Gas-phase formation and spectroscopic characterization of the disubstituted cyclopropenylidenes *c*-$C_3(C_2H)_2$, *c*-$C_3(CN)_2$, and *c*-$C_3(C_2H)(CN)$

Athena R. Flint[1], Alexandria G. Watrous[1], Brent R. Westbrook[1], Dev J. Patel[1], and Ryan C. Fortenberry[1]

[1]Department of Chemistry and Biochemistry, University of Mississippi, University, Mississippi 38677-1848, USA

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Abstract

Aims. The detection of *c*-C_3HC_2H and possible future detection of *c*-C_3HCN provide new molecules for reaction chemistry in the dense ISM where R-C_2 and R-CN species are prevalent. Determination of chemically viable *c*-C_3HC_2H and *c*-C_3HCN derivatives and their prominent spectral features can accelerate potential astrophysical detection for this chemical family. This work will characterize three such derivatives: *c*-$C_3(C_2H)_2$, *c*-$C_3(CN)_2$, and *c*-$C_3(C_2H)(CN)$.

Methods. Interstellar reaction pathways of small carbonaceous species are well-replicated through quantum chemical means. Highly-accurate cc-pVXZ-F12/CCSD(T)-F12 (X=D,T) calculations generate the energetics of chemical formation pathways as well as the basis for quartic force field and second-order vibrational perturbation theory rovibrational analysis of the vibrational frequencies and rotational constants of the molecules under study.

Results. The formation of *c*-$C_3(C_2H)_2$ is as thermodynamically and, likely, stepwise favorable as the formation of *c*-C_3HC_2H, rendering its detectability to be mostly dependent on the concentrations of the reactants. *c*-$C_3(C_2H)_2$ and *c*-$C_3(C_2H)(CN)$ will be detectable through radioastronomical observation with large dipole moments of 2.84 D and 4.26 D, respectively, while *c*-$C_3(CN)_2$ has an exceedingly small and likely unobservable dipole moment of 0.08 D. The most intense frequency for *c*-$C_3(C_2H)_2$ is ν_2 at 3316.9 cm^{-1} (3.01 μm) with an intensity of 140 km mol^{-1}. *c*-$C_3(C_2H)(CN)$ has one frequency with a large intensity, ν_1, at 3321.0 cm^{-1} (3.01 μm) with an intensity of 82 km mol^{-1}. *c*-$C_3(CN)_2$ lacks intense vibrational frequencies within the range that current instrumentation can readily observe.

Conclusions. *c*-$C_3(C_2H)_2$ and *c*-$C_3(C_2H)(CN)$ are viable candidates for astrophysical observation with favorable reaction profiles and spectral data produced herein, but *c*-$C_3(CN)_2$ will not be directly observable through any currently-available remote sensing means even if it forms in large abundances.