Structural phase transitions coupled with prominent dielectric anomalies and dielectric relaxation in $[(CH_3)_3NH]_2[KCo(CN)_6]$ and mixed $[(CH_3)_3NH]_2[KFe_xCo_{1-x}(CN)_6]$ double perovskite hybrids.

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Streszczenie

The crystals of pure $[(CH_3)_3NH]_2[KFe(CN)_6]$ (**TrMAFe**) and $[(CH_3)_3NH]_2[KCo(CN)_6]$ (**TrMACo**) as well as their mixed crystals (**TrMAFe$_x$Co$_{1-x}$**), with different ratios of $x = 0$, 0.12, 0.18, 0.49, 0.56, 0.73, 0.81, 1.0, have been grown from aqueous solutions. The structure of **TrMACo** has been determined at 360 K to be cubic (*Fmm*). In phase II (100 K), the **TrMACo** crystal is monoclinic (*C*2/*c*). The thermal stability of the pure and mixed crystals has been determined by using both DTA and TGA. Based on the DSC results, we have found a single phase transition (PT) for both pure and mixed crystals. The Fe(III) concentration was estimated by using the SEM technique. We have found a linear relationship between the PT temperature (T_c) and the molar concentration of Fe(III). Based on the obtained results, a phase diagram has been constructed. The mechanism of the structural PT has been discussed based on the results of dielectric relaxation and ^{1}H NMR and X-ray spectroscopy measurements. The results confirmed that the PT mechanism of both pure and mixed crystals is related to the change in the dynamic state of the $TrMA^+$ cations. The dielectric activation energy changes linearly with the mole fraction ranking from 35 to 38 kJ mol^{-1}, for the mixed crystals.

Adres publiczny

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