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Screening ferroelastic transitions in switchable cyano-bridged perovskites: $[CH_3C(NH_2)_2]_2[KM(CN)_6]$, M = Cr^{3+}, Fe^{3+}, Co^{3+} : crystal structure characterization, dielectric properties, ^1H NMR, and quasielastic neutron scattering studies

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Streszczenie

Here we report the dynamics of organic cations as guest molecules in the novel perovskite host framework. The novel switchable crystals from the coordination family [CH3C(NH2)2]2[KB″(CN)6] were constructed by employing acetamidinium cations (ACE = [CH3C(NH2)2]) as A-site and B″: Cr3+, Fe3+, Co3+ in the inorganic cage. The molecular motion of ACE+ as well as the effect of the trivalent metallic cation type on two-step transitions were studied using a combination of experimental methods: (i) X-ray diffraction experiments, (ii) thermal analysis, (iii) dielectric and electric studies, (iv) optical observations, (v) 1 H NMR spectroscopy, and (vi) quasielastic neutron scattering (QENS). On the basis of the X-ray analysis, transitions occur from a frozen-order phase (III, monoclinic, C2/m) to an in-plane rotational disorder state (II, trigonal, R$\bar{3}$m) and to a melt-like disorder one (I, cubic, Fm$\bar{3}$m). A markedly temperature-dependent dielectric constant indicates the tunable and switchable properties of all complexes. The QENS, as well as 1 H NMR spectroscopy, were applied to measure the dynamics of the organic cations residing in the inorganic framework. The ferroelastic nature of the phases III and II were proven based on the polarized light microscopy photographs. Also, the modified equation of the tolerance factor t was used to estimate the theoretical phase transition temperatures for a crystal with Mn3+.

Adres publiczny

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