Motions of Ethylammonium Ions in Solid Ethylammonium Chloranilate Studied by $^1$H Nuclear Magnetic Resonance

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The motions of the ethylammonium ion in solid ethylammonium chloranilate, $\text{C}_2\text{H}_5\text{NH}_3^+ \cdot \text{C}_6\text{H}_5\text{O}_4\text{Cl}_2^-$, are studied by $^1$H NMR second moment ($M_2$) and spin-lattice relaxation time ($T_1$) measurements. Reorientations of the CH$_3$ group about the C–C bond axis and the NH$_3^+$ group about C–N bond axis were observed and their motional parameters were evaluated. The internal rotational barriers of the CH$_3$ and NH$_3^+$ groups of an isolated C$_2$H$_5$NH$_3^+$ ion were estimated from ab initio molecular orbital calculations.

Key words: Nuclear Magnetic Resonance; Molecular Motion; Ethylammonium Ion; HF.