

LIF SPECTROSCOPY OF A CARBON CHAIN RADICAL PRODUCED BY A HC₃N DISCHARGE

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New electronic transitions of a carbon chain radical containing a nitrogen atom have been observed by LIF spectroscopy. The radical was produced in a supersonic jet by a pulsed discharge of HC₃N diluted to 0.3% with 3atm Ar. We confirmed that the radical contains a nitrogen atom from the fact that the spectrum was not observed when C₂H₂ was used as a precursor.

About ten vibronic bands with a 50nsec radiative lifetime have been observed in a region from 27000 to 27400 cm⁻¹. The observed bands could be classified as ²Π_{3/2}-²Π_{3/2} and ²Σ⁻-²Σ vibronic bands. The lower state rotational constants of the vibronic bands have been determined to be 0.07537(1) and 0.07932(5) cm⁻¹ for the Π and Σ states, respectively. The upper states of ²Σ⁻-²Σ bands have very large spin-rotation constants, which should be denoted as Σ^(±) subjected to a small Renner-Teller interaction. The new molecule has been tentatively assigned to be the C₄N radical. We performed an UMP2 level ab initio calculation with 6-311G** basis sets for the C₄N radical. The estimated rotational constant in the ground state was 0.077 cm⁻¹. This value agrees well with the observed rotational constants.