Electronic Supplementary Information (ESI) for:

Canted Antiferromagnetism and Spin Reorientation Transition in Layered Inorganic-Organic Perovskite $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$

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Table S1. Crystal data and structure refinement parameters for $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$.

Empirical formula	$C_{16}H_{24}MnN_2Cl_4$
Formula weight	441.11
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Cell Parameters	a = 7.2075(9) Å b = 7.3012(14) Å c = 39.413(6) Å
Volume	2074.0(6) $Å^3$
Z	4
Density (X-ray)	1. 413 gcm^{-3}
Absorption coefficient	1.151 mm^{-1}
Crystal size	0.55 x 0.4 x 0.1 mm^3
$\sin\theta_{max}/\lambda$	0.594 $Å^{-1}$
h, k, l range	$-1 \leq h \leq 8$ $-1 \leq k \leq 8$ $-46 \leq l \leq 1$
Total reflections	2339
Symmetry independent reflections	1726
R_{int}	0.030
R, wR	0.044, 0.109
Goodness of Fit	1.242
Parameters	119
Largest diff. peak and hole	0.369, –0.324 $eÅ^{-3}$

Table S2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$. $U_{eq} = 1/3(U_{11}+U_{22}+U_{33})$.

	x	**y**	**z**	**$U_{eq.}$**
Mn1	0	5000	5000	28(1)
Cl2	–352(1)	4922(2)	4373(1)	42(1)
Cl3	2363(1)	7633(1)	4946(1)	38(1)
C1	9837(7)	10273(7)	3444(1)	56(1)
C2	11235(9)	10926(8)	3246(1)	71(2)
C3	11380(10)	10378(10)	2908(2)	84(2)
C4	10168(10)	9148(10)	2782(2)	84(2)
C5	8834(11)	8454(10)	2973(2)	90(2)
C6	8655(9)	9017(10)	3305(2)	85(2)
C7	9588(9)	10915(8)	3809(1)	69(2)
C8	10390(7)	9630(7)	4062(1)	51(1)
N1	9917(6)	10154(7)	4413(1)	46(1)
H2	12096	11741	3336	85
H3	12308	10858	2770	101
H4	10273	8781	2557	101
H5	8021	7591	2883	108
H6	7708	8531	3437	102
H7A	10173	12104	3835	83
H7B	8274	11062	3855	83
H8A	9930	8405	4017	61
H8B	11729	9609	4037	61
H1	8740(90)	10030(80)	4436(15)	80(20)
H9	10220(80)	11250(90)	4567(15)	80(20)
H10	10450(70)	9360(80)	4582(14)	68(16)

Table S3. Selected bond lengths (Å) and angles (°) in the $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$ crystal at 296 K.

Atoms	Lengths (Å)	Atoms	Angles (°)
Mn1 – Cl2	2.4846(11)	Cl2 – Mn1 – Cl2 #1	180
Mn1 – Cl2 #1	2.4846(11)	Cl2 – Mn1 – Cl3	90.13(3)
Mn1 – Cl3	2.5773(9)	Cl2 #1 – Mn1 – Cl3	89.87(3)
Mn1 – Cl3 #1	2.5773(9)	Cl2 – Mn1 – Cl3 #1	89.87(3)
Mn1 – Cl3 #2	2.5776(9)	Cl2 #1 – Mn1 – Cl3 #1	90.13(3)
Mn1 – Cl3 #3	2.5776(9)	Cl3 – Mn1 – Cl3 #1	180
Mn1 #4 – Cl3	2.5776(9)	Cl2 – Mn1 – Cl3 #2	88.72(3)
C1 – C2	1.361(7)	Cl2 #1 – Mn1 – Cl3 #2	91.28(3)
C1 – C6	1.367(8)	Cl3 – Mn1 – Cl3 #2	90.34(1)
C1 – C7	1.524(7)	Cl3 #1 – Mn1 – Cl3 #2	89.66(1)
C2 – C3	1.393(8)	Cl2 – Mn1 – Cl3 #3	91.28(3)
C3 – C4	1.347(9)	Cl2 #1 – Mn1 – Cl3 #3	88.72(3)
C4 – C5	1.320(9)	Cl3 – Mn1 – Cl3 #3	89.66(1)
C6 – C7	1.378(8)	Cl3 #1 – Mn1 – Cl3 #3	90.34(1)
C7 – C8	1.486(7)	Cl3 #2 – Mn1 – Cl3 #3	180
N1 – C8	1.475(6)	Mn1 – Cl3 – Mn #4	168.66(4)
		C2 – C1 – C6	117.8(5)
		C2 – C1 – C7	121.4(5)
		C6 – C1 – C7	120.8(5)
		C1 – C2 – C3	120.2(6)
		C4 – C3 – C2	119.6(6)
		C5 – C4 – C3	121.3(6)
		C4 – C5 – C6	119.5(6)
		C1 – C6 – C5	121.5(6)
		C8 – C7 – C1	113.2(4)
		N1 – C8 – C7	112.0(4)

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Distances (Å) and angles of hydrogen bonds (°) in the $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$ crystal at 296 K.

N – H ··· Cl	Distance (Å) [N – H]	Distance (Å) [H ··· Cl]	Distance (Å) [N – Cl]	Angle (N – H ··· Cl)
N1 – H1 ··· Cl2	0.856	2.456(64)	3.298(4)	167.30(58)
N1 – H9 ··· Cl2	0.856	2.737(65)	3.490(5)	147.39(56)
N1 – H9 ··· Cl3	0.856	2.759(59)	3.396(4)	132.36(50)
N1 – H10 ··· Cl3	0.964	2.355(54)	3.303(4)	167.64(45)