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Synthesis, structure, and surface photovoltage and magnetic properties of a novel 3D homochiral manganese phosphonate with right–handed helical chains

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Table S1. Crystal data and structure refinement for compound **1.**

Empirical formula	$C_5H_{10}Mn_2NO_{12}P_2$
Formula weight	447.96
Temperature/K	295(2)
Crystal system	Tetragonal
Space group	$P4_2$
a (Å)	14.791(4)
c (Å)	5.696(3)
V (Å^3)	1246.1(8)
Z	4
D_c (g·cm^{-3})	2.388
Absorption coefficient	2.354
Reflections collected	8041
Independent reflections	2365（R_{int} = 0.0501）
Completeness to theta = 28.21	98.7 %
Goodness–of–fit on F^2	1.045
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0364, wR_2 = 0.0773
R indices (all data)	R_1 = 0.0488, wR_2 = 0.0827
Absolute structure parameter	−0.01(3)

$R_1 = \Sigma\,(|F_0|-|F_C|) / \Sigma\,|F_0|$; $wR_2 = [\Sigma\, w\,(|F_0|-|F_C|)^2 / \Sigma\, w\, F_0^2]^{1/2}$.

Table S2 Selected bond lengths (Å) and bond angles (°) in compound **1.**

Mn(1)–O(5)#1	2.136(4)	P(1)–O(1)	1.541(4)
Mn(1)–O(2)	2.153(4)	P(1)–O(2)	1.518(4)
Mn(1)−O(7)	2.155(3)	P(1)–O(3)	1.524(4)
Mn(1)−O(6)#2	2.156(4)	P(2)–O(7)	1.529(4)
Mn(1)−O(3)#2	2.177(4)	P(2)–O(8)	1.501(4)
Mn(1)−O(4)#1	2.321(4)	P(2)–O(9)	1.530(4)
Mn(2)−O(8)	2.113(4)	O(4)–C(1)	1.443(6)
Mn(2)−O(7)#3	2.148(4)	O(5)–C(2)	1.260(6)
Mn(2)−O(12)#4	2.148(4)	O(6)–C(2)	1.258(6)
Mn(2)−O(3)	2.198(3)	O(10)–C(3)	1.437(6)
Mn(2)−O(11)#3	2.256(4)	O(11)–C(4)	1.272(6)
Mn(2)−O(10)#4	2.321(4)	O(12)–C(4)	1.240(6)
O(5)#1–Mn(1)–O(2)	87.18(14)	O(8)–Mn(2)–O(7)#3	108.15(14)
O(5)#1–Mn(1)–O(7)	98.78(14)	O(8)–Mn(2)–O(12)#4	87.36(14)
O(2)–Mn(1)–O(7)	99.16(14)	O(7)#3–Mn(2)–O(12)#4	164.44(14)
O(5)#1–Mn(1)–O(6)#2	95.21(14)	O(8)−Mn(2)−O(3)	101.90(14)
O(2)–Mn(1)–O(6)#2	84.68(14)	O(7)#3−Mn(2)−O(3)	77.37(13)
O(7)–Mn(1)–O(6)#2	165.65(14)	O(12)#4−Mn(2)−O(3)	101.18(14)
O(5)#1–Mn(1)–O(3)#2	169.38(14)	O(8)–Mn(2)–O(11)#3	81.39(13)
O(2)–Mn(1)–O(3)#2	103.22(13)	O(7)#3–Mn(2)–O(11)#3	86.26(13)
O(7)–Mn(1)–O(3)#2	77.68(13)	O(12)#4–Mn(2)–O(11)#3	95.06(15)
O(6)#2–Mn(1)–O(3)#2	87.98(13)	O(3)–Mn(2)–O(11)#3	163.54(13)
O(5)#1–Mn(1)–O(4)#1	70.72(13)	O(8)–Mn(2)–O(10)#4	151.71(13)
O(2)–Mn(1)–O(4)#1	156.57(13)	O(7)#3–Mn(2)–O(10)#4	94.87(13)
O(7)–Mn(1)–O(4)#1	92.02(14)	O(12)#4–Mn(2)–O(10)#4	69.92(14)
O(6)#2–Mn(1)–O(4)#1	89.56(14)	O(3)–Mn(2)–O(10)#4	98.97(13)
O(3)#2–Mn(1)–O(4)#1	99.24(14)	O(11)#3–Mn(2)–O(10)#4	84.01(13)

Symmetry transformations used to generate equivalent atoms:

#1 –y+1, x, z+1/2 #2 x, y, z+1 #3 x, y,z–1 #4 –y+2, x, z–1/2

Figure S1 X–ray powder diffraction patterns of compound **1**. Simulated (lower trace) and experimental (upper trace).

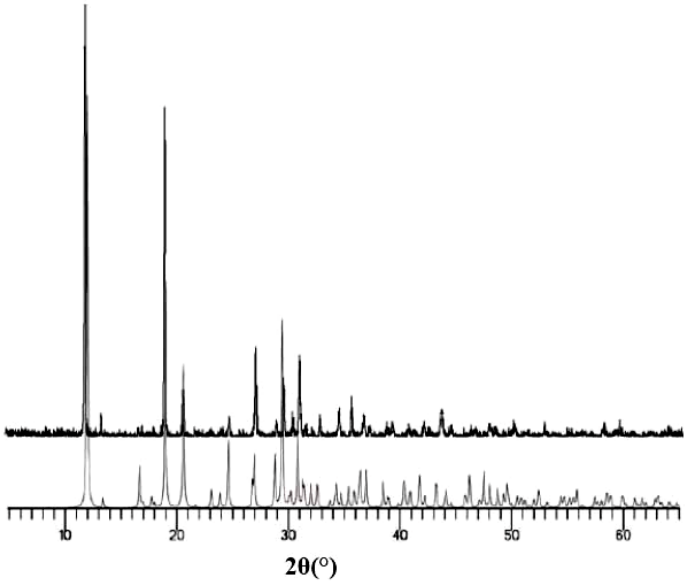

Figure S2 TG curve of compound **1.**

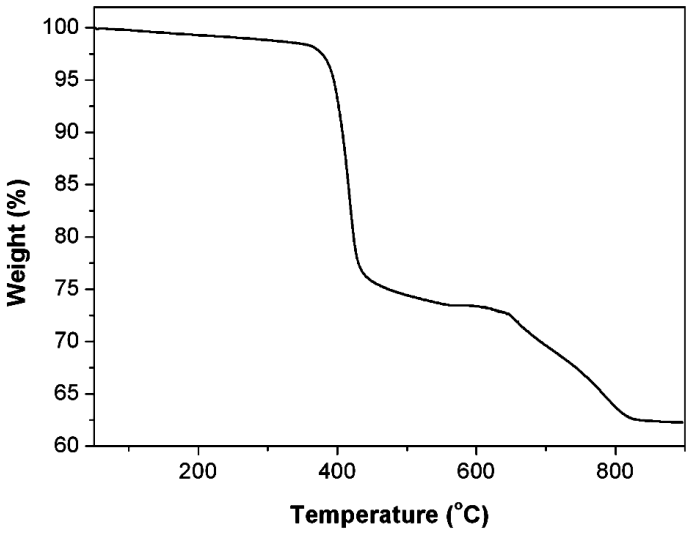

Figure S3 IR spectrum of compound **1.**

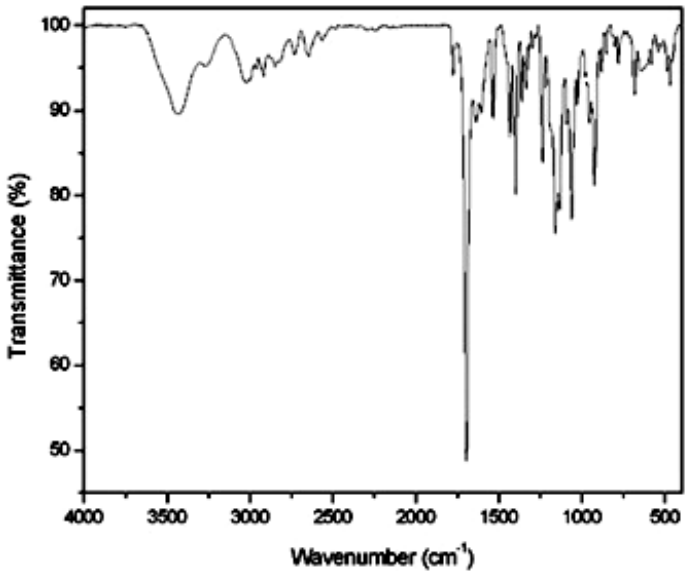

Figure S4 The FISPS of compound **1.** The intensities of the SPV response increase linearly with the external positive electric field.