Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Complex molecular dynamics of $(CH_3NH_3)_5Bi_2Br_{11}$ (MAPBB) protons from NMR relaxation and second moment of NMR spectrum.

Autorzy

L. Latanowicz

Wojciech Medycki

Ryszard Jakubas

Rok wydania

2011

Czasopismo

Journal of Magnetic Resonance

Numer woluminu

211

Strony

207-216

DOI

10.1016/j.jmr.2011.05.016

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Molecular dynamics of a polycrystalline sample of (CH(3)NH(3))(5)Bi(2)Br(11) (MAPBB) is studied on the basis of the proton T(1) (55.2 MHz) relaxation time and the proton second moment of NMR line. The T(1) (55.2 MHz) was measured for temperatures from 20K to 330 K, while the second moment M(2) for those from 40K to 330 K. The proton spin pairs of the methyl and ammonium groups perform a complex stochastic motion being a resultant of four components characterised by the correlation times τ(3)(T), τ(3)(H), τ(2), and τ(iso), referring to the tunnelling and over the barrier jumps in a triple potential, jumps between two equilibrium sites and isotropic rotation. The theoretical expressions for the spectral densities in the cases of the complex motion considered were derived. For τ(3)(H), τ(2), and τ(iso) the Arrhenius temperature dependence was assumed, while for τ(3)(T)-the Schrödinger one. The correlation times τ(3)(H) for CH(3) and NH(3) groups differ, which indicates the uncorrelated motion of these groups. The stochastic tunnelling jumps are not present above the temperature T(tun) at which the thermal energy is higher than the activation energy of jumps over the barrier attributed to the hindered rotation of the CH(3) and NH(3) groups. The T(tun) temperature is 54.6 K for NH(3) group and 46.5 K for CH(3) group in MAPBB crystal. The tunnelling jumps of the methyl and ammonium protons are responsible for the flattening of T(1) temperature dependence at low temperatures. The isotropic tumbling is detectable only from the M(2) temperature dependence. The isotropic tumbling reduces the second moment to 4 G(2) which is the value of the intermolecular part of the second moment. The motion characterised by the correlation time τ(2) is well detectable from both T(1) and M(2) temperature dependences. This motion causes the appearance of T(1) minimum at 130 K and reduction of the second moment to the 7.7 G(2) value. The small tunnelling splitting ω(T) of the same value for the methyl and ammonium groups was estimated as 226 MHz from the Haupt equation or 80 MHz from the corrected by us Haupt equation. These frequencies correspond to 0.93 μeV and 0.34 μeV tunnel splitting energy.

Słowa kluczowe

molecular dynamics, Proton spin–lattice relaxation time, Proton second moment of the NMR line, Spectral densities, Complex motion, Schrödinger equation

Adres publiczny

http://dx.doi.org/10.1016/j.jmr.2011.05.016

Plik został wygenerowany dnia 2026-11-09 18:28:54

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/JTZdpL-.