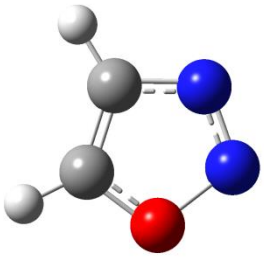
Electronic Supplementary Material (ESI) for RSC Advances.

Super/Hyperhalogen Aromatic Heterocyclic Compounds

Gorre Naaresh Reddy[a] and Santanab Giri[a]*

[a] Department of Chemistry, National Institute of Technology, Rourkela, 769008, India

Corresponding Author: giris@nitrkl.ac.in



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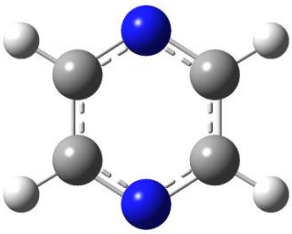

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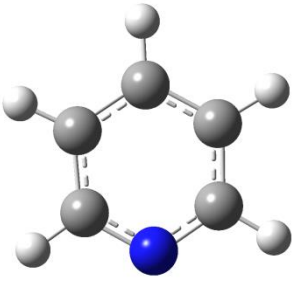

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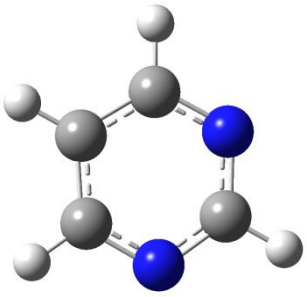

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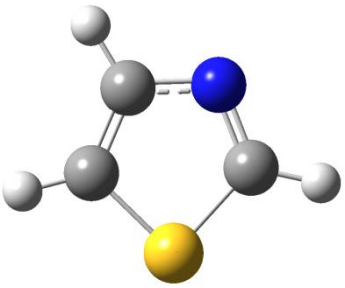

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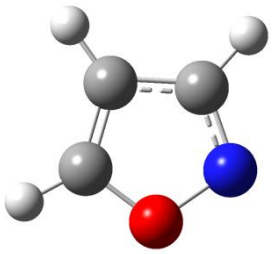

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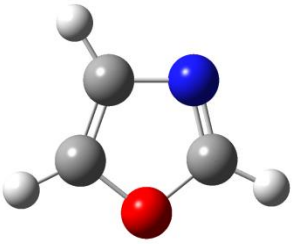

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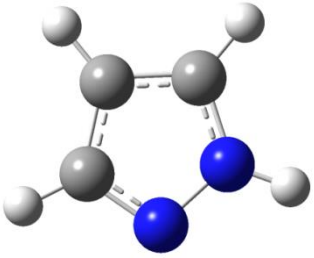

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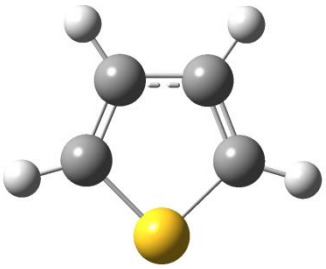

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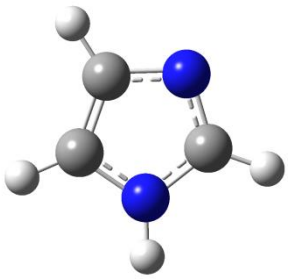

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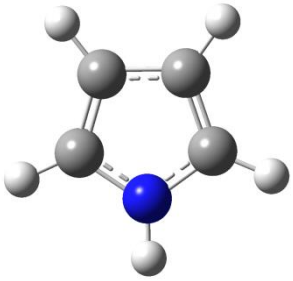
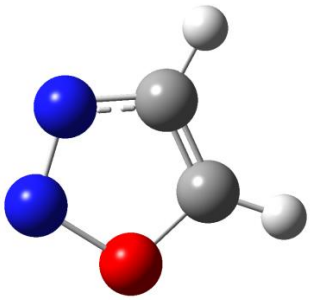


[C_4H_5N]

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



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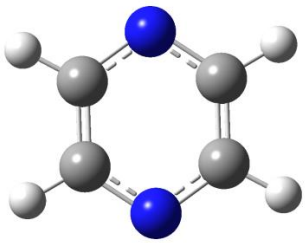

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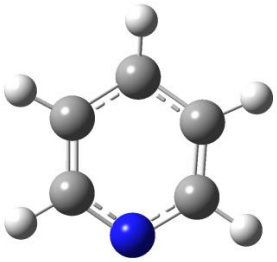

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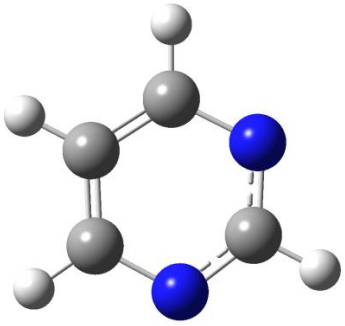

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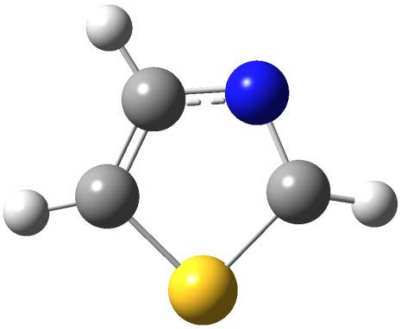

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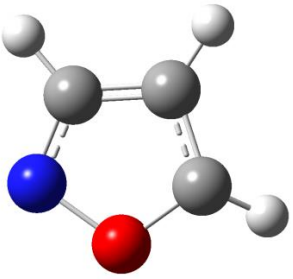

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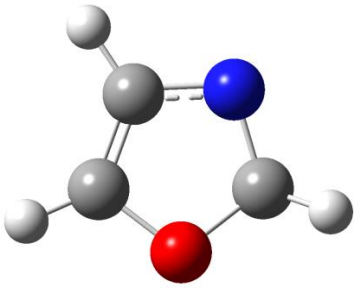

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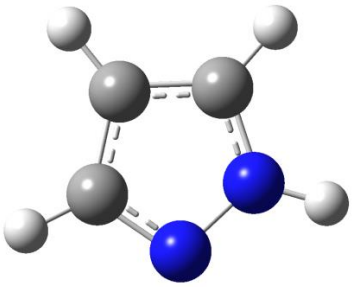

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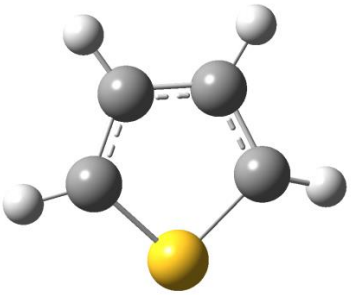

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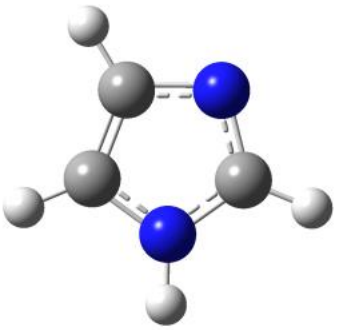

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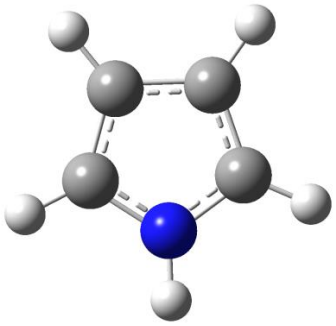
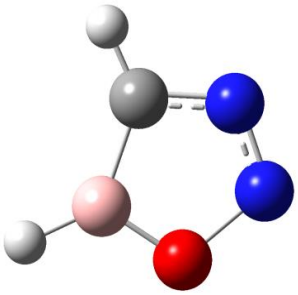


$[C_4H_5N]^-$

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



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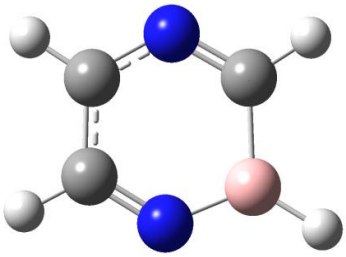

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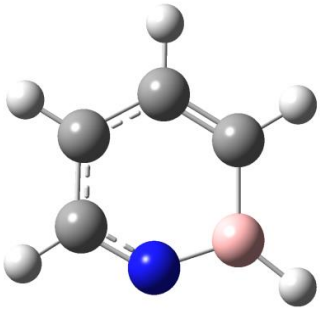

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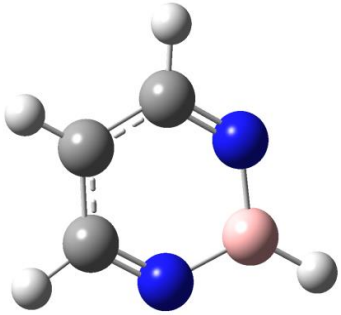

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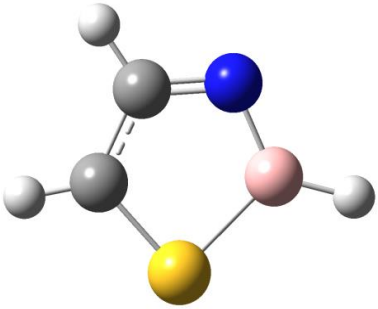

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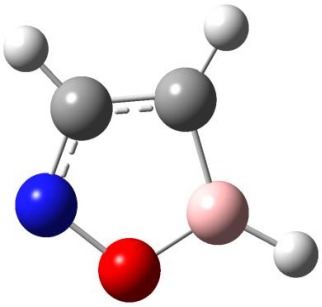

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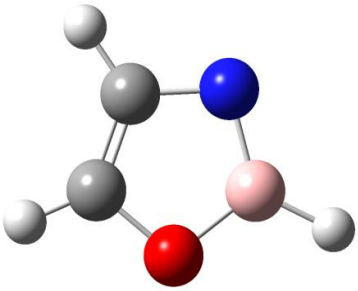

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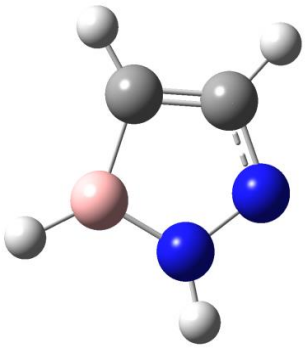

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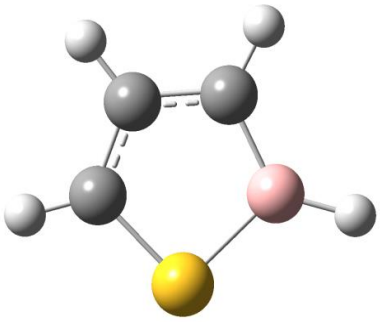

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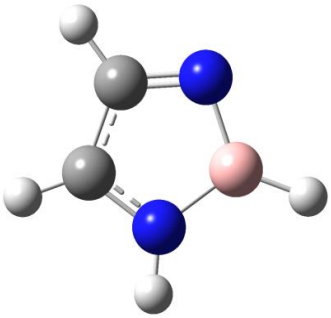

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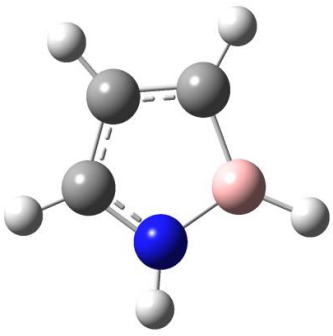
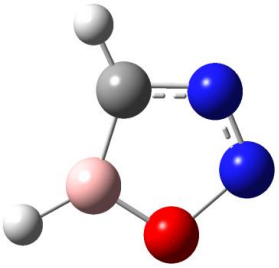


[C_3H_5BN]

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



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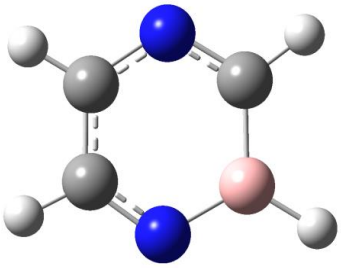

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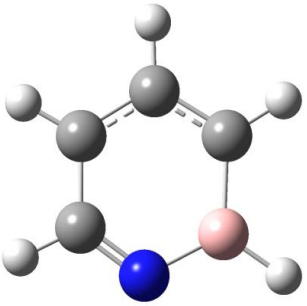

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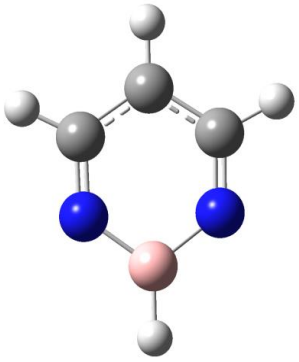

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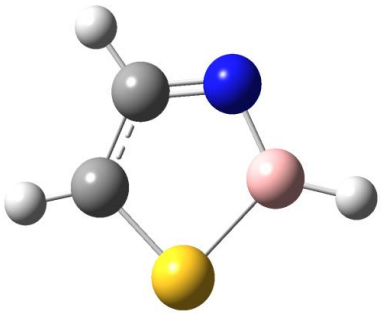

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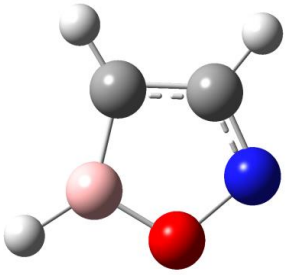

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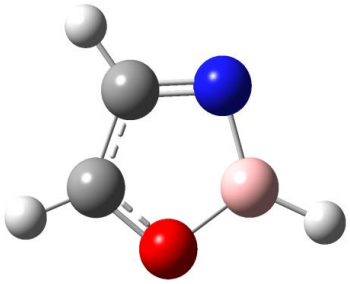

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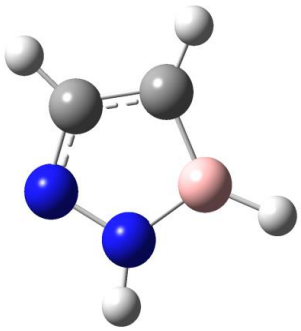

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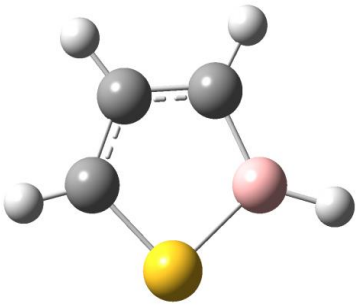

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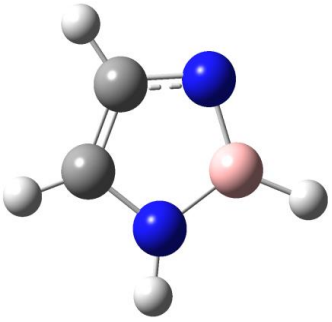

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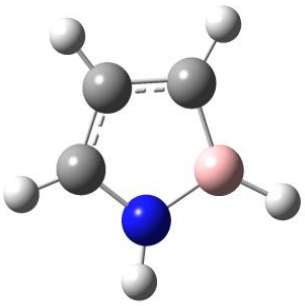
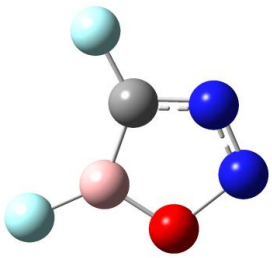


$[C_3H_5BN]^-$

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



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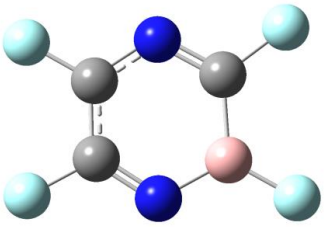

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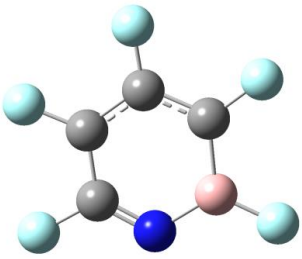

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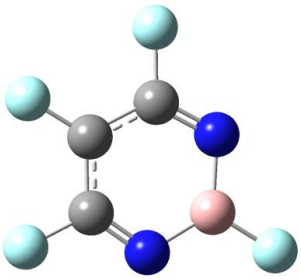

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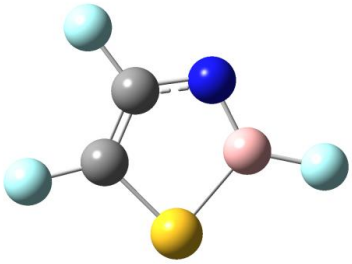

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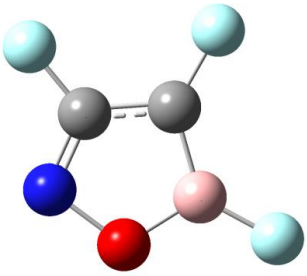

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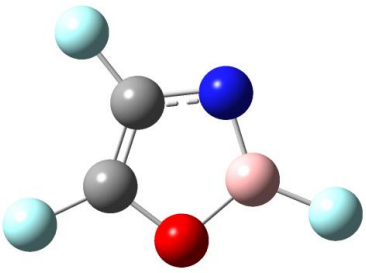

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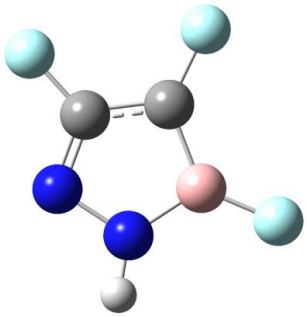

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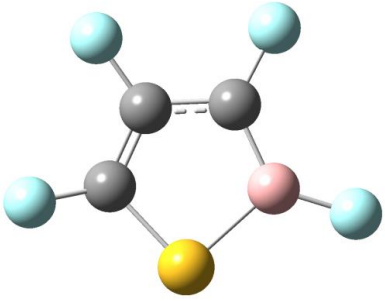

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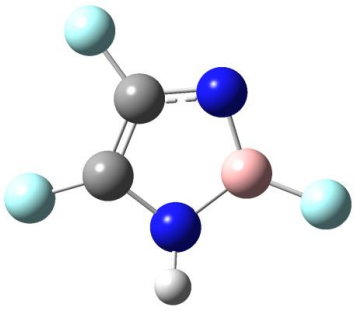

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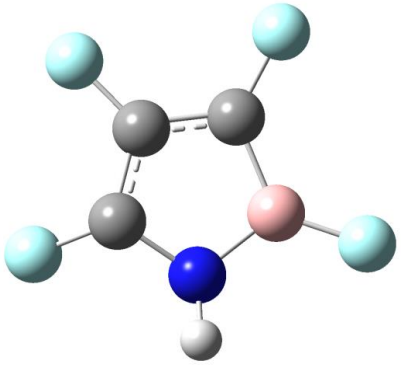
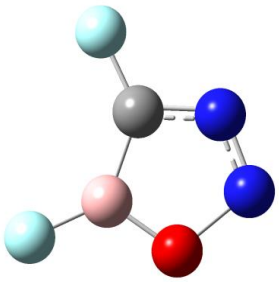
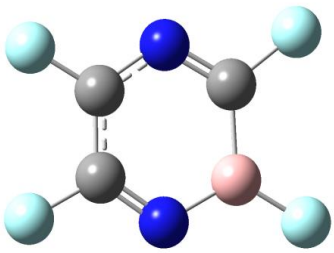


[C_3HF_4BN]

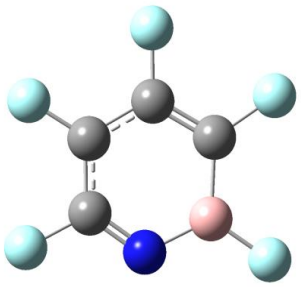
Figure S-V : Optimized geometries of F substituted aromatic heterocyclic neutral molecules



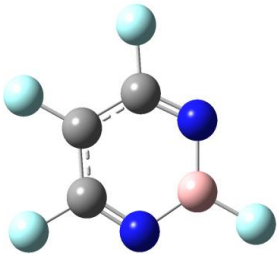
$[CF_2N_2BO]^-$



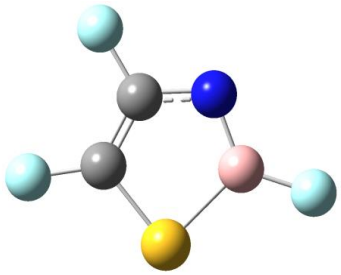
$[C_3F_4BN_2]^-$



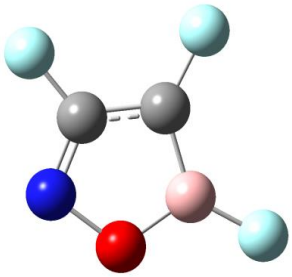
$[C_4F_5BN]^-$



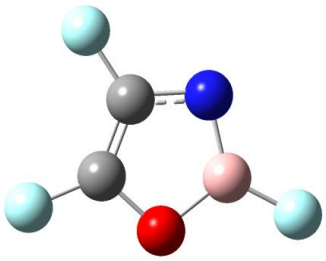
$[C_3F_4BN_2]^-$



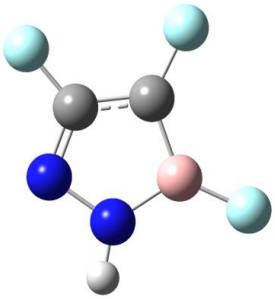
$[C_2F_3BNS]^-$



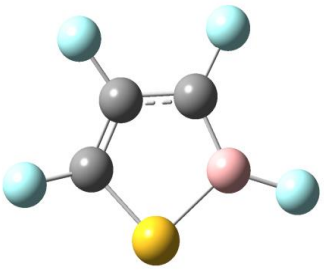
$[C_2F_3BNO]^-$



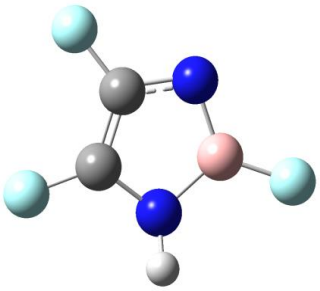
$[C_2F_3BNO]^-$



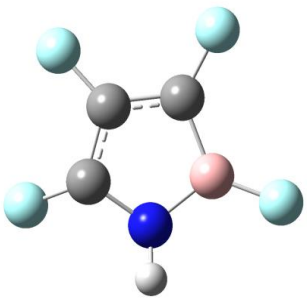
$[C_2HF_3BN_2]^-$



$[C_3F_4BS]^-$

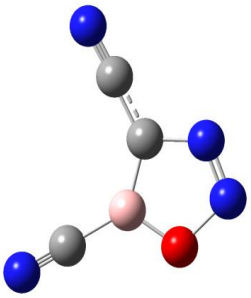


$[C_2HF_3BN_2]^-$

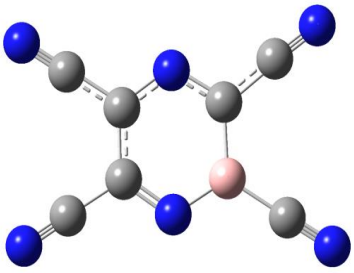


$[C_3HF_4BN]^-$

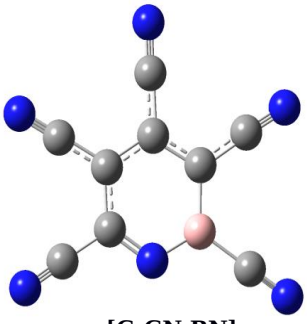
Figure S-VI : Optimized geometries of F substituted aromatic heterocyclic anion molecules



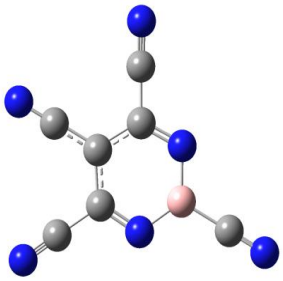
[CCN_2N_2BO]



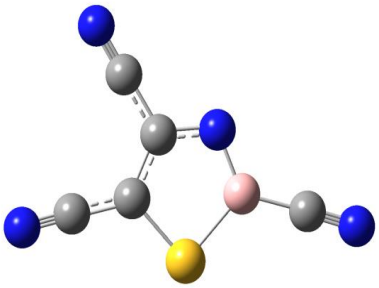
[$C_3CN_4BN_2$]



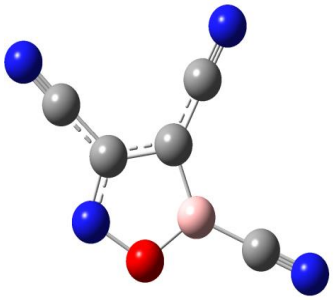
[C_4CN_5BN]



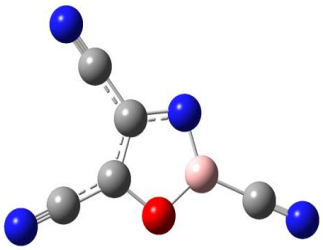
[$C_3CN_4BN_2$]



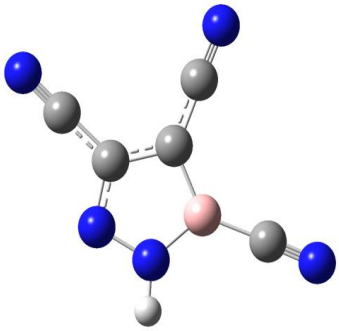
[C_2CN_3BNS]



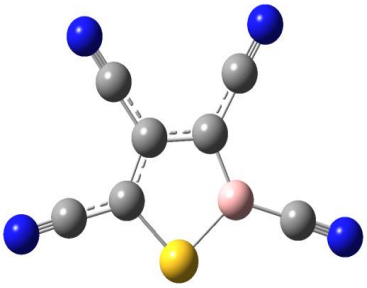
[C_2CN_3BNO]



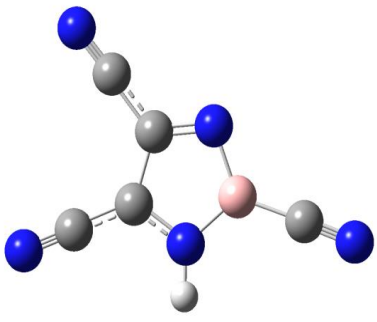
[C_2CN_3BNO]



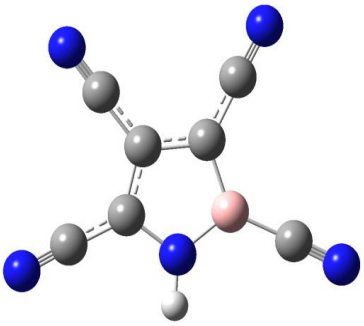
[$C_2HCN_3BN_2$]



[C_3CN_4BS]



[$C_2HCN_3BN_2$]



[C_3HCN_4BN]

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

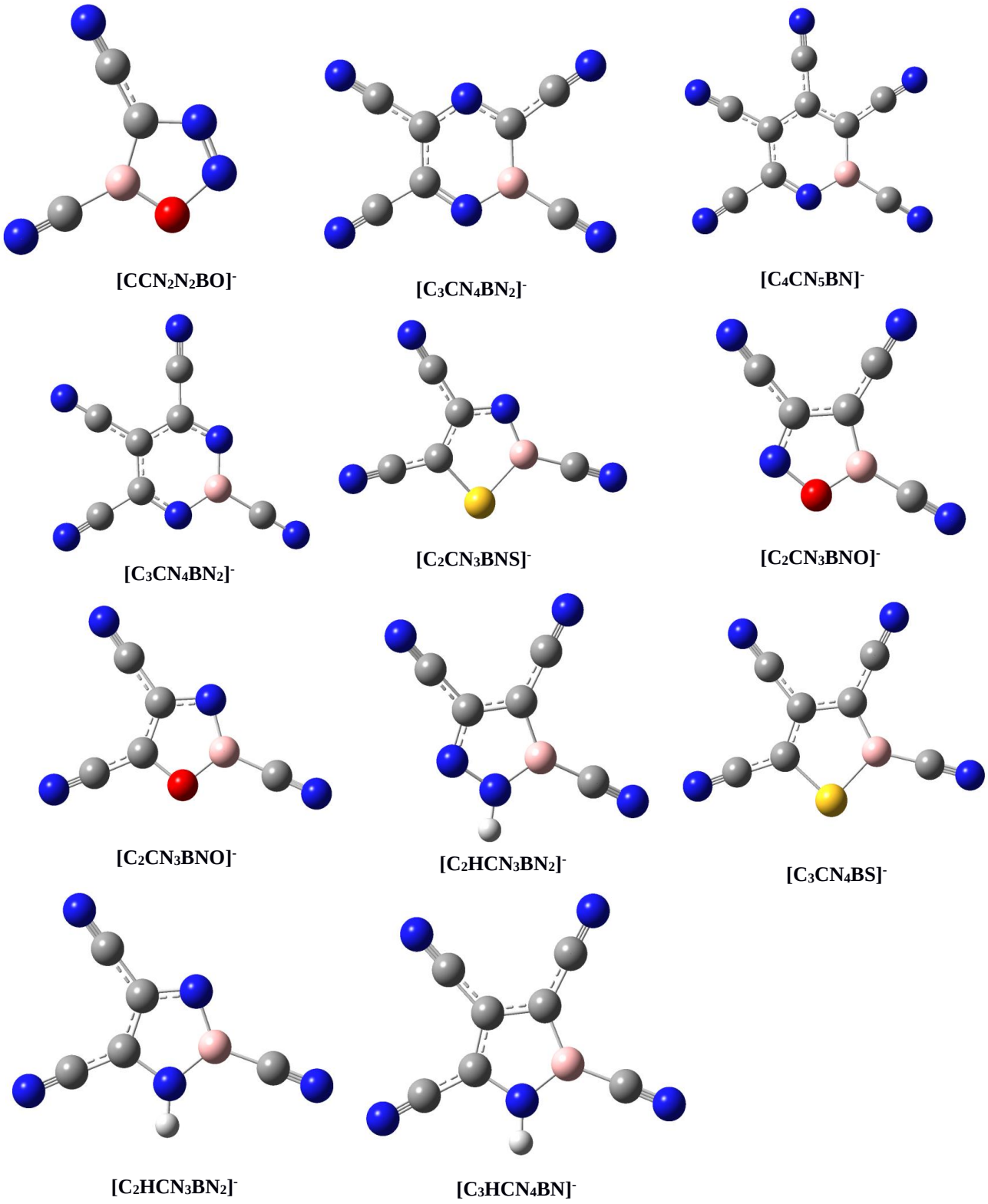


Figure S-VIII : Optimized geometries of CN substituted aromatic heterocyclic anion molecules