

Proton dynamics at low and high temperatures in a novel ferroelectric diammonium hypodiphosphate  $(\text{NH}_4)_2\text{H}_2\text{P}_2\text{O}_6$  (ADhP) as studied by  $^1\text{H}$  spin-lattice relaxation time and second moment of NMR line.

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Streszczenie

Proton spin–lattice relaxation times  $T_1$  at 24.7 MHz and 15 MHz and second moment of NMR line have been applied to study molecular dynamics of a novel ferroelectric  $(\text{NH}_4)_2\text{H}_2\text{P}_2\text{O}_6$  ( $T_c = 178$  K) in the temperature range 10–290 K. Low-temperature  $T_1$  behaviour below  $T_c$  is interpreted in terms of Haupt's theory and Schrödinger correlation time of tunnelling jumps. A shallow  $T_1$  minimum observed around 39 K is attributed to the  $C_3$  classical motion of “intra” proton–proton vectors of  $\text{NH}_3$  (ammonium groups may perform stochastic jumps about any of the four  $C_3$  symmetry axes). The tunnelling splitting of the ground state vibrational level,  $(\nu_T)_{\nu_0}$ , of the same frequency for both ammonium groups was estimated as high as 900 MHz. This tunnelling splitting exists only in the ferroelectric phase. Magnetisation recovery is found to be non-exponential in the temperature regime 63–48 K. The temperature of 63 K is the discovered  $T^{tun}$  above which the probability of stochastic tunnelling jumps equals zero. The  $T_1$  relaxation time is temperature independent below 25 K, which is related to a constant value of the correlation time characterising tunnelling jumps according to Schrödinger. The  $T_1$  minima observed in the paraelectric phase (204 K at 15 MHz and 213 K at 24.7 MHz) as well as second moment reduction at about 130 K are attributed to isotropic motion of all protons.

Słowa kluczowe

Solit state, Paraelectric and ferroelectric phases, Internal dynamics, Proton spin–lattice relaxation time, Proton second moment of NMR line, Complex motion, Schrödinger equation, Tunnelling splitting, Tunnelling jump

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