

SUPPLEMENTARY INFORMATION

The Onset of Electron-Induced Proton-Transfer in Hydrated Azabenzene Cluster Anions

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This supporting information contains the structures of cluster anions studied computationally using the M06-2X/6-31++G(*d,p*) method and basis set combination. Relative energetics are included for clusters of the same size in units of kcal mol⁻¹.

Figure S.1 - Select $\text{Py}^-(\text{H}_2\text{O})_3$ and $[\text{PyH}\cdot\text{OH}]^-(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.2 - Select $\text{Py}^-(\text{H}_2\text{O})_4$ and $[\text{PyH}\cdot\text{OH}]^-(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.3 - Select $\text{Py}^-(\text{H}_2\text{O})_5$ and $[\text{PyH}\cdot\text{OH}]^-(\text{H}_2\text{O})_4$ structures along with relative energies.

Figure S.4 - Select $\text{Py}^-(\text{H}_2\text{O})_6$ and $[\text{PyH}\cdot\text{OH}]^-(\text{H}_2\text{O})_5$ structures along with relative energies.

Figure S.5 - Select $\text{Pd}^-(\text{H}_2\text{O})$ and $\text{Pd}^-(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.6 - Select $\text{Pd}^-(\text{H}_2\text{O})_3$ and $[\text{PdH}\cdot\text{OH}]^-(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.7 - Select $\text{Pd}^-(\text{H}_2\text{O})_4$ and $[\text{PdH}\cdot\text{OH}]^-(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.8 - Select $\text{Pd}^-(\text{H}_2\text{O})_5$ and $[\text{PdH}\cdot\text{OH}]^-(\text{H}_2\text{O})_4$ structures along with relative energies.

Figure S.9 - Select $\text{Pd}^-(\text{H}_2\text{O})_6$ and $[\text{PdH}\cdot\text{OH}]^-(\text{H}_2\text{O})_5$ structures along with relative energies.

Figure S.10 - Select $\text{Pm}^-(\text{H}_2\text{O})$ and $\text{Pm}^-(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.11 - Select $\text{Pm}^-(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.12 - Select $\text{Pm}^-(\text{H}_2\text{O})_4$ structures along with relative energies.

Figure S.13 - Select $\text{Pm}^{\cdot-}(\text{H}_2\text{O})_5$ and $[\text{PmH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_4$ structures along with relative energies.

Figure S.14 - Select $\text{Pm}^{\cdot-}(\text{H}_2\text{O})_6$ and $[\text{PmH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_5$ structures along with relative energies.

Figure S.15 - Select $\text{Pz}^{\cdot-}(\text{H}_2\text{O})$ and $\text{Pz}^{\cdot-}(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.16 - Select $\text{Pz}^{\cdot-}(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.17 - Select $\text{Pz}^{\cdot-}(\text{H}_2\text{O})_4$ and $[\text{PzH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.18 - Select $\text{Pz}^{\cdot-}(\text{H}_2\text{O})_5$ and $[\text{PzH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_4$ structures along with relative energies.

Figure S.19 - Select $\text{Pz}^{\cdot-}(\text{H}_2\text{O})_6$ and $[\text{PzH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_5$ structures along with relative energies.

Figure S.20 - Select $\text{Tz}^{\cdot-}(\text{H}_2\text{O})$ and $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_2$ structures along with relative energies.

Figure S.21 - Select $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_3$ structures along with relative energies.

Figure S.22 - Select $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_4$ structures along with relative energies.

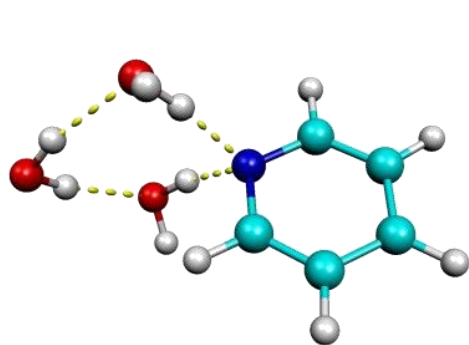
Figure S.23 - Select $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_5$ structures along with relative energies.

Figure S.24 - Select $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_6$ and $[\text{TzH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_5$ structures along with relative energies.

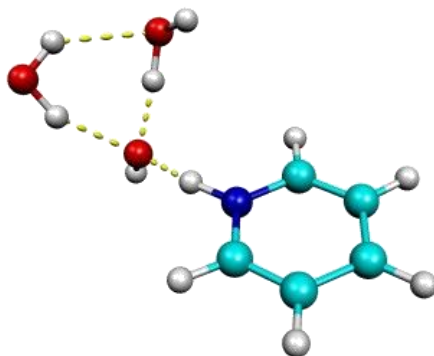
Figure S.25 - Photoelectron Spectra of $\text{Py}^{\cdot-}(\text{H}_2\text{O})_n$ and $[\text{PyH}\cdot\text{OH}]^{\cdot-}(\text{H}_2\text{O})_{n-1}$.

Figure S.26 - Photoelectron Spectra of $\text{Tz}^{\cdot-}(\text{H}_2\text{O})_n$.

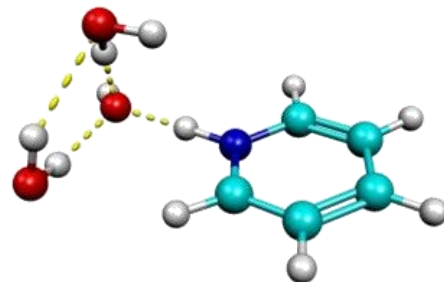
Figure S.1



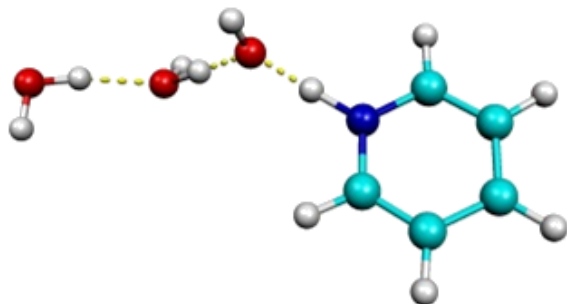
0.00 kcal mol⁻¹



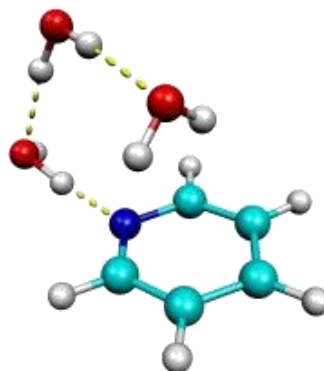
0.02 kcal mol⁻¹



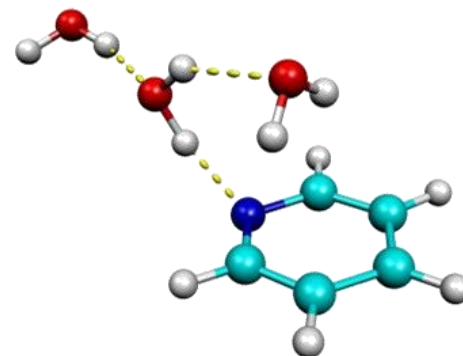
0.10 kcal mol⁻¹



3.77 kcal mol⁻¹

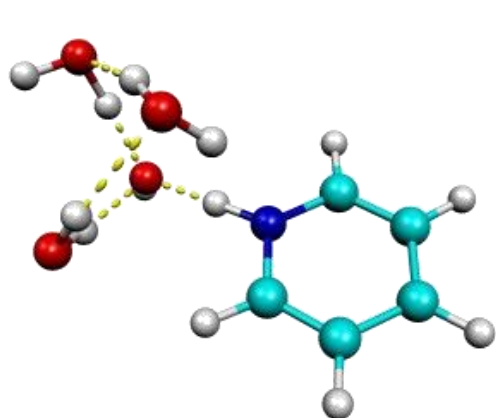


1.19 kcal mol⁻¹

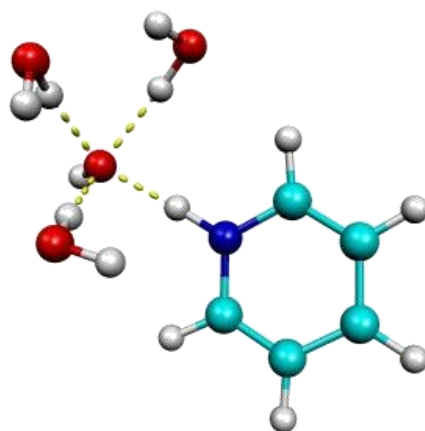


2.62 kcal mol⁻¹

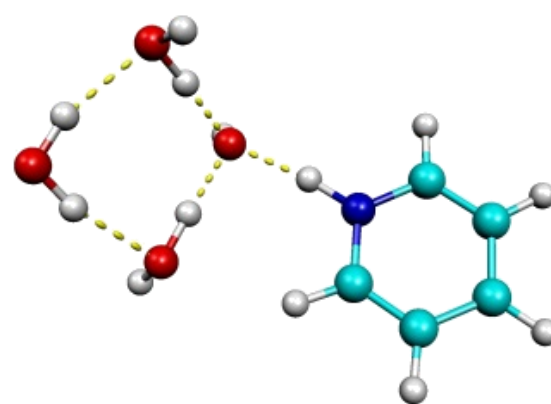
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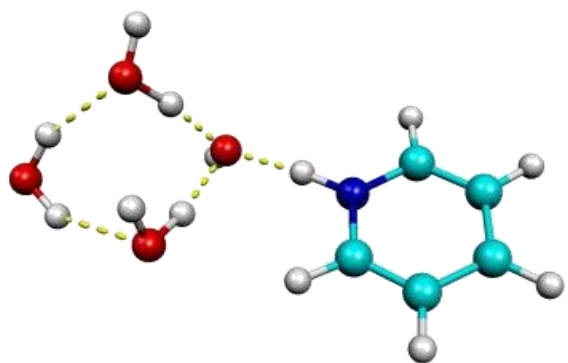
0.00 kcal mol⁻¹



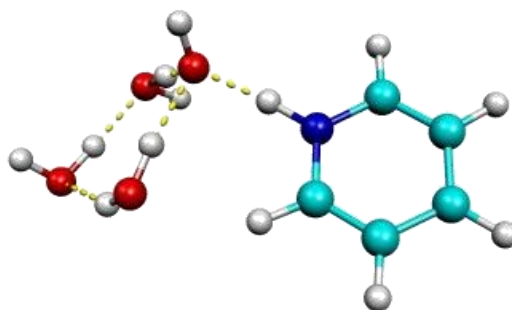
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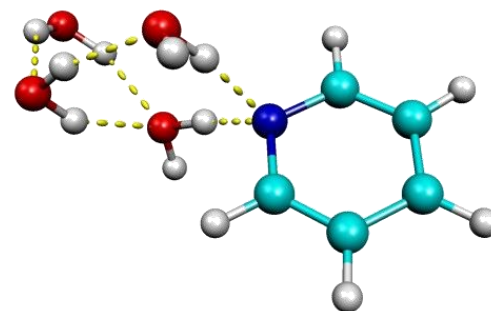
1.21 kcal mol⁻¹



1.53 kcal mol⁻¹

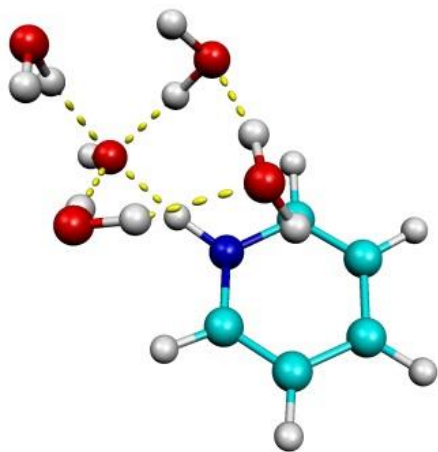


2.19 kcal mol⁻¹

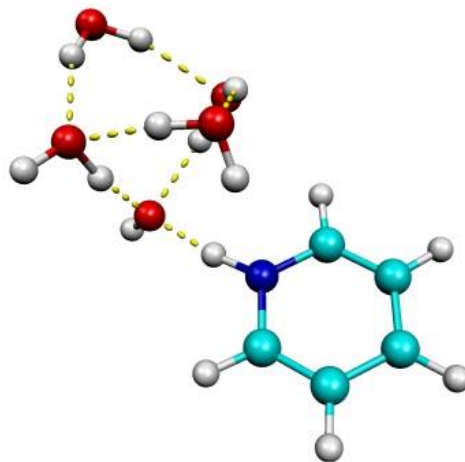


2.60 kcal mol⁻¹

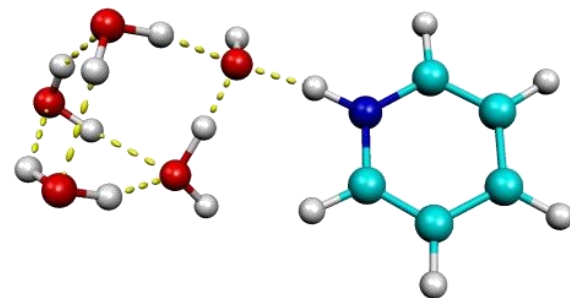
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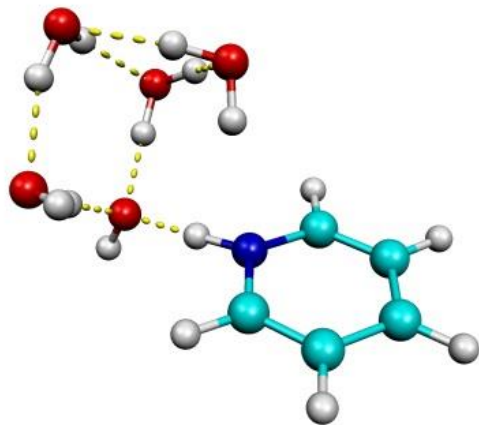
0.00kcal mol⁻¹



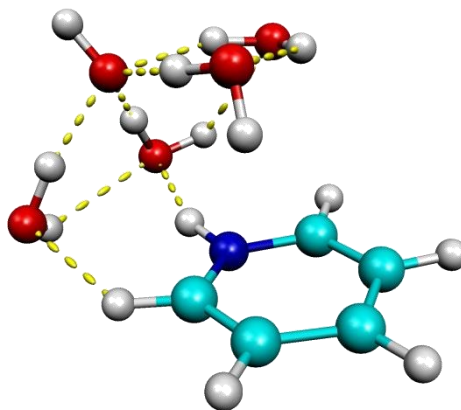
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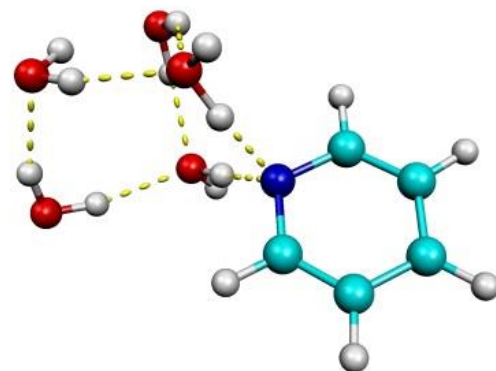
1.91kcal mol⁻¹



2.74 kcal mol⁻¹

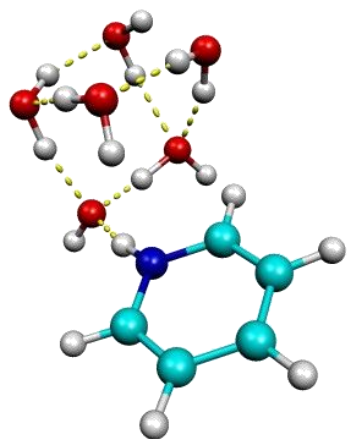


3.33 kcal mol⁻¹

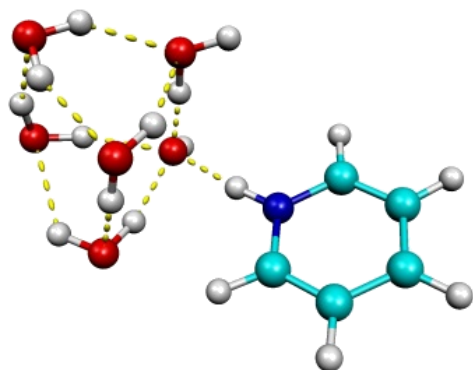


4.32 kcal mol⁻¹

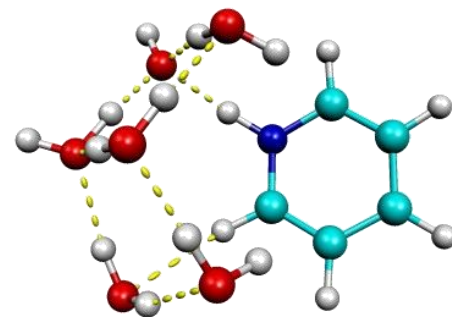
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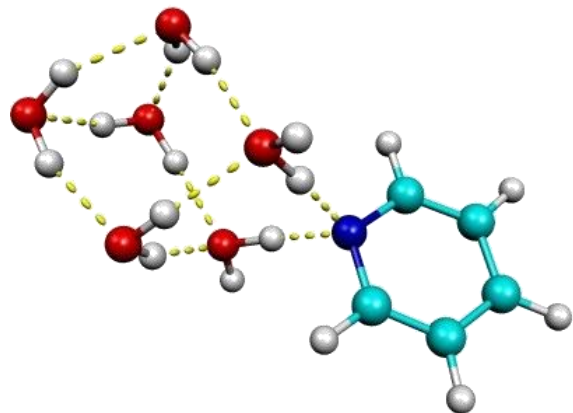
0.00 kcal mol⁻¹



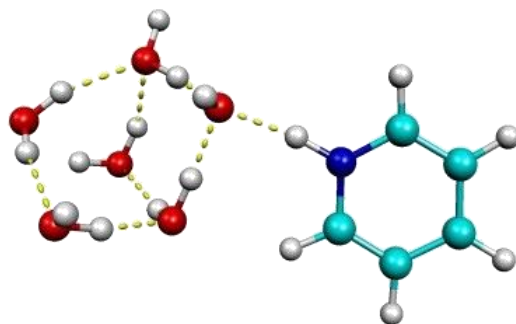
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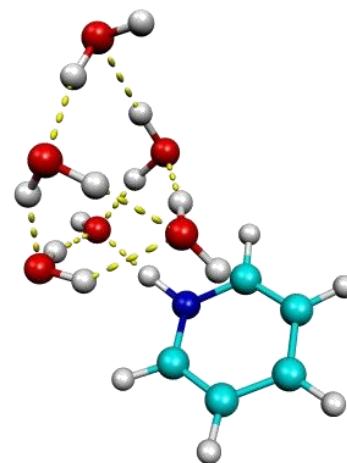
1.82 kcal mol⁻¹



1.96 kcal mol⁻¹

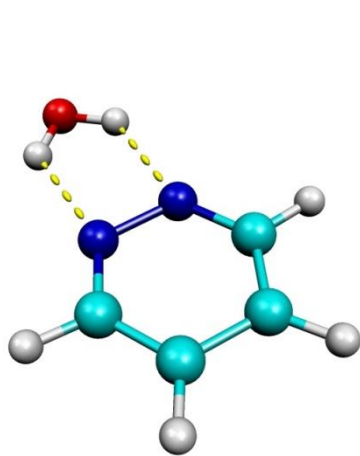


2.33 kcal mol⁻¹

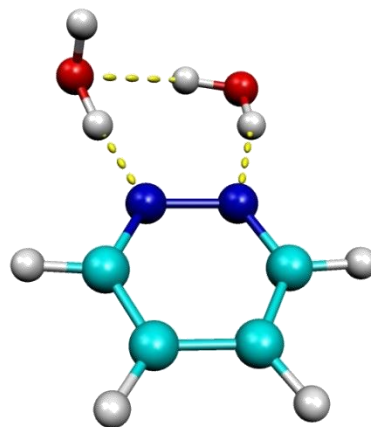


2.87 kcal mol⁻¹

Figure S.5

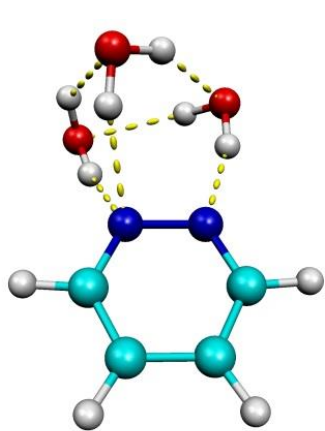


0.00 kcal mol⁻¹

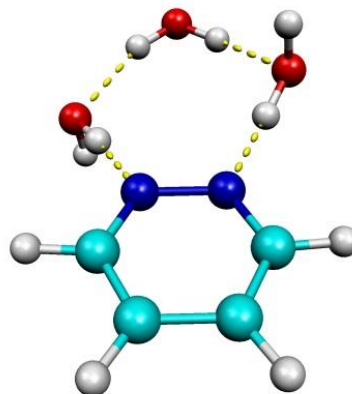


0.00 kcal mol⁻¹

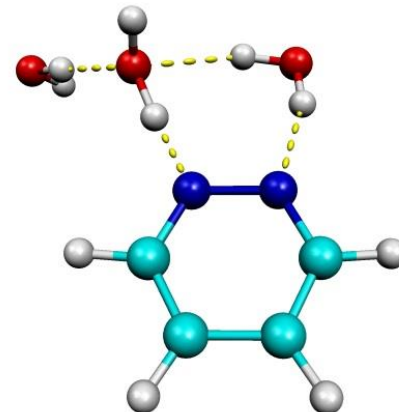
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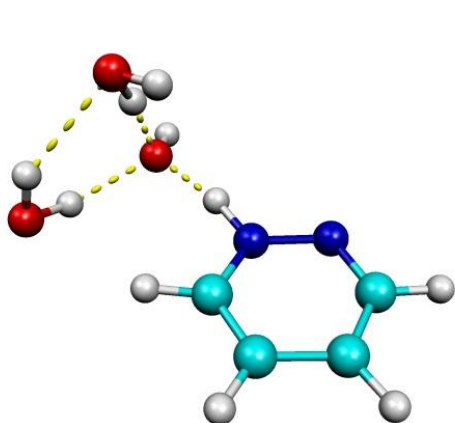
0.00 kcal mol⁻¹



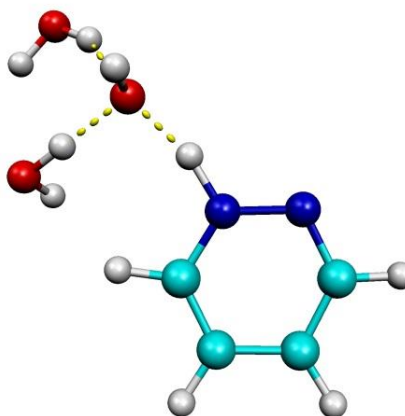
3.53 kcal mol⁻¹



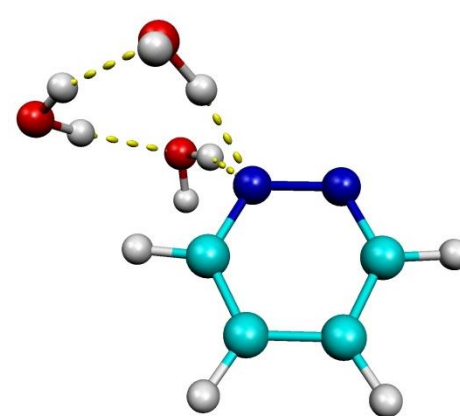
4.98 kcal mol⁻¹



6.48 kcal mol⁻¹

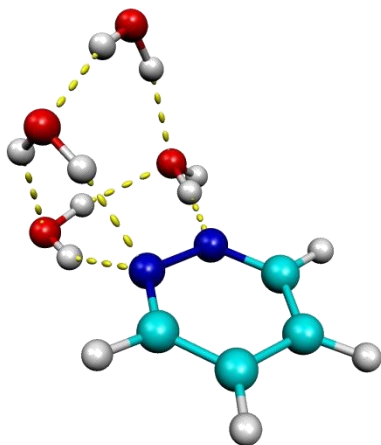


8.02 kcal mol⁻¹

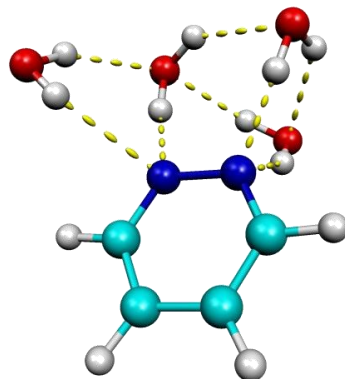


8.48 kcal mol⁻¹

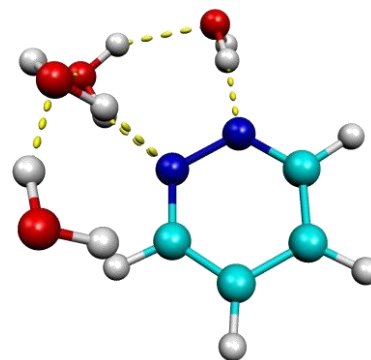
Figure S.7



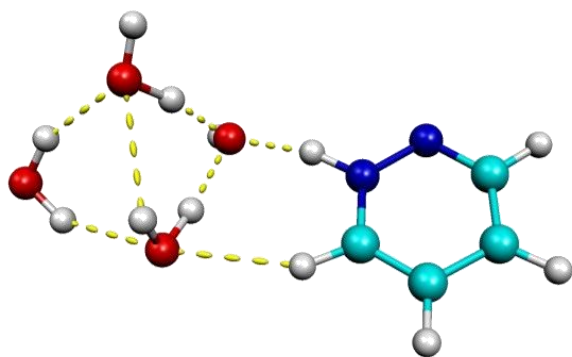
0.00 kcal mol⁻¹



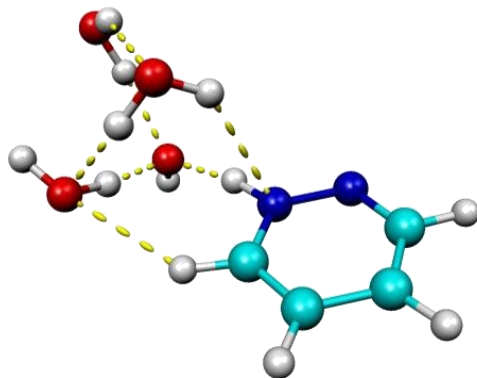
0.32 kcal mol⁻¹



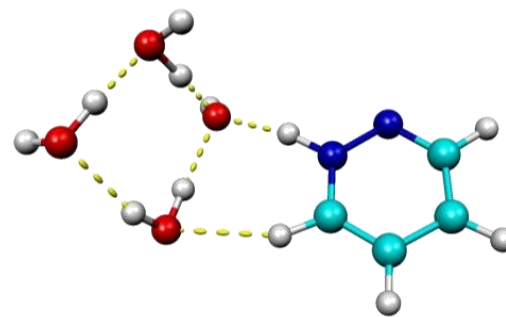
4.19 kcal mol⁻¹



4.50 kcal mol⁻¹

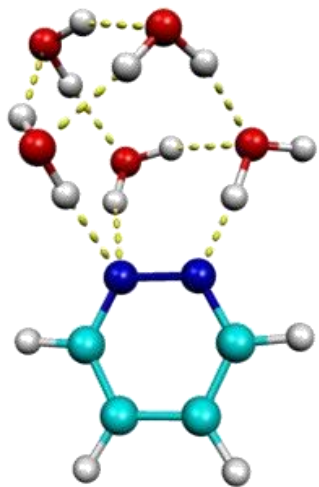


4.69 kcal mol⁻¹

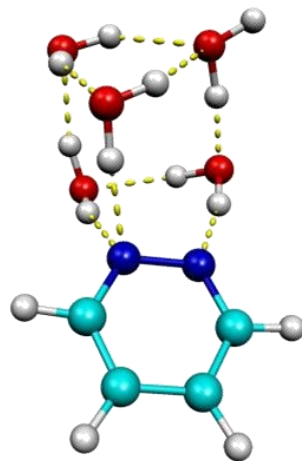


4.82 kcal mol⁻¹

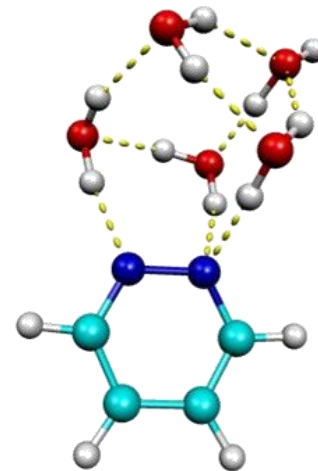
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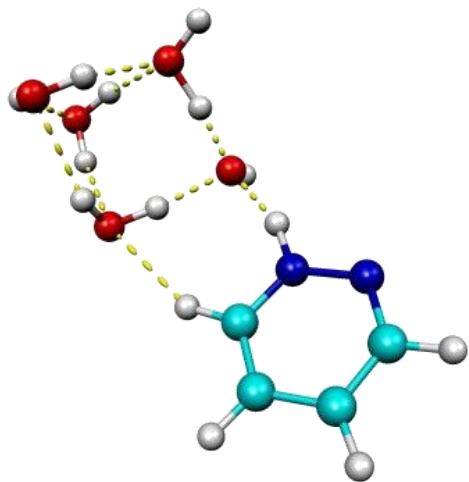
0.00 kcal mol⁻¹



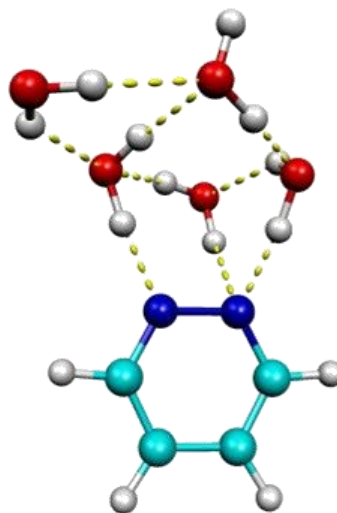
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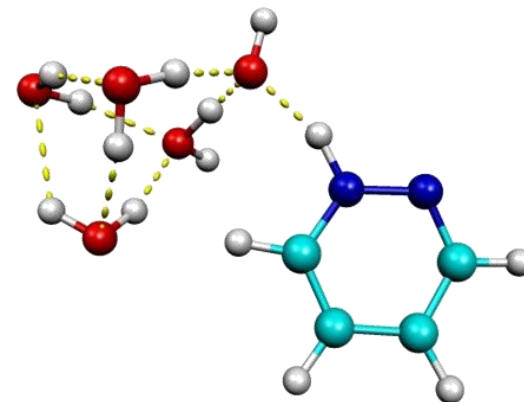
1.33 kcal mol⁻¹



4.14 kcal mol⁻¹

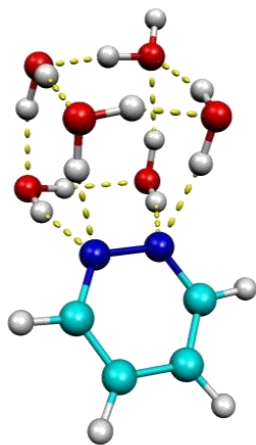


4.16 kcal mol⁻¹

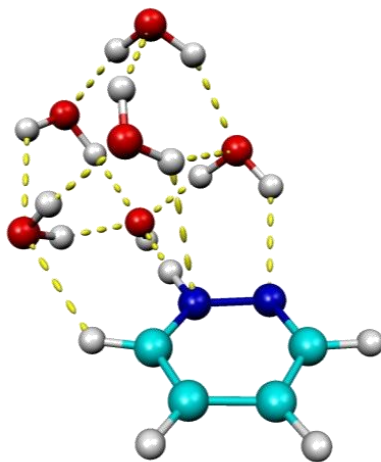


4.23 kcal mol⁻¹

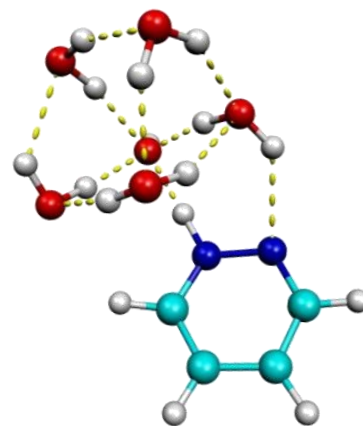
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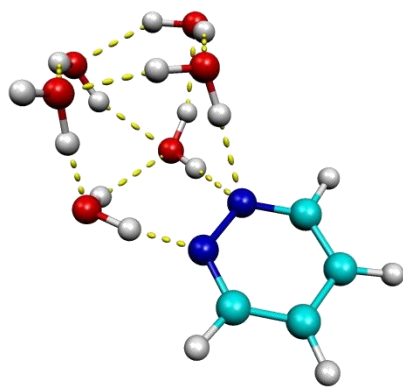
0.00 kcal mol⁻¹



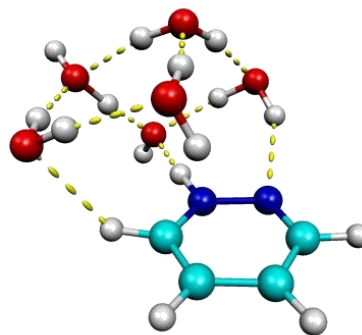
2.22 kcal mol⁻¹



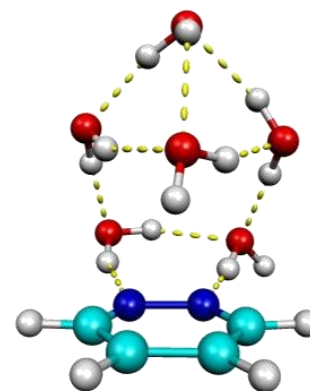
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2.97 kcal mol⁻¹

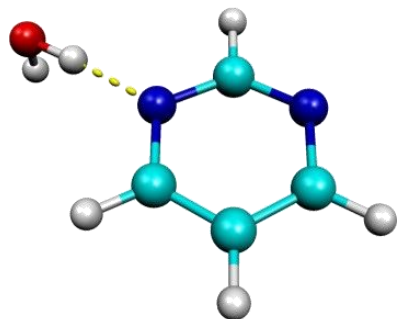


4.20 kcal mol⁻¹

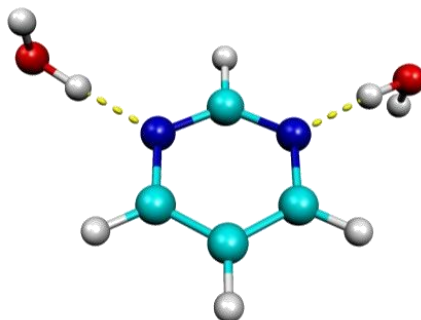


4.20 kcal mol⁻¹

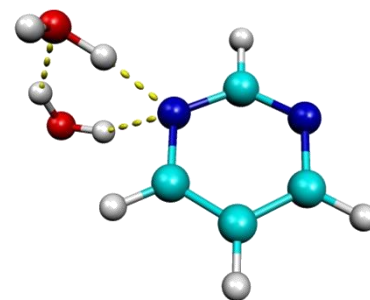
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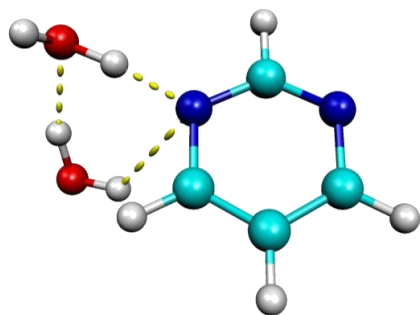
0.00 kcal mol⁻¹



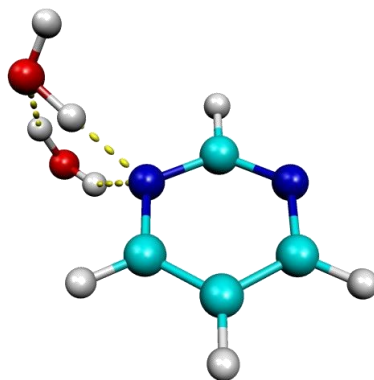
0.00 kcal mol⁻¹



0.64 kcal mol⁻¹

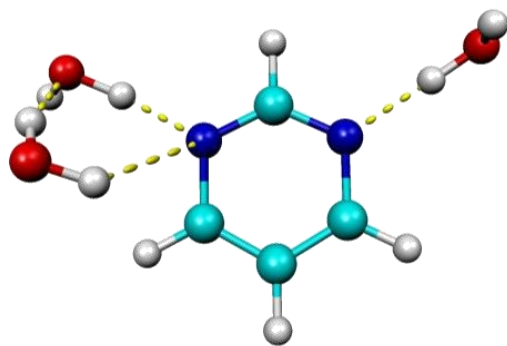


0.73 kcal mol⁻¹

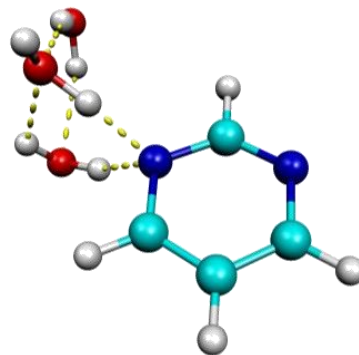


0.77 kcal mol⁻¹

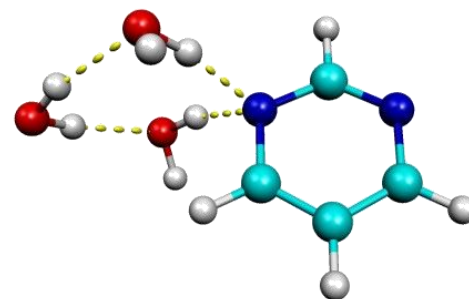
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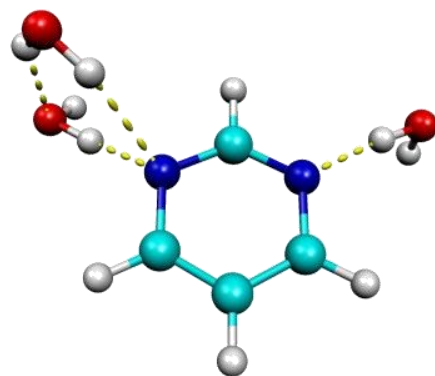
0.00 kcal mol⁻¹



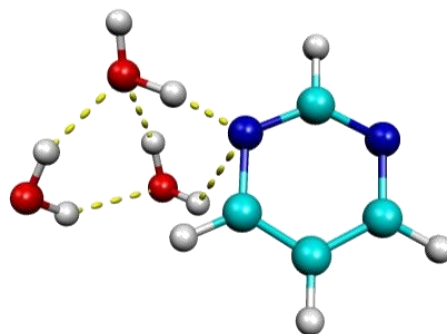
0.29 kcal mol⁻¹



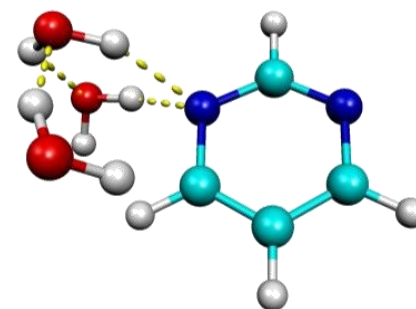
0.44 kcal mol⁻¹



0.50 kcal mol⁻¹

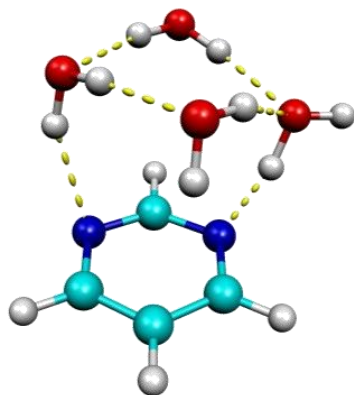


0.53 kcal mol⁻¹

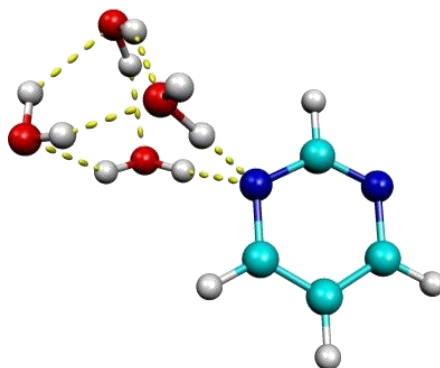


1.28 kcal mol⁻¹

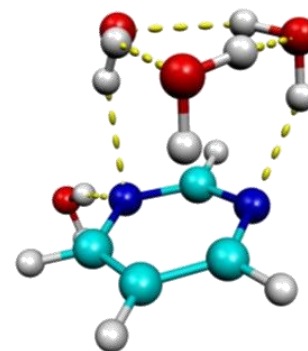
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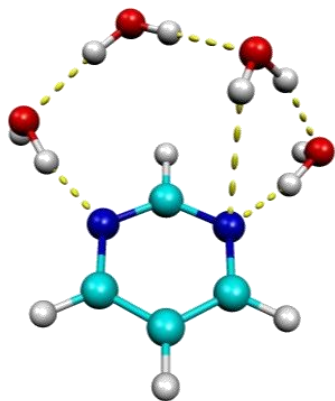
0.00 kcal mol⁻¹



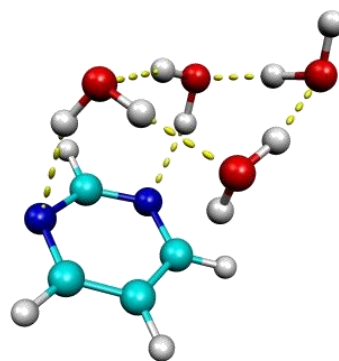
0.22 kcal mol⁻¹



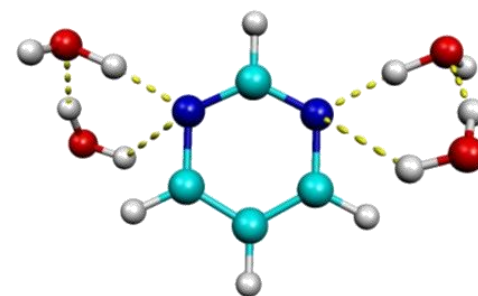
1.60 kcal mol⁻¹



1.92 kcal mol⁻¹

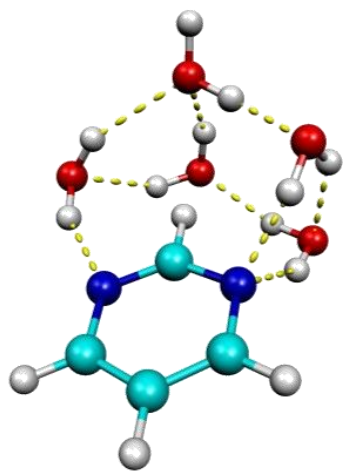


2.30 kcal mol⁻¹

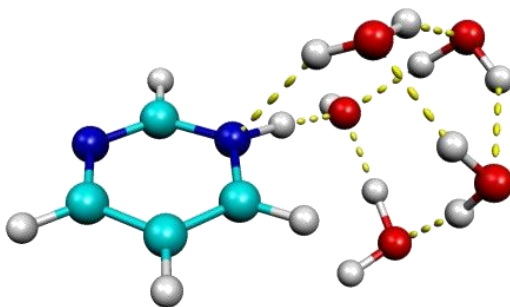


2.90 kcal mol⁻¹

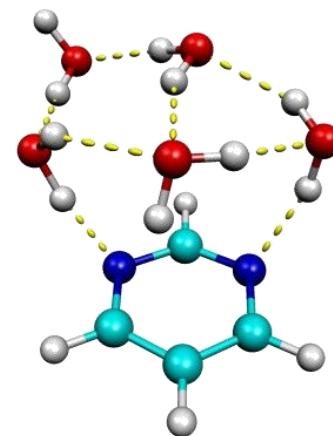
Figure S.13



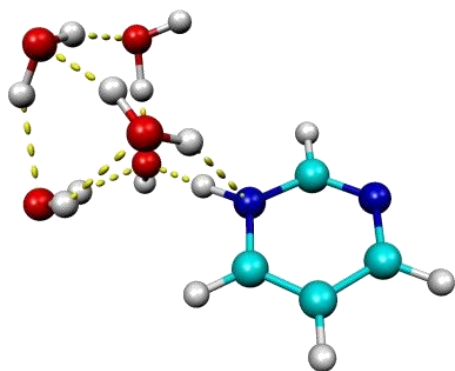
0.00 kcal mol⁻¹



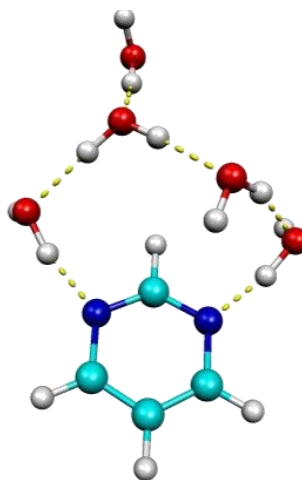
1.24 kcal mol⁻¹



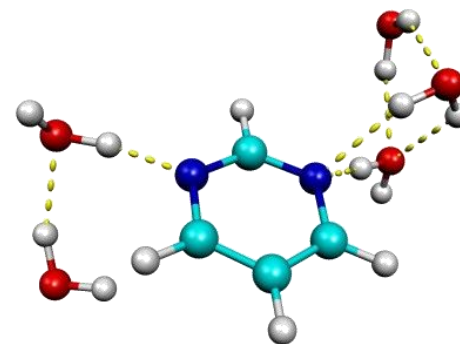
1.42 kcal mol⁻¹



1.43 kcal mol⁻¹

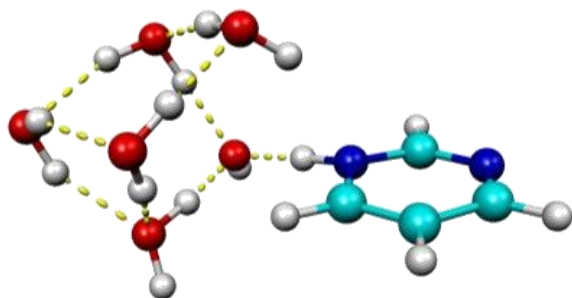


3.33 kcal mol⁻¹

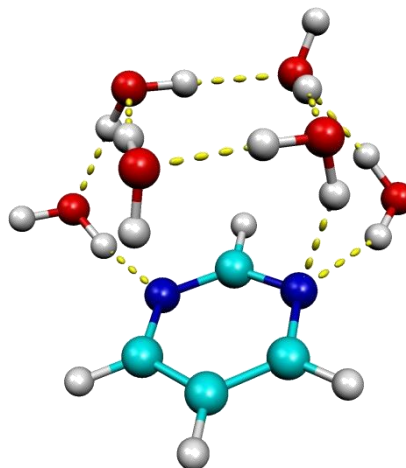


3.65 kcal mol⁻¹

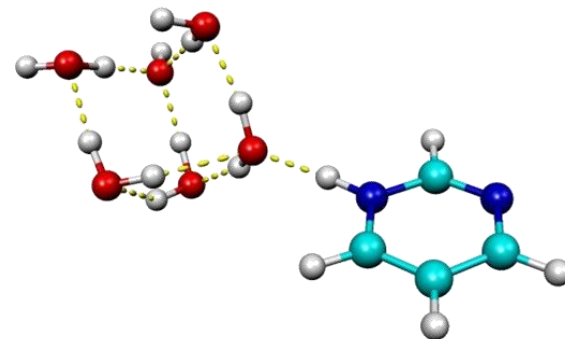
Figure S.14



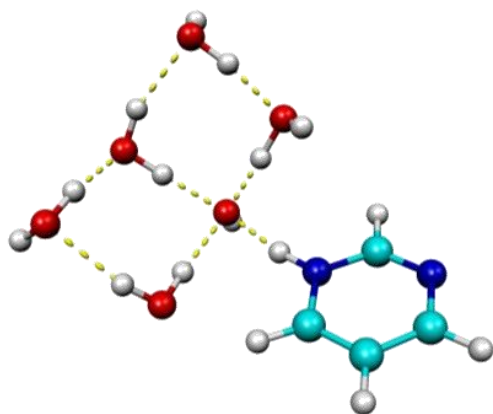
0.00 kcal mol⁻¹



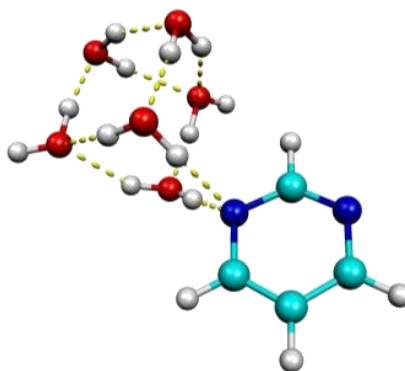
0.00 kcal mol⁻¹



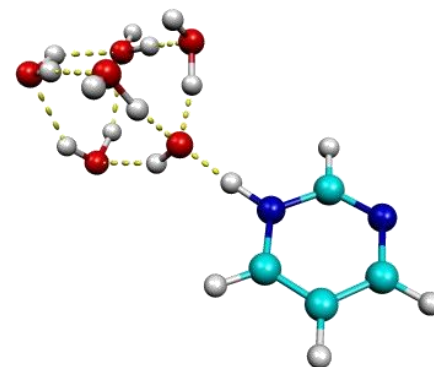
2.81 kcal mol⁻¹



3.87 kcal mol⁻¹

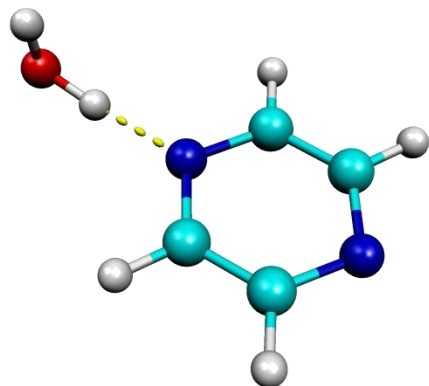


4.05 kcal mol⁻¹

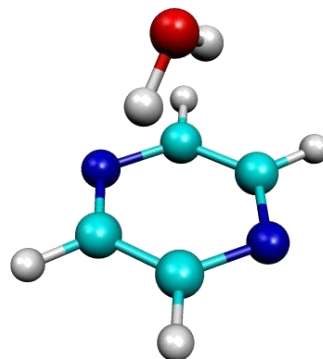


4.46 kcal mol⁻¹

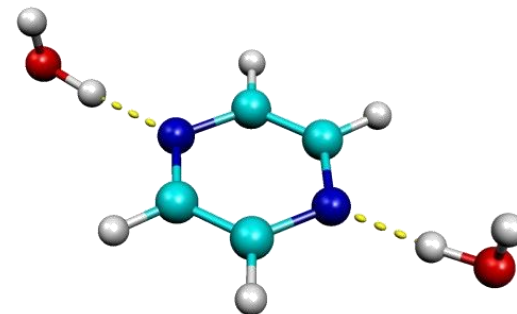
Figure S.15



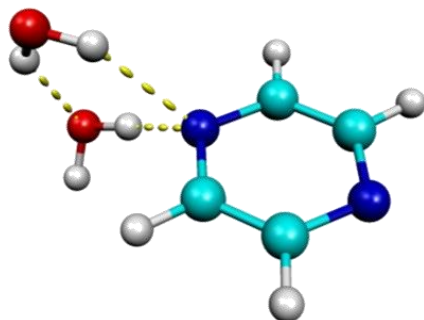
0.00 kcal mol⁻¹



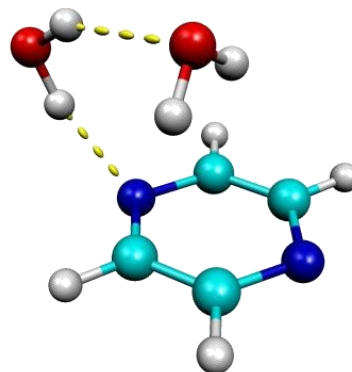
4.88 kcal mol⁻¹



0.00 kcal mol⁻¹

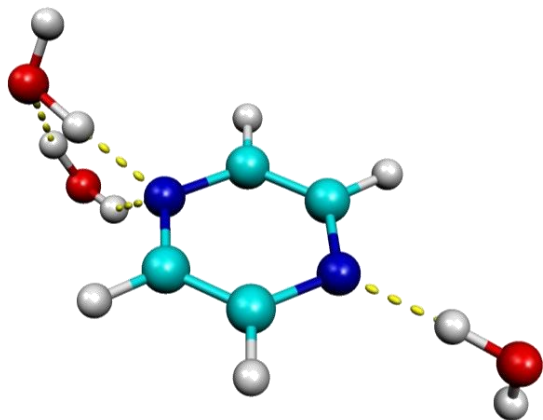


1.17 kcal mol⁻¹

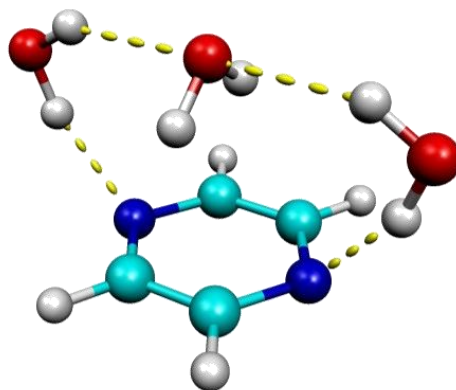


2.46 kcal mol⁻¹

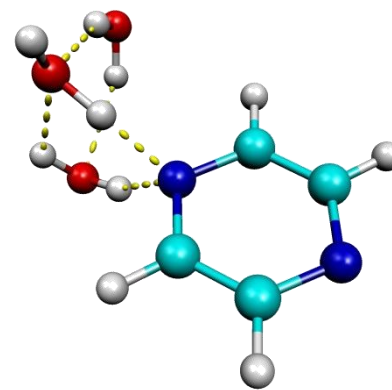
Figure S.16



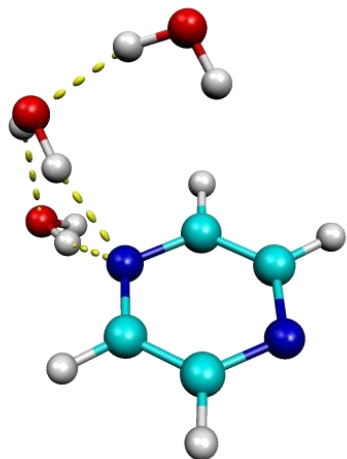
0.00 kcal mol⁻¹



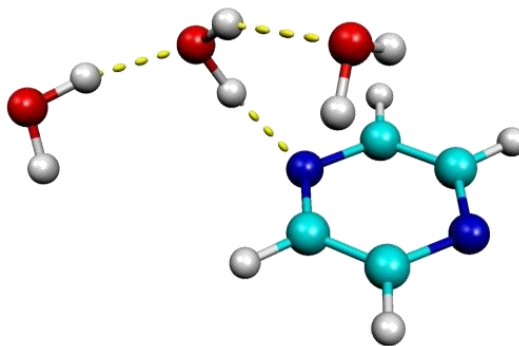
0.23 kcal mol⁻¹



0.80 kcal mol⁻¹

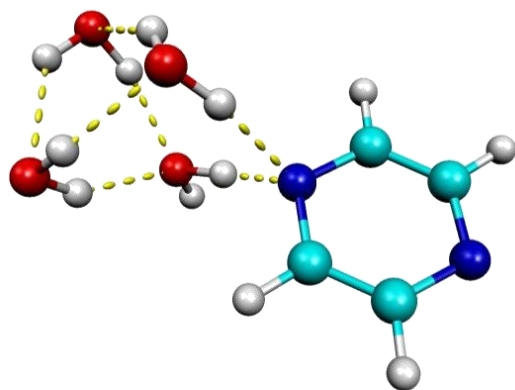


2.37 kcal mol⁻¹

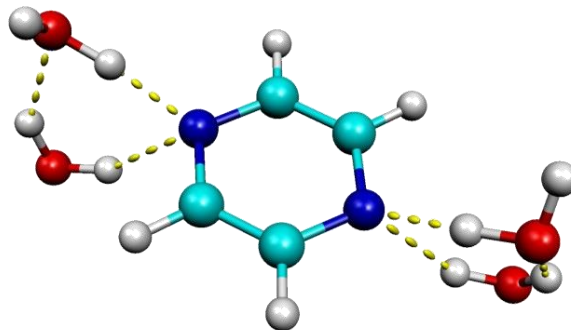


3.80 kcal mol⁻¹

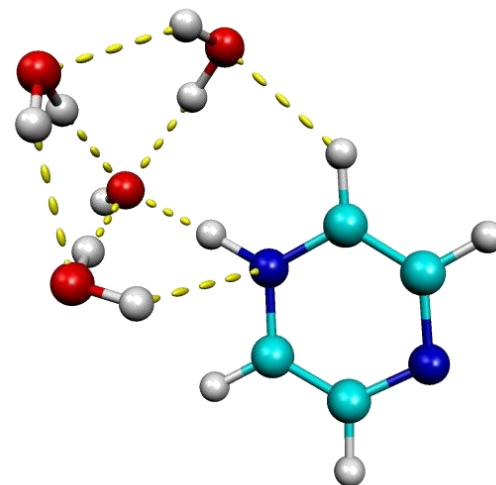
Figure S.17



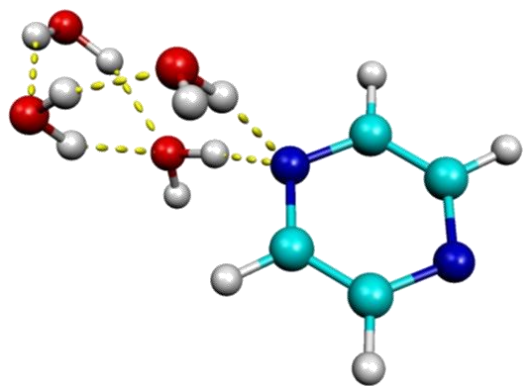
0.00 kcal mol⁻¹



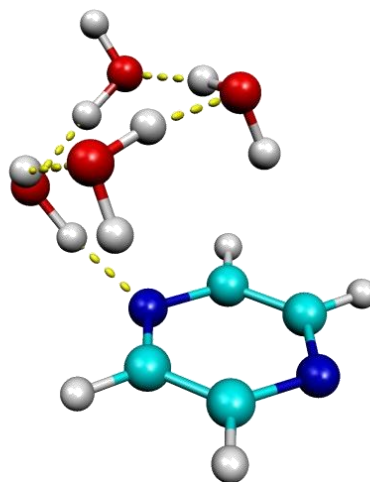
2.22 kcal mol⁻¹



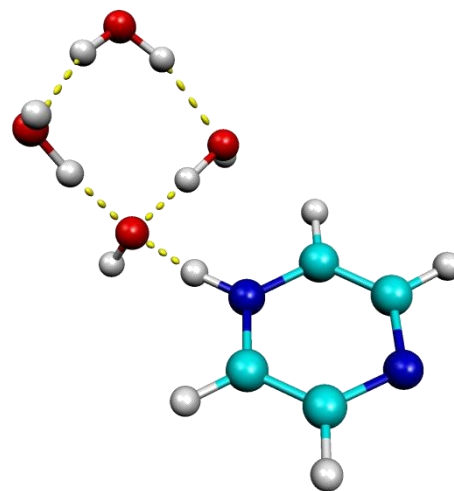
2.25 kcal mol⁻¹



2.87 kcal mol⁻¹

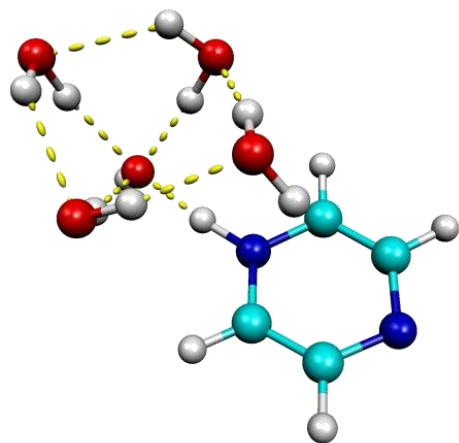


2.96 kcal mol⁻¹

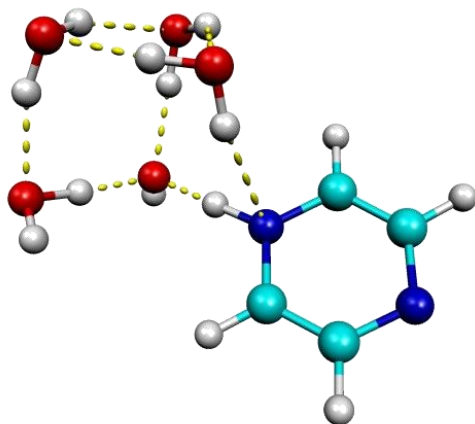


3.21 kcal mol⁻¹

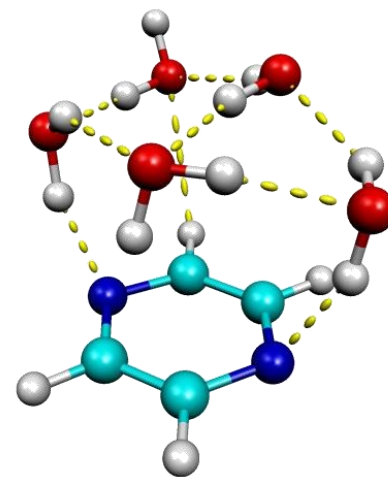
Figure S.18



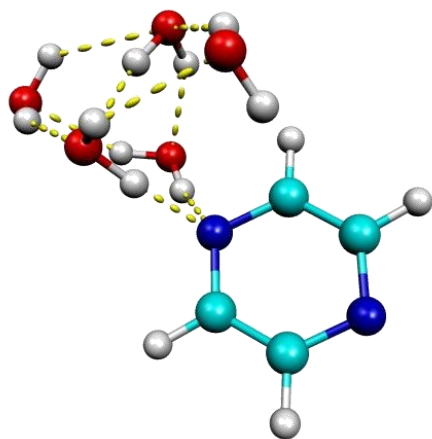
0.00 kcal mol⁻¹



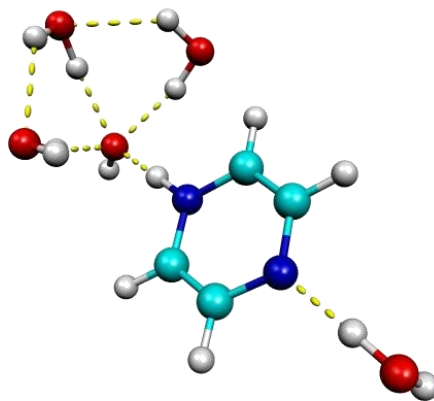
2.58 kcal mol⁻¹



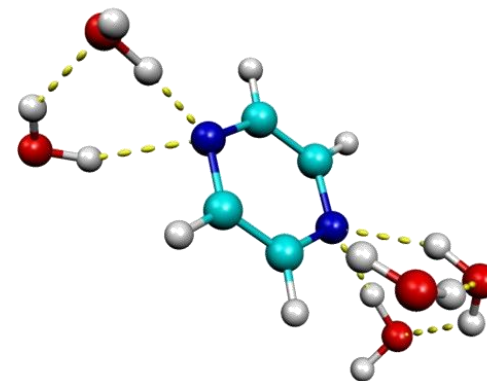
3.37 kcal mol⁻¹



3.50 kcal mol⁻¹

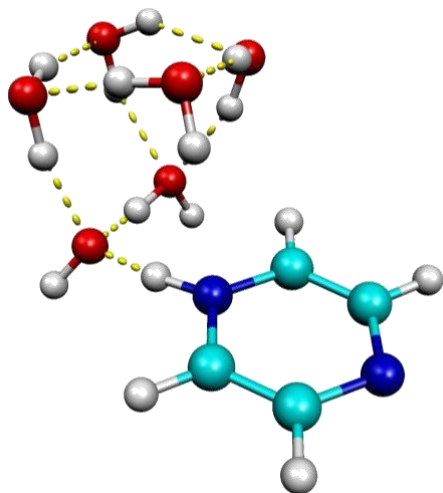


3.80 kcal mol⁻¹

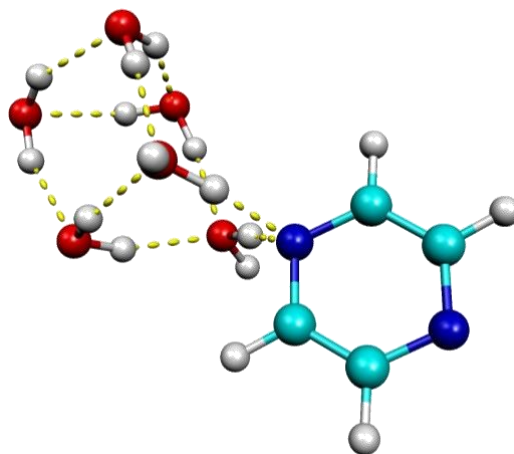


4.75 kcal mol⁻¹

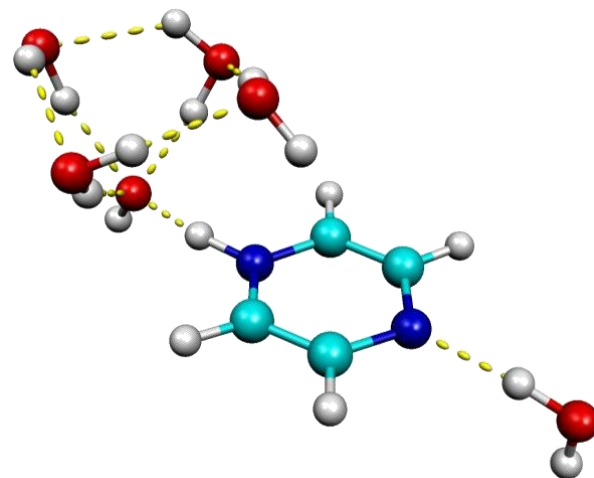
Figure S.19



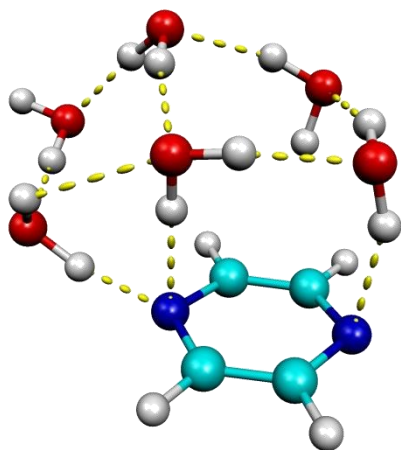
0.00 kcal mol⁻¹



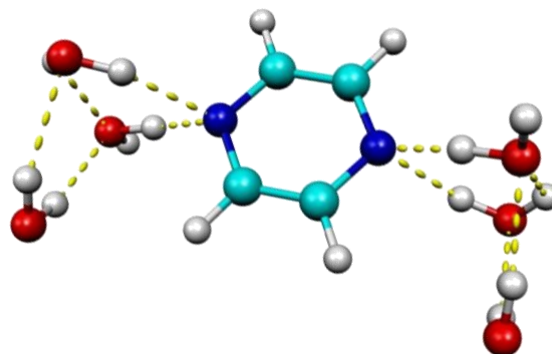
0.13 kcal mol⁻¹



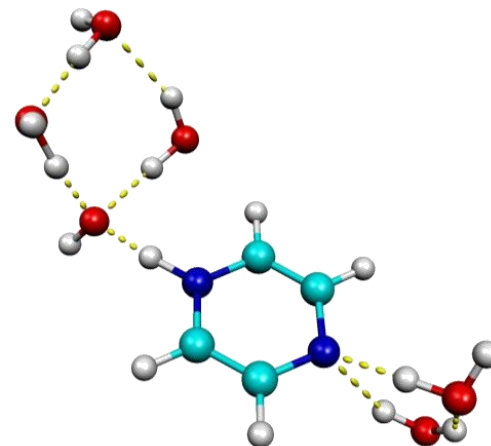
1.73 kcal mol⁻¹



2.11 kcal mol⁻¹

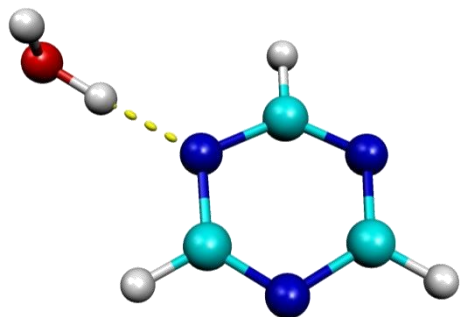


3.87 kcal mol⁻¹

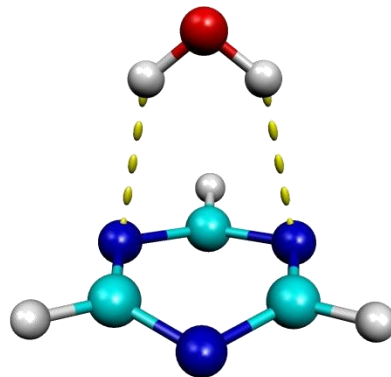


7.13 kcal mol⁻¹

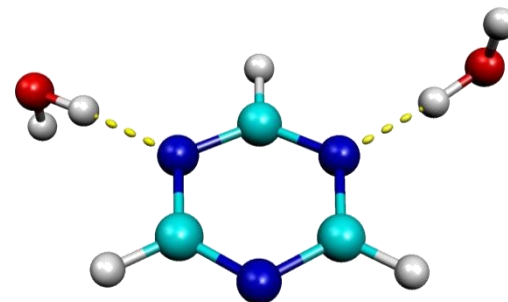
Figure S.20



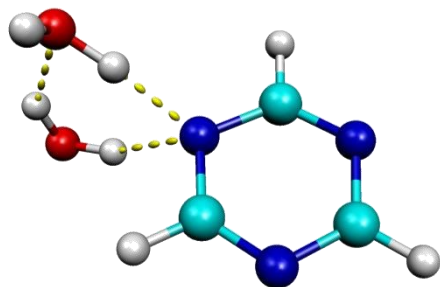
0.00 kcal mol⁻¹



3.57 kcal mol⁻¹

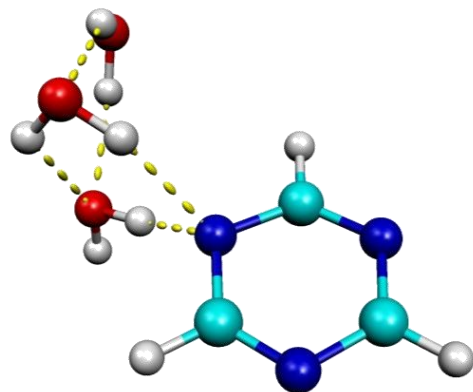


0.00 kcal mol⁻¹

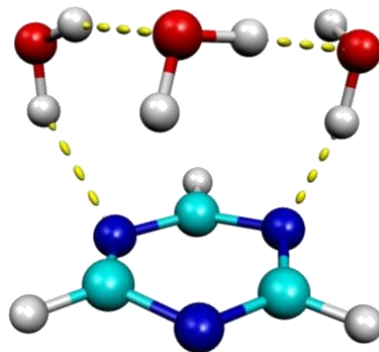


1.17 kcal mol⁻¹

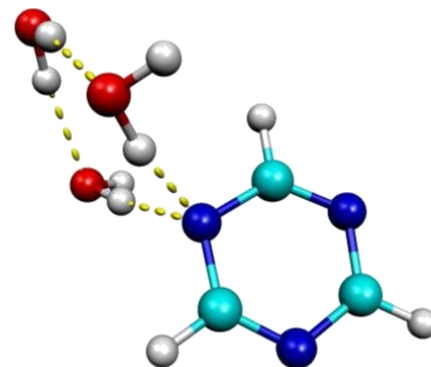
Figure S.21



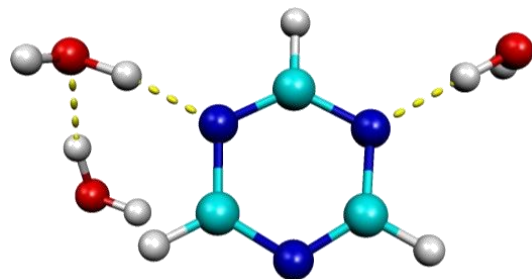
0.00 kcal mol⁻¹



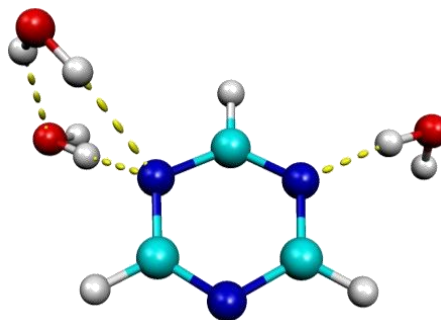
0.05 kcal mol⁻¹



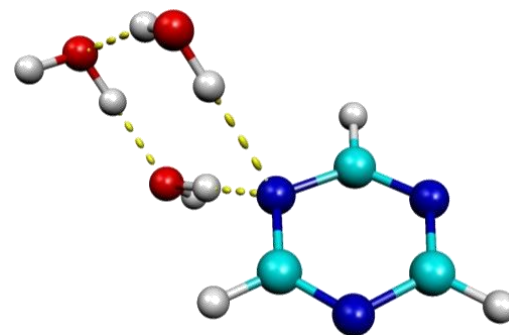
0.69 kcal mol⁻¹



1.29 kcal mol⁻¹

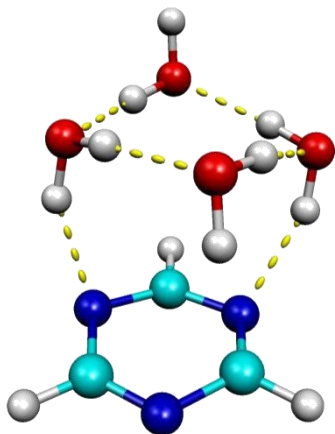


1.30 kcal mol⁻¹

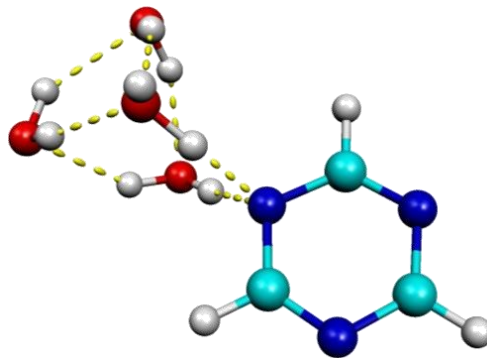


1.84 kcal mol⁻¹

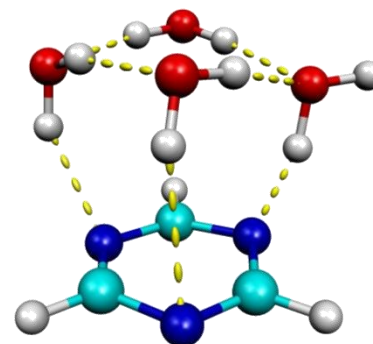
Figure S.22



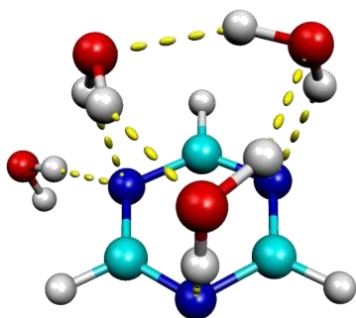
0.00 kcal mol⁻¹



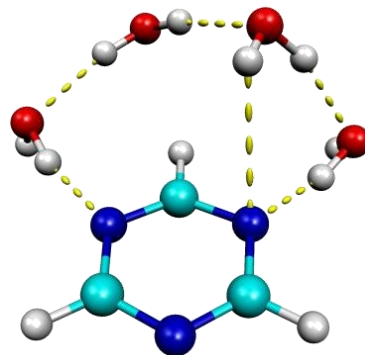
0.05 kcal mol⁻¹



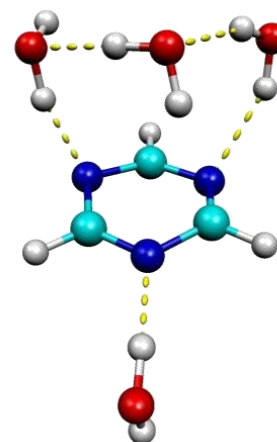
0.82 kcal mol⁻¹



1.37 kcal mol⁻¹

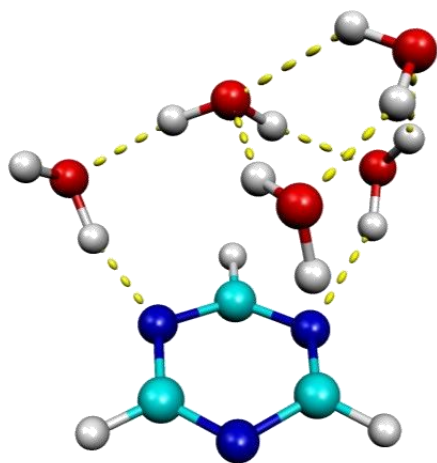


2.77 kcal mol⁻¹

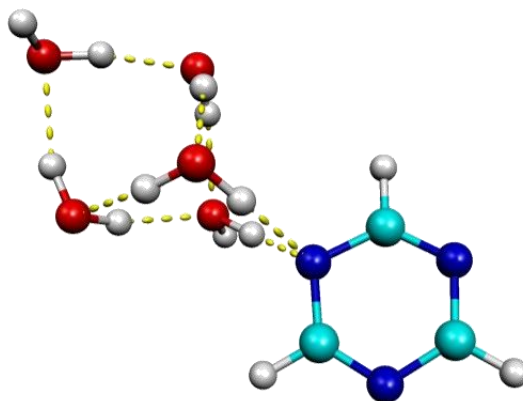


4.00 kcal mol⁻¹

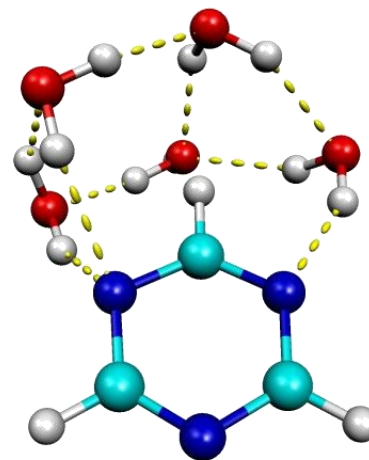
Figure S.23



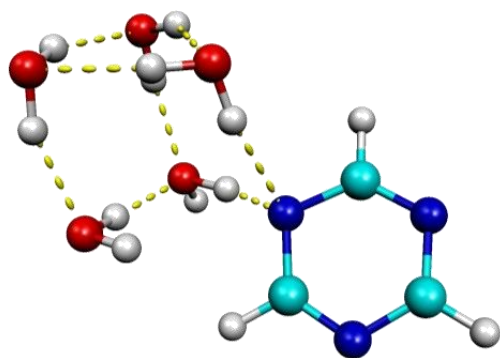
0.00 kcal mol⁻¹



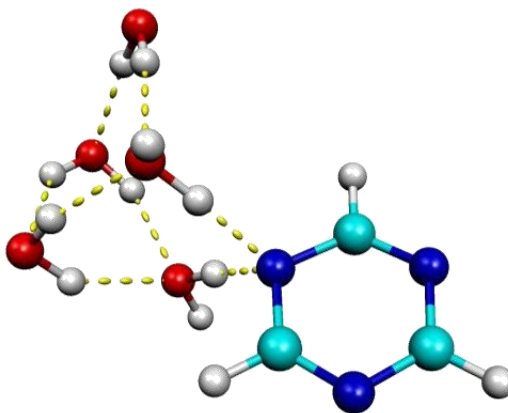
0.07 kcal mol⁻¹



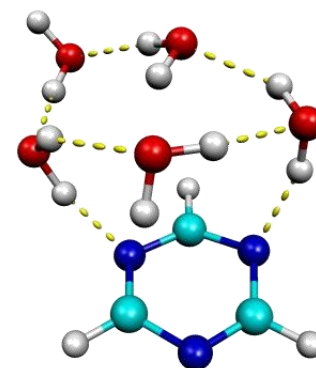
0.45 kcal mol⁻¹



2.02 kcal mol⁻¹

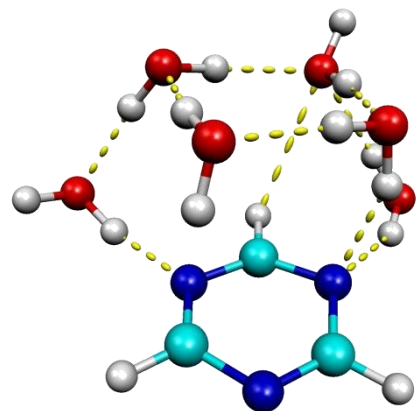


2.15 kcal mol⁻¹

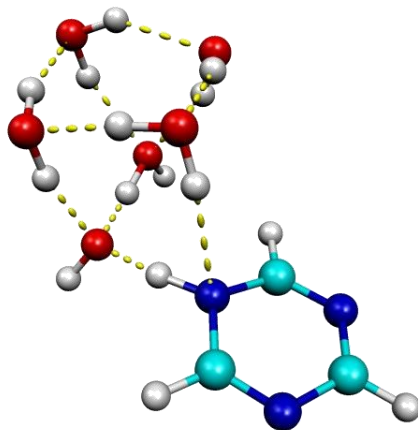


2.54 kcal mol⁻¹

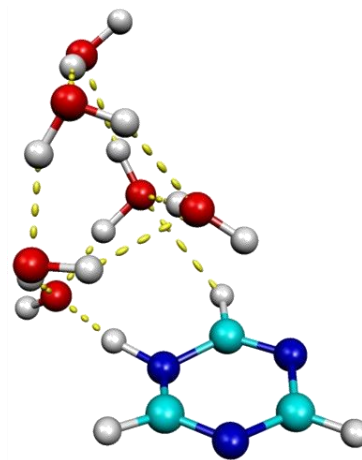
Figure S.24



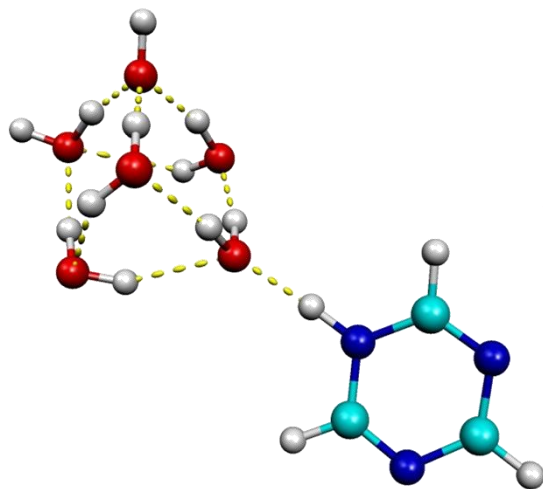
0.00 kcal mol⁻¹



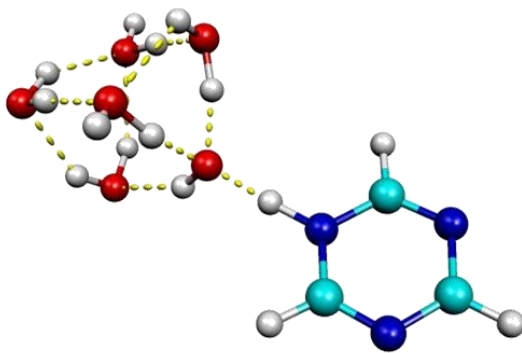
1.40 kcal mol⁻¹



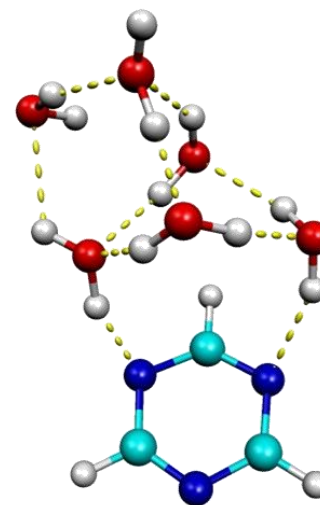
3.55 kcal mol⁻¹



4.12 kcal mol⁻¹



4.76 kcal mol⁻¹



4.85 kcal mol⁻¹

Figure S.25

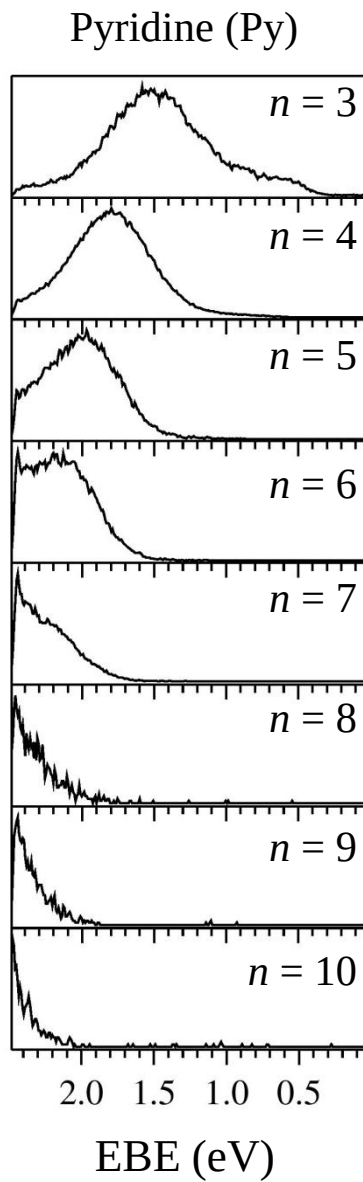


Figure S.26

