TUNNELING AND RING OPENING IN THE CYCLOPROPYL RADICAL AND CATION

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We report spectroscopic studies of the cyclopropyl radical and cation (c-C_3H_5). The cation especially is unstable towards ring-opening to allylic geometries, and the radical exhibits tunneling splitting due to inversion tunneling by the α-H atom that lies out of the C-C-C ring plane[1]. These large amplitude motion phenomena complicate the photoionization (and other) spectra and the determination of properties that are of interest due to ring strain in this fundamental cyclic radical. Through a multiscale reduced-dimension *ab initio* description of the potential energy surfaces of both the radical and the cation, the rotational and ionization spectra of the radical are simulated using advanced perturbative and variational rovibrational treatments. The results are compared with experimental photoionization data from the literature and new measurements[2].

[1] Dong *et al.*; J. Phys. Chem. A; 2006; 110; 3059-3070.
[2] Dyke *et al.*; J. Chem. Soc., Faraday Trans. 2; 1985; 81; 1573-1586.