PHOTOELECTRON IMAGING SPECTROSCOPY AS A WINDOW TO UNEXPECTED MOLECULES

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Targeting an anion with the formula CH_3O_3 for exploration with photoelectron imaging spectroscopy, we determine its identity to be dihydroxymethanolate, an anion largely absent in the literature, and the conjugate base of the hypothetical species orthoformic acid. Comparing the observed photoelectron spectrum to CCSD-EOM-IP and CCSD-EOM-SF calculations completed in QChem and Franck-Condon overlap simulations in PESCAL, we are able to determine with confidence the connectivity of the atoms in this molecule.