

Large Spontaneous Polarization and Clear Hysteresis Loop of a Room Temperature Hybrid Ferroelectric Based on Mixed Halide [BiI₃Cl₂] Polar Chains and Methylviologen Dication.

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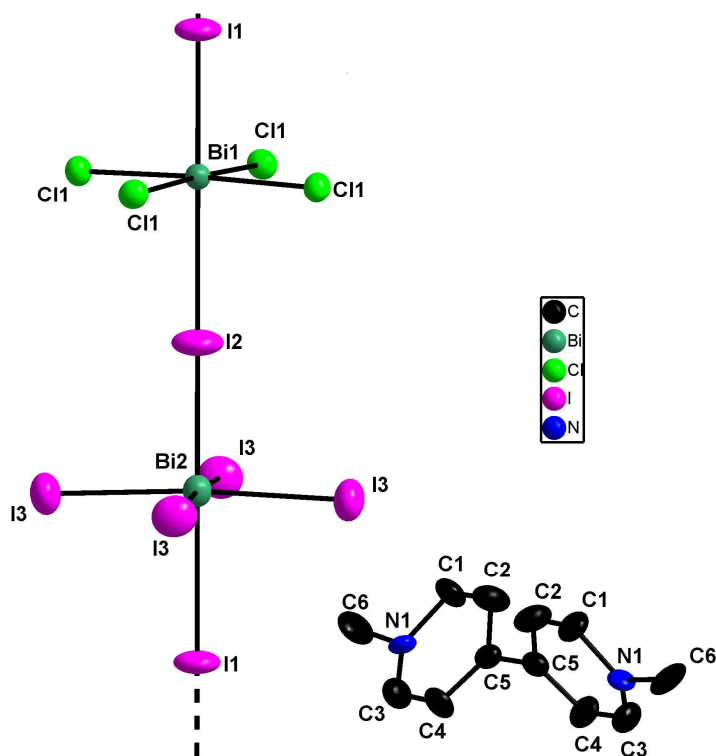
Supporting Information

I- X-ray single crystal study of (MV)[BiI₃Cl₂]

A- Summary of crystallographic data and structure refinement

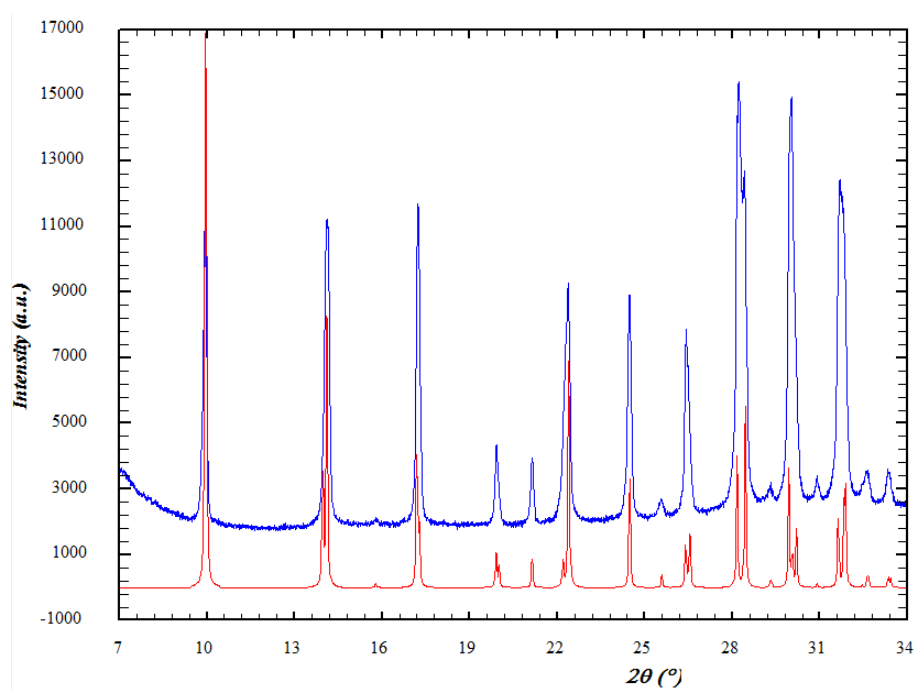
Empirical formula	C12 H14 Bi Cl2 I3 N2
Formula weight	846.83
Temperature	293(2) K
wavelength	0.71073 Å
Crystal system, space group	Tetragonal, P 4 n c
Unit cell dimensions	a = 12.5278(10) Å alpha = 90.00 deg. b = 12.5278(10) Å beta = 90.00 deg. c = 12.6511(7) Å gamma = 90.00 deg.
Volume	1985.5(3) Å ³
Z, Calculated density	4, 2.833 Mg/m ³
Absorption coefficient	13.806 mm ⁻¹
F(000)	1504
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	3.64 to 36.00 deg.
Limiting indices	-20<=h<=20, -17<=k<=20, -15<=l<=20
Reflections collected / unique	26088 / 4044 [R(int) = 0.0438]
Completeness to theta = 36.00	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.331 and 0.243
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4044 / 1 / 99
Goodness-of-fit on F ²	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0731
R indices (all data)	R1 = 0.0789, wR2 = 0.0840
Absolute structure parameter	0.464(8)
Largest diff. peak and hole	1.267 and -1.613 e.Å ⁻³

B- Thermal ellipsoid figure of the independent atoms in the structure of (MV)[BiI₃Cl₂]

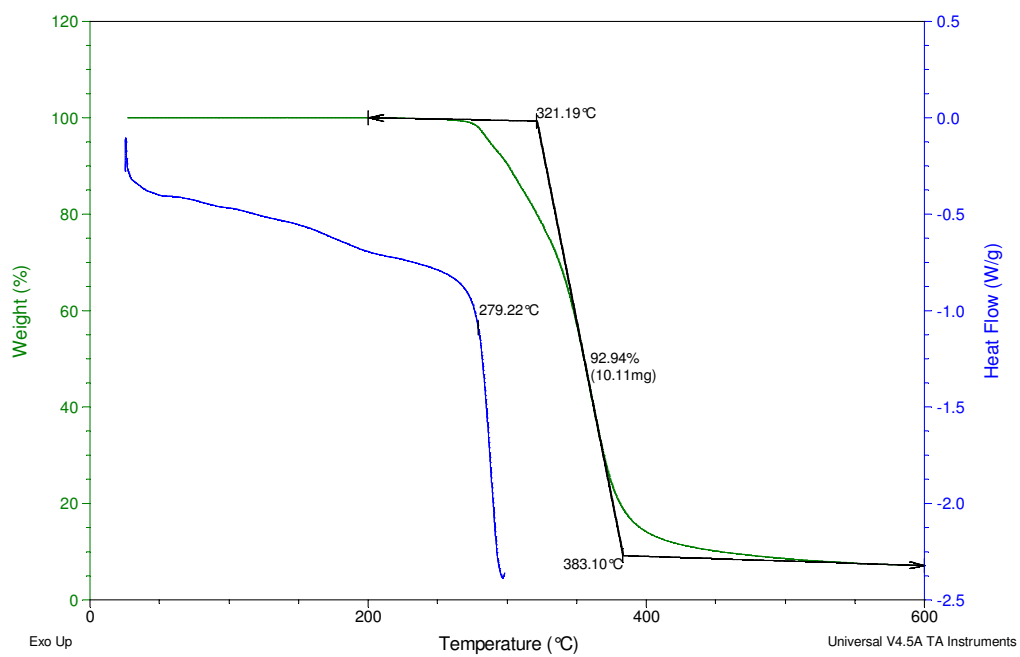


II- X-Ray Powder Diffraction pattern of (MV)[BiI₃Cl₂]

Theoretical (red) and experimental (blue)



III- TGA-DSC of (MV)[BiI₃Cl₂]



IV- UV-VIS spectra of (MV)[BiI₃Cl₂]

