

Molecular Motion and Crystal Structure of Solid Tetrapentylammonium Iodide

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The proton NMR spectra and spin-lattice relaxation times of tetrapentylammonium iodide have been measured between 100 K and the melting point. The room temperature crystal structure has been determined by X-ray diffraction as orthorhombic, space group $Ccca$, $Z = 4$ with $a = 10.811(2)$, $b = 22.771(5)$ and $c = 9.500(2)$ Å with fully ordered tetrapentylammonium cations. The existence of a solid-solid phase transition at 400 K has been confirmed by DTA. The onset of G_3 methyl group reorientations characterized by Arrhenius activation parameters has been evidenced. The intracation conformational motions in the pentyl chains start to manifest themselves already at lower temperatures. The appearance of an ionic plastic phase with coexisting liquid-like and solid-like cations has been discovered.

Key words: Nuclear Magnetic Resonance; Crystal Structure.