Possible Symmetry Breaking of the cyclic-C3 C2 H Radical

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Recently, theoretical work proposed the cyclic-C3 C2 H radical as a possible candidate for laboratory and/or interstellar observation. While this molecule has yet to be observed in the interstellar medium, the cyclic-C3 C2 H radical was subsequently synthesized and analyzed experimentally in the laboratory. Unfortunately, theoretical and experimental results disagree as to the correct geometric structure for this molecule. While previous theoretical work predicts the C2v structure shown in Fig. 1A, experimentalists concluded that the geometry for the cyclic-C3 C2 H radical is the Cs structure showin in Fig. 1B. We employed high-level coupled cluster methods including full inclusion of connected triple excitations to study the possibility of symmetry-breaking for the cyclic-C3 C2 H radical. We find evidence that the geometric structure for the cyclic-C3 C2 H radical should be a symmetry-borken Cs structure due to the presence of a second-order Jahn-Teller interaction between the ground and first excited states.