# Understanding the ionic liquid $[NC_{4111}][NTf_2]$ from individual building blocks: An IR-spectroscopic study

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**Abstract:**

This study explores at the molecular level the interactions underlying the IR spectra of the ionic liquid $[NC_{4111}][NTf_2]$ and its deuteratedisotopomer $[d_9\text{-}NC_{4111}][NTf_2]$ by first isolating the spectra of charged ionic building blocks using mass-selective CIVP spectroscopy and then following the evolution of these bands upon sequential assembly of the ionic constituents. The spectra of the (1,1) and (2,2) neutral ion pairs are recorded using superfluid helium droplets as well as a solid neon matrix, while those of the larger charged aggregates are again obtained with CIVP. In general, the cluster spectra are similar to that of the bulk, with the (2,2) system displaying the closest resemblance. Analysis of the polarization-dependent band intensities of the neutral ion pairs in liquid droplets as a function of external electric field yields dipole moments of the neutral aggregates. This information allows a coarse assessment of the packing structure of the neutral pairs to be antiparallel at 0.37 K, in contrast to the parallel arrangement found for the assembly of small, high-dipole neutral molecules with large rotational constants (e.g., HCN).