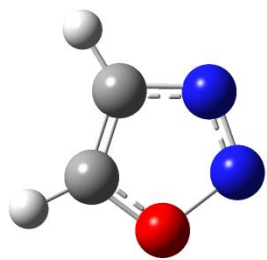


## Super/Hyperhalogen Aromatic Heterocyclic Compounds

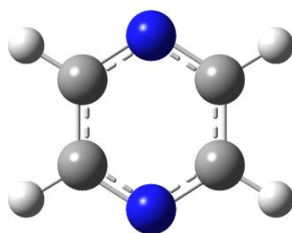
Gorre Naresh Reddy<sup>a</sup> and Santanab Giri<sup>a\*</sup>

<sup>a</sup> Department of Chemistry, National Institute of Technology, Rourkela, 769008, India

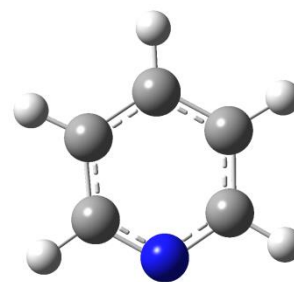
Corresponding Author: [giris@nitrkl.ac.in](mailto:giris@nitrkl.ac.in)



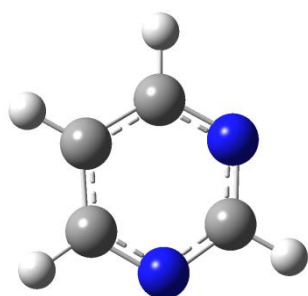
[C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>O]



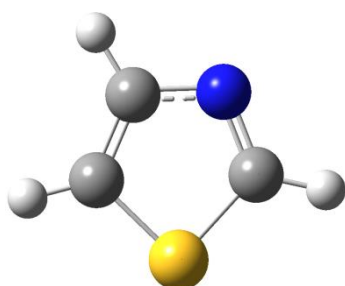
[C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>]



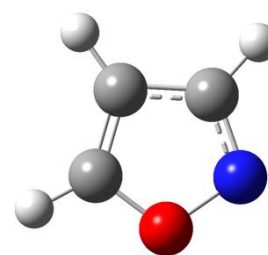
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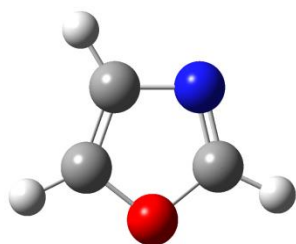
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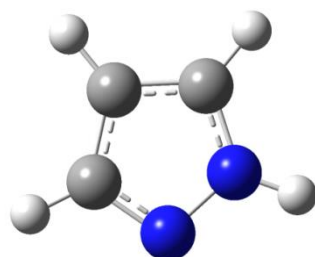
[C<sub>3</sub>H<sub>3</sub>NS]



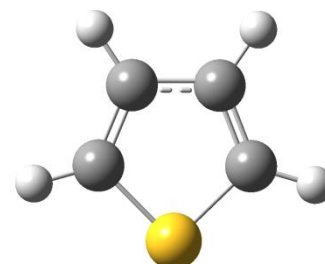
[C<sub>3</sub>H<sub>3</sub>NO]



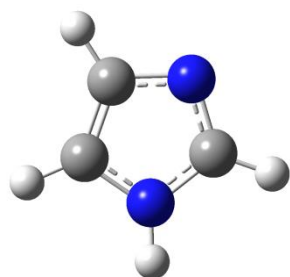
[C<sub>3</sub>H<sub>3</sub>NO]



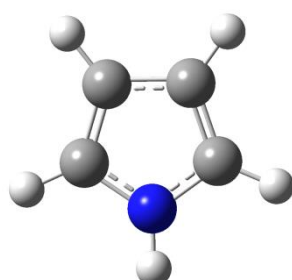
[C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>]



[C<sub>4</sub>H<sub>4</sub>S]

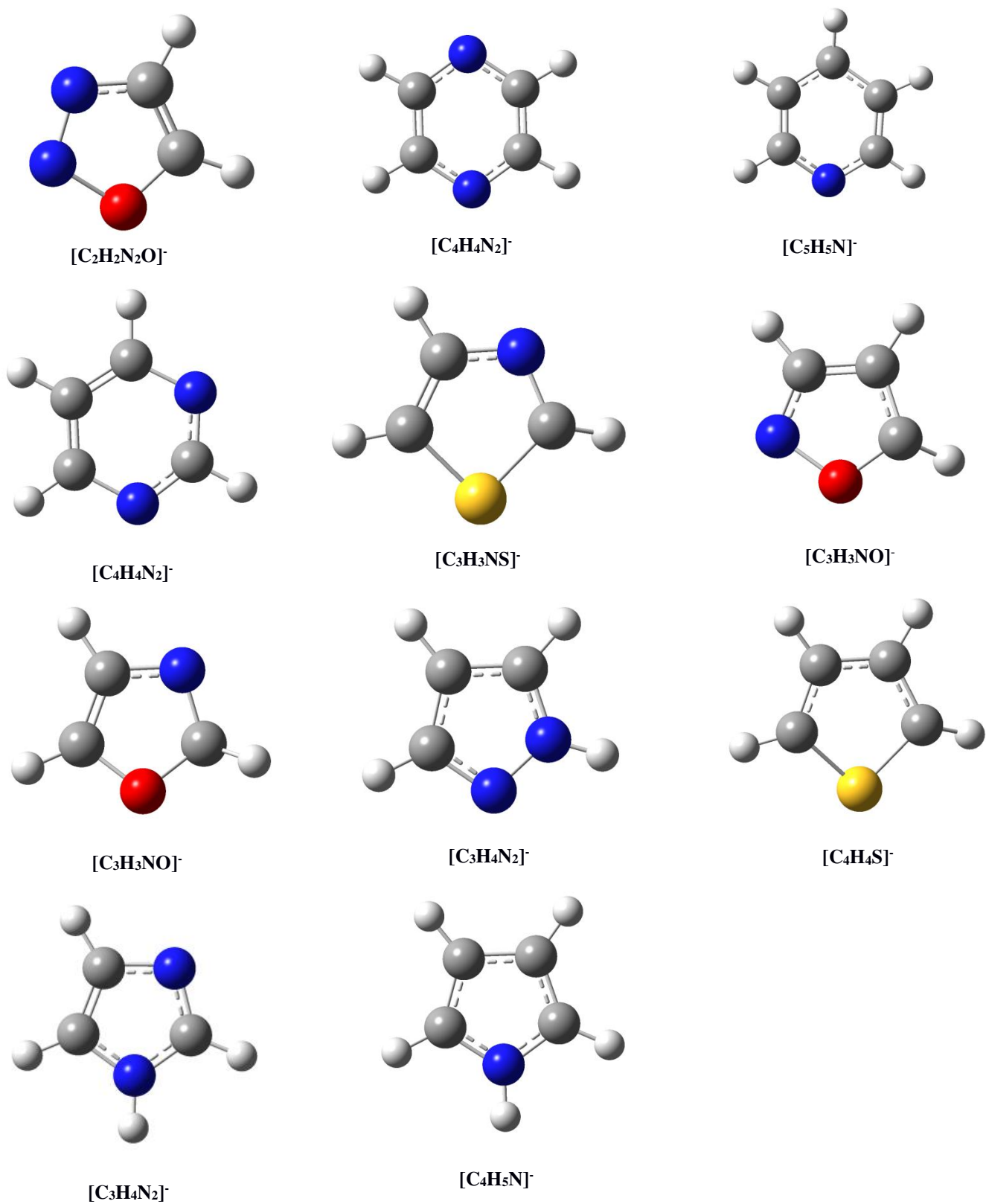


[C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>]

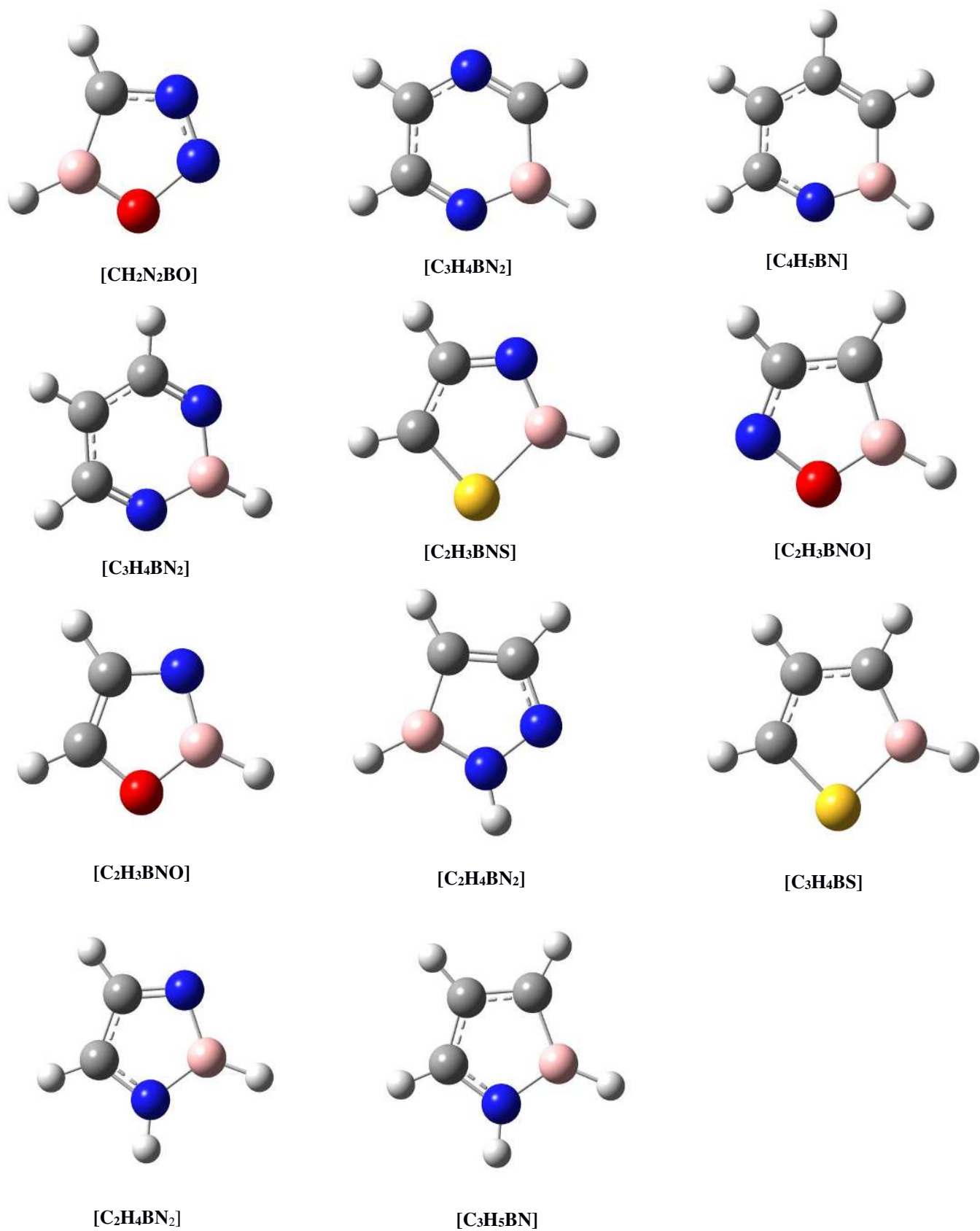


[C<sub>4</sub>H<sub>5</sub>N]

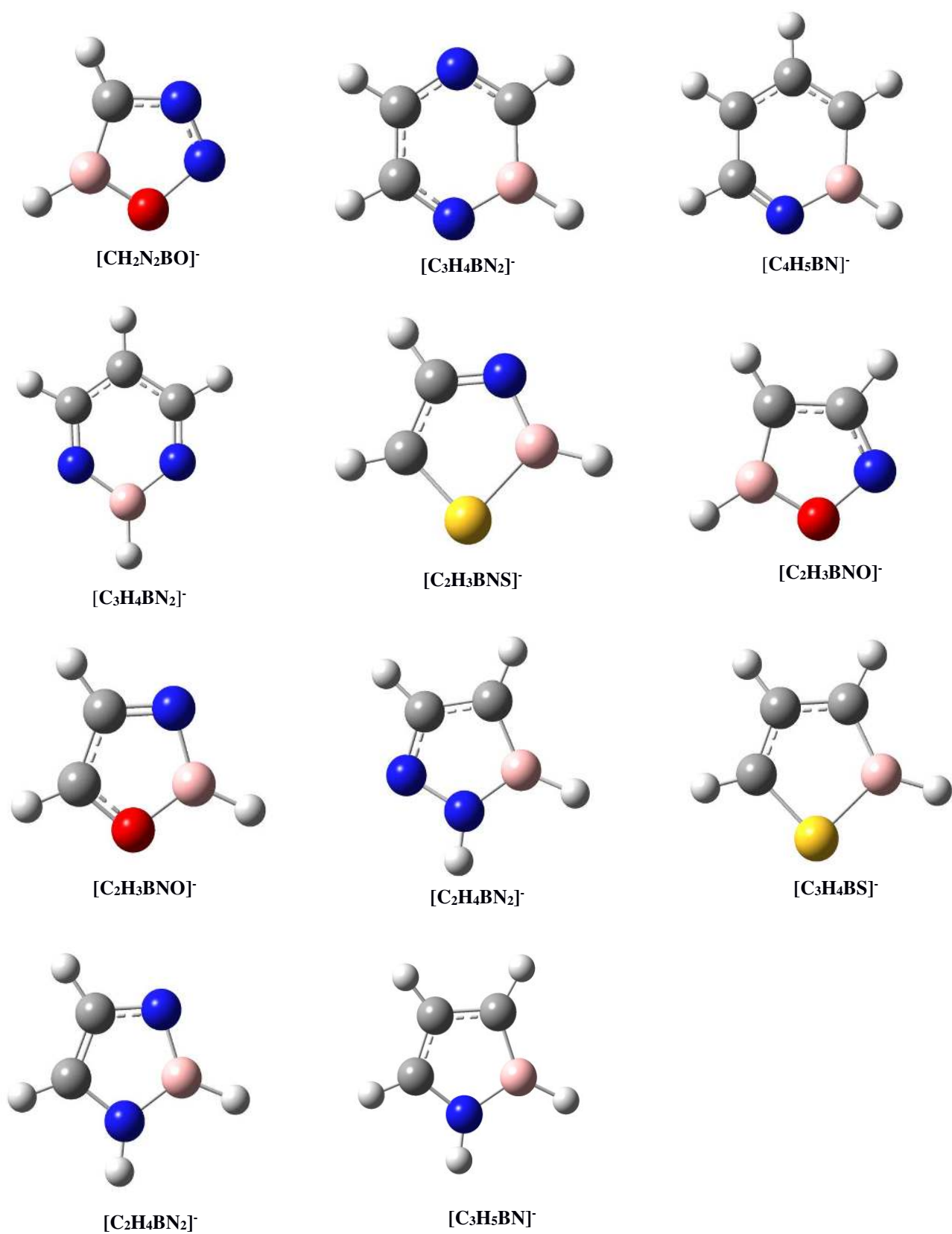
**Figure S-I** : Optimized geometries of neutral aromatic heterocyclic molecules



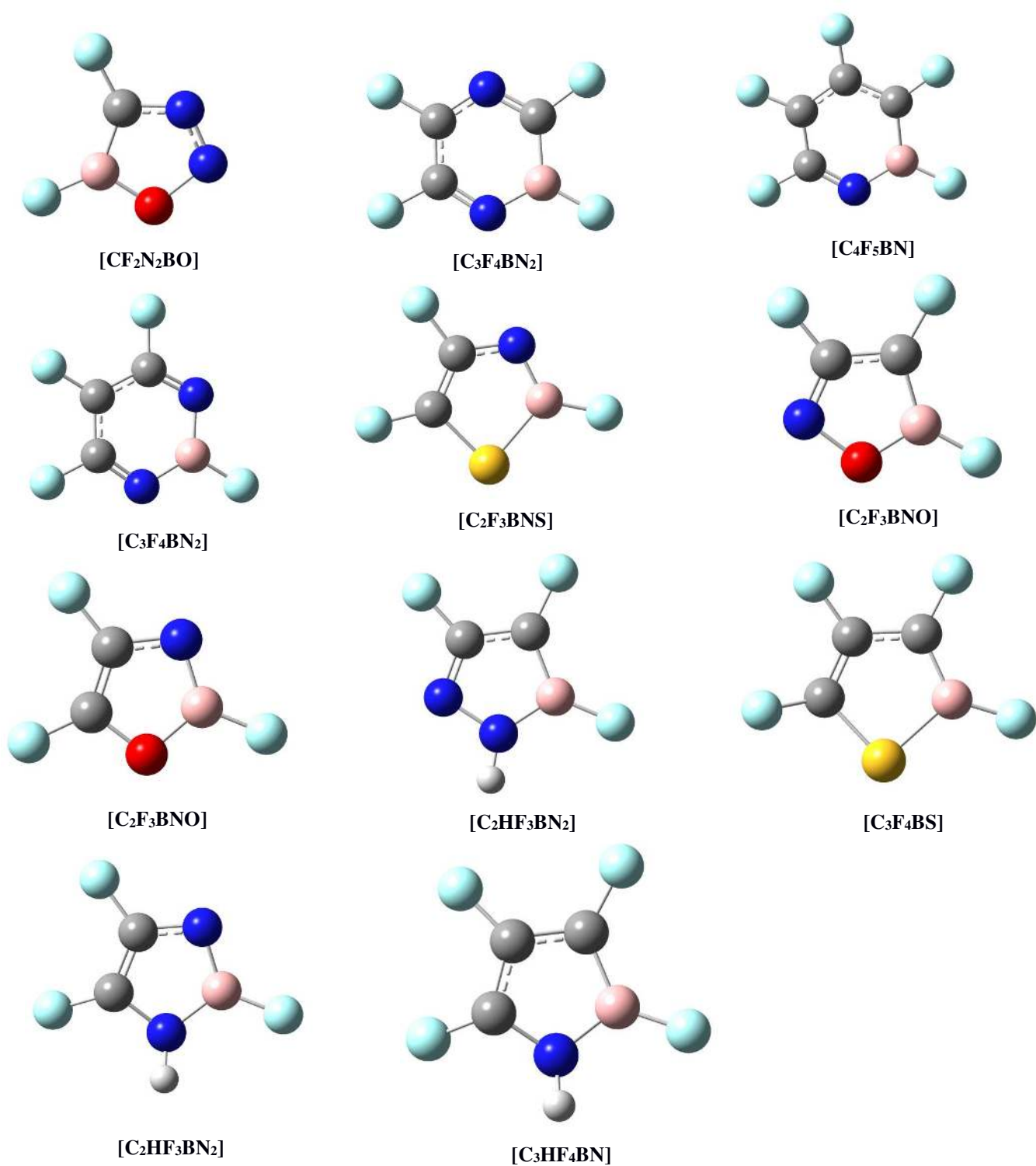
**Figure S-II:** Optimized geometries of anionic aromatic heterocyclic molecules



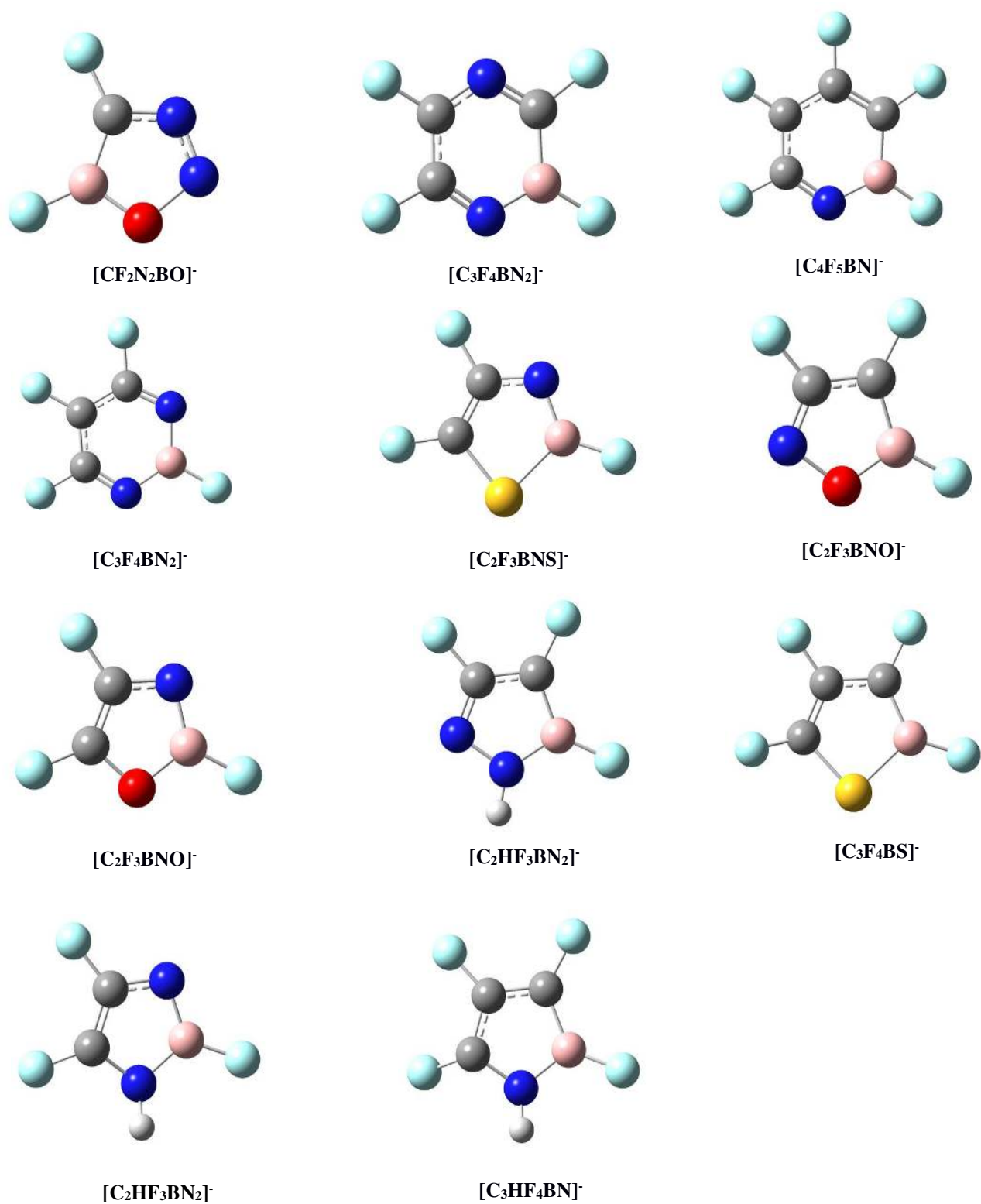
**Figure S-III** : Optimized geometries of B substituted neutral aromatic heterocyclic molecules



**Figure S-IV** : Optimized geometries of B substituted anionic aromatic heterocyclic molecules

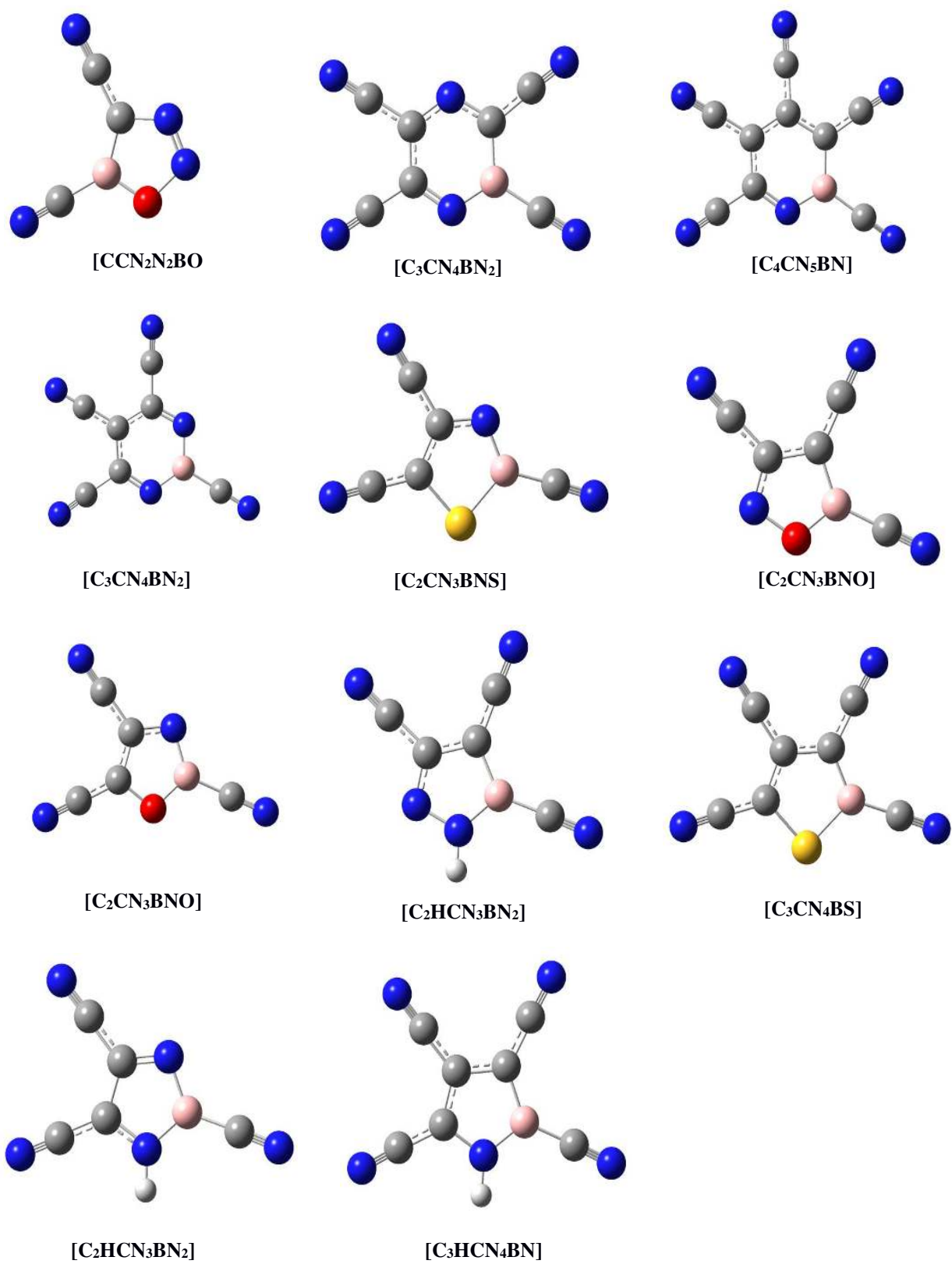


**Figure S-V** : Optimized geometries of F substituted aromatic heterocyclic neutral molecules



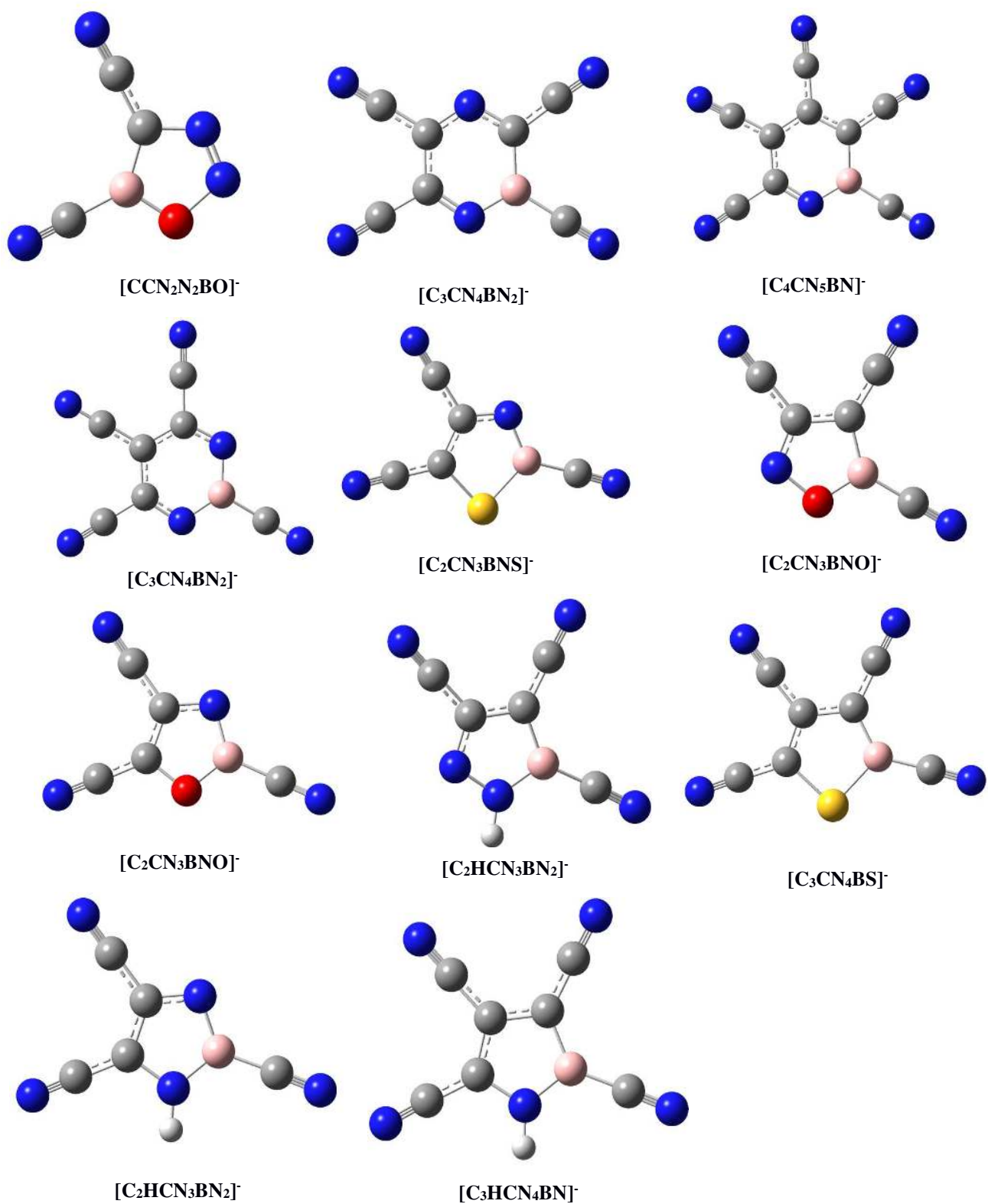
**Figure S-VI** : Optimized geometries of F substituted aromatic heterocyclic anion molecules





**Figure S-VII** : Optimized geometries of CN substituted aromatic heterocyclic neutral molecules





**Figure S-VIII** : Optimized geometries of CN substituted aromatic heterocyclic anion molecules