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Vibrational Spectroscopy of Benzonitrile-(Water)$_{1-2}$ cluster in Helium Droplets

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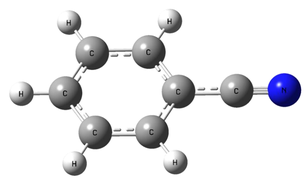
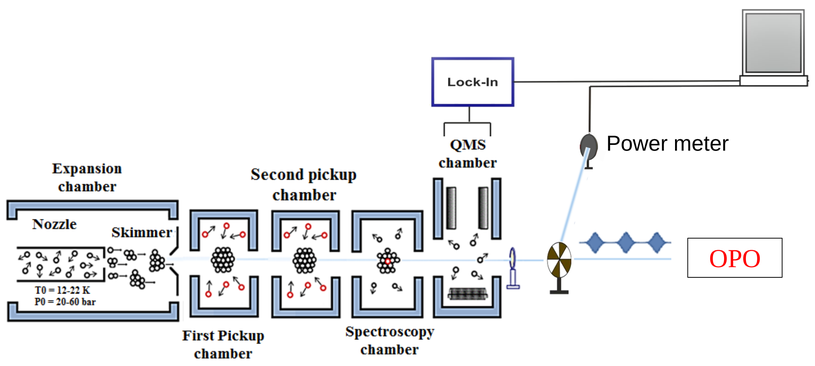
Abstract

Polycyclic aromatic hydrocarbons (PAH) are considered as primary carriers of the unidentified interstellar bands (UIRs). Despite its ubiquity, any specific PAH molecule has not been observed in the interstellar medium (ISM). Recently, the Benzonitrile molecule is observed in the interstellar medium[1]. Therefore, the Benzonitrile molecule can act as a precursor for these PAH molecules. Herein, we report the microhydration of Benzonitrile using mass-selective infrared spectroscopy inside the helium nanodroplets. By comparison of the experimental spectra with the ab-initio calculation at MP2/6-311++G(d,p) level of theory reveals the formation of different complexes of Benzonitrile-(water)$_{1-2}$.



He nanodroplet measurements...

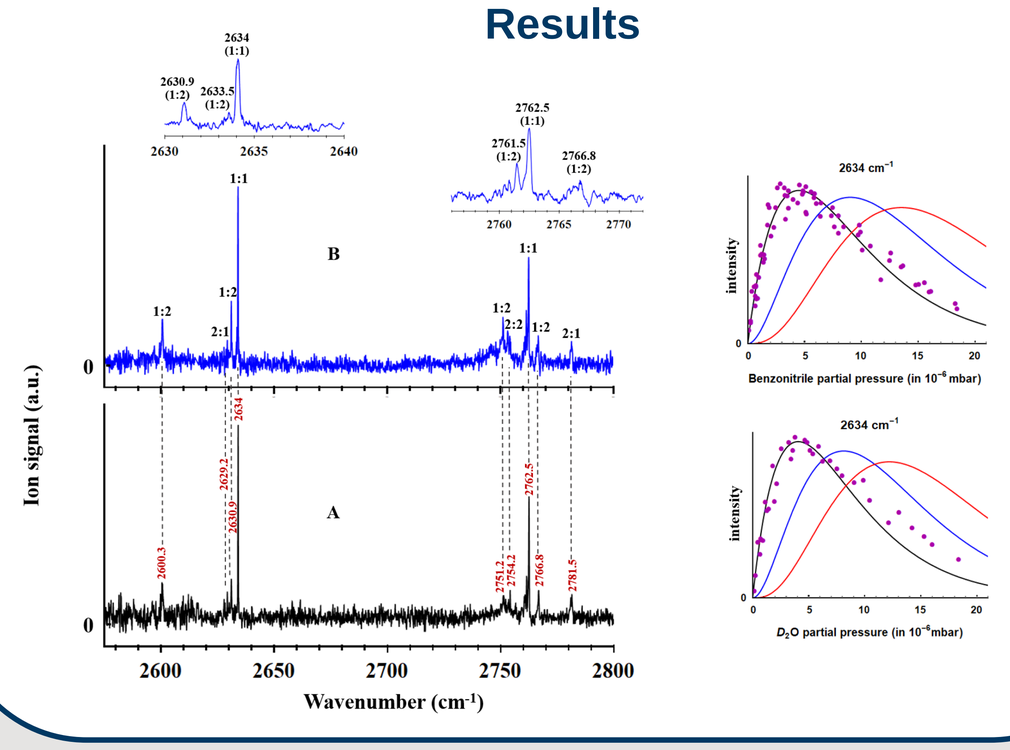


Pickup Curve

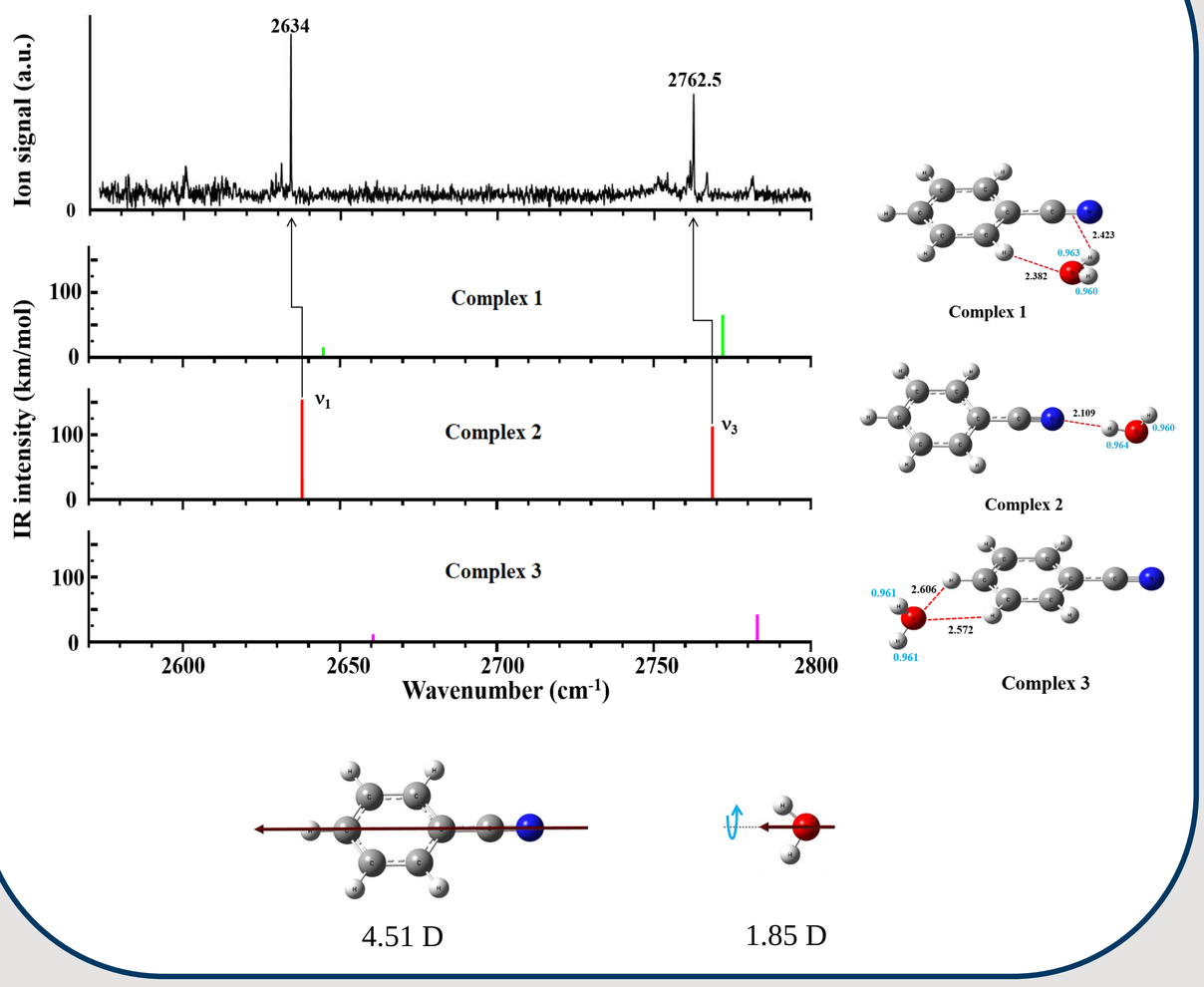
$$P_k = \frac{(\sigma\rho L)^k}{k!}\exp(-\sigma\rho L)$$

P_k: Probability of picking up k dopant molecules
σ: Cross section area of the droplets
ρ: Number density of the molecules in the pickup chamber
L: Length of the pickup region

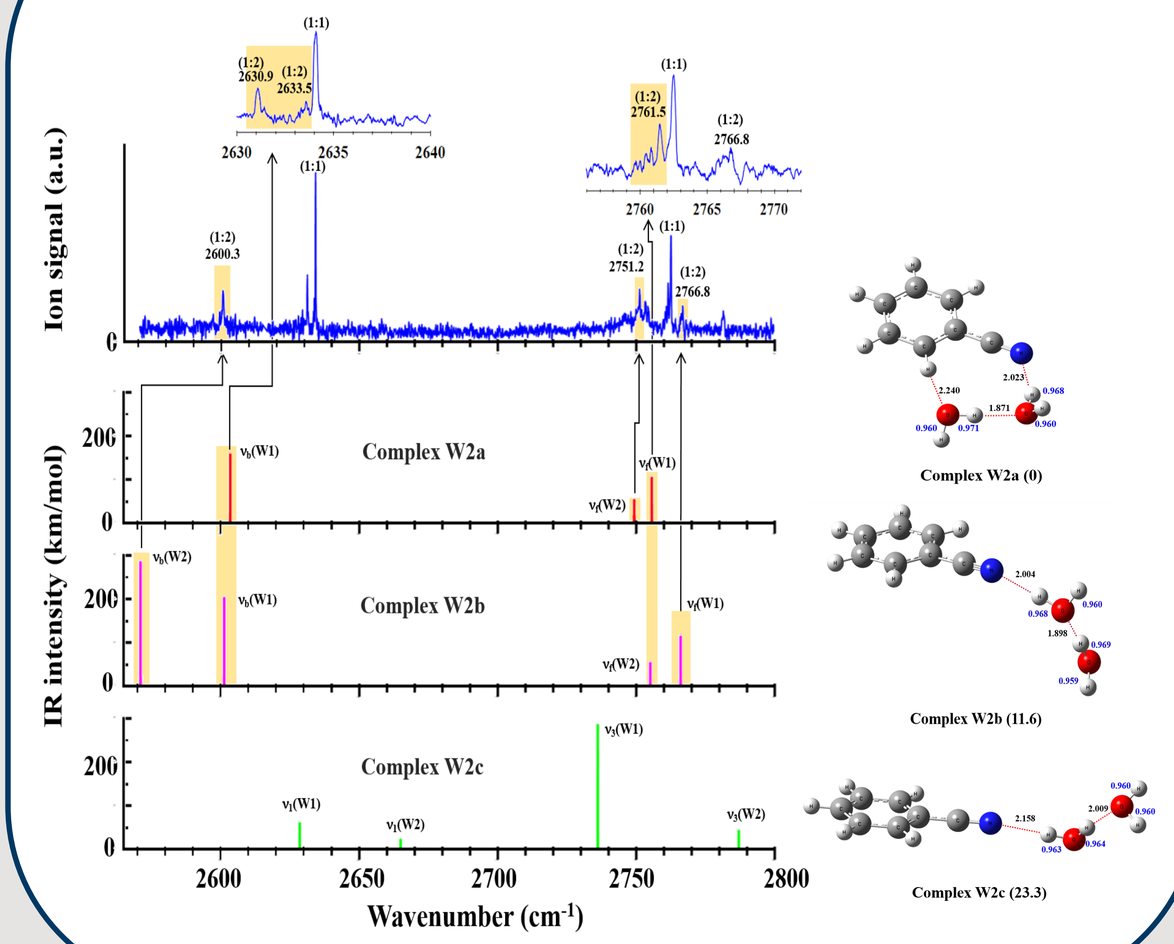
Results



Benzonitrile-D_2O complex



Benzonitrile-$(D_2O)_2$ complex



Summary

- IR spectra of Benzonitrile-(water)$_{1-2}$ complexes were studied and diffrent spectral feature were assigned to the corresponding cluster size of Benzonitrile and water using pickup curves.
- Only linear complex was found in case of Benzonitrile-(water)$_1$
- In Benzonitrile-(water)$_2$, two complex has been observed, most stable(ring type) and the linear complex.

Acknowledgement

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