Synthesis and Characterization of a New Ionic Liquid TMAFDOZ with New Method

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Room temperature ionic liquids, RTIL, (or “molten salts”) have generated considerable excitement in recent years as a new type of solvent media that possesses minimal vapor pressure. Ionic liquids, are liquids composed entirely of cations and anions within a wide temperature range (including room temperature). Tetramethylammonium fluoride, [NR₄]⁺[ZrO₂F]⁻, were prepared by dissolving powdered tetramethylammonium fluoride in MeCN and to this solution, a stoichiometric amount of ZrO₂ were added with stirring, maintaining the ratio of (R₄)NF: ZrO₂ as 1:1. This solution under stirring at room temperature until product was formed. After 7h stirring, the mixture was filtered. The product was washed with hexane and dried under vacuum for 1 h. The resulting salt is a light oily liquid. The reaction between and ZrO₂ produced a new ionic Liquid with tetramethylammonium cation. It is tetramethylammonium fluorodioxozirconate (IV), (CH₃)₄N[ZrO₂F], TMAFDOZ, that is easily synthesized in a nearly quantitative yield using a direct reaction of ZrO₂ and tetramethylammonium fluoride[1–5].

Synthesis of [R₄N]⁺[ZrO₂F]⁻ General method:

(CH₃)₄NF +ZrO₂ → (CH₃)₄N[ZrO₂F]

This compound was characterized by IR, UV/Visible, ¹⁹F-NMR, ¹³C-NMR and ¹H-NMR techniques. The electronic and vibrational spectra of TMAFDOZ has been measured and studied.

As thought, to discover a new ionic liquid is relatively easy, but to determine its usefulness as a solvent requires a much more substantial investment in determination of physical and chemical properties. The best trick would be a method for predicting an ionic liquid composition with a specified set of properties. That is an important goal that awaits a better fundamental understanding of structure–property relationships and the development of better computational tools.

REFERENCES: