

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

M. Steglich<sup>1</sup>, P. Hemberger<sup>1</sup>, V. B. Custodis<sup>2</sup>, A. Trevitt<sup>3</sup>, G. daSilva<sup>4</sup>, A. Bodi<sup>1</sup>

<sup>1</sup>Paul Scherrer Institute, <sup>2</sup>ETH Zürich, <sup>3</sup>University of Wollongong, <sup>4</sup>University of Melbourne

The meta-xylylene biradical *m*-C<sub>8</sub>H<sub>8</sub> 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*-C<sub>8</sub>H<sub>8</sub>I<sub>2</sub>) to produce *m*-C<sub>8</sub>H<sub>8</sub> 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.