

Supplementary Information S1

Figure shows the FT-IR spectrum of the $[\text{N}(\text{C}_2\text{H}_5)_4]_2\text{CdBr}_4$ single crystal recorded at 300 K over the range of 4000–500 cm^{-1} . The relatively weak absorption bands observed at 2991 and 2948 cm^{-1} correspond to the asymmetric and symmetric stretching vibrations of the CH_3 and CH_2 groups, respectively. Prominent peaks at 1455 and 1172 cm^{-1} are assigned to vibrational modes of the CH_3 group, while the bands at 1395 and 1367 cm^{-1} are attributed to vibrations of the CH_2 groups. The stretching vibration of the C–N bond is observed at 1004 cm^{-1} , and the characteristic bending mode of the C–N–C group appears at 788 cm^{-1} .

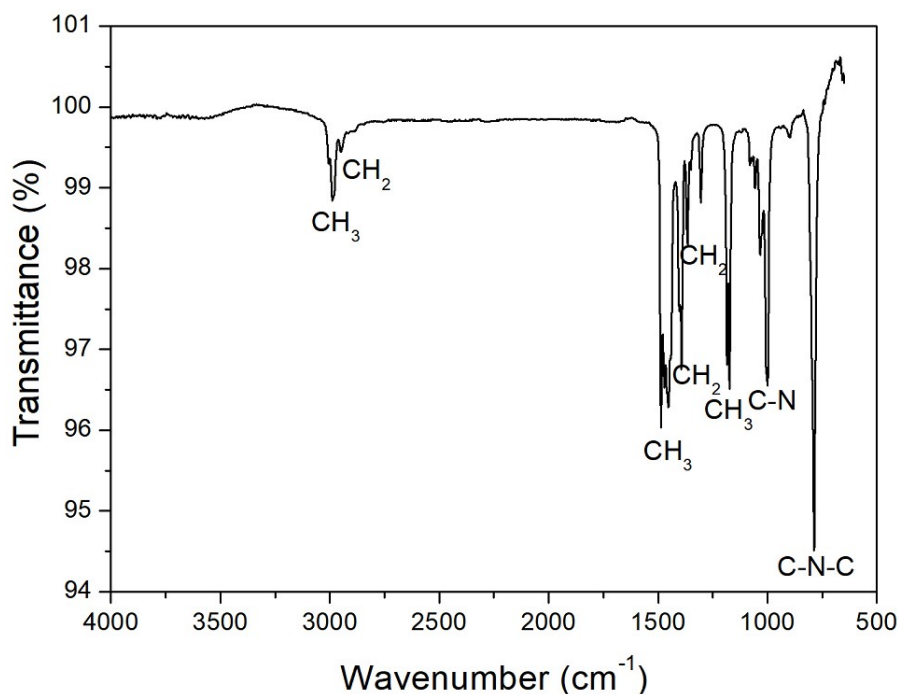


Figure FT-IR spectrum of $[\text{N}(\text{C}_2\text{H}_5)_4]_2\text{CdBr}_4$ measured in the range of 4000–500 cm^{-1} at 300 K.

Supplementary Information S2

Table. Crystal data and structure refinement for $[\text{N}(\text{C}_2\text{H}_5)_4]_2\text{CdBr}_4$ at 300 K.

Chemical formula	$\text{C}_{16}\text{H}_{40}\text{N}_2\text{CdBr}_4$
Weight	692.51
Crystal system	Tetragonal
Space group	$P4\bar{2}_1m$
Lattice constants	
a (Å)	13.4605(3)
b (Å)	13.4605(3)
c (Å)	14.4058(4)
Z	4
Volume (Å ³)	2610.12(14)
Radiation type	Mo-K α
Wavelength (Å)	0.71073

Supplementary Information S3

Table. The bond-length (Å) and bond-angle (°) of $[\text{N}(\text{C}_2\text{H}_5)_4]_2\text{CdBr}_4$ single crystals at 300 K.

Bond-length		Bond-angles	
Cd(1)-Br(1)	2.587(1)	Br(1)-Cd(1)-Br(2)	107.69(6)
Cd(1)-Br(2)	2.582(2)	Br(1)-Cd(1)-Br(3)	108.58(5)
Cd(1)-Br(3)	2.586(2)	Br(1)-Cd(1)-Br(1)	112.58(5)
Cd(1)-Br(1)	2.587(1)	Br(2)-Cd(1)-Br(3)	111.76(6)
N(1)-C(2)	1.46(2)	Br(2)-Cd(1)-Br(1)	107.69(6)
N(1)-C(3)	1.49(2)	Br(3)-Cd(1)-Br(1)	108.58(5)
N(1)-C(6)	1.48(2)	C(2)-N(1)-C(3)	102(1)
N(1)-C(6)	1.48(2)	C(2)-N(1)-C(6)	112(1)
N(2)-C(8)	1.5	C(3)-N(1)-C(6)	111(1)
C(1)-C(2)	1.58(4)	C(6)-N(1)-C(6)	109(1)
C(3)-C(4)	1.48(3)	C(8)-N(2)-C(8)	108.4
C(5)-C(6)	1.53(2)	C(8)-N(2)-C(8)	111.6
C(8)-C(9)	1.54(2)	N(1)-C(3)-C(4)	115(2)
C(1)-H	0.96	N(1)-C(6)-C(5)	114(1)
C(2)-H	0.97	N(2)-C(8)-C(9)	114
C(3)-H	0.97		
C(4)-H	0.96		
C(5)-H	0.96		
C(6)-H	0.97		
C(8)-H	0.97		
C(9)-H	0.96		