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Supporting Information



Figure S1. Isomers of $C_5H_3N_2O_4^-$ are listed in order of increasing electronic energies (ZPE corrected) relative to the most stable isomer. These energies (kcal mol⁻¹) are calculated at the B3LYP/6-311++G(d,p) level of theory and shown beneath each structure.



Figure S2. Tautomerization of $C_5H_3N_2O_4^-$ involves many low energy H transfers throughout the ion. This potential energy surface (kcal mol⁻¹) is calculated at the B3LYP/6-311++G(d,p) level of theory and displays the barriers to the conversion between several $C_5H_3N_2O_4^-$ structures.



Figure S3. Isomers of $C_4H_3N_2O_2^-$ are listed in order of increasing electronic energies (ZPE corrected) relative to the most stable isomer. These energies (kcal mol⁻¹) are calculated at the B3LYP/6-311++G(d,p) level of theory and shown beneath each structure.