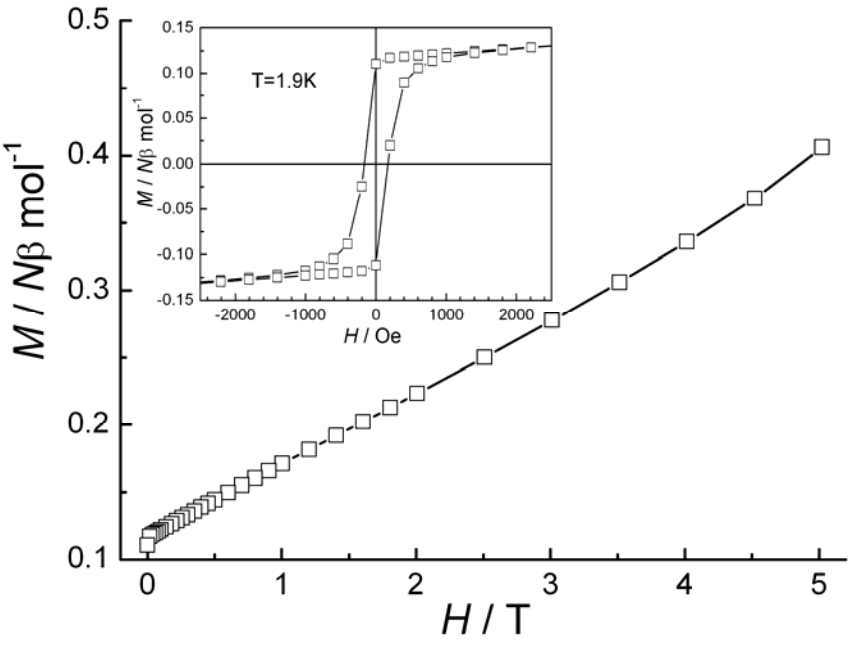

Fig. S10

Table S1 Crystal data and details for the structure determination for **1**.

	Compound **1**
Empirical formula	C6 H16 Co N2 O6 P2
Formula weight	333.08
Temperature (K)	293(2)
Wavelength (Å)	0.71069
Crystal system	*Orthorhombic*
Space group	$P2_12_12_1$
a (Å)	10.1040(4)
b (Å)	10.8100(5)
c (Å)	10.9930(5)
β (°)	90
Volume (Å^3)	1200.70(9)
Z	4
D_{calc} (g cm^{-3})	1.843
Absorption coefficient (mm^{-1})	1.713
F(000)	684
Crystal size (mm)	0.21 x 0.18 x 0.16
θ range (°)	2.64 –26.07
Limiting indices	$-12 \le h \le 12$, $-13 \le k \le 13$, $-8 \le l \le 13$
Reflections collected / unique	6673 / 2368 [R(int) = 0.0180]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2368 / 2 / 168
Goodness-of-fit on F^2	1.084
Absolute structure parameter	0.034(14)
Final *R* indices [$I>2\sigma(I)$]	$R_1 = 0.0209$, $wR_2 = 0.0603$
R indices (all data)	$R_1 = 0.0221$, $wR_2 = 0.0608$
Largest diff. peak and hole (e Å^{-3})	0.607 and -0.300

Table S2 Selected bond lengths [Å] and angles [˚] for **1**.

Co(1)-O(1)#1	1.9581(17)	P(1)-O(1)	1.5128(18)
Co(1)-O(2)#2	1.9337(18)	P(1)-O(4)	1.5170(17)
Co(1)-O(4)	1.9538(16)	P(1)-O(5)	1.5189(17)
Co(1)-O(6)	1.9403(17)	P(2)-O(2)	1.5066(19)
P(1)-H(1)	1.360(10)	P(2)-O(3)	1.5160(19)
P(2)-H(2)	1.371(10)	P(2)-O(6)	1.5104(17)
O(1)#1-Co(1)-O(2)#2	111.88(9)	O(1)-P(1)-O(4)	111.96(10)
O(1)#1-Co(1)-O(6)	111.83(9)	O(1)-P(1)-O(5)	113.26(11)
O(1)#1-Co(1)- O(4)	110.15(7)	O(4)-P(1)-O(5)	110.08(10)
O(2)#2-Co(1)-O(4)	102.10(8)	O(2)-P(2)-O(3)	113.91(12)
O(2)#2-Co(1)-O(6)	109.77(8)	O(2)-P(2)-O(6)	108.85(11)
O(4)-Co(1)-O(6)	110.71(8)	O(3)-P(2)-O(6)	113.18(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y,z-1/2 #2 -x+1,y+1/2,-z+1/2