Organic-inorganic hybrid crystals, $(2,4,6\text{-}CH_3PyH)_3Sb_2Cl_9$ and $(2,4,6\text{-}CH_3PyH)_3Bi_2Cl_9$. Crystal structure characterization and tunneling of CH_3 groups studied by ^{1}H NMR and neutron spectroscopy.

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The crystal structures of $(2,4,6\text{-}CH_3PyH)_3Sb_2Cl_9$ (TMPCA) and $(2,4,6\text{-}CH_3PyH)_3Bi_2Cl_9$(TMPCB) (Py – pyridine) have been determined at 100K by the single crystal X-ray diffraction method. TMPCA and TMPCB crystallize in the monoclinic *C2/c* and triclinic *P*1 polar space group, respectively. In both cases the asymmetric part is comprised of three nonequivalent 2,4,6-trimethylpyridinium cations and a discrete $M_2Cl_9{}^{3-}$ anion. The $Bi_2Cl_9{}^{3-}$moiety forms a face-sharing bi-octahedron, whereas in a case of $Sb_2Cl_9{}^{3-}$ we deal with two pyramids connected by a corner. The inelastic neutron scattering spectra (INS) were recorded for TMPCA at low temperatures (4–50K). Two peaks on each side of the central elastic line have been observed at *ca.* 4.8 and 2.9μeV, the high energy peak exhibits an excitation energy value equal to *ca.* 6meV. For TMPCA and TMPCB the ^{1}H NMR spin–lattice relaxation times, T_1, have been measured in the temperature region 15–410K. The flattening of the T_1 (spin–lattice) *vs.* reciprocal temperature, $1/T$, dependence between 30K and 15K indicates the incoherent tunneling effect of the methyl group being treated as the quantum rotor. The conclusions drawn from the ^{1}H NMR results as regards to the tunneling of the CH_3 groups in the pyridinium cations are consistent with the tunneling peaks observed in the INS spectra.

Słowa kluczowe

Haloantimonates(III), Halobismuthates(III), Inelastic neutron scattering, atom, CH3 tunneling

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