

## GROUND STATE POTENTIAL ENERGY SURFACE AND ROVIBRATIONAL STRUCTURE OF $C_3H^-$

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The detection of molecular anions in the laboratory by spectroscopic methods and the interpretation of these spectra is greatly aided by accurate theoretical calculations for the geometries and relative stabilities of the different isomers. This contribution describes a six dimensional *ab initio* potential energy surface (PES) for the singlet ground state of  $C_3H^-$  calculated at the CCSD(T)/aug-cc-pVQZ level. In agreement with previous studies<sup>a</sup>, the global potential minimum corresponds to a planar cyclic isomer. A local minimum is also located about  $2500\text{ cm}^{-1}$  higher in energy, corresponding to a planar *trans* bent isomer. The PES, represented by a fitted analytical form in the region of the two minima, is used in variational calculations to determine anharmonic rovibrational term values ( $J \leq 2$ ) for both isomers and their deuterated analogues. Rotational, centrifugal distortion and vibration-rotation constants are evaluated. The implications of the theoretical calculations for future investigations of  $C_3H^-$  and  $C_3D^-$  using microwave, infrared and photodetachment spectroscopies are discussed.

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<sup>a</sup>K. Aoki, K. Hashimoto, S. Ikuta and O. Nomura *Chem. Phys. Lett.* **242**, 527 (1995).