

Experimental and Theoretical Study between CN radical and Acetonitrile CH₃CN Relevant to Astrochemical Environments

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Acetonitrile (CH₃CN) has been detected in molecular clouds (Sgr B2) and in hot cores in regions of massive star formation. The CH₃CN abundance in these objects which was found to be 10⁻⁹ or larger was explained by evaporation of molecular material from ice mantles of interstellar grains.

The gas phase reactivity of CH₃CN was studied in the literature in the presence of OH, NO₃, Cl and CN. However, no data are available at temperatures below 256 K. For this reason, a kinetic study of acetonitrile in the presence of the CN radical in interstellar conditions has been carried out below 168 K using the CRESU technique (Cinétique de Réaction en Ecoulement Supersonique Uniforme / Reaction Kinetics in a Uniform Supersonic Expansion) which generates a low temperature flow reactor. The study was completed by a series of measurements in the temperature range 258 - 354 K using a cryogenic cell or the CRESU apparatus in its subsonic configuration. In order to determine the rate coefficient, Pulsed Laser photolysis (PLP) and Laser Induced Fluorescence (LIF) techniques have been used. A first laser produced CN radicals by photolysis of ICN at 266 nm, while the second one, delayed with respect to the photolysis pulse, probed the fluorescence of these radicals by excitation at 387 nm. The rate coefficients of the studied reactions were determined from the temporal evolution of the fluorescence signal as a function of the CH₃CN concentration.

Whereas at temperatures higher than 200 K, the rate coefficient presents a usual Arrhenius behavior, a dramatic increase by *two orders of magnitude* in the temperature range 168 - 123 K occurs. At temperatures lower than 120 K, the rate coefficient still increases but at a lower level, reaching a value of $(5.08 \pm 0.86) \times 10^{-11} \text{ cm}^3 \text{ molec.}^{-1} \text{ s}^{-1}$ at 23 K. Interestingly, the rate coefficient was no pressure dependent at room temperature whereas this was observed below 168 K indicating a very different reactive mechanism according to the temperature range. More specifically, at 132 K and 52 K, measurements indicated that the stabilization of the adduct was competing with tunneling through an activation barrier confirmed by theoretical calculations. At 132 K, the tunneling contribution was precisely determined to be $(2.04 \pm 0.12) \times 10^{-12} \text{ cm}^3 \text{ molec.}^{-1} \text{ s}^{-1}$ and seems to increase at lower temperatures. This is the first time that this kind of behavior is identified at very low temperature for the CN radical reactivity in the gas phase.

References

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