

Supplementary Material:

Table S1. Crystal data and structure refinement for $(C_5H_{14}N_2)[MnCl_4(H_2O)_2]$.

Empirical formula	$(C_5H_{14}N_2)[MnCl_4(H_2O)_2]$
Crystal color /shape	Plate, colourless
Formula weight (g mol ⁻¹)	334.95
Volume (Å ³)	1270.2 (3)
ρ_{cal} (Mg m ⁻³)	1.752
Crystal system	monoclinic
Space group	P2/c
Z	4
a(Å)	12.394 (14)
b(Å)	9.408 (11)
c(Å)	11.879 (14)
α (°)	90
β (°)	113.518 (4)
γ (°)	90
θ range for data collection (°)	2.2< θ < 27.6
Temperature (k)	150
λ (Moka) (Å)	0.71073
Absorption correction	Multi-scan
Crystal size (mm ³)	0.46*0.44*0.09
h.k.l range	-16<h<16, -12<k<10, -15<l<15
Diffractometer	D8 VENTURE Bruker AXS
Programs systems	SHELXT- 2015 and SHELXL-2018
No.of reflections collected	10704
No. of independant reflection	2925
No. of reflections observed ($I > 2s(I)$)	2681
Rint	0.061
F(000)	684
No.of parameters	152
Goodness of fit	0.95
Transmission factors	$T_{\text{max}} = 0.846$, $T_{\text{min}} = 0.490$
Rindices	R= 0.042, WR= 0.106

Table S2. Main distances (Å) and angles (°) for (C₅H₁₄N₂)[MnCl₄(H₂O)₂] atomic arrangement.

MnCl ₄ (H ₂ O) ₂ octahedron anion		C ₅ H ₁₄ N ₂ organic cation	
Parameter	value	Parameter	value
Mn1—O1	2.1838 (15)	C1—N2	1.494 (3)
Mn1—O1 ⁱ	2.1838 (15)	C1—C7	1.510 (3)
Mn1—Cl1 ⁱ	2.4929 (6)	N2—C3	1.496 (3)
Mn1—Cl2	2.5909 (6)	C3—C4	1.520 (3)
Mn1—Cl2 ⁱ	2.5909 (6)	C4—C5	1.510 (3)
Mn2—O11	2.2331 (16)	C5—N6	1.514 (3)
Mn2—O11 ⁱⁱ	2.2331 (16)	N6—C7	1.495 (3)
Mn2—Cl11 ⁱⁱ	2.4888 (6)	N2—C1—C7	114.34 (18)
Mn2—Cl11	2.4888 (6)	C1—N2—C3	115.12 (17)
Mn2—Cl12 ⁱⁱ	2.6049 (6)	N2—C3—C4	111.65 (18)
Mn2—Cl12	2.6049 (6)	C5—C4—C3	115.40 (18)
O1—Mn1—O1 ⁱ	171.81 (10)	C4—C5—N6	115.01 (17)
O1—Mn1—Cl1 ⁱ	91.42 (5)	C7—N6—C5	117.94 (16)
O1i—Mn1—Cl1 ⁱ	94.37 (5)	N6—C7—C1	112.32 (18)
O1—Mn1—Cl1	94.37 (5)		
O1i—Mn1—Cl1	91.42 (5)		
Cl1i—Mn1—Cl1	90.00 (3)		
O1—Mn1—Cl2	89.12 (5)		
O1i—Mn1—Cl2	84.89 (5)		
Cl1i—Mn1—Cl2	92.13 (2)		
Cl1—Mn1—Cl2	175.865 (18)		
O1—Mn1—Cl2 ⁱ	84.89 (5)		
O1i—Mn1—Cl2 ⁱ	89.12 (5)		
Cl1i—Mn1—Cl2 ⁱ	175.865 (18)		
Cl1—Mn1—Cl2 ⁱ	92.13 (2)		
Cl2—Mn1—Cl2 ⁱ	85.96 (3)		
O11—Mn2—O11 ⁱⁱ	85.60 (8)		
O11—Mn2—Cl11 ⁱⁱ	87.92 (4)		
O11ii—Mn2—Cl11 ⁱⁱ	170.86 (4)		
O11—Mn2—Cl11	170.86 (4)		
O11ii—Mn2—Cl11	87.92 (4)		
Cl11ii—Mn2—Cl11	99.21 (3)		
O11—Mn2—Cl12 ⁱⁱ	91.63 (4)		
O11ii—Mn2—Cl12 ⁱⁱ	84.83 (4)		
Cl11ii—Mn2—Cl12 ⁱⁱ	88.915 (17)		
Cl11—Mn2—Cl12 ⁱⁱ	88.915 (17)		
Cl12ii—Mn2—Cl12	175.18 (3)		

Table S3. Observed vibration frequencies (cm^{-1}) and band assignments for $(\text{C}_5\text{H}_{14}\text{N}_2)[\text{MnCl}_4(\text{H}_2\text{O})_2]$.

observed	Assignment
3118	$\nu_{\text{as}}(\text{N-H})$
3051	$\nu_{\text{s}}(\text{N-H})$
2805	$\nu_{\text{s}}(\text{C-H})$
1647	$\nu_{\text{a}}(\text{C-H})$
1570	$\delta(\text{NH}_2)$
1450	$\delta_{\text{as}}(\text{C-N-H})$
1385	$\delta(\text{CH}_2)$
1333	$\delta(\text{CH}_2)$
1103	$\nu_{\text{as}}(\text{C-N})$
1065	$\nu_{\text{as}}(\text{C-N})$
1021	$\nu_{\text{as}}(\text{C-C})$
976	$\rho(\text{NH}_2)$
880	$\delta(\text{C-C-C})$
780	$\delta(\text{C-C-N})$
529	$\delta(\text{C-N-C})$

Abbreviations: ν - stretching; δ - bending; ρ - rocking; s: Symmetric; as: Asymmetric.

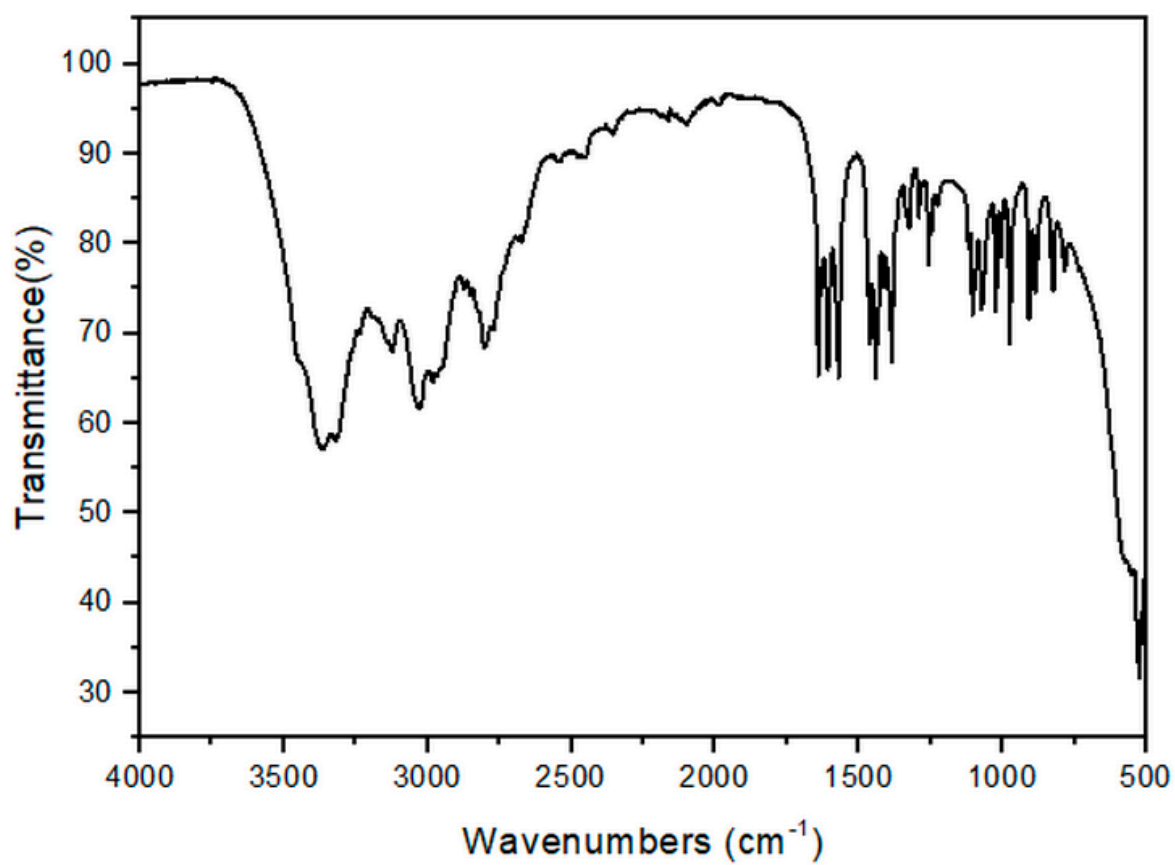


Figure S1. Infrared absorption spectra of the studied compound