Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Organic Heterocyclic Molecules go to Superalkali

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Neutral and Cations [At b3lyp/6-31+G(d,p)]

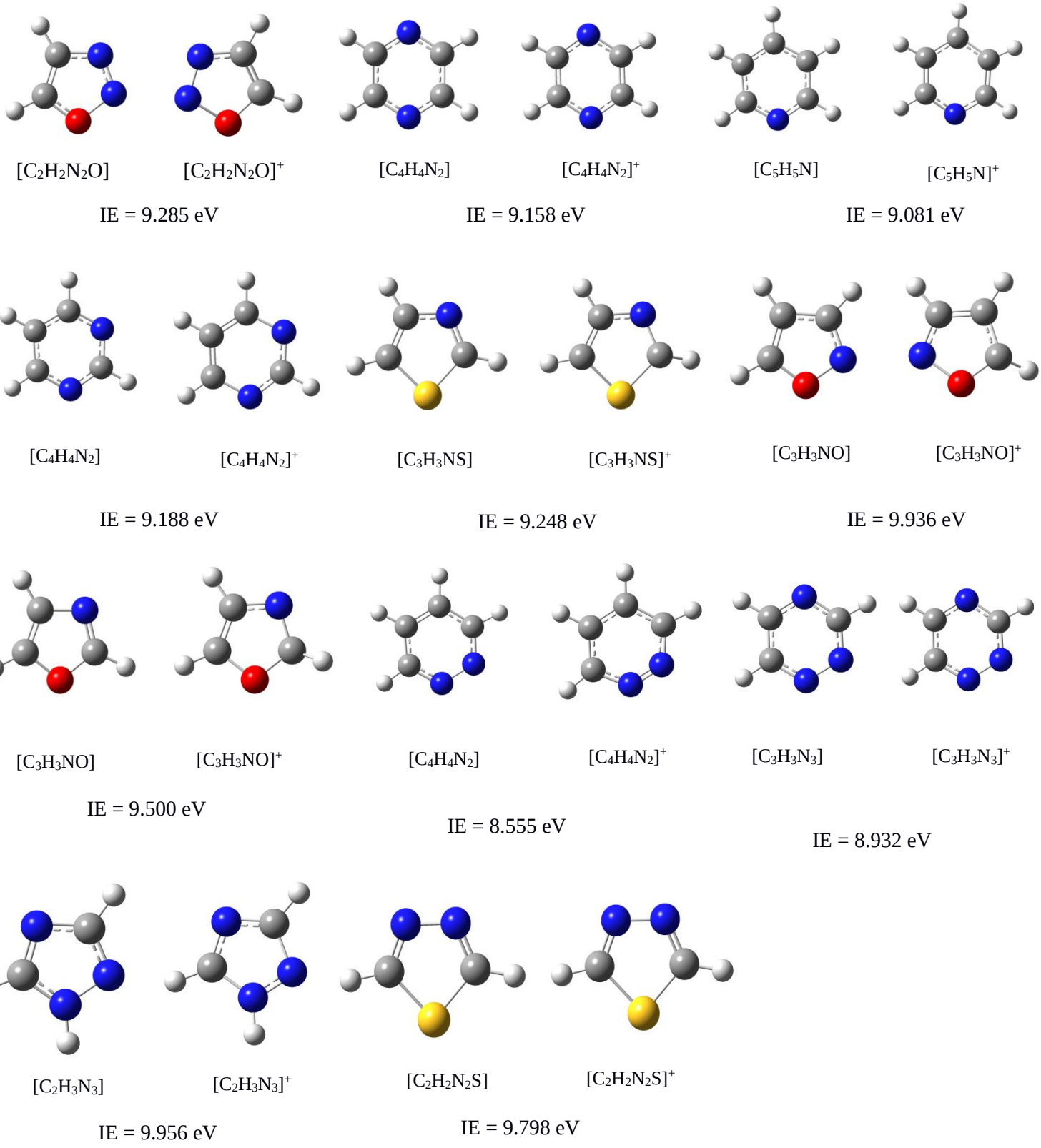
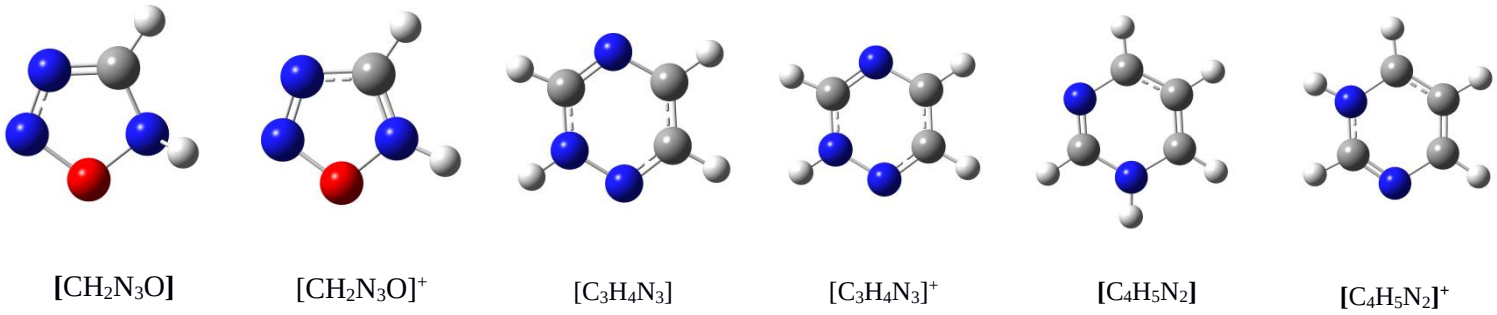
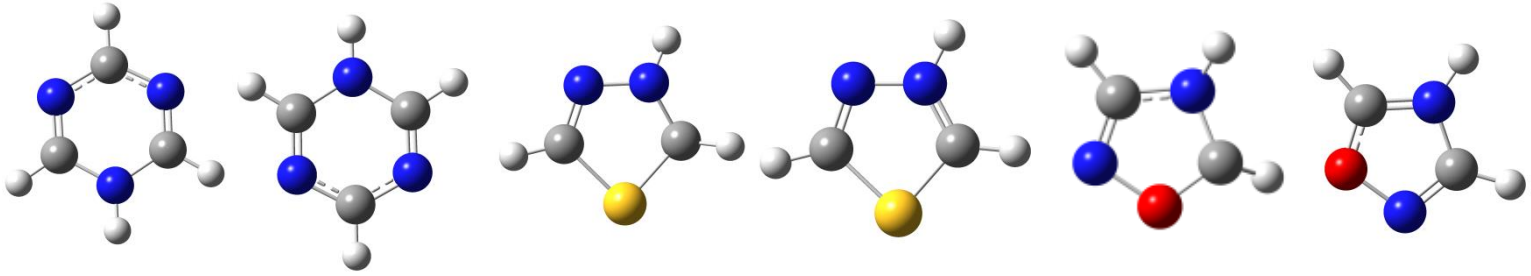


Figure S-I: Optimized geometries, Ionization energies of neutral and cations of aromatic heterocyclic molecules.



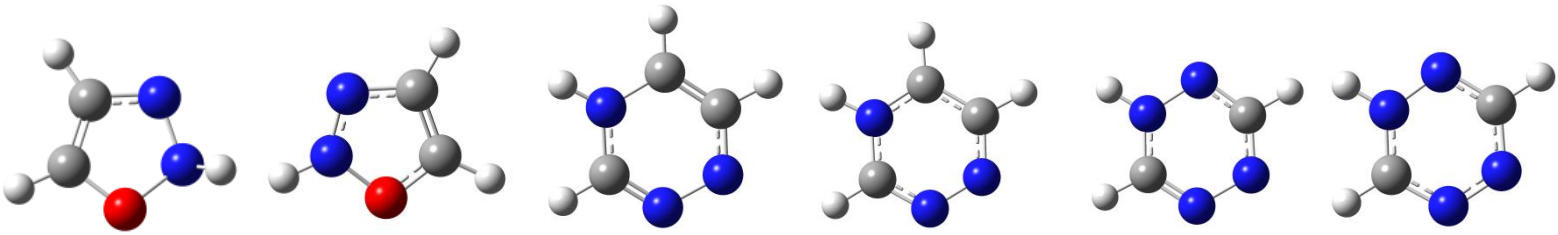
[CH_2N_3O] $[CH_2N_3O]^+$ $[C_3H_4N_3]$ $[C_3H_4N_3]^+$ **[$C_4H_5N_2$]** **[$C_4H_5N_2$]$^+$**

IE = 7.515 eV IE = 6.638 eV IE = **5.**700 eV



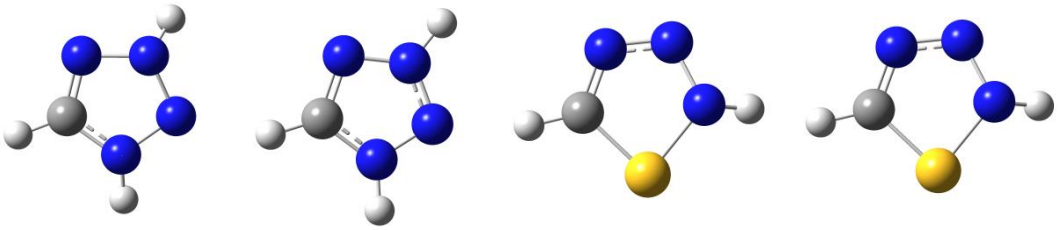
$[C_3H_4N_3]$ $[C_3H_4N_3]^+$ $[C_2H_3N_2S]$ $[C_2H_3N_2S]^+$ $[C_2H_3N_2O]$ $[C_2H_3N_2O]^+$

IE = 6.231 eV IE = 5.728 eV IE = 5.951 eV



$[C_2H_3N_2O]$ $[C_2H_3N_2O]^+$ $[C_3H_4N_3]$ $[C_3H_4N_3]^+$ $[C_2H_3N_4]$ $[C_2H_3N_4]^+$

IE = 6.756 eV IE = 6.767 eV IE = 7.737 eV

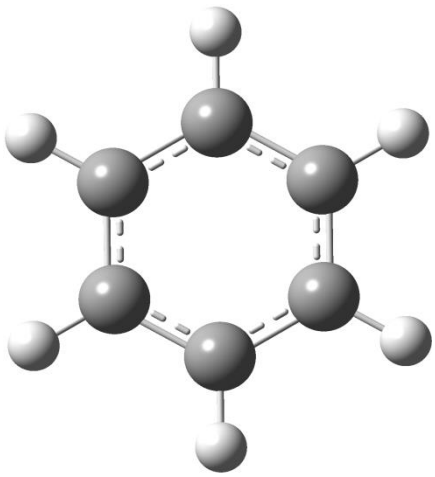


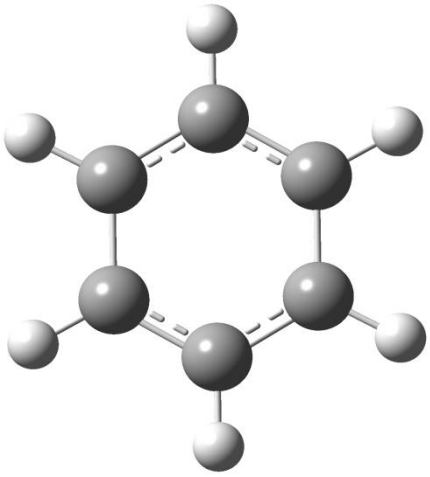
$[CH_3N_4]$ $[CH_3N_4]^+$ $[CH_2N_3S]$ $[CH_2N_3S]^+$

IE = 5.943 eV IE = 7.065 eV

Figure S-II: Optimized geometries, Ionization energies of neutral and cations of one C by N substituted aromatic heterocyclic molecules.

Neutrals **Cations**

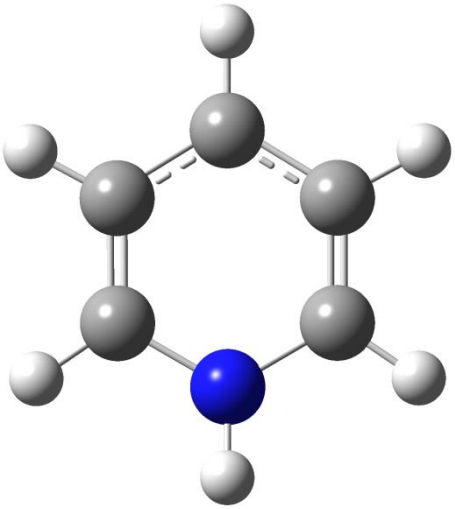


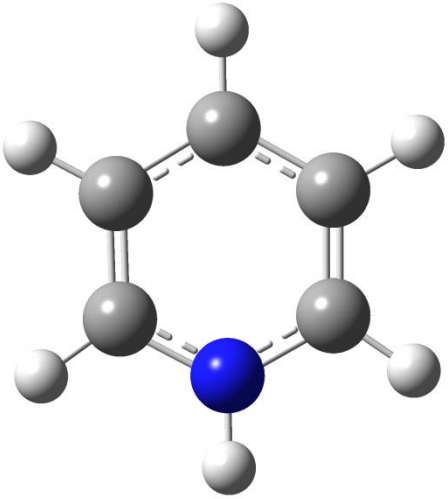


[C_6H_6] **[C_6H_6]$^+$**

IE = 9.065 eV [at b3lyp/6-31+G(d,p)]

Figure S-III: Optimized geometries, Ionization energy of neutral and cation of benzene.



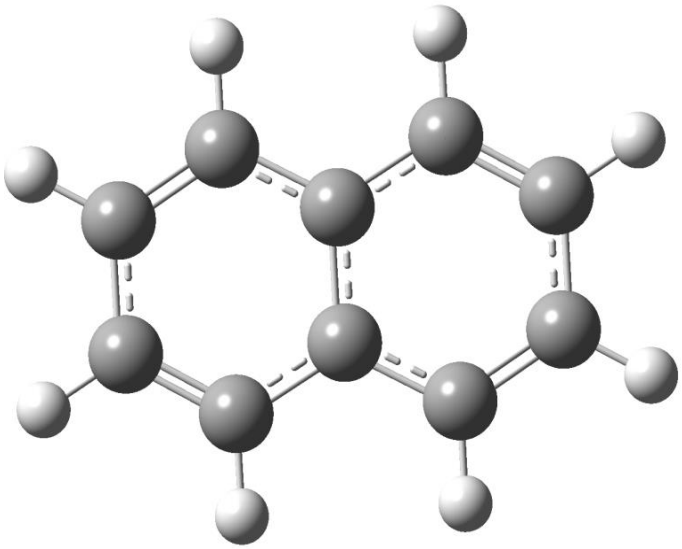


[C_5H_6N] **[C_5H_6N]$^+$**

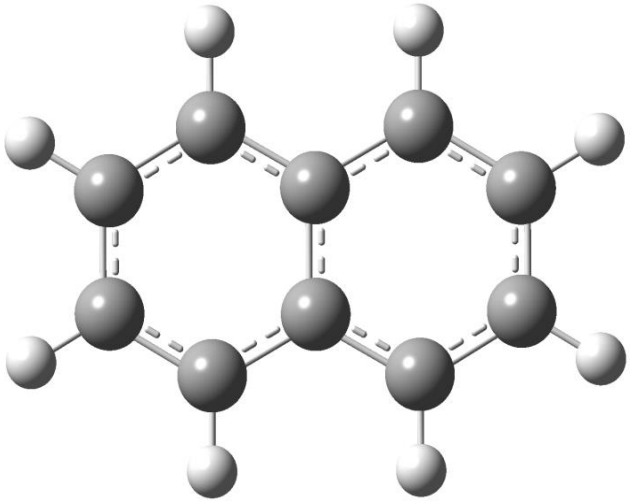
IE = 5.158 eV [at b3lyp/6-31+G(d,p)]

Figure S-IV: Optimized geometries, Ionization energy of neutral and cation of [C_5H_6N].

Neutrals **Cations**



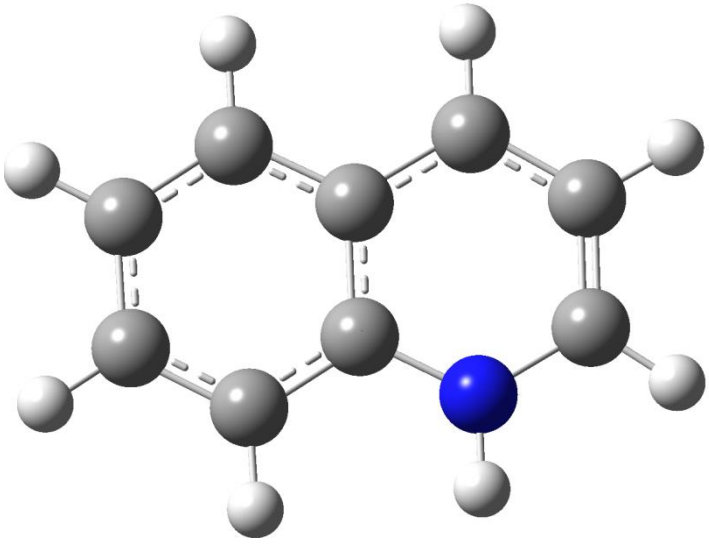
[$C_{10}H_8$]



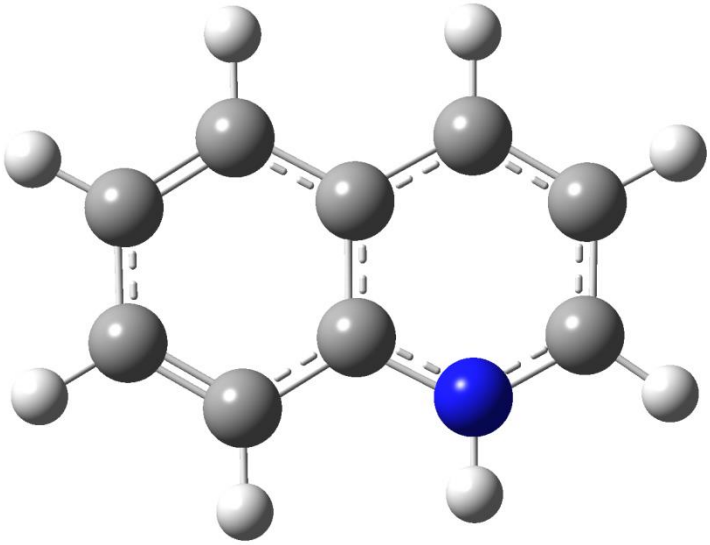
[$C_{10}H_8$]$^+$

IE = 7.816 eV [at b3lyp/6-31+G(d,p)]

Figure S-V: Optimized geometries, Ionization energy of neutral and cation of naphthalene



[C_9H_8N]

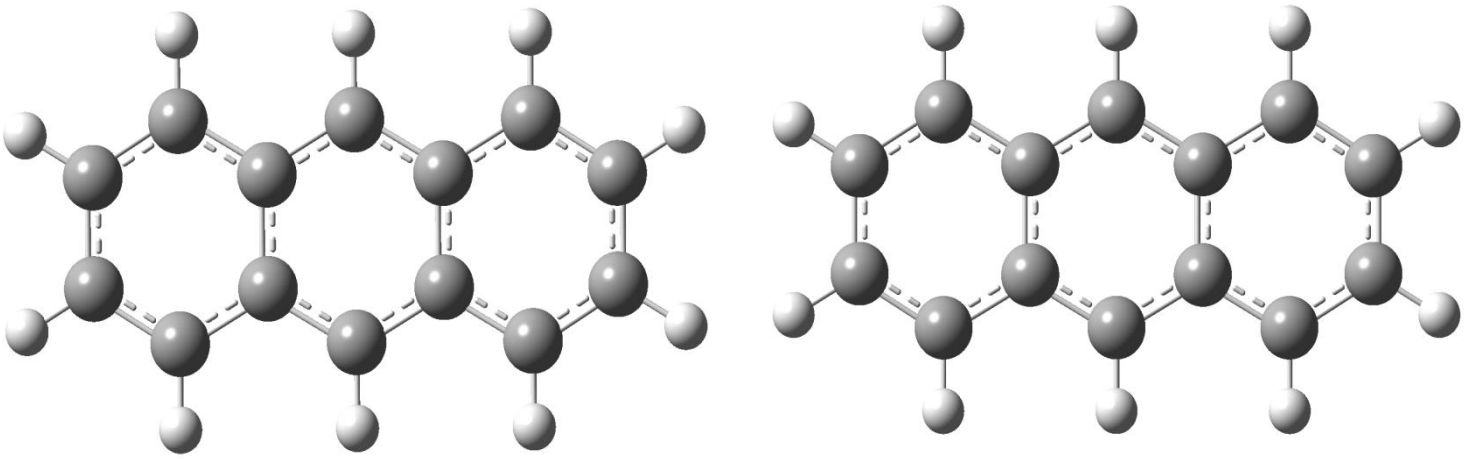


[C_9H_8N]$^+$

IE = 5.303 eV [at b3lyp/6-31+G(d,p)]

Figure S-VI: Optimized geometries, Ionization energy of one C by N substituted neutral and cation of naphthalene.

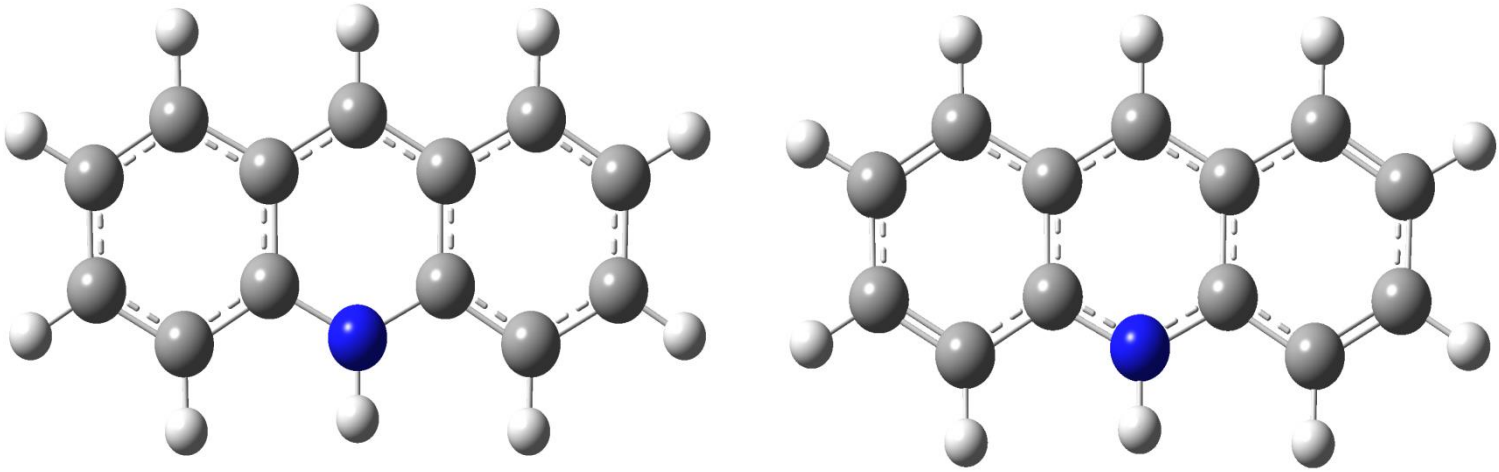
Neutrals **Cations**



[$C_{14}H_{10}$] **[$C_{14}H_{10}$]$^{+}$**

IE = 7.034 eV [at b3lyp/6-31+G(d,p)]

Figure S-VII: Optimized geometries, Ionization energy of neutral and cation of anthracene.



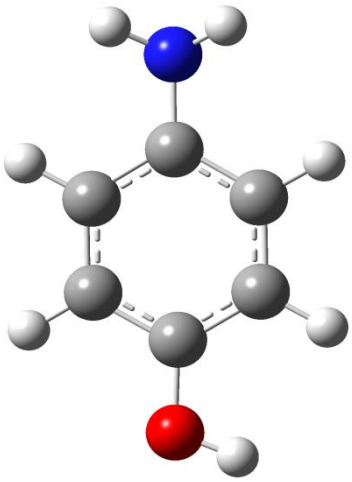
[$C_{13}H_{10}N$] **[$C_{13}H_{10}N$]$^{+}$**

IE = 5.459 eV [at b3lyp/6-31+G(d,p)]

Figure S-VIII: Optimized geometries, Ionization energy of one C by N substituted neutral and cation of anthracene.

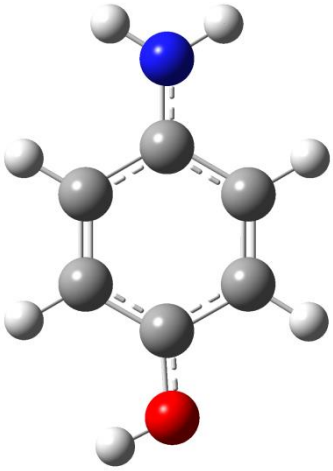
Organic Reducing agents

Neutrals



$[C_6H_4(NH_2)(OH)]$

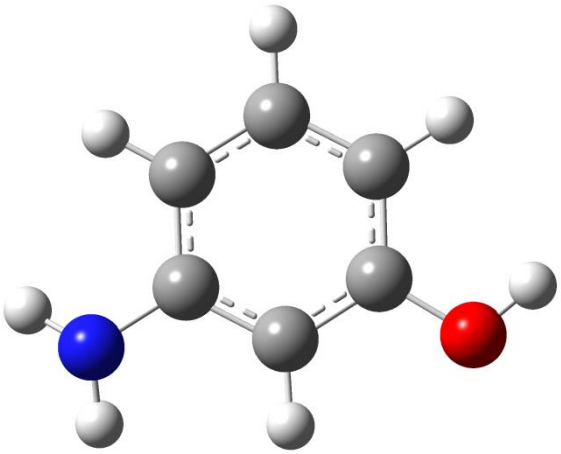
Cations



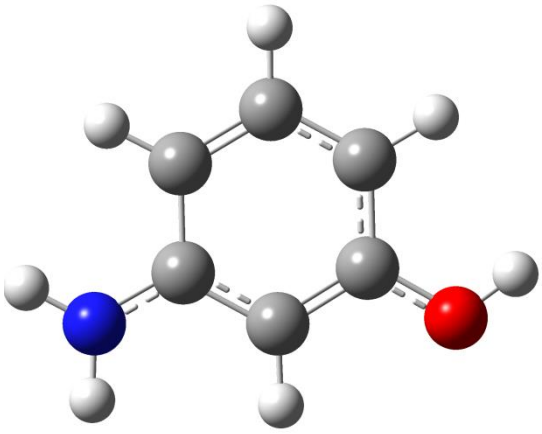
$[C_6H_4(NH_2)(OH)]^+$

IE = 6.982 eV [at b3lyp/6-31+G(d,p)]

Figure S-IX: Optimized geometries, Ionization energy of neutral and cation of 4-aminophenol



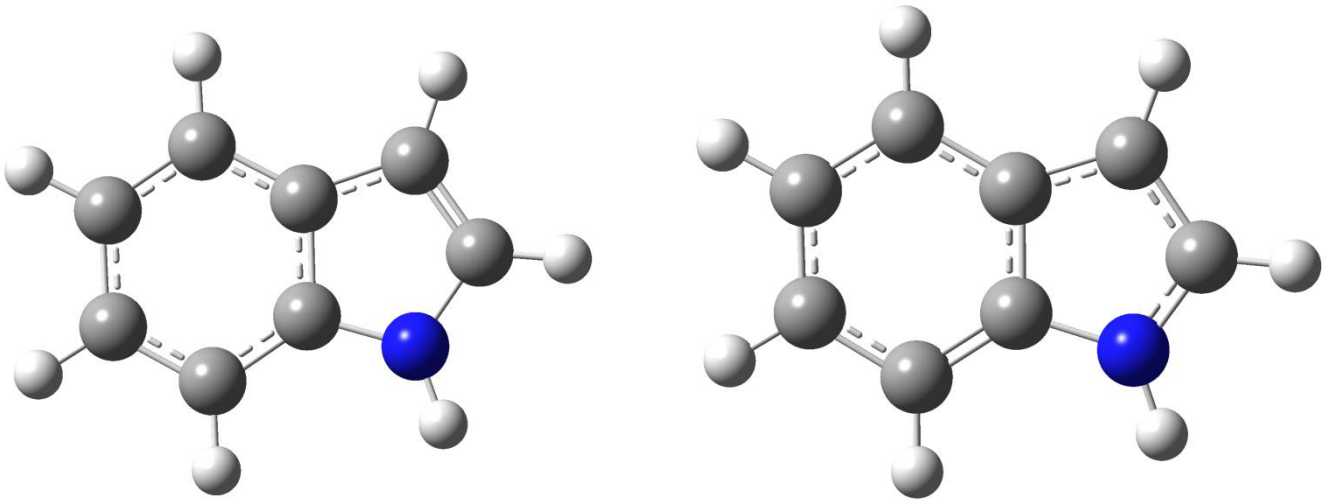
$[C_6H_4(NH_2)(OH)]$



$[C_6H_4(NH_2)(OH)]$

IE = 7.397 eV [at b3lyp/6-31+G(d,p)]

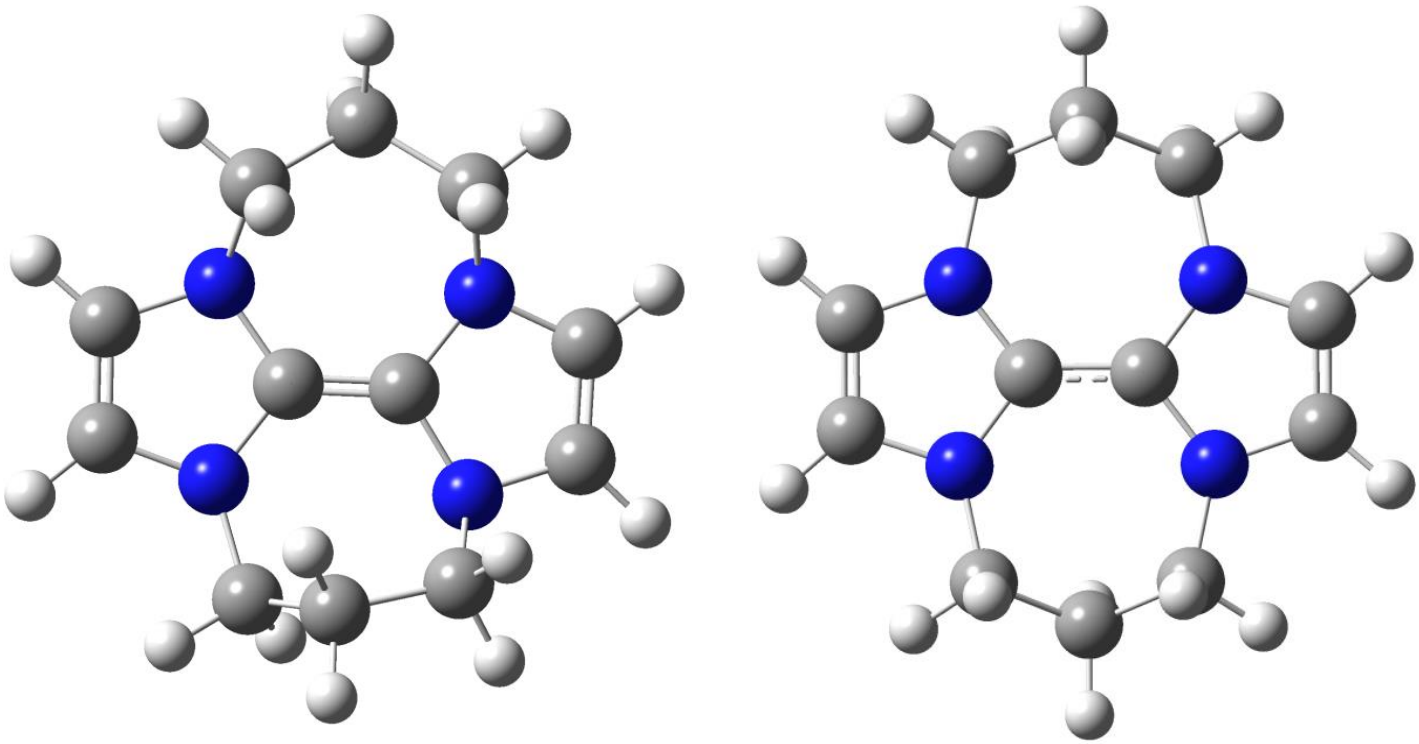
Figure S-X: Optimized geometries, Ionization energy of neutral and cation of 3-aminophenol.



$[C_8H_7N]$ $[C_8H_7N]^+$

IE = 7.512 eV [at b3lyp/6-31+G(d,p)]

Figure S-XI: Optimized geometries, Ionization energy of neutral and cation of indole.



$[C_{12}H_{16}N_4]$ $[C_{12}H_{16}N_4]^+$

IE = 4.210 eV [at b3lyp/6-31+G(d,p)]

Figure S-XII: Optimized geometries, Ionization energy of neutral and cation of $[C_{12}H_{16}N_4]$.