BROADBAND ROTATIONAL SPECTROSCOPY OF 2,4,6-CYCLOHEPTATRIENE-1-CARBONITRILE: A POTENTIAL INTERSTELLAR MOLECULE

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The recent astronomical observations of the simplest aromatic nitrile benzonitrile, *c*-C_6H_5CN, followed by a five-membered [1], [2] and a bicyclic [3] CN functionalized ring in TMC-1 have opened up a new field of complex organic molecules (COMs) in space. These new findings provided an impetus for the laboratory rotational spectroscopy studies of larger -CN functionalized rings. One such example is 2,4,6-cycloheptatriene-1-carbonitrile (2,4,6-CHT-1-CN), a seven-membered ring with a -CN group attached to the sp^3-hybridized carbon atom. With a permanent electric dipole moment of 4.3 D and a low boiling point, the molecule is an excellent candidate for laboratory rotational spectroscopy.

Experiments were performed in the 18-26 GHz and 75-110 GHz frequency ranges in a supersonic expansion setup and a room temperature flow cell setup, respectively. The measurements across the 18-110 GHz region enabled the identification and assignment of the vibronic ground state, singly substituted rare-atom isotopologues, and vibrationally excited states. In this work, we report the precise determination of the rotational constants, quartic centrifugal distortion constants, as well as nitrogen nuclear quadrupole coupling constants for the vibronic ground state. The rotational spectroscopy study of 2,4,6-CHT-1-CN presented here forms the basis for future astronomical detection of this molecule.

[1] M. C. McCarthy et al., "Interstellar detection of the highly polar five-membered ring cyanocyclopentadiene," Nat Astron, vol. 5, no. 2, pp. 176–180, Feb. 2021, doi: 10.1038/s41550-020-01213-y.

[2] K. L. K. Lee et al., "Interstellar Detection of 2-cyanocyclopentadiene, C5H5CN, a Second Five-membered Ring toward TMC-1," ApJL, vol. 910, no. 1, p. L2, Mar. 2021, doi: 10.3847/2041-8213/abe764.

[3] B. A. McGuire et al., "Detection of two interstellar polycyclic aromatic hydrocarbons via spectral matched filtering," Science, vol. 371, no. 6535, pp. 1265–1269, Mar. 2021, doi: 10.1126/science.abb7535.