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Crystal structures and phase transitions of inorganic-organic hybrid layered materials (C6H5CH2CH2NH3)2MCl4 (M = Cu2+ and Mn2+)

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Because of the combination of the hydrogen bonds between halogen atoms in an inorganic part and nitrogen atoms in an organic part, a layered inorganic-organic hybrid perovskite (C6H5CH2CH2NH3)2MeCl4 (Me = Cu2+, Mn2+, Fe2+) shows a various crystal structures [1, 2, 3]. To understand an interlayer spacing effect on a magnetic property, various systems have been developed. All three Cu-, Mn- and Fe-compounds crystallized in the same orthorhombic space group (Pbca, No. 61) at room temperature (a = 7.207Å, b = 7.301Å, c = 39.413Å for Mn-compound, a = 7.302Å, b = 7.327Å, c = 38.635Å for Cu-compound, and a = 7.171Å, b = 7.279Å, c = 39.106Å for Fe-compound, respectively). However, in the recent study [1], it is reported that Cu-compound should be ferroelectric, although the inversion center in the point group mmm prevents the spontaneous polarization. In addition, it is also claimed that Mn-compound should have an additional phase transition at 100K and below 100K the point group of Mn-compound is mm2 (Pbc21), where the ferroelectric property is allowed [4]. But from our own investigations on Mn- and Cu-compounds [2, 5] and also a recent study on Fe-compound [3] strongly suggest that Cu-, Mn- and Fe-compounds are not ferroelectric at room temperature but ferroelastic. In this study, we will show crystal structures of Mn- and Cu-compounds not only from neutron single crystal diffraction techniques but also other methods including temperature dependent X-ray powder diffraction results and domain structures under polarized microscope.

Reference
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