

Photoelectron Spectroscopy of Deprotonated Methane Diol

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We report photoelectron spectra of deprotonated methane diol, or the hydroxymethoxide anion, ($\text{H}_2\text{C}(\text{OH})\text{O}^-$). A vibrational progression is observed in the photoelectron spectra, primarily consisting of combination bands of the OCO symmetric and asymmetric stretches with lower frequency modes in the hydroxymethoxy radical. A high-resolution photoelectron spectrum aids in the experimental assignment of several neutral vibrational frequencies, including an experimental determination of the lowest frequency mode, the H-atom torsion in the HOCO moiety (110 cm^{-1}). The electron affinity of the hydroxymethoxy radical is determined to be $2.220(5)\text{ eV}$. In addition, the first excited state of the radical neutral is observed, which has a vertical detachment energy only $\sim 0.75\text{ eV}$ above the neutral ground state. The photoelectron spectrum resulting from electron detachment to the hydroxymethoxy radical excited state is broad and unstructured, which could be a result of spectral congestion or the strong coupling between the neutral ground and excited state surfaces. The gas-phase acidity of methane diol is calculated to be $366(2)\text{ kcal/mol}$, which results in $D_0(\text{H}_2\text{C}(\text{OH})\text{O}-\text{H}) = 104(2)\text{ kcal/mol}$ using the experimentally determined electron affinity of the hydroxymethoxy radical.

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