

ON THE STABILITY OF GLYCINE-WATER CLUSTERS
WITH EXCESS ELECTRON : IMPLICATIONS FOR
PHOTOELECTRON SPECTROSCOPY

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Calculations are presented for the glycine-(H₂O)_n⁻(n=0-2) anionic clusters with excess electron, with the glycine core in the canonical or zwitterion form. A variety of conformers are predicted, and their relative energy is examined to estimate thermodynamic stability. The dynamic (proton transfer) pathways between the anionic clusters with the canonical and the zwitterion glycine core are examined. Small barrier heights for isomerization from the zwitterion glycine-(H₂O)₂⁻ anion to those with canonical glycine core suggest that the former conformers may be kinetically unstable and unfavorable for detection of neutral glycine zwitterion-(H₂O)_n(n=1,2) clusters by photodetachment, in accordance with the photoelectron spectroscopic experiments by Bowen and co-workers [Xu et al., J. Chem. Phys. 119, 10696 (2003)]. The calculated stability of the glycine-(H₂O)_n⁻ anion clusters with canonical glycine core relative to those with zwitterion core indicates that the observation of the anionic conformers with the canonical glycine core would be much more feasible, as revealed by Johnson and co-workers [Diken et al. J. Chem. Phys. 120, 9902 (2004)].