

Switchable dielectric constant, structural and vibrational studies of double perovskite organic–inorganic hybrids: (azetidinium)₂[KCr(CN)₆] and (azetidinium)₂[KFe(CN)₆].

Autorzy

Magdalena Rok

Marcin Moskwa

Joanna Hetmańczyk

Łukasz Hetmańczyk

Grażyna Bator

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Artykuł

We have synthesized and characterized two novel organic–inorganic hybrid crystals: $(C_3H_8N)_2[KCr(CN)_6]$ (**AZECr**) and $(C_3H_8N)_2[KFe(CN)_6]$ (**AZEFFe**). Thermal DSC, TG and DT analyses indicate that each compound undergoes one structural phase transition (PT). **AZECr** and **AZEFFe** undergo a structural phase transition each upon cooling at 171 and 186 K, respectively. The crystal structures are refined for **AZECr-high-temperature**, **AZECr-low-temperature**, and **AZEFFe-high-temperature** at 210 K, 120, and 240 K, respectively. **AZECr** and **AZEFFe** are isomorphous at the high-temperature (HT) phase and are characterized by a three-dimensional framework consisting of $[X_4K_4(CN)_{12}]$ (where X are Cr^{III} or Fe^{III}) cages formed by X–CN–K fragments, which are filled by guest azetidinium (AZE⁺) cations. The crystal system changes during the PT in **AZECr** from the HT phase to the low-temperature (LT) phase, as shown at 120 K, where the crystal adopts the $P2_1/c$ monoclinic space group. The AZE⁺ cations and the CN[−] bridges, which were highly disordered in the HT phase, are fully ordered in the LT one. **AZEFFe-LT** diffraction data reveal extensive twinning of the crystal, and, unfortunately, our attempts to solve the structure of the crystal were unsuccessful. To compare and obtain insight into the mechanisms of PTs in these crystals, we measured the infrared (IR) spectra in a wide wavenumber range from middle IR (MIR) to far IR (FIR). IR measurements fully confirm that both samples are isomorphous at the HT phase. However, in the LT phase, the spectra are different, which means that the LT phases are not identical and may suggest that **AZECr-LT** and **AZEFFe-LT** are not isomorphous. Additionally, to confirm the change in dynamical states of molecules in PT, dielectric measurements were carried out between 150 and 300 K in the frequency range of 25 Hz to 2 MHz. It was shown that the permittivity value can be switched between two states: ON (a high ϵ' value, HT) and OFF (a low ϵ' value, LT).

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