STRUCTURE AND DYNAMICS OF THE CYCLOPROPENE RADICAL CATION STUDIED BY HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPY

<u>KONSTANTINA VASILATOU</u>, JULIE M. MICHAUD, DENITSA BAYKUSHEVA, GUIDO GRASSI and FREDERIC MERKT, *Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland.*

High-resolution photoelectron spectra of cyclopropene (c-C₃H₄) and several of its deuterated isotopomers have been recorded. From the analysis of the almost fully resolved rotational structure of the origin of the $\widetilde{X}^{+2}B_2 \leftarrow \widetilde{X}^{1}A_1$ ionizing transition of c-C₃H₄, c-C₃H₃D, c-C₃H₂D₂, c-C₃HD₃ and c-C₃D₄ and the observation of several low-lying vibrational levels of the corresponding cations, we conclude that the cyclopropene cation has an equilibrium structure deviating from C_{2v} symmetry. We believe that the cation is subject to a large-amplitude tunnelling motion along a mode of a₂ symmetry involving a twist of the CH₂ group and an asymmetric out-of-plane bending of the CH units. The reasons for this belief and also currently unresolved aspects of our analysis will be discussed.