

Experimental and theoretical study of the CN + CH₃CN reaction at very low temperature: Evidence of a competition between tunnelling and adduct stabilization at temperatures below 160 K ?

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A kinetic study of acetonitrile (CH₃CN) in the presence of the CN radical was performed in interstellar conditions (23 - 168 K) using the CRESU technique (Cinétique de Réaction en Ecoulement Supersonique Uniforme / Reaction Kinetics in a Uniform Supersonic Expansion). 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.

Whereas at temperatures higher than 200 K, the measured rate coefficient presents a usual Arrhenius behavior, a dramatic increase by *two orders of magnitude* in the temperature range 168 – 123 K occurs. At $T \leq 120$ 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, a series of measurements which have been carried out for different pressures indicated that the stabilization of the adduct may compete with tunneling through an energy barrier confirmed by theoretical calculations. This is the first time that such a behavior is observed at very low temperature for the CN radical gas phase reactivity.