Supporting Informaion:

Designing Aromatic Heterocyclic Superacids in Brønsted and Lewis Perspectives

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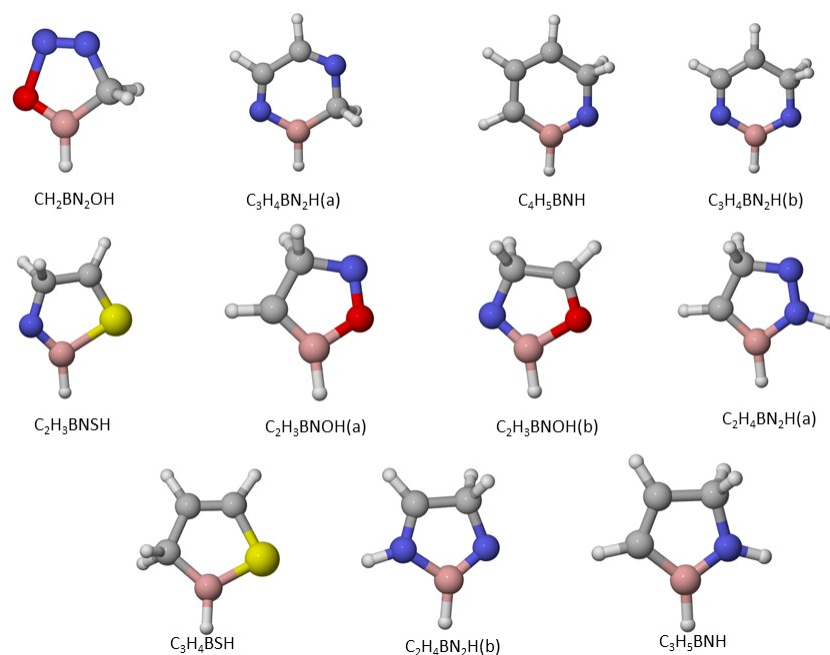[b]Department of Chemistry, National Institute of Technology Rourkela, Odisha 769008.

Figure S1. Optimized geometries of normal heterocyclic compounds with H-atom at carbon centre.

Table T1. Free energy changes due to deprotonation, NICS and pKa of normal heterocyclic molecules. (When H at Carbon centre).

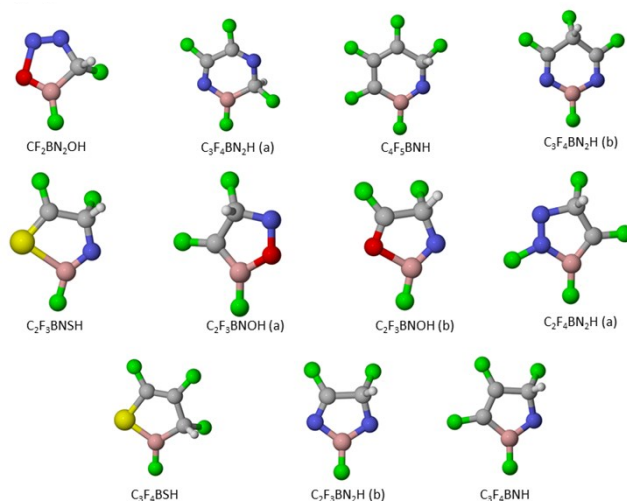| Molecule	Free energy change due to deprotonation ΔG (kcal/mol)	NICS (0)	NICS (1)	pK_a
CH_2BN_2O	331.78	-10.5	-9.1	12.57
$C_3H_4BN_2$ (a)	313.09	-3.1	-7.6	-0.41
C_4H_5BN	288.74	-4.3	-7.2	-17.54
$C_3H_4BN_2$ (b)	270.69	-2.9	-6.7	-32.32
C_2H_3BNS	300.78	-10.1	-7.9	-8.62
C_2H_3BNO (a)	288.88	-9.2	-7.6	-21.78
C_2H_3BNO (b)	308.16	-7.8	-6.3	-4.09
$C_2H_4BN_2$ (a)	313.26	-10.8	-8.7	-3.37
C_3H_4BS	340.67	-10.2	-7.9	19.41
$C_2H_4BN_2$ (b)	324.01	-10.05	-7.4	8.35
C_3H_5BN	359.45	-10.5	-7.3	31.10

Figure S2. Optimized neutral geometries of F-Substituted heterocyclic complex with H-atom at carbon Centre.

Table T2. Free energy changes due to deprotonation, NICS and pK_a of F-substituted Heterocyclic Molecules. (When H at Carbon centre).

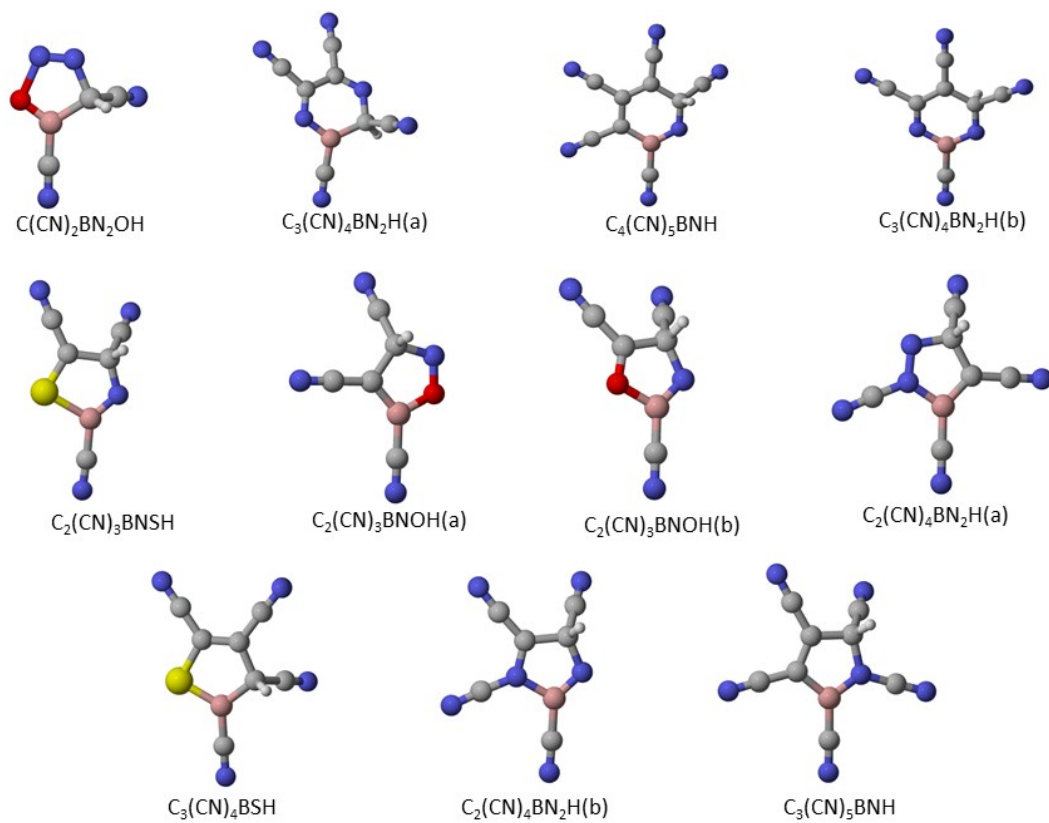| Molecule	Free energy change due to deprotonation (ΔG) (kcal/mol)	NICS (0)	NICS (1)	pK_a
CF_2BN_2O	317.05	-9.2	-6.4	3.85
$C_3F_4BN_2$ (a)	290.66	-10.8	-8.7	-10.94
C_4F_5BN	258.95	-14.2	-8.9	-33.36
$C_3F_4BN_2$ (b)	296.47	-9.2	-6.9	-6.88
C_2F_3BNS	289.42	-11.5	-5.1	-13.24
C_2F_3BNO (a)	262.03	-14.4	-5.9	-37.30
C_2F_3BNO (b)	300.55	-10.9	-4.1	-6.45
$C_2F_4BN_2$ (a)	287.20	-18.9	-7.2	-16.82
C_3F_4BS	327.09	-16.9	-8.2	15.56
$C_2F_3BN_2$ (b)	293.79	-2.8	-2.0	-34.29
C_3F_4BN	300.41	-9.0	-2.0	-22.26

Figure S3. Optimized neutral geometries of CN-Substituted heterocyclic complex with H-atom at carbon centre.

Table S3. Free energy changes due to deprotonation, NICS and pK_a of CN-substituted Heterocyclic Molecules. (When H at Carbon centre).

Molecule	Free energy change due to deprotonation ΔG (kcal/mol)	NICS (0)	NICS (1)	pK_a
$C(CN)_2BN_2O$	282.70	-10.9	-9.0	-13.24
$C_3(CN)_4BN_2$ (a)	243.00	-6.1	-8.7	-65.99
$C_4(CN)_5BN$	208.41	-7.5	-8.3	-38.57
$C_3(CN)_4BN_2$ (b)	202.51	-6.0	-8.1	-49.93
$C_2(CN)_3BNS$	242.50	-11.1	-8.7	-39.61
$C_2(CN)_3BNO$ (a)	229.66	-10.6	-8.1	-46.02
$C_2(CN)_3BNO$ (b)	242.26	-10.0	-7.7	-18.98
$C_2(CN)_4BN_2$ (a)	230.83	-12.7	-8.6	-40.23
$C_3(CN)_4BS$	266.15	-12.4	-8.5	-17.71
$C_2(CN)_4BN_2$ (b)	238.22	-11.6	-7.9	-37.03
$C_3(CN)_5BN$	265.04	-13.5	-7.9	-60.14