Poster 12

Charge Distribution Change in Nb_2PS_{10} due to Incorporation of K: Solid State ^{31}P NMR Study

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^{31}P isotropic chemical shift (δ_i) and chemical shift anisotropy ($\Delta\delta$) of KNb_2PS_{10} are, respectively, smaller and wider than those of Nb_2PS_{10}: these results are explained based on the shorter average P-S bond length and the bigger average $\angle$S-P-S deviation from 109.5° of KNb_2PS_{10} than those of Nb_2PS_{10}, respectively. The smaller δ_i value indicates higher electron density in π orbitals of P in the P-S bonds if the known semiempirical relationship between δ_i, P-O bond length, and the number of electrons in π orbitals of P in P-O bond for orthophosphate similarly holds for PS_4 units. Thus, solid state ^{31}P magic angle spinning (MAS) nuclear magnetic resonance (NMR) data of metal thiophosphates, Nb_2PS_{10} and KNb_2PS_{10} indicate that presence of potassium results in increase of electron density at phosphorous sites.