HELIUM NANODROPLET ISOLATION OF IONIC LIQUID VAPOR: INRARED LASER SPECTROSCOPY OF [EMIM][Tf_2N]

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The Infrared spectrum of the vapor produced upon thermal vaporization of the [emim][Tf_2N][a] ionic liquid has been obtained using the helium nanodroplet isolation method. Despite the low vapor pressure of [emim][Tf_2N], sufficient gas phase densities are produced, allowing for efficient helium nanodroplet pick-up. The mass spectrum of the emim[Tf_2N] doped droplet beam shows signatures[b] that have been attributed in gas phase measurements to the presence of isolated, intact [emim][Tf_2N] ion-pairs. Furthermore, the mass spectrometry results indicate that emim[Tf_2N] does not undergo thermal decomposition at 410 K. Comparisons are made between the experimental measurements and *ab initio* calculations (mp2/6-311++g(d,p)) of the CH stretch vibrational bands and permanent electric dipole moments for several [emim][Tf_2N] low energy isomers. The helium nanodroplet infrared spectrum of this species provides rather definitive support to the previously suggested vaporization mechanism of ionic liquids.[c]

[a] [emim][Tf_2N] is defined as 1-ethyl-3-methylimidazolium[bis(trifluoromethylsulfonyl)imide]

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