

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

Hiroyuki Ishida, Naoki Kumagae, and Setsuko Sato^a

Department of Chemistry, Faculty of Science, Okayama University, Okayama 700-8530, Japan

^a Department of Chemistry, Faculty of Education, Gifu University, Gifu 501-1193, Japan

Reprint requests to Dr. H. I.; Fax +81-86-251-8497; E-mail: ishidah@cc.okayama-u.ac.jp

Z. Naturforsch. **56a**, 523–526 (2001); received April 30, 2001

The motions of the ethylammonium ion in solid ethylammonium chloranilate, $\text{C}_2\text{H}_5\text{NH}_3^+ \cdot \text{C}_6\text{HO}_4\text{Cl}_2^-$, are studied by ^1H 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 $\text{C}_2\text{H}_5\text{NH}_3^+$ ion were estimated from *ab initio* molecular orbital calculations.

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