Supplementary information

Peroxy self-reaction leading to the formation of furfural

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No literature data are available on 2-hydroxymethylfuran and a FC simulation on this molecule was performed for both the ground state (neutral)-to-ground state (cation) and ground state (neutral)-to-excited state (cation) electronic transitions. The optimized AIE is 8.55 eV based on the best fit agreement and the term energy of the excited electronic state of the cation is optimized to be 0.2 eV by shifting the ground state (neutral)-to-excited state (cation) transition to have the best fit with the experimental data.
Due to the low signal-to-noise ratio for this m/z, the assignment cannot be conclusive. For 2-hydroperoxymethylfuran the adiabatic ionization energy is optimized as 8.80 eV and the term energy of the excited electronic state of the cation is calculated to be 0.75 eV using the same procedures as described above for m/z = 98 PI spectrum.

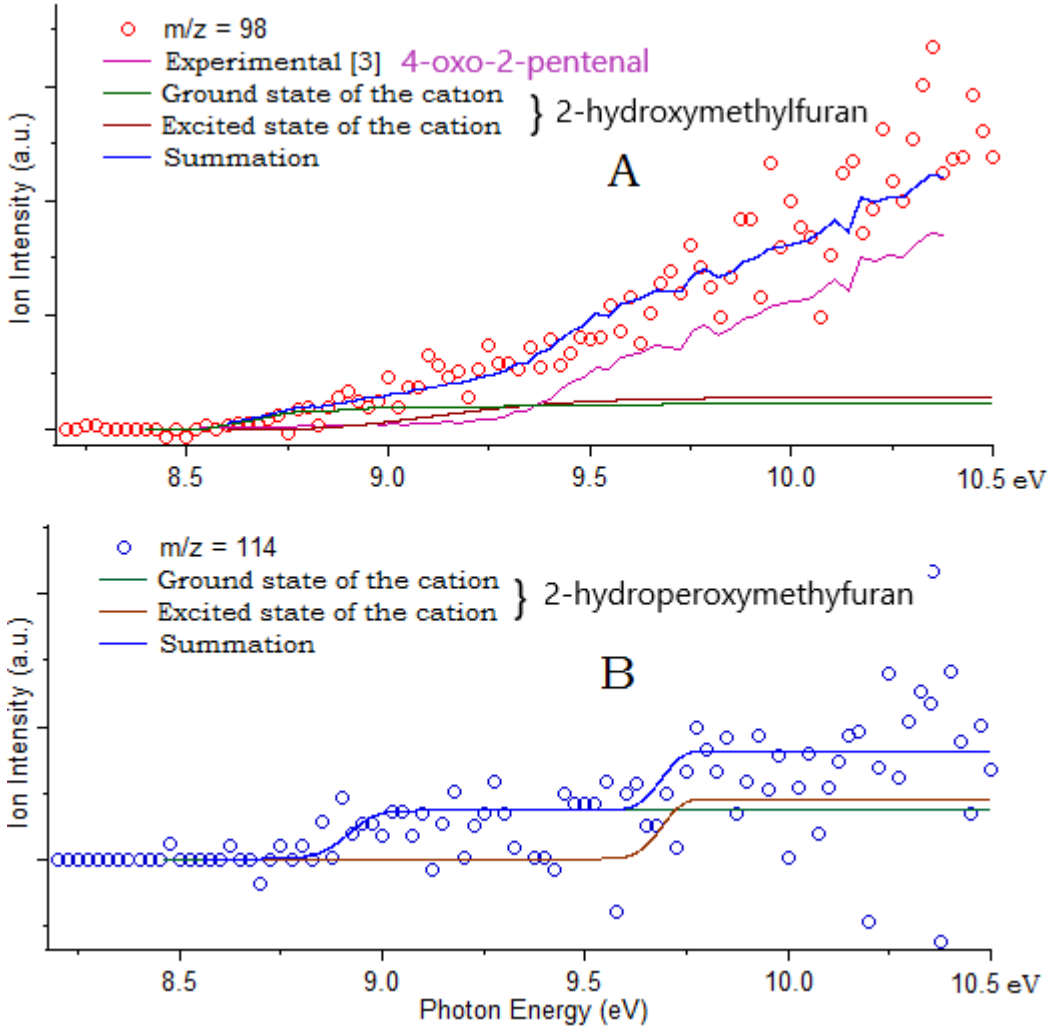

Figure S1. Photoionization spectra of m/z=98 (A) and m/z=114 (B) species.