

On the Photoelectron Spectrum and Heat of Formation of the meta-Xylylene Biradical

M. Steglich¹, P. Hemberger¹, V. B. Custodis², A. Trevitt³, G. daSilva⁴, A. Bodi¹

¹Paul Scherrer Institute, ²ETH Zürich, ³University of Wollongong, ⁴University of Melbourne

The meta-xylylene biradical *m*-C₈H₈ represents a prototypical organic triplet that serves as a model compound for the test and refinement of quantum theoretical calculations and is a promising building block for organic molecule-based magnets. We used flash vacuum pyrolysis of 1,3-bisiodomethyl-benzene (*m*-C₈H₈I₂) to produce *m*-C₈H₈ in the gas phase and photoelectron spectroscopy to probe the first two electronic states of the radical cation. The ionization energy was found to be (7.27±0.01) eV. From that, the heat of formation of the biradical is derived indirectly by investigating the C-I bond dissociation behavior of the precursor ion. We obtain $\Delta H_{f,298K} = (321.3 \pm 10)$ kJ/mol, which is slightly below the value of a previous study applying a different experimental approach.