

Formation of Benzonitrile Anions in Low Temperature Matrices and their Microsolvation in Water

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The discovery of benzonitrile (PhCN) molecule in Taurus Molecular Cloud - 1 in 2018, has led to a pursuit of research for neutral and protonated benzonitrile molecules, aggregates and their interaction with water molecules. However, literature reports on PhCN anion (PhCN⁻), a probable candidate yet to be identified in space, are scarce. Here we report the novel synthesis and spectroscopic characterization of PhCN⁻ in LDA water ices and inert gas matrices at 4K using matrix isolation FTIR, UV-Vis and EPR spectroscopy. PhCN⁻ is a curious case because preparing an anion out of PhCN is challenging owing to the negative electron affinity (~ -4.5 kcal mol⁻¹) of the molecule!

The synthesis of PhCN⁻ involved the use of an alkali metal, such as sodium as a source of electrons¹. Hydrated electrons are produced after co-deposition of water with sodium. These electrons are easily transferred to a PhCN molecule to produce PhCN⁻. PhCN⁻ is thermally stable, but photolabile and gets converted to the neutral molecule during photolysis. The thermal stability of PhCN⁻ anion in inert gas matrix also provides an opportunity to probe the non-covalent interactions of PhCN⁻ with solvent molecules such as water. However, in Ar matrix, photoactivation is necessary to cause the transfer of electron from sodium to the PhCN molecule. But due to the photolabile nature, the anion gives up its electron to the matrix in presence of visible light and forms neutral PhCN again.

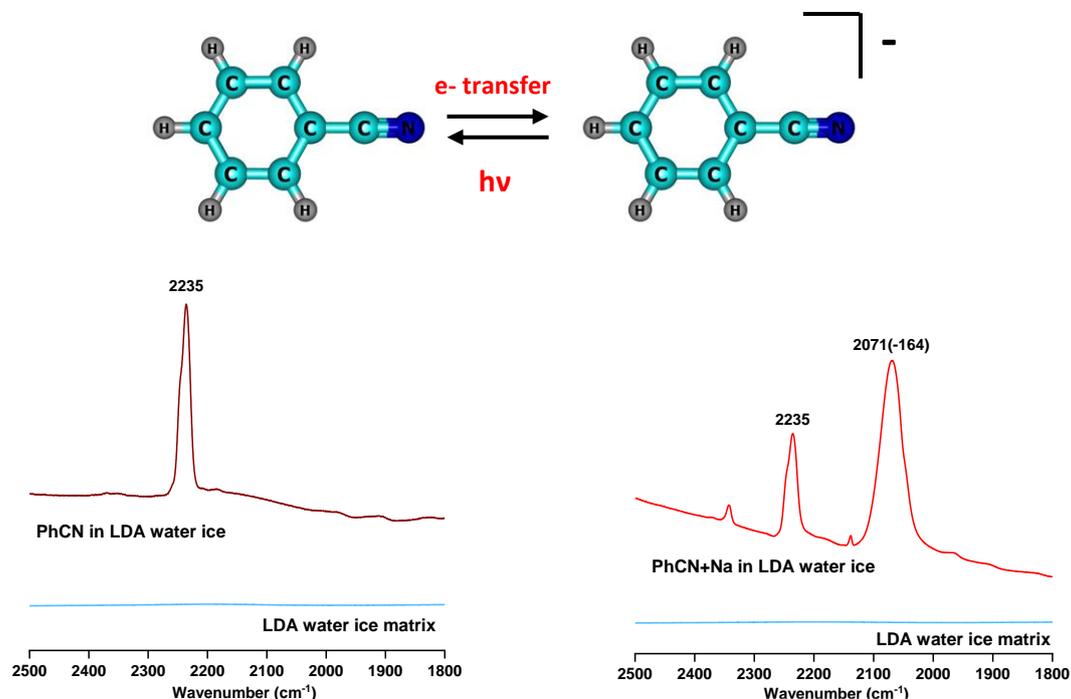


Figure1. C≡N stretching mode of PhCN in LDA water ice matrix before Na deposition.

Figure2. C≡N stretching mode of PhCN in LDA water ice matrix after Na deposition.