SPECTROSCOPIC AND COMPUTATIONAL CHARACTERIZATION OF 2-AZA-1,3-BUTADIENE, A MOLECULE OF ASTROCHEMICAL SIGNIFICANCE

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Being N-substituted unsaturated species, azabutadienes are molecules of potential relevance in astrochemistry, ranging from the interstellar medium to Titan's atmosphere. 2-azabutadiene and butadiene share a similar conjugated π system, thus allowing the investigation of the effects of heteroatom substitution. More interestingly, 2-azabutadiene can be used to proxy the abundance of interstellar butadiene. To enable future astronomical searches, the rotational spectrum of 2-azabutadiene has been investigated up to 330 GHz. Experiment has been supported and guided by an accurate computational characterization of the molecular structure, energetics, and spectroscopic properties of the two possible forms, *trans* and *gauche*. The *trans* species, more stable by about 7 kJ/mol than *gauche*-2-azabutadiene, has been experimentally observed and its rotational and centrifugal distortion constants obtained with remarkable accuracy, while theoretical estimates of the spectroscopic parameters are reported for *gauche*-2-azabutadiene.