

# Structure and phase transition of ferroelectric quinuclidinium copper(II) bromide

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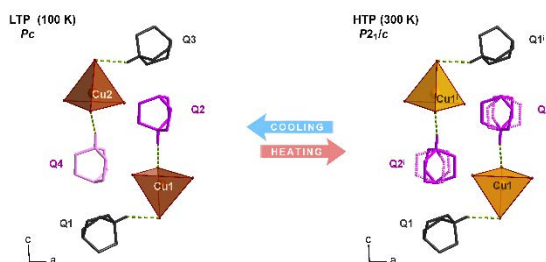
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Hybrid organic-inorganic compounds (HOICs) are of increasing interest due to their multifunctional properties arising from the synergy between organic cations and inorganic frameworks. Among these, quinuclidinium-based metal halides have shown promising applications in dielectric switching, ferroelectricity, and optoelectronics [1-3]. Particularly, their phase transitions are often associated with dynamic reorientations of the organic cations and reorganization of the hydrogen-bonding (HB) network, affecting the material's electric and optical behaviour.

Recent studies have demonstrated that quinuclidine-like molecules, such as dabco [4], are effective in designing switchable dielectric and ferroelectric materials due to their ability to undergo reversible structural phase transitions. In the high-temperature phase (HTP), these materials typically exhibit a high-dielectric "ON" state, linked to the dynamic reorientation of dipolar cations. Upon cooling, the transition to the low-temperature phase (LTP) freezes this motion, resulting in a low-dielectric "OFF" state.

Here, we report on a newly synthesized compound,  $(C_7H_{14}N)_2CuBr_4$  ( $Q_2CuBr_4$ ), where the inorganic component is copper(II) bromide [5]. This compound was expected to show distinct phase behavior based on analogies with previously studied Mn, Co, and Cd analogs [3]. A combination of thermal (DSC), structural (X-ray diffraction), and spectroscopic (IR, Raman) techniques was used to characterize the phase transition and its effects. Our results reveal temperature-induced structural changes involving ordering of the quinuclidinium (Q) cation and rearrangement of the HB network, which is strongly tied to the material's dielectric response. Fig. 1 illustrates the structural differences between the two phases, highlighting cation ordering.

These findings contribute to the broader understanding of structure–property relationships in HOICs and underscore the potential of  $Q_2CuBr_4$  as a candidate for switchable dielectric applications.



**Figure 1.** Fragment of  $Q_2CuBr_4$  structure viewed along the  $b$ -axis, showing Q cation ordering across the phase transition. The Q ions are presented in two different colors to differentiate two positions. The disordered cations are presented with dotted pink lines. For clarity, C—H hydrogen atoms are omitted. N—H $\cdots$ Br hydrogen bonds are marked with green dashed lines.

- [1] Wojcik, N. A., Kowalska, D. A., Trzebiatowska, M., Jach, E., Ostrowski, A., Bednarski, W., Gusowski, M., Staniorowski, P. & Ciżman, A. (2021). *J. Phys. Chem. C* **125**, 16810-16818.
- [2] Jach, E., Kowalska, D. A., Gusowski, M. A., Trzebiatowska, M., Krupinski, M., Medycki, W., Jędryka, J., Staniorowski, P. & Ciżman, A. (2023). *J. Phys. Chem. C* **127** (5), 2589-2602.
- [3] Jach, E., Kowalska, D. A., Trzebiatowska, M., Medycki, W., Ostrowski, A., Bednarski, W., Gusowski, M., Staniorowski, P., Bartoszewicz, A., Diu, U. & Ciżman, A. (2025). *Inorg. Chem.* **64**, 7422-7436.
- [4] Ciżman, A., Kowalska, D. A., Trzebiatowska, M., Medycki, W., Krupiński, M., Staniorowski, P. & Poprawski, R. (2020) *Dalton Trans.* **49**, 10394-10401.
- [5] Ciżman, A., Kowalska, D. A., Szarek, P., Medycki, W., Wójcik, N. A., Gusowski, M., Trzebiatowska, M., Bartosiewicz, A., Filevskaya, L., Staniorowski, P. & Jach, E. (submitted 2025).