Electronic Supplementary Information

High Stability and Moderate Second-Order Nonlinear Optical Properties of Hybrid Lead-Free Perovskite $[(CH_3)_3NCH_2Cl]CdCl_3$ Bulk Crystals

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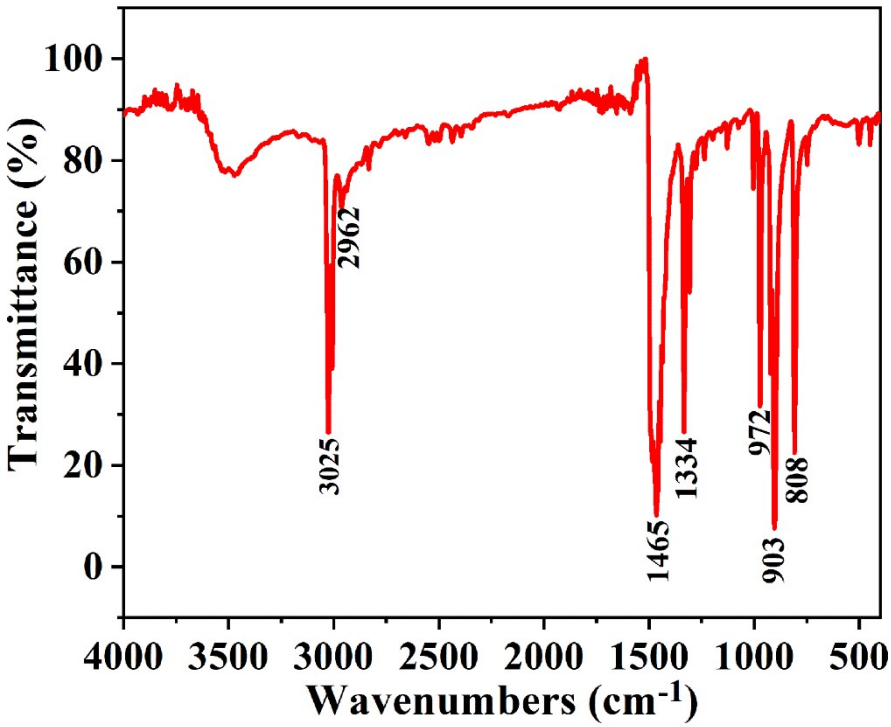

Fig. S1 The IR spectrum of (TMCM)$CdCl_3$.

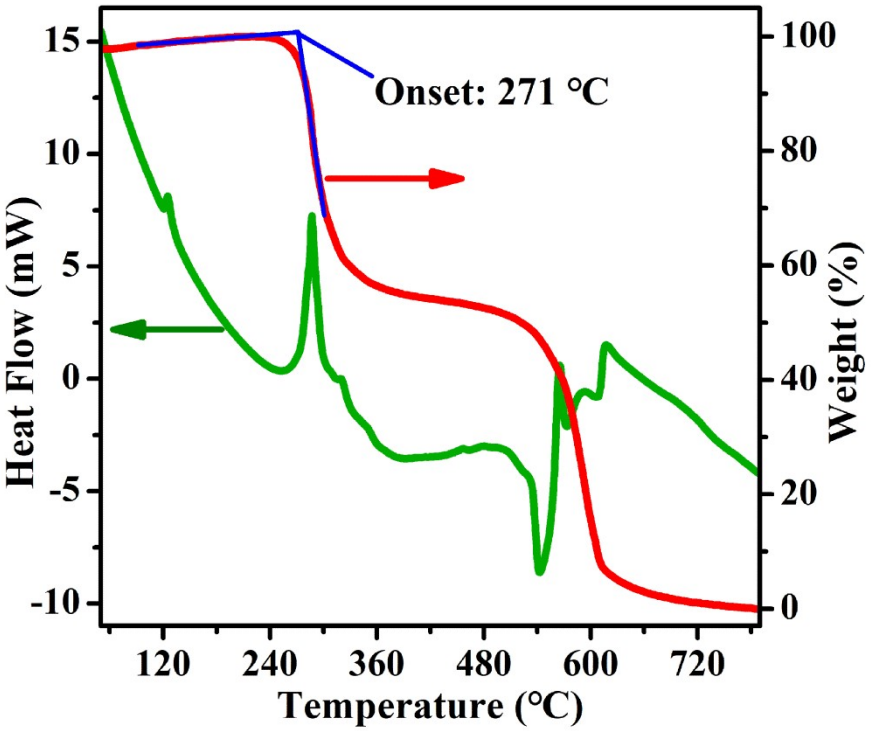

Fig. S2 The thermal stability analysis of DTA and TG curves of (TMCM)$CdCl_3$.

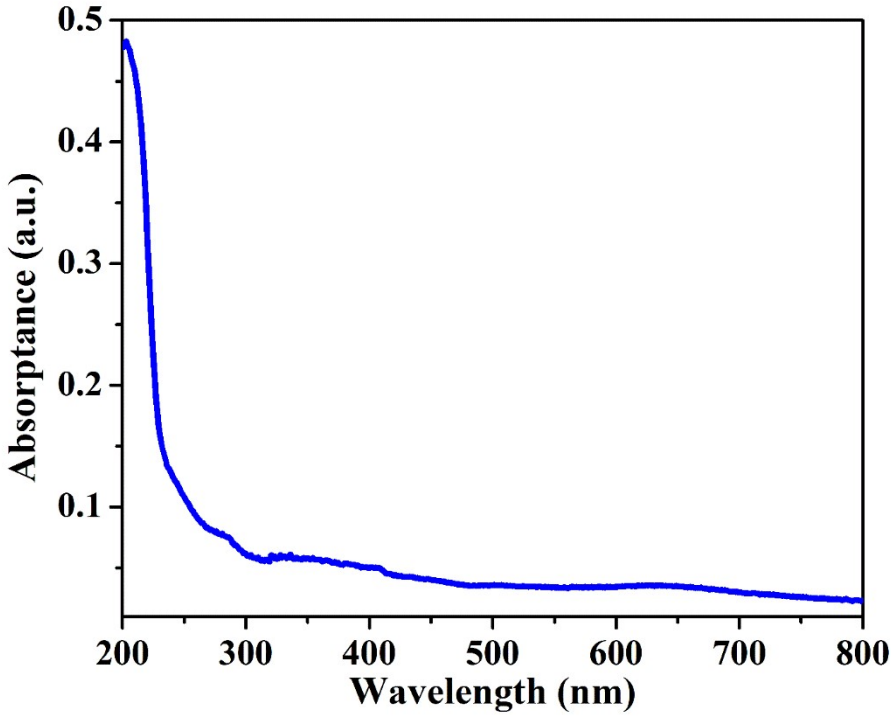

Fig. S3 The absorption spectrum of (TMCM)$CdCl_3$.

Table S1. The crystallographic parameters for (TMCM)$CdCl_3$.

Empirical formula	$C_4H_{11}CdCl_4N$
formula weight /g·mol^{-1}	327.34
temperature/K	273.15
wavelength/Å	0.71073
crystal system	Monoclinic
space group	Cc
a/Å	9.4797(10)
b/Å	15.7695(16)
c/Å	6.7960(8)
α/°	90
β/°	94.474(4)
γ/°	90
volume/Å^3	1012.84(19)
Z	4
density/mg·m^{-3}	2.147
Absorption coefficient (mm^{-1})	3.145
F(000)	632
Measured theta range (º)	3.788-28.315
Absorption correction	Semi-empirical from equivalents
Data/restraints/parameters	2431/2/95
GOF on F^2	1.069
R, wR [I>2sigma(I)]	0.0180, 0.0386
R, wR [all data]	0.0223, 0.0401
Absolute structure parameter	0.04(2)
Extinction coefficient	0.0094(4)
Largest diff. peak and hole	0.386 and -0.442 e.Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for (TMCM)$CdCl_3$.

Cd(1)-Cd(1)#1	3.3981(4)
Cd(1)-Cd(1)#2	3.3981(4)
Cd(1)-Cl(2)	2.6417(14)
Cd(1)-Cl(2)#1	2.6839(15)
Cd(1)-Cl(3)	2.6391(12)
Cd(1)-Cl(3)#1	2.6508(13)
Cd(1)-Cl(1)#2	2.6451(16)
Cd(1)-Cl(1)	2.6106(14)
Cl(4)-C(1)	1.755(5)
N(1)-C(2)	1.495(5)
N(1)-C(1)	1.491(6)
N(1)-C(4)	1.489(5)
N(1)-C(3)	1.503(6)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600

Cd(1)#1-Cd(1)-Cd(1)#2	179.04(2)
Cl(2)-Cd(1)-Cd(1)#2	50.90(3)
Cl(2)#1-Cd(1)-Cd(1)#2	129.73(3)
Cl(2)#1-Cd(1)-Cd(1)#1	49.81(3)
Cl(2)-Cd(1)-Cd(1)#1	129.55(3)
Cl(2)-Cd(1)-Cl(2)#1	95.10(5)
Cl(2)-Cd(1)-Cl(3)#1	98.06(4)
Cl(2)-Cd(1)-Cl(1)#2	82.85(4)
Cl(3)-Cd(1)-Cd(1)#1	128.86(4)
Cl(3)#1-Cd(1)-Cd(1)#2	131.08(3)

Cl(3)#1-Cd(1)-Cd(1)#1	49.88(3)
Cl(3)-Cd(1)-Cd(1)#2	50.18(3)
Cl(3)-Cd(1)-Cl(2)#1	97.24(4)
Cl(3)-Cd(1)-Cl(2)	83.70(5)
Cl(3)#1-Cd(1)-Cl(2)#1	82.67(5)
Cl(3)-Cd(1)-Cl(3)#1	178.24(7)
Cl(3)-Cd(1)-Cl(1)#2	83.33(5)
Cl(1)#2-Cd(1)-Cd(1)#2	49.27(3)
Cl(1)-Cd(1)-Cd(1)#1	50.16(4)
Cl(1)#2-Cd(1)-Cd(1)#1	131.23(3)
Cl(1)-Cd(1)-Cd(1)#2	129.33(4)
Cl(1)-Cd(1)-Cl(2)	176.95(6)
Cl(1)#2-Cd(1)-Cl(2)#1	177.80(6)
Cl(1)-Cd(1)-Cl(2)#1	82.69(4)
Cl(1)-Cd(1)-Cl(3)#1	83.77(5)
Cl(1)-Cd(1)-Cl(3)	94.47(4)
Cl(1)#2-Cd(1)-Cl(3)#1	96.83(5)
Cl(1)-Cd(1)-Cl(1)#2	99.39(6)
Cd(1)-Cl(2)-Cd(1)#2	79.29(4)
Cd(1)-Cl(3)-Cd(1)#2	79.94(2)
Cd(1)-Cl(1)-Cd(1)#1	80.56(4)
C(2)-N(1)-C(3)	109.1(3)
C(1)-N(1)-C(2)	110.8(3)
C(1)-N(1)-C(3)	105.8(4)
C(4)-N(1)-C(2)	108.7(4)
C(4)-N(1)-C(1)	113.2(3)
C(4)-N(1)-C(3)	109.2(4)
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Cl(4)-C(1)-H(1A)	109.3
Cl(4)-C(1)-H(1B)	109.3
N(1)-C(1)-Cl(4)	111.4(3)
N(1)-C(1)-H(1A)	109.3
N(1)-C(1)-H(1B)	109.3

H(1A)-C(1)-H(1B)	108.0
N(1)-C(4)-H(4A)	109.5
N(1)-C(4)-H(4B)	109.5
N(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(1)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
N(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5

Symmetry transformations used to generate equivalent atoms:

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