

## The effect of low-temperature dynamics of the dimethylammonium group in $[(\text{CH}_3)_2\text{NH}_2]_3\text{Sb}_2\text{Cl}_9$ on proton spin-lattice relaxation and narrowing of the proton NMR.

### Autorzy

L. Latanowicz

Wojciech Medycki

Ryszard Jakubas

### Rok wydania

2005

### Czasopismo

Journal of Physical Chemistry  
A

### Numer woluminu

109

### Strony

3097-3104

### DOI

10.1021/jp045080y

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

This paper reports the temperature dependence of the relaxation time  $T_1$  (55.2 and 90 MHz) and the second moment of the NMR line for protons in a polycrystalline sample of  $[\text{NH}_2(\text{CH}_3)_2]_3\text{Sb}_2\text{Cl}_9$  (DMACA). The fundamental aspects of molecular dynamics from quantum tunneling at low temperatures to thermally activated reorientation at elevated temperatures have been studied. The experimentally observed spin-lattice relaxation rate is a consequence of dipolar interactions between the spin pairs inside the methyl group ( $1/T_{1AE}$  contribution) as well as the spins belonging to neighboring methyl groups and pairs, methyl spin-outer methyl spin ( $1/T_{1EE}$  contribution). These contributions are considered separately. Two methyl groups in the dimethylammonium (DMA) cations are dynamically inequivalent. The values of the tunnel splitting of separate methyl groups are obtained from the  $T_1$  (55.2 MHz) experiment. The tunneling dynamics taking place below the characteristic temperatures 74 and 42 K for separate methyl groups are discussed in terms of the Schrödinger equation. These temperatures point to the one at which thermal energy  $C_p T$  and potential barrier take the same value. It is established that the second moment of the proton NMR line below 74 K up to liquid helium temperature is much lower than the rigid lattice value, which is due to a tunneling stochastic process of the methyl groups.

### Adres publiczny

<https://doi.org/10.1021/jp045080y>

### Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>