

Piezoelectric and pyroelectric properties of organic MDABCO-NH₄Cl₃ Perovskite for Flexible Energy Harvesting

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SI1. DSC and TGA

In Figure S1, the measured differential scanning calorimetry (DSC) of synthesized MDABCO-NH₄Cl₃ perovskite crystals reveals that the ferroelectric-paraelectric phase transition occurs at 428 K, at a lower temperature than that found for MDABCO-NH₄I₃, which was 443 K. Also, the structural changes involved in the transition manifests themselves through two other peaks, one at 425 K and other at 438 K, while for MDABCO-NH₄I₃, there is a single peak with a 10 K width. Cooling down from 470 K, an exothermic peak at 369 K is observed, correspondent to the inverse phase transition accompanied by a hysteresis temperature of around 60 K. The DSC spectra supports the dielectric measurements, where two side bands were also observed during the measurements of the dielectric permittivity as a function of temperature. Thermogravimetric analysis (TGA), Figure S2, demonstrates that the crystals remain stable up to 473 K, confirming that the phenomena observed in the DSC are related to changes in the structural properties of the perovskite crystals at the ferroelectric-paraelectric transition and not to any mass losses. Degradation begins beyond 473 K, marked by subtle peaks at 559 K and 588 K, eventually progressing to complete degradation at 623 K.

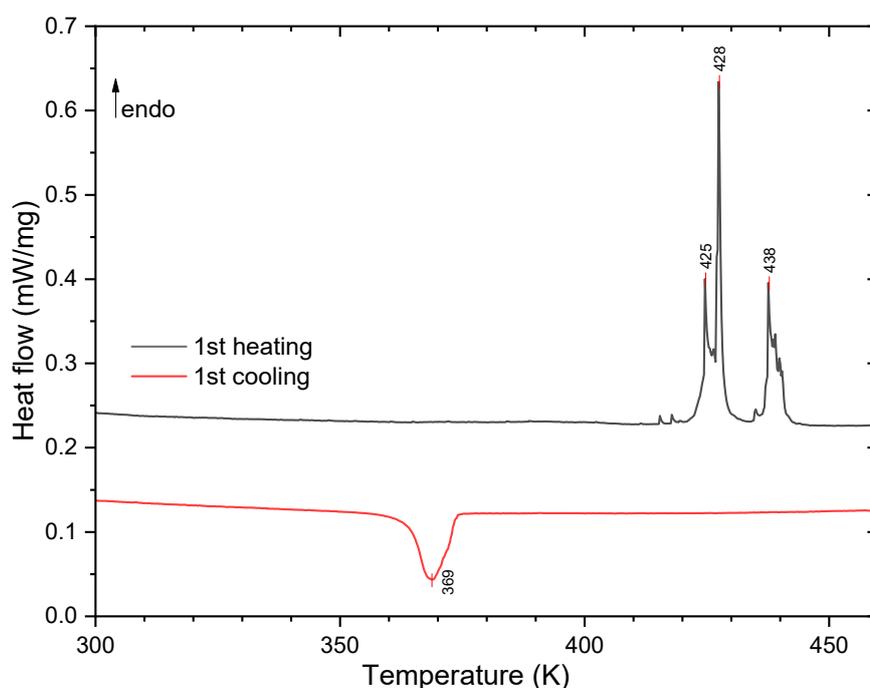


Figure S1. DSC spectrum of MDABCO-NH₄Cl₃ crystals.

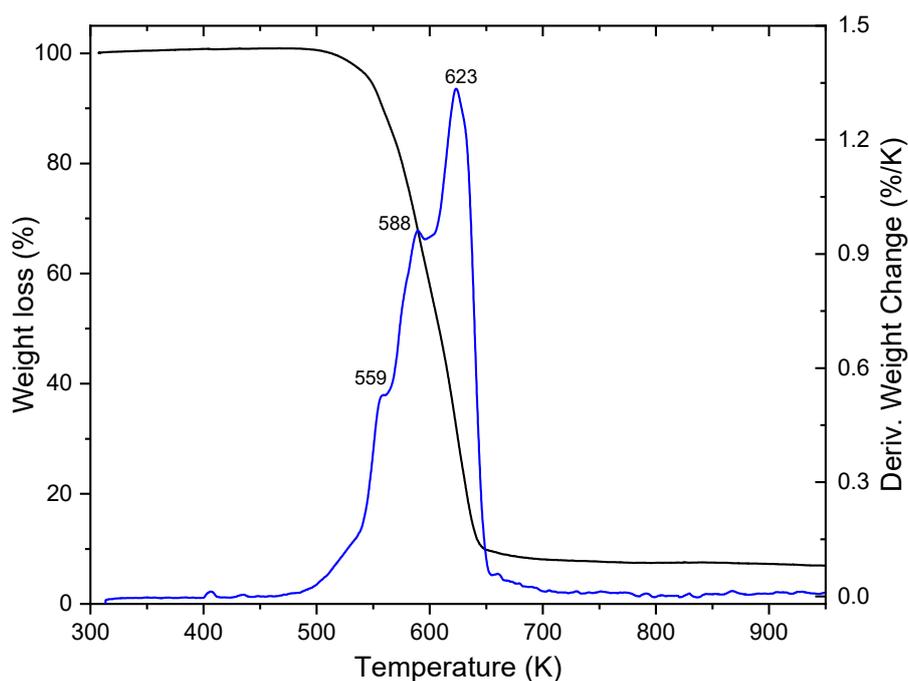


Figure S2. TGA spectrum of MDABCO-NH₄Cl₃ crystals.

SI 2. XRray powder diffraction

Analysis of the X-ray diffraction (XRD) powder diffraction spectra reveals that the MDABCO-NH₄Cl₃ perovskite has a similar powder spectra (similar Bragg peak positions) to that of the previously published MDABCO-NH₄I₃ perovskite and therefore must have a similar crystal structure [26]. Variations in the intensity of certain peaks are observed as a result of the presence of Chlorine (Cl) instead of Iodine (I) atoms, as shown in Figure S3.

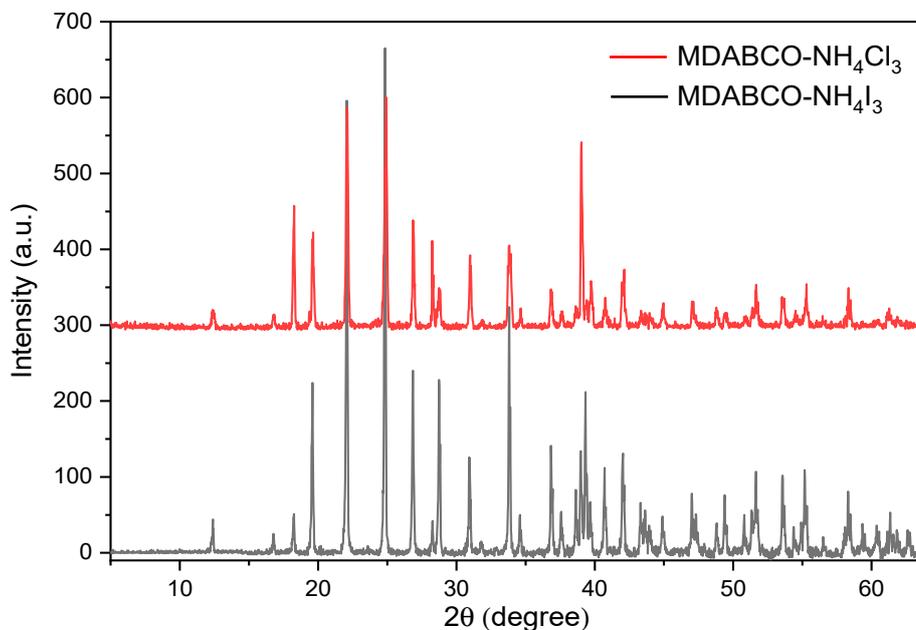


Figure S3. XRD spectrum of MDABCO-NH₄Cl₃ crystal powder.

SI 3. FTIR-ATR

Figure S4 displays the FTIR-ATR spectrum between 3500-600 cm^{-1} for a polycrystalline sample of MDABCO- NH_4Cl_3 and MDABCO- NH_4I_3 perovskites. The spectrum exhibits similar bands, and the most intense and broad band shows a sharp peak at 2991 cm^{-1} . This band can be attributed to hydrogen bonds between the N atom of NH_4^+ group and H and Cl^- or I^- ions. The intense and sharp band at 1382 cm^{-1} is a typical region where vibrations associated with N-H bonds and angular deformations in ammonium ions (NH_4^+) can occur. Other intense bands appear at 1454 cm^{-1} , 1047 cm^{-1} , and 845 cm^{-1} in both spectra, confirming the structural similarities between both perovskites.

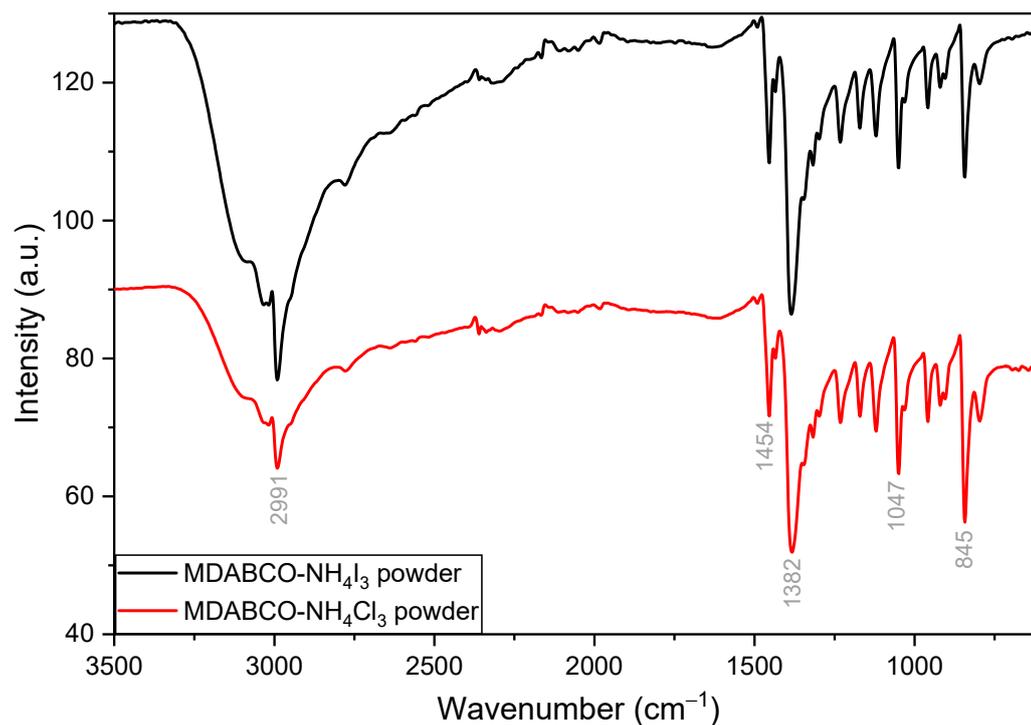


Figure S4. FTIR-ATR spectrum of MDABCO- NH_4Cl_3 and MDABCO- NH_4I_3 crystal powders.