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The strange spectroscopy and fragmentation dynamics of the X 2B2 ground state of CH2F2+

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At low resolution, the first photoelectron band of CH2F2, first recorded in the 1970s at a resolution of ca. 800 cm-1 (or 0.1 eV), shows an apparently simple progression in the HCH bending mode. This is consistent with the large reduction in HCH bond angle, from ca. 113o to 85o, predicted by ab initio calculations. As new technologies and photon sources have evolved over the last 40 years and the resolution has improved to better than 1 cm-1, this apparently simple spectrum has 'changed'to reveal a complex structure of overlapping symmetric and non-symmetric vibrational modes. Interpretation is only possible allowing for coupling between anharmonic vibrations.1 In part, the complexity of the spectrum arises due to the very low dissociation limit of CH2F2+ 2B2 by H-atom loss to CHF2+ + H (D0 = 2650 cm-1). Experiments performed at the X04DB vacuum-ultraviolet beamline of the Swiss Light Source have re-recorded both the photoelectron spectrum and the coincidence fragmentation spectrum by imaging threshold photoelectron photoion coincidence spectroscopy at a resolution of ca. 15 cm-1 (or 0.002 eV).2,3 They shed new light both on the spectroscopy and fragmentation of the ground state of CH2F2+. These results will be presented and discussed at PTPC 2014.

see attached Word file

Primary author: Prof. TUCKETT, Richard (University of Birmingham)

Co-authors: Dr BODI, Andras (Paul Scherrer Institute, Switzerland); Dr HARVEY, Jonelle (University of Birmingham UK); Dr HEMBERGER, Patrick (Paul Scherrer Institute, Switzerland)

Presenter: Prof. TUCKETT, Richard (University of Birmingham)

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