A106 Hydrophobic and Hydrophilic Ionic Liquid Mixtures Used for Explosive Analytes

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After attending this presentation, attendees will have a general understanding of the potential applications afforded by mixtures of hydrophobic and hydrophilic ionic liquids, specifically their contributions to improved rate, specificity, and yield with forensic sampling of explosive analytes.

This presentation will impact the forensic science community by leading to the identification of homogenous ionic liquid mixtures that are able to collect a wide range of analytes of drugs and explosives, which is important to the forensic and chemical investigative community in ensuring relative ease and quickness when collecting field evidence.

Within the last decade, ionic liquids have become an increasingly popular topic within all disciplines of science because their unique physical and chemical properties have sparked interest in potential applications and innovative developments. Ionic liquids (ILs) are low-melting salts in their liquid state which are completely comprised of cations and anions. The development of room-temperature ILs in the early 1990s by chemists Wilkes and Zaworotko opened up a gateway toward more specified properties and functional possibilities, most notably advantages such as negligible vapor pressure, extreme thermal stability, customizable tailorability, and recyclability.[1] Especially with today's push for the Green Chemistry movement, it has become a higher priority to reduce or even eliminate the use of hazardous substances within chemical processes. Therefore the utilization of ionic liquids as a replacement for common solvents has been the focus of much research in recent years.[2,3] Depending on the specific ionic liquid, characteristics can range according to hydrophobicity, hydrophilicity, visoscity, conductivity, solubility, and electrochemical window.[3] With over 1,000 ionic liquids reported in literature today, there may be about 10^{18} possible cation/anion combinations—the properties and application possibilities are endless. The purpose of this study is to create homogenous ionic liquid mixtures consisting of a hydrophobic and hydrophilic component in an effort to maximize the range of analytes to be collected, retained, and analyzed quantitatively and qualitatively.

In investigative laboratories, specifically those pertaining to forensic sampling, it is in one's best interest to identify an optimum solvent for a group of compounds, i.e., one solvent for drugs and another for explosives; however, when examiners are working within the field, they are not able to distinguish one from another. For example, if an investigator comes across an unknown white powder, he is unable to tell whether it is cocaine, Triactetone Triperoxide (TATP), or simply powdered sugar. By using an essentially universal solvent, not only will the field agents reduce the amount of items they must carry onto the field, but they also minimize the risk of destroying the sample by using the wrong solvent and, due to the negligible vapor pressure, preserve the sample for analysis.

The approach of this study included tests for homogenous mixtures, solubility tests with four different explosives (TNT, Compound B, RDX, and PETN), which were then analyzed via Direct Analysis in Real Time-Mass Spectrometry (DART®-MS). It is common to have difficulty mixing molecular solvents, but it is considerably more complex when dealing with ionic liquids (salts) since each mixture could result in a binary mixture composed of three or four components as each salt must have an anion and a cation. In order to reduce unnecessary complexity, two ionic liquids with a common ion were selected for the homogenous tests. Out of the 27 mixtures tested, 17 were determined to be homogenous. Solubility tests with TNT were then conducted on the homogenous mixtures, in which six mixtures showed an immediate color change from clear and colorless to a dark purple which turned into a deep blood-red color over time. It is interesting to note that all six mixtures contained the $EMIM\text{-}BF_4$ ion. From previous studies, this drastic color change is suspected to be the cause of a charge transfer complex which reacts only with the TNT molecule. Nine of the remaining homogenous mixtures showed a slight or delayed color change. When the initial six mixtures, containing the $EMIM\text{-}BF_4$ ion, were tested with the other explosives, Compound B and RDX were deemed soluble, whereas PETN was considered only partially soluble or had limited solubility. Compound B was the only other explosive to display a color change within the mixtures, which is expected because it contains 40% TNT and 60% RDX. These samples were characterized via DART-MS, which confirmed the presence of TNT, RDX, and PETN within seconds. It is important to note that all analyte peaks were clean and there was no matrix interference from the collection swab, suggesting that the ionic liquid mixtures were able to not only retain the analyte, but also preserve the swab during analysis. This is an extremely important finding because this shows great potential for improved rate, specificity, and yield for forensic sampling.

The opinions or assertions contained herein are the private views of the author and are not to be construed as official or as reflecting the views of the Department of the Army or the Department of Defense.

References:

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