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Anion photoelectron spectroscopy of ZnOH, combined experimental and theoretical study IVAN IORDANOV, Department of Physics, Pennsylvania State University, K.D.D. GUNARATNE, Department of Chemistry, Pennsylvania State University, JORGE SOFO, Department of Physics, Pennsylvania State University, A.W. CASTLEMAN JR., Department of Chemistry, Pennsylvania State University — Information about ZnOH anion has been obtained for the first time using TOF mass spectrometry combined with the Velocity Map Imaging Apparatus. Vertical detachment energies (VDE), nature of the HOMO and LUMO, photoelectron angular distributions of the studied species are reported. Combined with our experimental study, we report on first-principles calculations of ZnOH using density functional theory (DFT) with the Perdew-Burke-Ernzerhof (PBE) functional and also calculations using couple-cluster singles, doubles and triples (CCSD(T)) method. The calculations are used to determine the ground state geometry, vibrational modes and detachment energies of the neutral and anion ZnOH cluster. These results are used to explain the characteristics of the experimental ZnOH spectrum.

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