

Supporting Information for

(1,4-Butyldiammonium)CdBr₄: A Layered Organic-Inorganic Hybrid Perovskite with Visible-blind Ultraviolet Photoelectric Response

*Yuyin Wang,^{ab} Chengmin Ji,^a Xitao Liu,^a Shiguo Han,^a Jing Zhang,^a Zhihua Sun,^{*a} Asma Khan,^{ab} and Junhua Luo^{*,a}*

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P.R.China

^bUniversity of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100039, P.R. China

**To whom correspondence should be addressed. E-mail: sunzhihua@fjirsm.ac.cn;*

jhluo@fjirsm.ac.cn

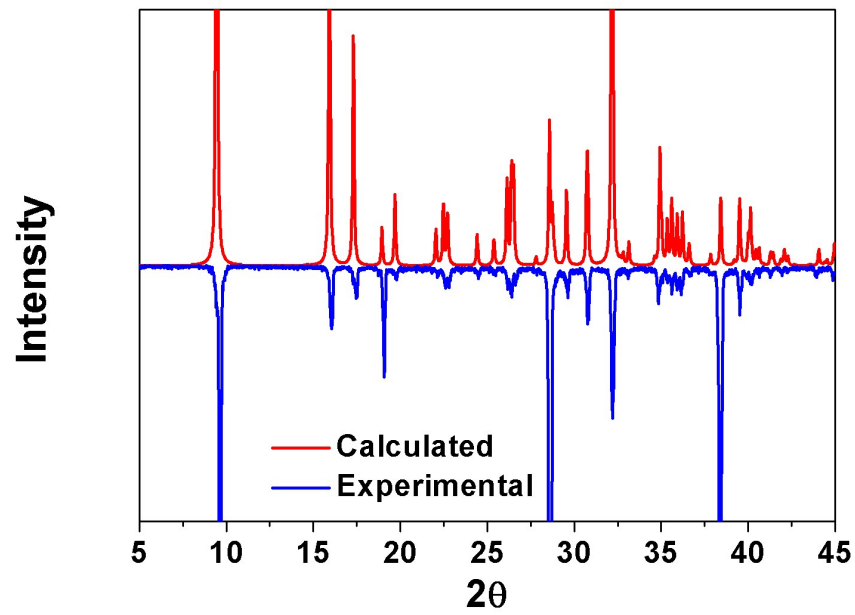


Figure S1. Powder X-ray Diffraction (PXRD) patterns of experimental data and the calculated data.

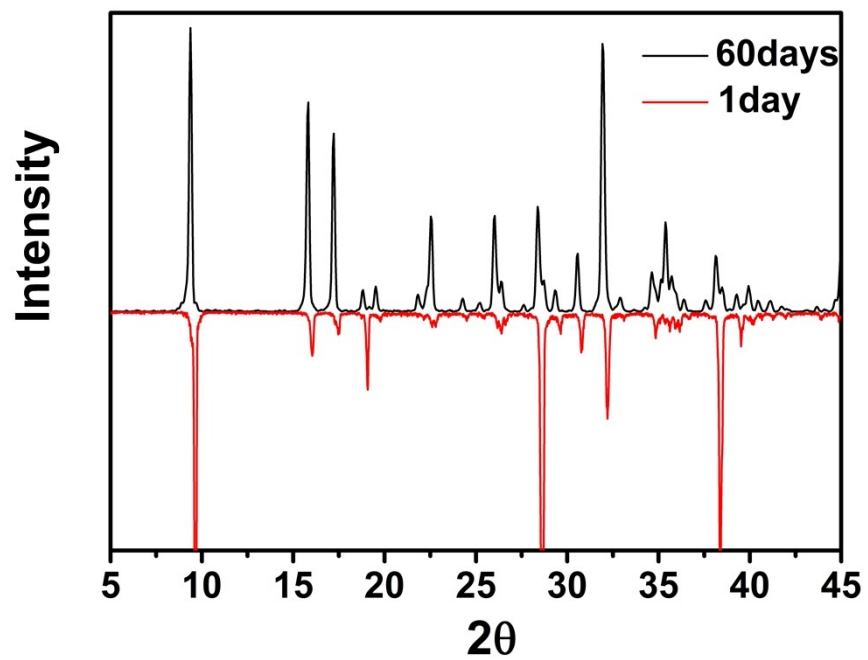


Figure S2. PXRD patterns of 1 recorded on the freshly - prepared sample (1 day) and after 60 days.

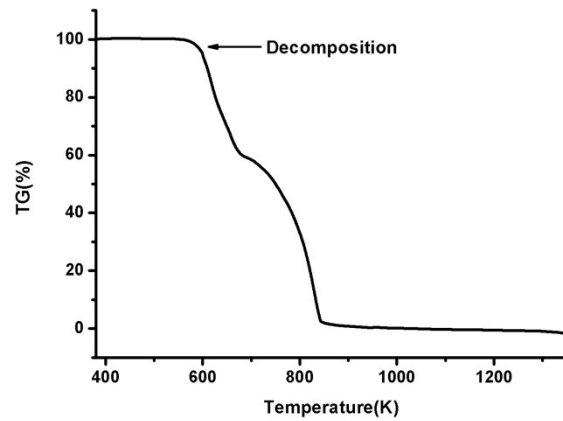


Figure S3. TG curves for **1**.

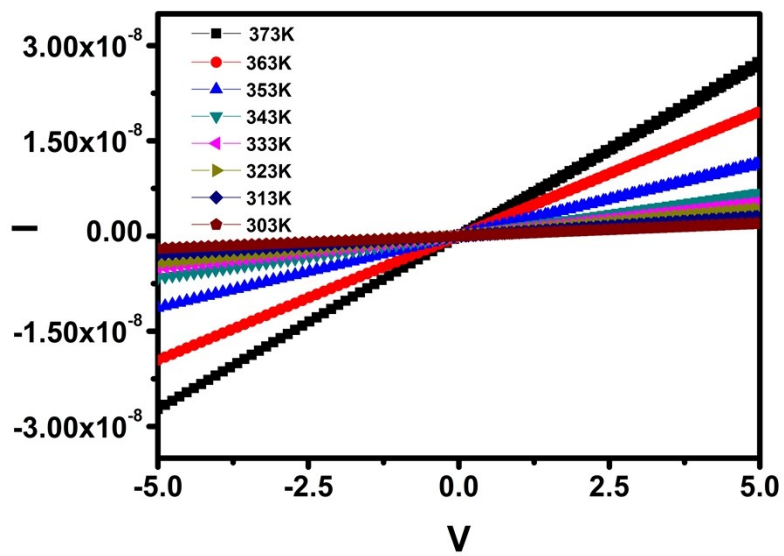


Figure S4. Temperature-dependent I-V curves of 1.

Table S1. Crystal Data and Structure Refinements for **1**

Temperature (K)	100
Formula	C ₄ H ₁₄ N ₂ CdBr ₄
Crystal system, Space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Cell parameters (Å)	<i>a</i> = 9.5648 (6); <i>b</i> = 7.9073 (4); <i>c</i> = 7.9960(5)
<i>V</i> (Å ³)	591.99(2)
<i>Z</i>	2
ρ_c (g/cm ³)	2.930
<i>F</i> (000)	480
Theta range (°)	3.9780- 29.1180
Limiting indices	-11 ≤ <i>h</i> ≤ 9, -9 ≤ <i>k</i> ≤ 9, -9 ≤ <i>l</i> ≤ 8
Reflections collected / unique	1192 / 1099 [<i>R</i> _{int} = 0.041]
Completeness	99.15%
GOF.	1.044
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0277, <i>wR</i> ₂ = 0.0632
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0308, <i>wR</i> ₂ = 0.0647

Table S2. Bond Lengths of compound **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cd1	Br2	2.6409 (5)	Cd1	Br3 ³	2.8543 (4)
Cd1	Br2 ¹	2.6409 (5)	Br3	Cd1 ⁴	2.8543 (4)
Cd1	Br3 ¹	2.8257 (4)			
Cd1	Br3	2.8257 (4)			
Cd1	Br3 ²	2.8543 (4)			

Table S3. Bond Angles of compound **1**.

Atom	Atom	Atom	Angle/	Atom	Atom	Atom	Angle/
Br2	Cd1	Br2 ¹	180.0	Br3	Cd1	Br3 ²	89.677 (5)
Br2	Cd1	Br3 ¹	90.152 (14)	Br2	Cd1	Br3 ³	87.964 (14)
Br2 ¹	Cd1	Br3 ¹	89.848 (14)	Br2 ¹	Cd1	Br3 ³	92.036 (14)
Br2	Cd1	Br3	89.848 (14)	Br3 ¹	Cd1	Br3 ³	89.676 (5)
Br2 ¹	Cd1	Br3	90.152 (14)	Br3	Cd1	Br3 ³	90.323 (5)
Br3 ¹	Cd1	Br3	180.0	Br3 ²	Cd1	Br3 ³	180.000 (12)
Br2	Cd1	Br3 ²	92.036 (14)	Cd1	Br3	Cd1 ⁴	163.714 (18)
Br2 ¹	Cd1	Br3 ²	87.964 (14)				
Br3 ¹	Cd1	Br3 ²	90.324 (5)				