Supplementary information for

Acidic stabilization of the dual-aromatic heterocyclic anions

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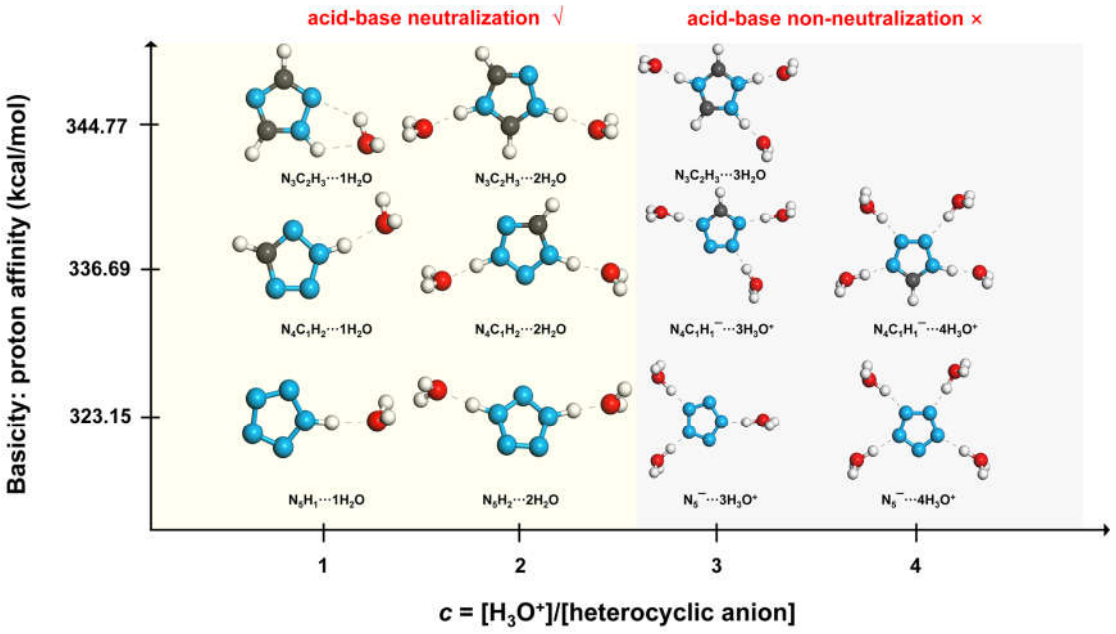

Figure S1. Reactivity of $N_3C_2H_2^-$, $N_4C_1H_1^-$, and N_5^- with increasing concentration of H_3O^+.

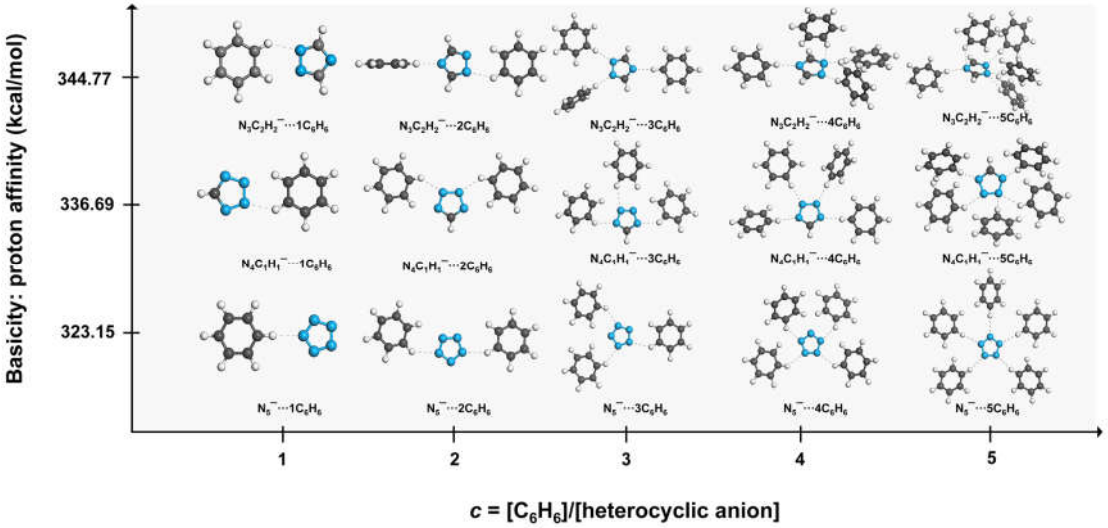

Figure S2. Reactivity of $N_3C_2H_2^-$, $N_4C_1H_1^-$, and N_5^- with increasing concentration of benzene.

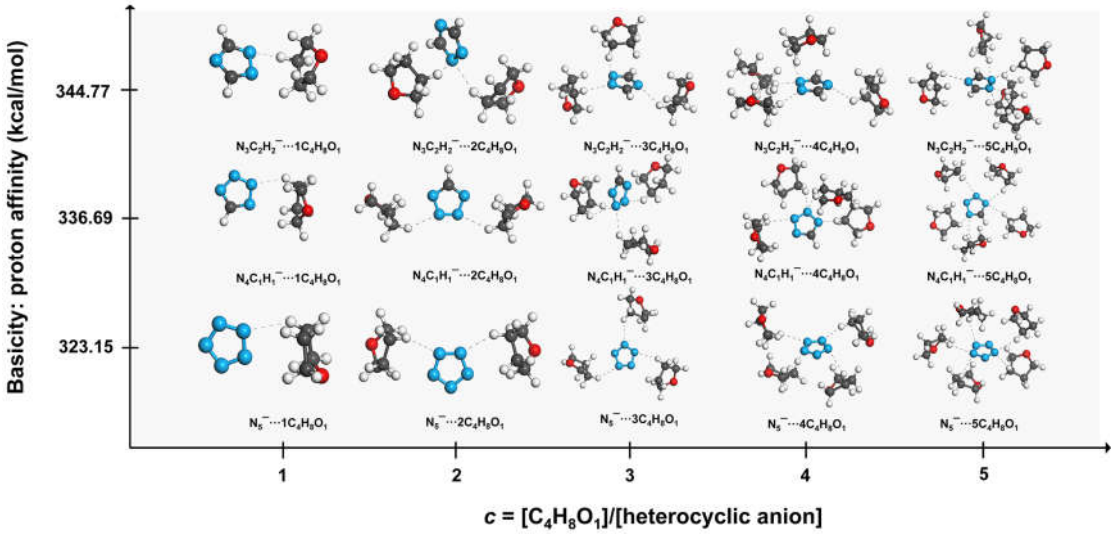

Figure S3. Reactivity of $N_3C_2H_2^-$, $N_4C_1H_1^-$, and N_5^- with increasing concentration of THF.

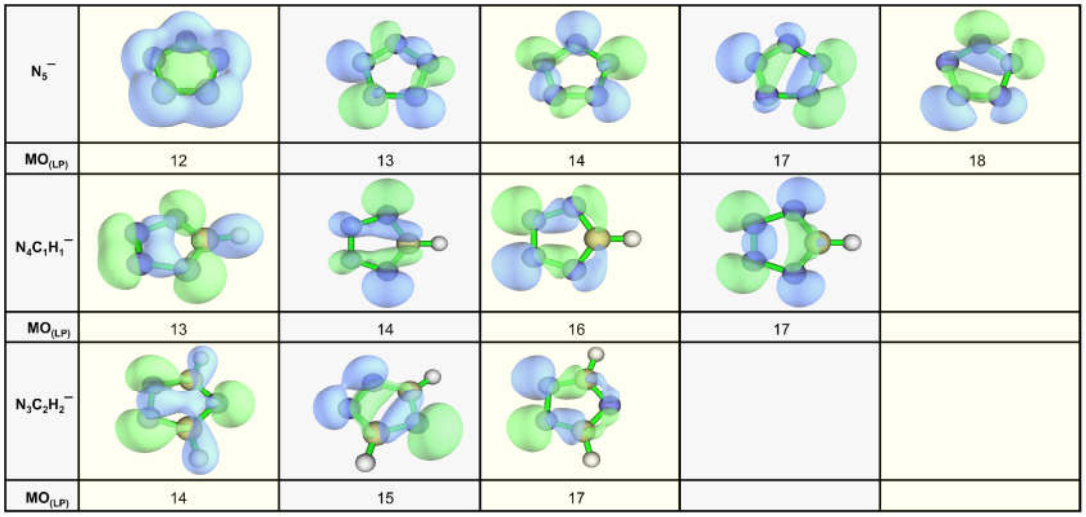

Figure S4. Isosurfaces (0.05) of σ MO containing nitrogen lone pairs ($MO_{min\text{-}\sigma(LP)}$) of $N_3C_2H_2^-$, $N_4C_1H_1^-$, and N_5^-. The number under each isosurface is the corresponding MO index.

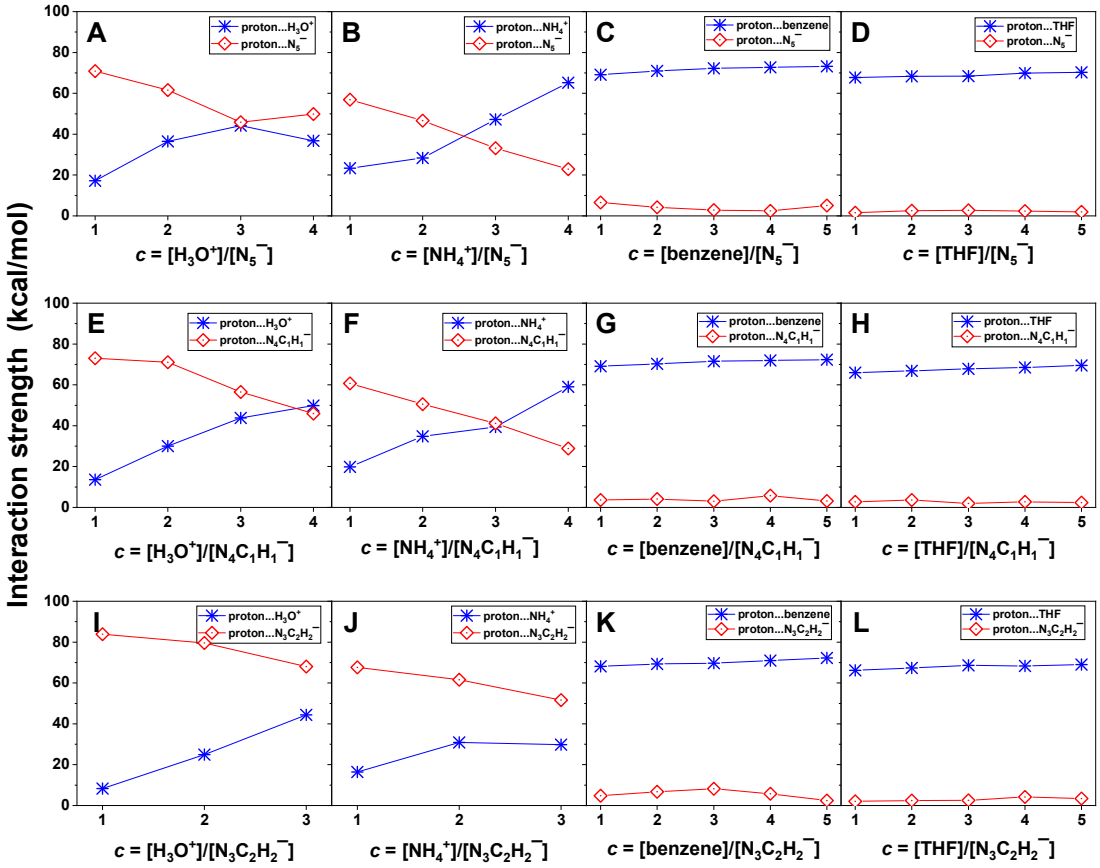

Figure S5. Interaction strengths of the proton with heterocyclic anions and with solvent species.

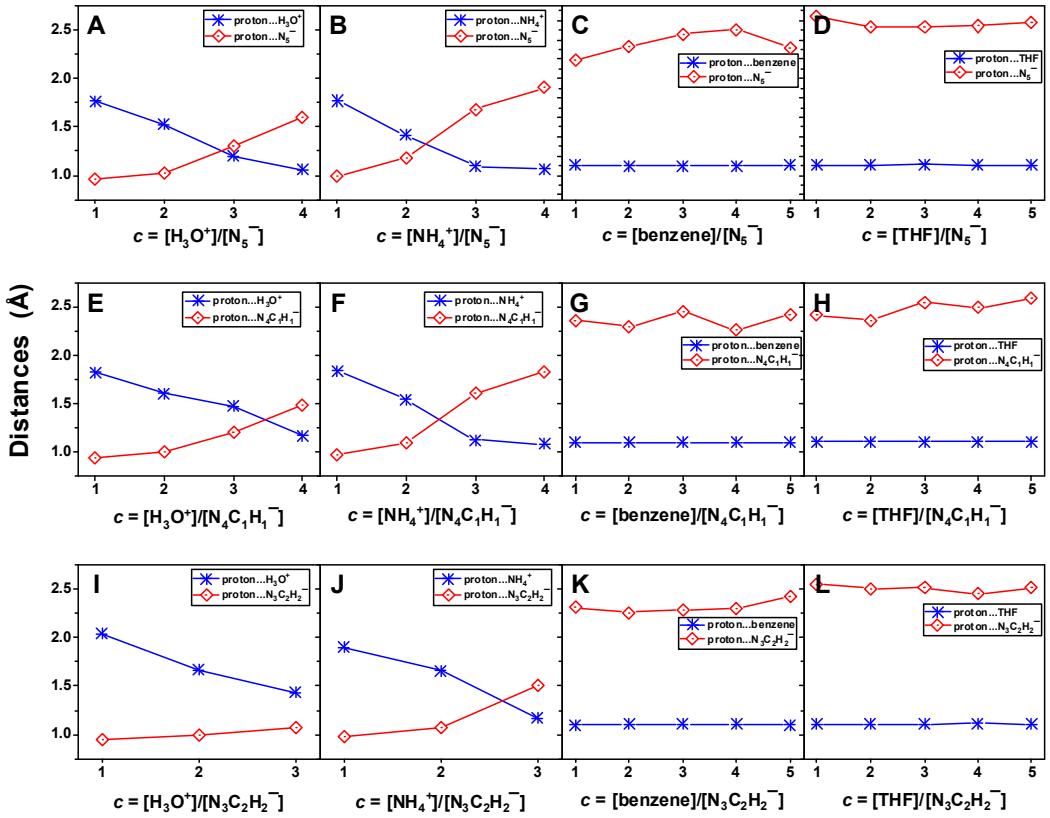

Figure S6. Distances of the proton from heterocyclic anions and from solvent species.

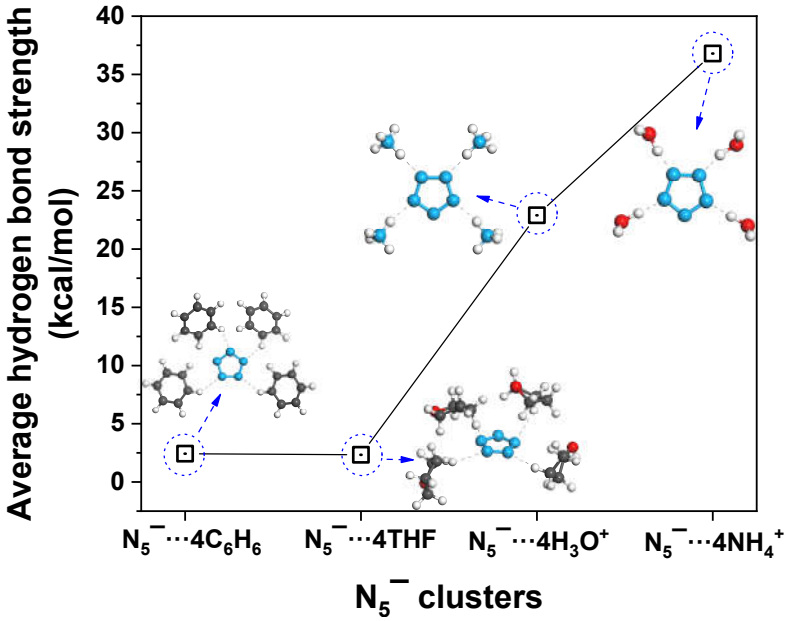

Figure S7. Comparison of strengths of the intermolecular hydrogen bonding in $N_5^-\cdots4H_3O^+$, $N_5^-\cdots4NH_4^+$, $N_5^-\cdots$4benzene, and $N_5^-\cdots$4THF complexes.

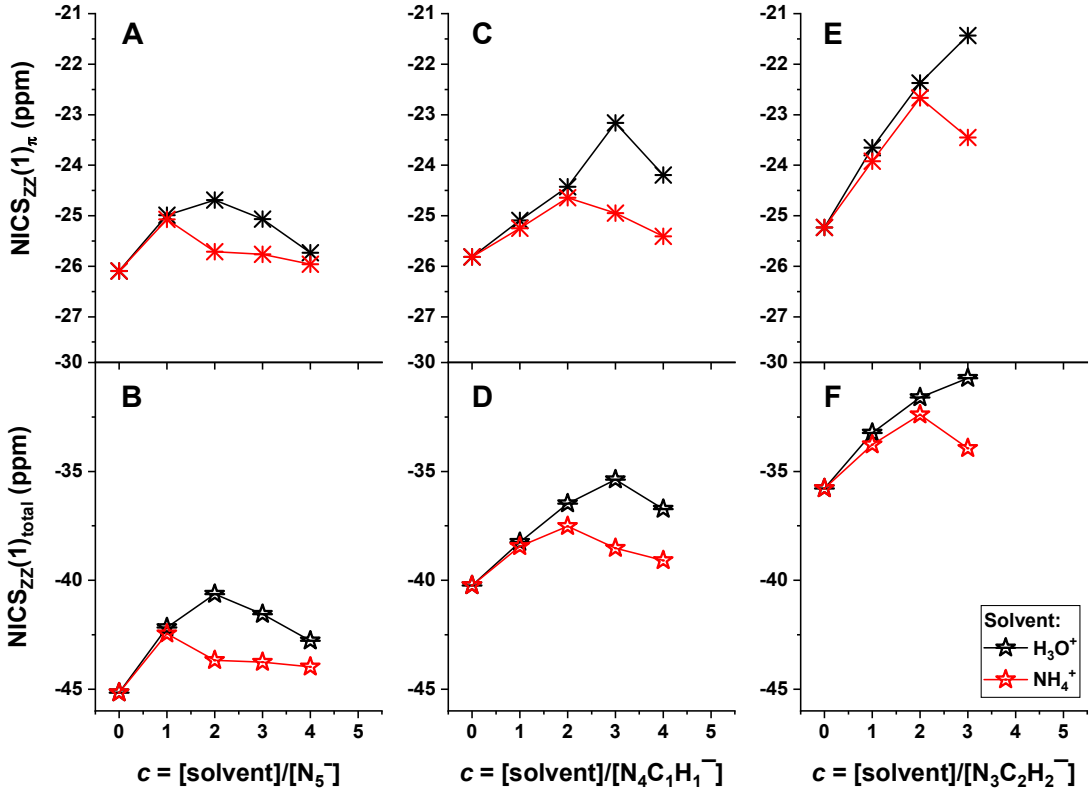

Figure S8. $NICS_{zz}(1)_\pi$ and $NICS_{zz}(1)_{total}$ of **(A-B)** N_5^-, **(C-D)** $N_4C_1H_1^-$, and **(E-F)** $N_3C_2H_2^-$ with increasing concentration of H_3O^+ and NH_4^+.

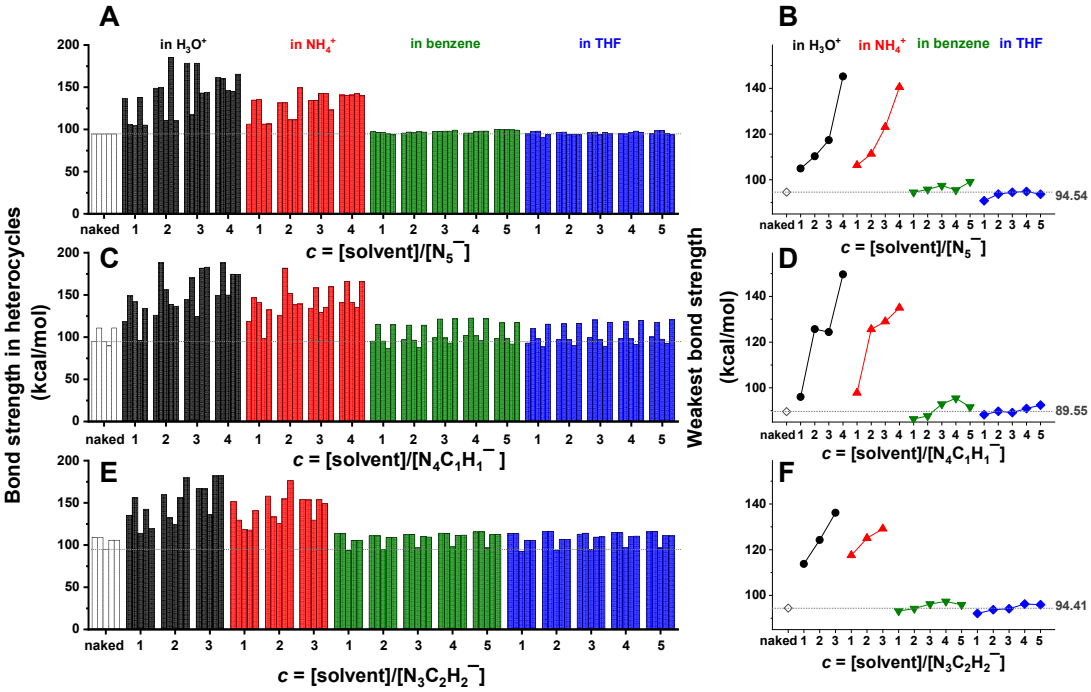

Figure S9. All bond strengths and weakest bond strengths in the rings of (A-B) N_5^-, (C-D) $N_4C_1H_1^-$, and (E-F) $N_3C_2H_2^-$ in variant concentration of solvents. The weakest bond strength in the ring of each naked heterocyclic anion is marked by a dashed line for comparison.