

# Laboratory rotational spectroscopy and astronomical search of ethynyl-substituted naphthalene

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Polycyclic aromatic hydrocarbons (PAHs) constitute one of the most abundant forms of interstellar carbon in the universe. They are proposed as carriers of the infrared emission features that dominate the spectra of most galactic and extragalactic sources. However, the formation processes of these species have been poorly understood due to the inability to detect individual PAH molecules. The recent interstellar detections of the first pure PAH indene [1] and the two isomers of the PAH cyanonaphthalene [2] renew interest in related molecular species that could be present in similar astronomical environments. In this context, 1- and 2-ethynyl-naphthalene are promising candidates to be observed in the Taurus molecular cloud (TMC-1), where 1- and 2-cyanonaphthalene have been detected. To enable the interstellar search of these species, their pure rotational spectra need to be investigated in the laboratory. We report the rotational spectra of 1- and 2-ethynyl-naphthalene using a broadband Fourier transform microwave spectrometer in the 2-8 GHz frequency range. The experimental investigation has been supported by quantum chemical calculations. Accurate spectroscopic parameters have been derived from the analysis of the experimental spectra, allowing for reliable predictions for astronomical searches. Our searches in TMC-1 for both isomers provide upper limits for the abundances of these species.

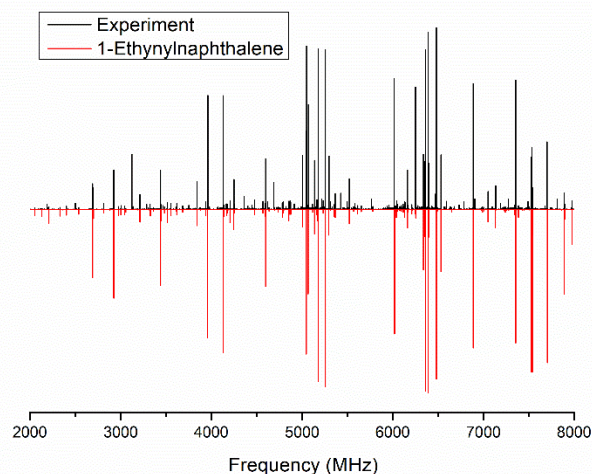


Figure 1: Rotational spectrum of 1-ethynyl-naphthalene.

**Index Terms:** astrochemistry, polycyclic aromatic hydrocarbons, structural determination, computational chemistry, ISM.

- [1] Cernicharo, J., Agúndez, M., Cabezas, C., et al. “Pure hydrocarbon cycles in TMC-1: Discovery of ethynyl cyclopropenylidene, cyclopentadiene, and indene”, *A&A*, 649, L15, 2021; Burkhardt, A. M., Lee, L. K., Changala, P. B., et al., Discovery of the Pure Polycyclic Aromatic Hydrocarbon Indene (c-C<sub>9</sub>H<sub>8</sub>) with GOTHAM Observations of TMC-1”, *ApJ*, 913, L18, 2021.
- [2] McGuire, B.A., Loomis, R.A., Burkhardt, A.M., et al. “Detection of two interstellar polycyclic aromatic hydrocarbons via spectral matched filtering”, *Science*, 371, 1265, 2021.