TRIGGERING INTRA-CLUSTER ELECTRON CAPTURE WITH VIBRATIONAL EXCITATION: AN IR STUDY OF THE $CH_3NO_2(H_2O)_6$ ANION

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Nitromethane (NM), the simplest of the nitro-containing organic molecules, possesses a large dipole moment of 3.46 D[a]. Nagata and co-workers[b] have demonstrated that Ar-mediated condensation of NM can trap a significant fraction of the collision complexes in a situation where the electron is retained in a diffuse hydrated electron configuration. This raises the possibility of triggering the electron capture onto NM to form the NM^- radical anion, releasing the substantial exothermicity of the reaction by evaporation of water molecules and allows the barrier to evaporation to be probed. We report vibrational predissociation spectra of both the product $NM^-(H_2O)_n$ anions as well as the high energy species that features a diffuse electron cloud. Interestingly, the spectra indicate that the high energy isomer has a neutral NM moiety and occurs with the same spectral signature of the excess electron binding site as that in the isolated water hexamer anion, indicating that it is attached in a position remote from the charge. Detailed comparison of the C-H and N-O stretching regions suggests that the reactive isomer occurs with the NM molecule attached to the backside of the water network via accepting H-bonds rather than attachment of the methyl group to the electron cloud, where the NM and water network would share the electron cloud.

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[a] R. N. Compton, et. al. *J. Chem. Phys.* **105** (9), September 1996.
[b] R. Nakanishi and T. Nagata *J. Chem. Phys.* **130** (22), June 2009.