

Supporting Information

Nitrenium ion $\leftrightarrow$ Nitreone Resonance in Fused Cyclic Five-Membered Triazolium Ions (*f*CFTIs): A Quantum Chemical Study

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Table S1. Benchmarking of quantum chemical methods for ^{15}N chemical shift (δ) calculations at N^2 center.

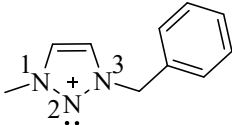
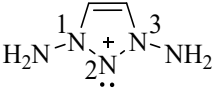
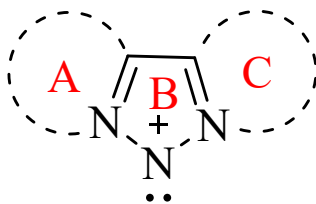
S. No.	Method	^{15}N δ (ppm)	^{15}N δ (ppm)
			
1	Experiment	-42.00¹	-50.00²
2	B3LYP/6-31+G (d, p)	-45.49	-34.06
3	B3LYP/6-311++G(2d,2p)	-42.96	-30.96
4	M06/6-31+G (d, p)	-41.21	-28.55
5	M06/6-311++G(2d,2p)	-39.67	-7.54
6	M06-2x/6-31+G (d, p)	-48.01	-45.99
7	M06-2x/6-311++G(2d,2p)	-52.32	-10.25
8	MP2/6-31+G (d, p)	-16.88	-9.70
9	MP2/6-311++G(2d,2p)	-24.18	-15.53
10	TPSSH/def2-TZVP	-42.05	-51.28

Table S2. Estimation of lone pairs using NBO analysis at different levels of quantum chemical methods in Gaussian 16 suite of programs.

Methods	No. of lone pairs	
	F9	F17
B3LYP/6-31+G(d,p)	1	2
B3LYP/6-311++G(3d,2p)	1	2
M06/6-31+G(d,p)	1	2
M06-2x/6-311++G(3d,2p)	1	2
M06-2x/aug-cc-pvdz	1	2
MP2/6-31+G(d,p)	1	2
CCSD/6-31+G(d,p)	1	2
QCISD/6-31+G(d,p)	1	2

Table S3. NICS(1) values of *f*CFTIs **F1-F24**. All values are in ppm. A, B, and C rings are labelled in *f*CFTI.



ID	A	B	C
F1	12.13	5.88	12.13
F2	19.45	19.59	19.45
F3	4.45	-0.51	4.45
F4	5.93	-0.26	5.93
F5	13.34	11.69	13.34
F6	17.12	6.50	17.12
F7	-1.19	3.41	-1.19
F8	-1.49	4.36	-1.49
F9	-7.98	-11.10	-7.98
F10	-7.25	-11.12	-7.25
F11	-5.87	-9.86	-5.87
F12	-5.87	-9.86	-5.87
F13	1.44	-6.84	1.44
F14	-1.48	-10.53	-1.48
F15^[a]	-11.98	-10.93	-11.98
F16	8.15	2.65	8.15
F17	-9.59	-11.77	-9.59
F18	-9.85	-12.30	-9.85
F19	-9.42	-11.96	-9.42
F20	-9.57	-12.58	-9.57
F21	-8.88	-10.96	-8.88
F22	-9.93	-7.10	-9.93
F23	-10.41	-5.98	-10.41
F24	-9.28	-5.07	-9.28

^[a]In **F15**, the NICS (1) value of the fourth ring is -7.11 ppm.

Table S4. Bond Stretch Isomerism explored at various quantum chemical levels methods for *f*CFTI **F1**.

Method	NLP ^[a]	C ⁴ -C ⁵ ^[b] (Å)	E1 ^[c] (Hartree)	NLP ^[a]	C ⁴ -C ⁵ ^[b] (Å)	E2 ^[c] (Hartree)	ΔE = (E1-E2)*627.5 (kcal/mol)
B3LYP/6-31+G(d,p)	2	1.34	-472.211694	1	1.44	-472.238342	-16.72
B3LYP/Aug-cc-pVTZ	2	1.34	-472.351847	1	1.44	-472.378403	-16.66
M06/6-31+G(d,p)	2	1.34	-471.873436	1	1.44	-471.899498	-16.35
M06/Aug-cc-pVTZ	2	1.33	-472.006651	1	1.44	-472.033158	-16.63
M062x/6-31+G(d,p)	-	-	-	1	1.44	-472.036165	-
M062x/Aug-cc-pVTZ	-	-	-	1	1.44	-472.028023	-
HF/6-31+G(d,p)	-	-	-	1	1.45	-469.300574	-
MP2/Aug-cc-pVTZ	-	-	-	1	1.44	-469.446640	-
G2-MP2	-	-	-	1	1.43	-471.515806	-
CBS-QB3	2	1.34	-471.519599	1	1.44	-471.545124	-16.01

^[a] NLP denotes number of lone pair at the N² center; ^[b] Bond length of C⁴-C⁵ bond; ^[c] E1 and E2 represents the sum of electronic energy and zero-point energy. (-) denotes the structures are not optimised at bond length (1.34 Å).

Table S5. Computed T1 diagnostic values for *f*CFTIs **F1-F8** at CCSD(T)/cc-pVTZ//CBS-QB3 level of theory.

ID	T1 diagnostic
F1	0.015
F2	0.016
F3	0.017
F4	0.017
F5	0.016
F6	0.016
F7	0.017
F8	0.018

Table S6. Quantum chemically estimated Weiberg Bond Index (WBI) in *f*CFTIs **F1-F24** (at B3LYP/6-311++G(3d,2p) level of theory) and energy of LUMO (at CBS-QB3 level of theory).

ID	WBI N-N	LUMO (eV)
IX	1.35	-2.24
X	1.35	-2.73
F1	1.39	-5.08
F2	1.39	-6.12
F3	1.40	-5.83
F4	1.36	-5.82
F5	1.36	-4.84
F6	1.36	-4.14
F7	1.35	-5.56
F8	1.37	-6.07
F9	1.23	-2.87
F10	1.23	-2.92
F11	1.24	-2.77
F12	1.22	-2.34
F13	1.33	-4.25
F14	1.31	-3.57
F15	1.32	-2.26
F16	1.20	-3.19
F17	1.21	-2.59
F18	1.23	-3.29
F19	1.21	-3.20
F20	1.22	-3.57
F21	1.20	-1.88
F22	1.40	-1.71
F23	1.15	-2.73
F24	1.13	-2.47

Table S7. Quantum chemically estimated energies (at CBS-QB3 level of theory) of all optimised structures of **IX**, **X** and *f*CFTIs considered in this study (**F1-F24**). All the values are in Hartrees (Energy = electronic energy + zero-point energy correction; Enthalpy = electronic energy + thermal enthalpy correction).

ID	Energy of singlet species	Energy of triplet species	Enthalpy of singlet species	Enthalpy of Hydride complex	Enthalpy of NHC complex
IX	-320.659933	-320.515085	-320.651786	-321.417185	-624.904031
X	-474.026074	-473.920837	-474.015568	-474.786276	-778.282102
F1	-471.545124	-471.537491	-471.536830	-472.395324	-775.865184
F2	-503.595129	-503.592564	-503.586909	-504.495350	-807.952045
F3	-503.608452	-503.601636	-503.600395	-504.494154	-807.950621
F4	-1076.133727	-1076.132238	-1076.124589	-1076.988030	-1380.451856
F5	-621.840763	-621.829503	-621.829982	-622.673757	-926.145307
F6	-658.138796	-658.137360	-658.126372	-658.974964	-962.454215
F7	-697.933581	-697.907787	-697.921924	-698.783285	-1002.232504
F8	-730.000520	-729.972596	-729.988920	-730.877862	-1034.320041
F9	-1189.849321	-1189.741779	-1189.840446	-1190.588980	-1494.059538
F10	-544.572640	-544.454856	-544.564780	-545.322850	-848.790086
F11	-1496.602964	-1496.497740	-1496.588508	-1497.341167	*
F12	-811.635320	-811.536172	-811.620948	-812.356464	*
F13	-620.652172	-620.555978	-620.642091	-621.460953	-924.927548
F14	-580.913018	-580.802913	-580.902855	-581.692931	-885.169960
F15	-624.988704	-624.916737	-624.978492	-625.675562	*
F16	-737.847421	-737.798246	-737.831409	-738.586914	*
F17	-548.912208	-548.802483	-548.902712	-549.629816	*
F18	-580.963696	-580.844764	-580.954414	-581.708499	-885.169361
F19	-580.975763	-580.865226	-580.966542	-581.711069	-885.175309
F20	-580.971938	-580.873716	-580.962610	-581.726161	-885.195723
F21	-583.341545	-583.234513	-583.329527	-584.045923	*
F22	-583.335103	-583.229092	-583.323074	-584.003749	*
F23	-1189.825227	-1189.722301	-1189.816364	-1190.529323	*
F24	-544.549932	-544.436312	-544.542004	-545.263893	*

*These structure gets deformed.

The electronic parameters were estimated using the equations given below.

$$\Delta E_{S-T} = E_{\text{singlet}} - E_{\text{triplet}} \dots \dots \dots (S1)$$

E is the sum of the electronic energy and zero-point energy.

$$\text{Hydride ion affinity} = - (H_{\text{CFTIH}} - (H_{\text{CFTI}}^+ - 0.517252)) \dots \dots \dots (S2)$$

The H_{CFTIH} , and H_{CFTI}^+ are the sum of electronic energy and thermal enthalpy correction values of a hydride complex, and *f*CFTI molecule respectively.

$$\Delta H_{\text{NHC}} = (H_{[\text{fCFTI-NHC}]}^+ - (H_{\text{fCFTI}}^+ - 304.234936)) \dots \dots \dots (S3)$$

The $H_{\text{fCFTI-NHC}}$ and H_{fCFTI}^+ are the sum of electronic energy and thermal enthalpy correction values of an NHC complex and *f*CFTI molecule respectively.

$$\omega = \mu^2 / 2\eta \dots \dots \dots (S4)$$

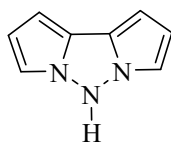
Where μ is chemical potential and η is the hardness of molecules obtained using equations (i) and (ii).

$$\mu = (E_{\text{HOMO}} + E_{\text{LUMO}}) / 2 \dots \dots \dots (i) \quad \eta = E_{\text{LUMO}} - E_{\text{HOMO}} \dots \dots \dots (ii)$$

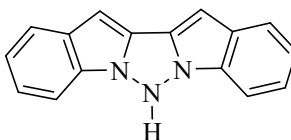
The ^{15}N chemical shift value (δ) were estimated using equation S5.

$$\delta \text{ (ppm)} = -145.37 - \sigma_{\text{iso}}(^{15}\text{N}) \dots \dots \dots (S5)$$

σ_{iso} denotes the absolute chemical shielding value of the N^2 center in *f*CFTIs **F1-F24** and -145.37 (σ_{ref}) is the absolute chemical shielding value of the nitrogen in CH_3NO_2 .



XXV



XXVI
CAS No. 241-15-6

Figure S1. 1,2,3-Triazole ring containing bipyrrrole and biindole.

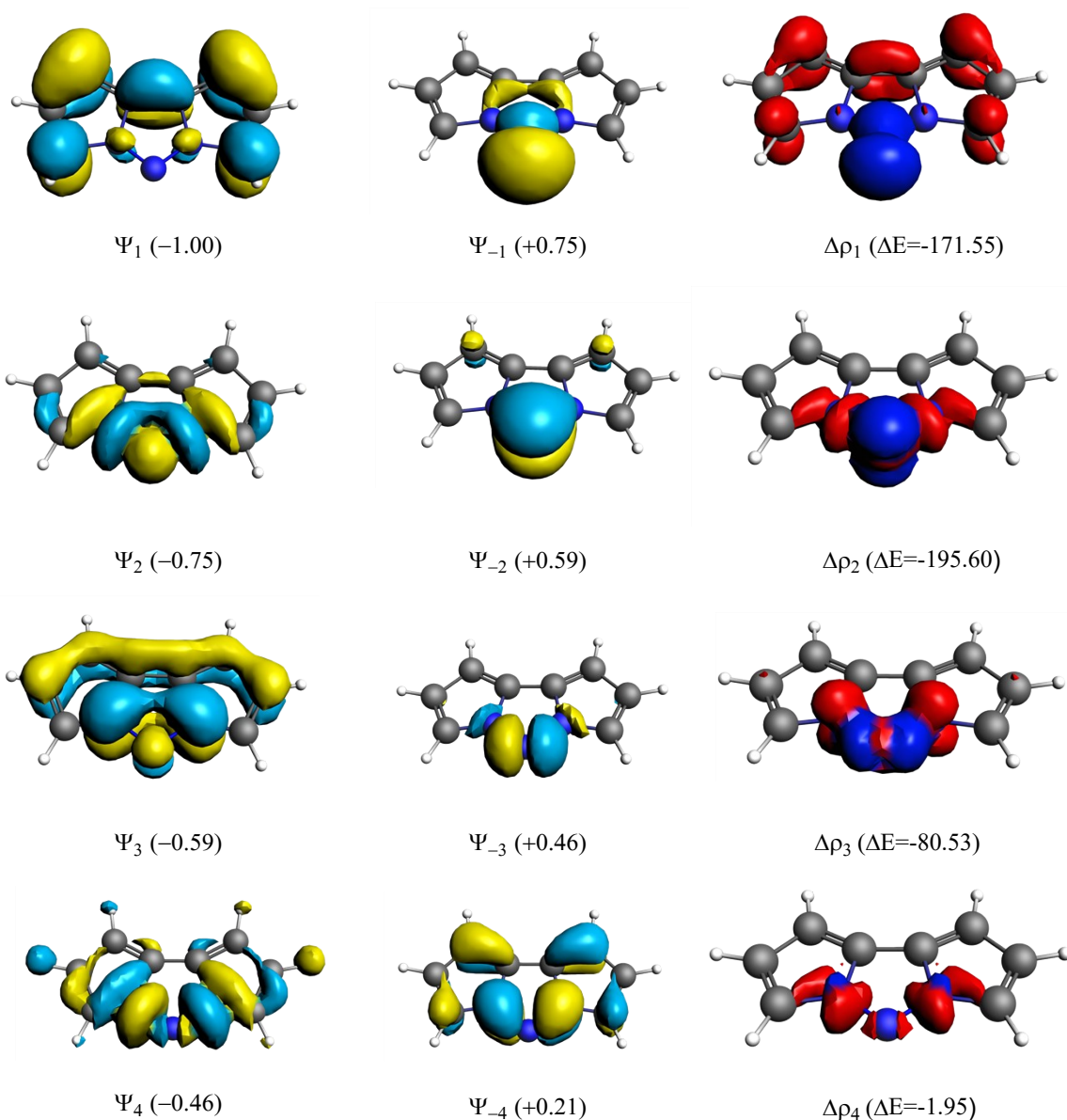


Figure S2a Plots of important NOCV pair of orbitals Ψ_n/Ψ_n of best bonding possibility in **F1** with their Eigen values in the parenthesis, the associated deformation densities $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue. The isosurface values for NOCV orbitals and deformation densities are 0.03 and 0.003, respectively. $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue.

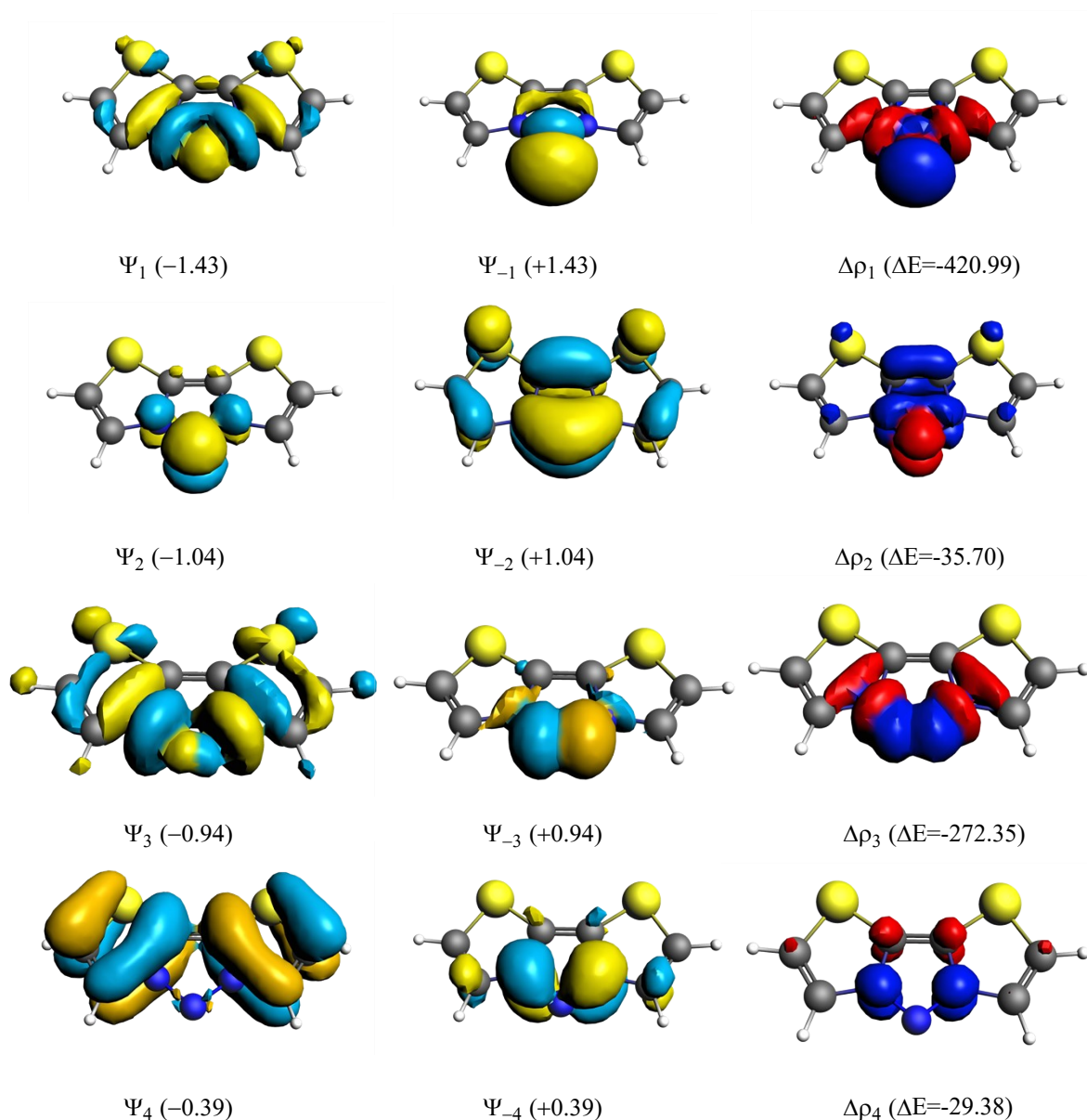


Figure S2b. Plots of important NOCV pair of orbitals Ψ_n/Ψ_{-n} of best bonding possibility in **F9** with their Eigen values in the parenthesis, the associated deformation densities $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue. The isosurface values for NOCV orbitals and deformation densities are 0.03 and 0.003, respectively. $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue.

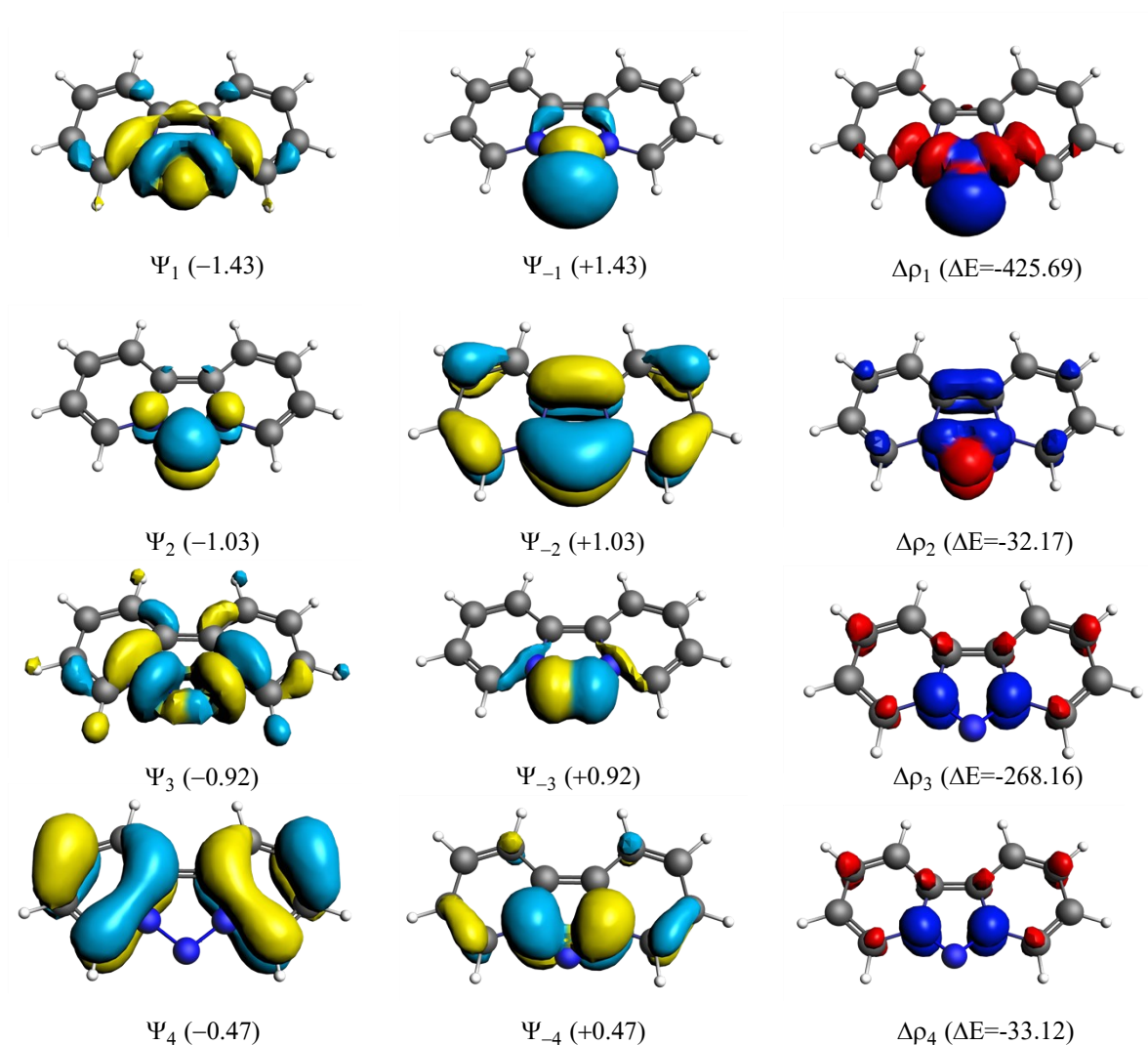


Figure S2c. Plots of important NOCV pair of orbitals Ψ_n/Ψ_{-n} of best bonding possibility in **F17** with their Eigen values in the parenthesis, the associated deformation densities $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue. The isosurface values for NOCV orbitals and deformation densities are 0.03 and 0.003, respectively. $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue.

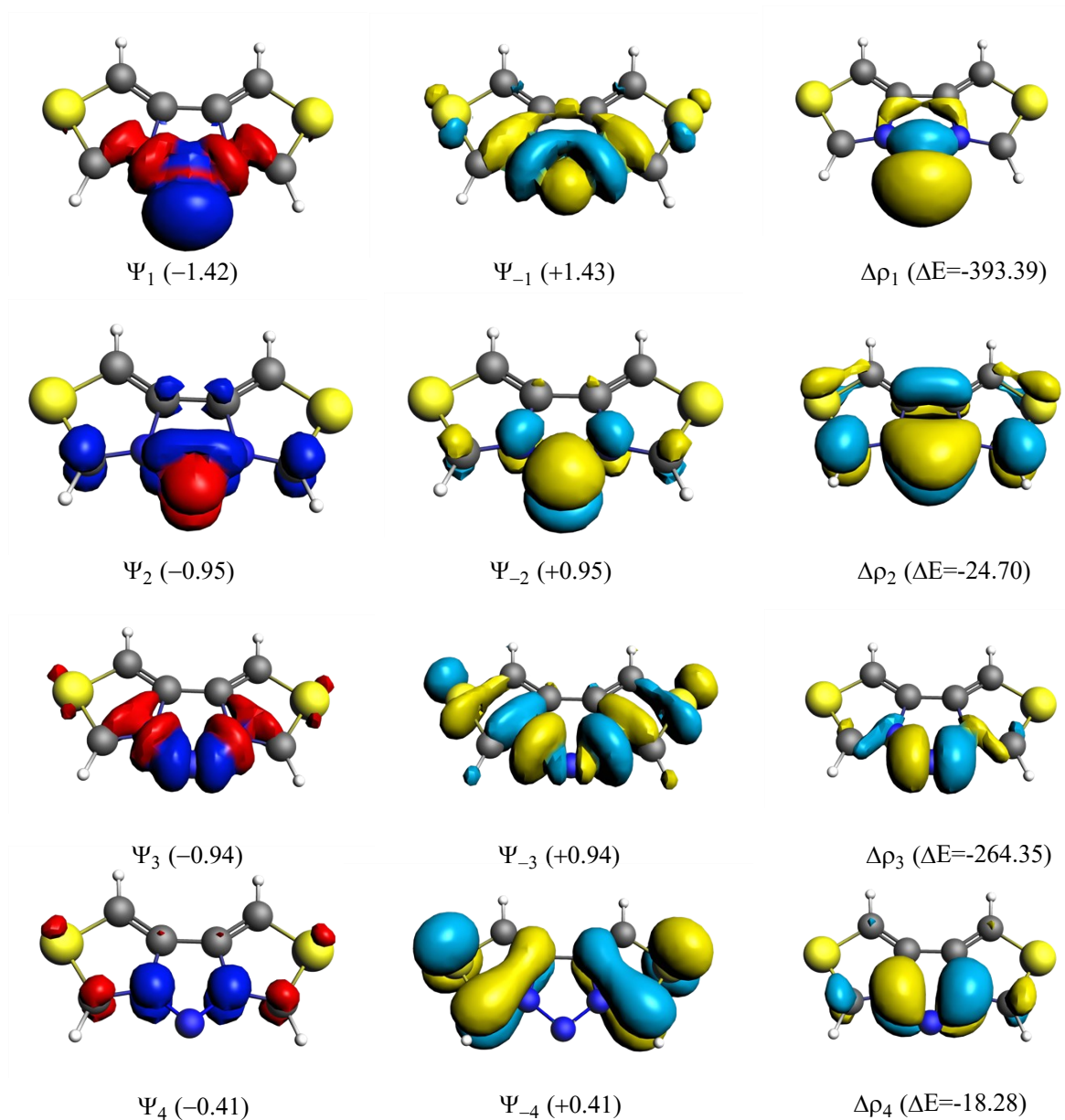
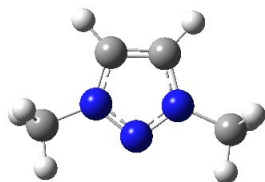


Figure S2d. Plots of important NOCV pair of orbitals Ψ_n/Ψ_n of best bonding possibility in **F23** with their Eigen values in the parenthesis, the associated deformation densities $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue. The isosurface values for NOCV orbitals and deformation densities are 0.03 and 0.003, respectively. $\Delta\rho_n$ and the orbital stabilization energies ΔE (kcal/mol) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot $\Delta\rho_n$ is from red to blue.

Cartesian coordinates of all the optimized geometries of CFTI IX, and X, β CFTIs (F1-F24), and their complexes with H⁻, NHC considered in this study

IX-Singlet



1 1			
C	0.68470700	-1.25175500	0.00000000
C	-0.68470700	-1.25175500	-0.00000700
N	1.04327100	0.06051700	0.00000600
H	1.39944800	-2.05749200	0.00002600
H	-1.39944800	-2.05749200	-0.00001800
N	0.00000000	0.85908400	-0.00003600
N	-1.04327100	0.06051700	-0.00000500
C	-2.39888600	0.63489200	0.00001800
H	-2.92450400	0.30586900	-0.89544400
H	-2.92448200	0.30586100	0.89549100
H	-2.29420500	1.71653000	0.00002100
C	2.39888600	0.63489200	0.00001100
H	2.92450000	0.30584800	-0.89544600
H	2.29420500	1.71653000	-0.00001100
H	2.92448700	0.30588200	0.89548900

IX-Triplet

1 3			
C	-0.70371200	1.22499400	0.03173600
C	0.70355600	1.22491600	0.03136700
N	-1.12016800	-0.04087100	-0.14721500
H	-1.37523700	2.06515500	0.12998200
H	1.37523700	2.06489600	0.13005100
N	0.00029200	-0.90717700	0.12722500
N	1.11996900	-0.04124200	-0.14856200
C	2.45150500	-0.61526900	0.01951000
H	3.18462700	0.15723200	-0.20715400
H	2.58418400	-0.97434900	1.04342700
H	2.56756000	-1.44208200	-0.68021900
C	-2.45148700	-0.61552200	0.01905900
H	-2.56724700	-1.44077800	-0.68259400
H	-2.58416000	-0.97710000	1.04210700
H	-3.18478800	0.15734700	-0.20577100

IX.H⁻

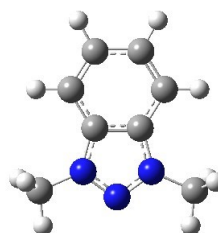
0 1			
C	0.66661900	1.26594500	-0.14685500
C	-0.66661900	1.26594500	-0.14685600
N	1.17838600	0.05342500	0.40247200
H	1.34539900	2.03391700	-0.48589500
H	-1.34539900	2.03391700	-0.48589500
N	0.00000000	-0.62627200	0.92890600
N	-1.17838600	0.05342500	0.40247200
C	-1.92528600	-0.77812500	-0.55041300
H	-2.79589200	-0.21091500	-0.89015700
H	-1.32855500	-1.06881200	-1.42622000

H	-2.27358000	-1.67569500	-0.03951000
C	1.92528500	-0.77812500	-0.55041300
H	2.79589200	-0.21091500	-0.89015700
H	2.27358000	-1.67569600	-0.03951100
H	1.32855400	-1.06881200	-1.42622000
H	0.00000000	-0.37487100	1.91382900

IX.NHC

1 1			
C	2.25381000	1.11125400	0.14040700
C	2.17712300	0.31973000	1.20633400
N	1.31576700	0.72602600	-0.86720200
H	2.89283100	1.96374100	-0.02914400
H	2.74619400	0.35682800	2.12212600
N	0.56247100	-0.34423900	-0.23855900
N	1.20051200	-0.71107800	1.03575000
C	1.78529300	-2.06685800	1.01186300
H	0.99214000	-2.80992100	0.94194700
H	2.49949500	-2.20305600	0.19268500
H	2.30029100	-2.21421100	1.96271600
C	1.91528100	0.31358000	-2.15223500
H	2.47337400	1.16597200	-2.54326000
H	2.59107300	-0.54103200	-2.04355200
H	1.12110300	0.07211500	-2.85798700
C	-0.77740700	0.00084500	-0.05790900
N	-1.76355100	-0.90722000	-0.21429000
N	-1.35538600	1.18283800	0.24963300
C	-2.97972500	-0.29698500	0.01027700
C	-1.58703500	-2.31891100	-0.57230700
C	-2.72460300	1.00670900	0.28590600
C	-0.69246400	2.46926800	0.51175300
H	-3.91043900	-0.83354700	-0.05162700
H	-2.38465800	-2.60598800	-1.25552100
H	-0.62260200	-2.43309800	-1.06042700
H	-1.62704400	-2.94029600	0.32261700
H	-3.39479500	1.82082700	0.50095200
H	-1.45339800	3.16837000	0.85079300
H	0.06063700	2.34570100	1.28659000
H	-0.22452500	2.83151400	-0.40077800

X-Singlet



1 1			
C	0.21905400	-0.70200900	-0.00003000
C	0.21906100	0.70200600	-0.00002500
C	1.40710100	1.44350300	0.00003300
C	2.57671500	0.70858000	0.00008400
C	2.57670900	-0.70859500	0.00008200

C	1.40709100	-1.44351100	0.00003000
H	1.41279300	2.52527200	0.00005000
H	3.52665200	1.22819900	0.00012900
H	3.52664400	-1.22822000	0.00012900
H	1.41277700	-2.52528000	0.00004900
N	-1.11185500	1.05365500	-0.00006200
N	-1.89384500	0.00000900	-0.00005200
N	-1.11185800	-1.05365700	-0.00009600
C	-1.70064900	2.39678800	-0.00000600
H	-1.38079400	2.92972700	0.89537800
H	-1.37905400	2.93050700	-0.89429400
H	-2.78132700	2.28187900	-0.00111200
C	-1.70066900	-2.39677100	0.00001500
H	-1.37866800	-2.93071100	-0.89399500
H	-1.38125000	-2.92951800	0.89567100
H	-2.78134700	-2.28185300	-0.00163400

X-Triplet

1 3			
C	-0.19203300	-0.70514600	-0.00874000
C	-0.19204600	0.70513800	-0.00874100
C	-1.39605800	1.43463700	0.00127900
C	-2.64135600	0.67775400	0.00312300
C	-2.64134500	-0.67779200	0.00312400
C	-1.39602600	-1.43466100	0.00128100
H	-1.40973000	2.51623100	0.01015900
H	-3.57236500	1.22896000	0.00619200
H	-3.57234300	-1.22901600	0.00619300
H	-1.40968800	-2.51625600	0.01016600
N	1.11078500	1.07024900	-0.01776900
N	1.96484600	0.00001500	-0.01380400
N	1.11081200	-1.07023000	-0.01776900
C	1.69550400	2.40570900	0.01873800
H	1.02059300	3.10803500	-0.46768000
H	1.86987400	2.70687100	1.05399800
H	2.64237200	2.37125300	-0.51637400
C	1.69555500	-2.40568000	0.01873700
H	1.86997000	-2.70682300	1.05399400
H	1.02063500	-3.10802300	-0.46764300
H	2.64240000	-2.37122000	-0.51641400

X.H⁻

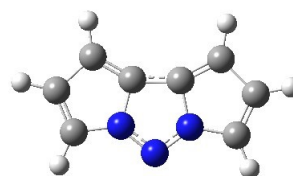
0 1			
C	-0.21917900	0.70316200	-0.14246600
C	-0.21917100	-0.70316500	-0.14246200
C	-1.39868600	-1.41748200	-0.02177400
C	-2.59738300	-0.69498000	0.09420000
C	-2.59739000	0.69496100	0.09419600
C	-1.39869700	1.41747100	-0.02178300
H	-1.40459100	-2.50083000	-0.01845500
H	-3.53257400	-1.23359900	0.19291900
H	-3.53258500	1.23357200	0.19291300
H	-1.40461000	2.50081900	-0.01847100
N	1.11052600	-1.11977400	-0.35523900
N	1.93935300	0.00001100	0.04858900
N	1.11052000	1.11978200	-0.35524800
C	1.59221100	-2.37282600	0.18137900
H	1.54592600	-2.40940600	1.28392200
H	0.98861700	-3.18756000	-0.21988500
H	2.62490400	-2.51705800	-0.13719500
C	1.59218300	2.37283700	0.18138800
H	0.98861200	3.18757200	-0.21990700
H	1.54584900	2.40942000	1.28392900

H	2.62489100	2.51706400	-0.13714000
H	1.90944100	0.00001100	1.09459800

X.NHC

1 1			
C	1.52730300	0.16047100	0.05380100
N	1.68522100	1.46957700	-0.24801000
N	2.66736600	-0.47874300	-0.28130900
C	2.95131900	1.64207300	-0.78702100
C	0.73539100	2.58675800	-0.09885200
C	3.55491000	0.43184800	-0.82151500
C	2.93280900	-1.90773400	-0.10177600
H	3.30403000	2.61078400	-1.09435400
H	1.20838000	3.46612400	-0.53075000
H	-0.18683100	2.37317600	-0.63395700
H	0.51821400	2.75477600	0.95220900
H	4.52948600	0.13990700	-1.17148100
H	2.46631100	-2.48177200	-0.90155000
H	4.01025600	-2.05787500	-0.11737700
H	2.53647300	-2.22280300	0.86207100
N	0.47105000	-0.51888700	0.66405800
N	-0.22471700	-1.37637700	-0.30072900
N	-0.46251500	0.37795600	1.29945300
C	-1.43892200	-0.63982300	-0.53724100
C	-1.60033800	0.34925600	0.43138700
C	-0.69911600	0.04466100	2.71776500
C	-2.39929500	-0.85755100	-1.51237400
C	-2.73192800	1.15182200	0.45996100
H	0.24603900	0.09802800	3.25653300
H	-1.37201300	0.79854700	3.12736800
C	-3.53945300	-0.04940400	-1.49381400
H	-2.27126000	-1.62667400	-2.26410900
C	-3.70507100	0.93598400	-0.52003200
H	-2.86285900	1.91857000	1.21403000
H	-4.30237000	-0.18987800	-2.24940900
H	-4.59677400	1.55056900	-0.52604600
C	-0.48456100	-2.72718300	0.24497100
H	0.45775300	-3.23126800	0.45000000
H	-1.09684900	-2.70686800	1.15222800
H	-1.14703500	-0.94483700	2.85272700
H	-1.01406600	-3.29025000	-0.52392500

F1-Singlet



1 1			
C	-0.00000100	-0.69927500	0.71925100
N	-0.00000100	1.47856800	0.00000000
N	0.00000200	0.68657600	-1.02794400
N	0.00000200	0.68657600	1.02794400
C	-0.00000100	-0.69927500	-0.71925100
C	-0.00000100	-1.35255100	1.91267500
C	0.00001400	0.90192600	2.42910200
C	-0.00001200	-0.33475300	2.97438100
H	-0.00002300	-0.55012900	4.03151100
H	0.00002300	1.89696600	2.84082400

H	-0.00000500	-2.41994100	2.06918900
C	-0.00000100	-1.35255100	-1.91267500
H	-0.00000500	-2.41994100	-2.06918900
C	0.00001400	0.90192600	-2.42910200
C	-0.00001200	-0.33475300	-2.97438100
H	-0.00002300	-0.55012900	-4.03151100
H	0.00002300	1.89696600	-2.84082400

F1-Triplet

1 3			
C	0.69390100	-0.64563200	0.00000300
N	0.00000000	1.57587500	0.00000100
N	-1.03422900	0.71701400	0.00000000
N	1.03422900	0.71701400	0.00000300
C	-0.69390100	-0.64563200	0.00000000
C	1.91852000	-1.36555700	0.00000700
C	2.39612000	0.87534400	0.00000700
C	2.94588700	-0.41729800	-0.00001100
H	4.00416300	-0.62725100	-0.00002400
H	2.85760300	1.85018900	0.00000800
H	2.02401400	-2.43874700	0.00000800
C	-1.91852000	-1.36555700	0.00000200
H	-2.02401400	-2.43874700	0.00000300
C	-2.39612000	0.87534400	-0.00000100
C	-2.94588700	-0.41729800	-0.00000800
H	-4.00416300	-0.62725100	-0.00001400
H	-2.85760300	1.85018900	-0.00000200

F1.H-

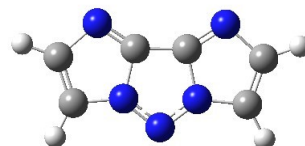
0 1			
C	-0.72067200	0.64943300	0.07748700
N	-0.00006100	-1.59906700	0.00011800
N	1.08771900	-0.68087600	0.01942300
N	-1.08783500	-0.68096200	0.02136800
C	0.72063600	0.64943000	0.07667700
C	-1.88789800	1.38999200	0.02408500
C	-2.44444000	-0.82691500	-0.08919800
C	-2.96034100	0.45837700	-0.06916500
H	-4.01032300	0.69967700	-0.12678500
H	-2.91622300	-1.79177000	-0.16169300
H	-1.96323800	2.46492800	0.03057900
C	1.88796100	1.38996700	0.02479600
H	1.96337000	2.46489300	0.03213200
C	2.44440800	-0.82692700	-0.08956900
C	2.96038000	0.45835500	-0.06851800
H	4.01038500	0.69961900	-0.12586600
H	2.91613000	-1.79175300	-0.16284700
H	0.00094300	-2.06952600	0.90854100

F1.NHC

1 1			
C	2.01905200	0.71284300	0.13929300
N	-0.08690300	0.13104300	-0.76314400
N	0.76533700	-1.00474300	-0.60750600
N	0.76189500	1.16420200	-0.24854400
C	2.00407500	-0.71289400	-0.06024400
C	2.77789400	1.83428000	0.39679000
C	0.72211300	2.54089900	-0.32529600
C	1.95673000	2.96655500	0.11871400
H	2.24339700	4.00022700	0.23195600
H	-0.15697600	3.08315600	-0.62868700

H	3.80648600	1.84806100	0.71748300
C	2.69284000	-1.90684200	0.00980000
H	3.70151300	-2.04188600	0.36379900
C	0.63414200	-2.34353500	-0.89950400
C	1.82969000	-2.91605900	-0.50723600
H	2.06858900	-3.96284200	-0.61020800
H	-0.24369300	-2.75764000	-1.36519100
C	-1.29151100	0.00887600	-0.03860400
N	-2.48803100	0.19594500	-0.62412700
N	-1.49379000	-0.29814100	1.25790400
C	-3.47201000	0.00790900	0.32058900
C	-2.71838000	0.54529000	-2.03644000
C	-2.85021200	-0.30286700	1.49174500
C	-0.45463900	-0.59409000	2.26260700
H	-4.51800700	0.10765000	0.08661700
H	-3.37002100	-0.20392600	-2.48426300
H	-3.18657000	1.52766600	-2.09114600
H	-1.75988200	0.55985600	-2.54789000
H	-3.25924100	-0.52531900	2.46261600
H	-0.95095200	-0.73002400	3.22038500
H	0.07447700	-1.50483400	1.98542600
H	0.24262200	0.23952100	2.32375800

F2-Singlet



1 1			
C	0.00000000	-0.68429700	0.72734300
N	-0.00000200	1.50746300	0.00000000
N	0.00000000	0.71471200	-1.02941400
N	0.00000000	0.71471200	1.02941400
C	0.00000000	-0.68429700	-0.72734300
C	0.00000300	0.84739300	2.43882700
C	-0.00000100	-0.43266600	2.87315400
H	-0.00000300	-0.78769100	3.89132700
H	0.00000500	1.80461500	2.93249900
C	0.00000300	0.84739300	-2.43882700
C	-0.00000100	-0.43266600	-2.87315400
H	-0.00000300	-0.78769100	-3.89132700
H	0.00000500	1.80461500	-2.93249900
N	0.00000000	-1.38265800	-1.79717200
N	0.00000000	-1.38265800	1.79717200

F2- Triplet

1 3			
C	0.63995100	-0.00000200	0.69800800
N	-1.60522800	0.00001000	0.00000000
N	-0.73596500	0.00000200	-1.03505800
N	-0.73596500	0.00000200	1.03505800
C	0.63995100	-0.00000200	-0.69800800
C	-0.83458700	-0.00001300	2.38947100
C	0.51879900	0.00001700	2.82254900
H	0.85402100	0.00002300	3.84981400
H	-1.77142400	-0.00001900	2.92463900
C	-0.83458700	-0.00001300	-2.38947100
C	0.51879900	0.00001700	-2.82254900
H	0.85402100	0.00002300	-3.84981400

H	-1.77142400	-0.00001900	-2.92463900
N	1.39178200	-0.00001000	-1.79805900
N	1.39178200	-0.00001000	1.79805900

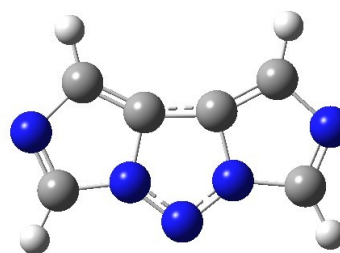
F2.H⁻

0 1			
C	0.72269000	-0.63378700	0.07187600
N	0.00006600	1.61403800	-0.03882600
N	-1.08150600	0.69414400	0.03005300
N	1.08155200	0.69419000	0.03125000
C	-0.72267300	-0.63376800	0.07143700
C	2.44809600	0.77353400	-0.07981800
C	2.84443800	-0.54987300	-0.05867700
H	3.85707400	-0.91976800	-0.10351000
H	2.98630600	1.70274300	-0.14591200
C	-2.44807400	0.77355300	-0.08018000
C	-2.84447700	-0.54984600	-0.05804300
H	-3.85714900	-0.91970700	-0.10233000
H	-2.98623700	1.70274900	-0.14680100
N	-1.77812700	-1.41499200	0.02218700
N	1.77807500	-1.41500900	0.02192900
H	-0.00041500	2.14850300	0.83283100

F2.NHC

1 1			
C	-2.02524100	-0.72311300	0.03153200
N	0.08856600	0.00691500	-0.74647300
N	-0.76542900	1.09605400	-0.38423700
N	-0.76442100	-1.08888100	-0.40320300
C	-2.02686100	0.72105700	0.04201300
C	-0.73947200	-2.45948600	-0.57743600
C	-1.99883700	-2.84531400	-0.16924200
H	-2.38061300	-3.85331000	-0.12564300
H	0.11594100	-3.00553200	-0.93504800
C	-0.74703700	2.46826800	-0.54820300
C	-2.00845900	2.84513900	-0.13870700
H	-2.39407900	3.85118600	-0.08513000
H	0.10754600	3.02147100	-0.89667100
N	-2.79232100	1.76711500	0.20998600
N	-2.78610500	-1.77396400	0.19157600
C	1.31247900	0.00125500	-0.04844900
N	2.49398700	0.01020200	-0.69188800
N	1.54710800	-0.01342300	1.27966200
C	3.50117100	0.00123800	0.24566500
C	2.68998500	0.02740200	-2.15274300
C	2.90946600	-0.01361600	1.47306500
C	0.53483400	-0.02722400	2.35429800
H	4.54175800	0.00600700	-0.03064000
H	3.23949800	0.92721200	-2.42698300
H	3.25301300	-0.85796500	-2.44578000
H	1.71513700	0.02511900	-2.63242400
H	3.34438600	-0.02421400	2.45816300
H	1.06206400	-0.03572600	3.30500700
H	-0.08552100	0.86494400	2.28750400
H	-0.08099000	-0.92096400	2.26891800

F3-Singlet



1 1			
C	0.69502800	-0.00000900	0.71934200
N	-1.48694300	0.00010500	0.00000000
N	-0.68751700	0.00001600	-1.02323400
N	-0.68751700	0.00001600	1.02323400
C	0.69502800	-0.00000900	-0.71934200
C	1.30784000	-0.00001300	1.93561600
C	-0.82661300	-0.00009600	2.45629300
H	-1.79318800	-0.00009600	2.93811400
H	2.35953500	0.00000000	2.17419100
C	1.30784000	-0.00001300	-1.93561600
H	2.35953500	0.00000000	-2.17419100
C	-0.82661300	-0.00009600	-2.45629300
H	-1.79318800	-0.00009600	-2.93811400
N	0.34186400	0.00004600	-2.97292900
N	0.34186400	0.00004600	2.97292900

F3-Triplet

1 3			
C	0.64740300	0.00000300	0.69446600
N	-1.57058600	-0.00000100	0.00000000
N	-0.70557500	0.00000200	-1.03236800
N	-0.70557500	0.00000200	1.03236800
C	0.64740300	0.00000300	-0.69446600
C	1.31601300	0.00000500	1.96009100
C	-0.80620700	0.00000400	2.41325700
H	-1.74975300	-0.00000200	2.93864500
H	2.37936500	0.00000200	2.14870800
C	1.31601300	0.00000500	-1.96009100
H	2.37936500	0.00000200	-2.14870800
C	-0.80620700	0.00000400	-2.41325700
H	-1.74975300	-0.00000200	-2.93864500
N	0.40903100	-0.00001100	-2.95115400
N	0.40903100	-0.00001100	2.95115400

F3.H⁻

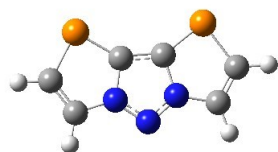
0 1			
C	0.72094100	0.65849300	0.08490600
N	0.00003600	-1.60078400	-0.00089900
N	-1.08840500	-0.67733700	0.02290700
N	1.08844900	-0.67734300	0.02332900
C	-0.72094800	0.65848000	0.08474500
C	1.91351100	1.34384800	0.02114100
C	2.44526000	-0.75731800	-0.09444500
H	2.98316500	-1.68814700	-0.17005900
H	2.07703800	2.40884500	0.02649400
C	-1.91354600	1.34382600	0.02138000
H	-2.07710400	2.40881700	0.02696800
C	-2.44523100	-0.75731700	-0.09464700

H	-2.98311200	-1.68814500	-0.17044400
N	-2.95931500	0.45588900	-0.07656600
N	2.95929200	0.45591000	-0.07675900
H	-0.00030800	-2.07579000	0.90446500

F3.NHC

1 1			
N	0.77291600	1.10164200	-0.41822300
N	-0.08550200	0.00058200	-0.75790000
N	0.77308000	-1.10082300	-0.41986500
C	2.02743200	-0.72009900	0.05117400
C	2.02735200	0.72038600	0.05220000
C	0.75566800	-2.46493300	-0.59039000
H	-0.09316500	-3.01602200	-0.96223800
C	0.75550600	2.46594600	-0.58721200
H	-0.09338600	3.01746900	-0.95827900
C	-1.29864000	-0.00006700	-0.04121100
N	-2.48798600	0.00081800	-0.67110200
N	-1.51924300	-0.00168800	1.28955500
C	-3.48455700	-0.00019400	0.27735100
C	-2.70256400	0.00284800	-2.12968300
C	-2.87919200	-0.00179900	1.49810400
C	-0.49731300	-0.00316800	2.35451000
H	-4.52817100	0.00027300	0.01271200
H	-3.26437200	-0.88835400	-2.40692100
H	-3.26069900	0.89693300	-2.40509700
H	-1.73419000	0.00137900	-2.62206900
H	-3.30315500	-0.00300600	2.48800000
H	-1.01578700	-0.00391000	3.31000800
H	0.12019600	-0.89591000	2.27141300
H	0.12090000	0.88925100	2.27320100
N	1.90602300	2.95495600	-0.19449000
N	1.90618200	-2.95437700	-0.19817800
C	2.71027700	1.90503000	0.18850500
H	3.72371500	2.06375100	0.51810200
C	2.71037200	-1.90489100	0.18614600
H	3.72378700	-2.06397700	0.51563600

F4-Singlet



1 1			
C	0.00000000	0.71676400	-0.43165400
N	0.00000000	0.00000000	1.73760100
N	0.00000000	-1.03004900	0.93934800
N	0.00000000	1.03004900	0.93934800
C	0.00000000	-0.71676400	-0.43165400
C	0.00000000	2.40379900	1.26818500
C	0.00000000	3.13716100	0.14218300
H	0.00000000	4.21818000	0.13731100
H	0.00000000	2.68789300	2.30977900
C	0.00000000	-2.40379900	1.26818500
C	0.00000000	-3.13716100	0.14218300

H	0.00000000	-4.21818000	0.13731100
H	0.00000000	-2.68789300	2.30977900
P	0.00000000	2.14628600	-1.39842700
P	0.00000000	-2.14628600	-1.39842700

F4-Triplet

1 3			
C	0.00000000	0.69370500	-0.37729300
N	0.00000000	0.00000000	1.81355500
N	0.00000000	-1.03338800	0.96817400
N	0.00000000	1.03338800	0.96817400
C	0.00000000	-0.69370500	-0.37729300
C	0.00000000	2.39608900	1.24021700
C	0.00000000	3.12947600	0.08354200
H	0.00000000	4.21084000	0.08791300
H	0.00000000	2.72457500	2.26972200
C	0.00000000	-2.39608900	1.24021700
C	0.00000000	-3.12947600	0.08354200
H	0.00000000	-4.21084000	0.08791300
H	0.00000000	-2.72457500	2.26972200
P	0.00000000	2.18017600	-1.41073900
P	0.00000000	-2.18017600	-1.41073900

F4.H-

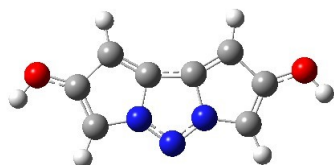
0 1			
C	0.72048700	-0.38332400	0.05624800
N	-0.00001800	1.85331300	0.01297400
N	-1.09180500	0.93861500	0.01263600
N	1.09182600	0.93861600	0.01303200
C	-0.72048400	-0.38332800	0.05604700
C	2.42969100	1.19804300	-0.07539800
C	3.13894500	0.02310400	-0.06545300
H	4.21767700	-0.00588100	-0.12021500
H	2.77617400	2.21831600	-0.14197500
C	-2.42968100	1.19805100	-0.07540600
C	-3.13894100	0.02310700	-0.06557900
H	-4.21766300	-0.00586800	-0.12056500
H	-2.77617200	2.21830500	-0.14216900
P	2.11563400	-1.43021300	0.01135100
P	-2.11564800	-1.43020500	0.01161700
H	0.00006600	2.31368000	0.92715900

F4.NHC

1 1			
C	-1.68786000	0.71971700	-0.06860500
N	0.43464800	-0.00005300	-0.79675600
N	-0.43721400	-1.10333700	-0.50459100
N	-0.43722500	1.10325900	-0.50472400
C	-1.68785800	-0.71975100	-0.06852400
C	-0.22744200	2.44814500	-0.68343700
C	-1.35160500	3.14052600	-0.31981200
H	-1.41215100	4.21810200	-0.37136400
H	0.71582500	2.80905900	-1.06501500
C	-0.22744700	-2.44823900	-0.68320700
C	-1.35162000	-3.14058100	-0.31954400
H	-1.41217300	-4.21816100	-0.37100800

H	0.71582500	-2.80919400	-1.06473200
P	-2.70824300	2.10662400	0.19487400
P	-2.70825100	-2.10662800	0.19505900
C	1.60801100	0.00000400	-0.01792200
N	1.75518100	0.00016300	1.32278400
N	2.83121900	-0.00009500	-0.58067400
C	3.10112300	0.00016700	1.60680500
C	0.67313400	0.00032200	2.32709900
C	3.77373200	0.00001100	0.42183300
C	3.12420100	-0.00027000	-2.02463200
H	3.46915500	0.00028400	2.61875600
H	0.06010800	-0.89152100	2.20787100
H	1.13577700	0.00026600	3.31081600
H	0.06035300	0.89233300	2.20785000
H	4.83037000	-0.00004000	0.21565700
H	3.69835100	0.89208400	-2.27140700
H	3.69822900	-0.89275400	-2.27122100
H	2.18324800	-0.00026300	-2.56779600

F5-Singlet



l 1			
C	-0.72003900	-0.57513600	0.00012800
N	0.00000500	1.60176500	-0.00005800
N	1.03411000	0.81079700	-0.00021200
N	-1.03411000	0.81079200	0.00016800
C	0.72003800	-0.57514000	-0.00013400
C	-1.89758500	-1.24318100	-0.00003200
C	-2.42292600	1.02986500	0.00017100
C	-2.96632100	-0.22375800	0.00001300
H	-2.84297700	2.02036500	0.00028100
H	-2.06820700	-2.30846300	-0.00014400
C	1.89758000	-1.24318300	0.00009000
H	2.06821300	-2.30846200	0.00022900
C	2.42293200	1.02986800	-0.00007100
C	2.96632200	-0.22375300	-0.00000400
H	2.84297300	2.02037300	-0.00014400
O	4.23220700	-0.62910200	0.00001800
H	4.85190800	0.11238300	-0.00006700
O	-4.23221400	-0.62909500	-0.00009500
H	-4.85190200	0.11240000	0.00022200

F5-Triplet

l 3			
C	-0.69895900	-0.53647200	0.00005400
N	0.00000100	1.69804400	0.00000200
N	1.03707000	0.84138000	-0.00006100
N	-1.03706900	0.84138000	0.00005900
C	0.69895900	-0.53647200	-0.00006000
C	-1.89141100	-1.25671400	0.00003100
C	-2.38194300	1.01194500	0.00005700

C	-2.93136600	-0.30015600	0.00004400
H	-2.84832400	1.98408300	0.00007400
H	-2.01586000	-2.32702300	0.00003300
C	1.89141100	-1.25671400	-0.00002700
H	2.01586000	-2.32702300	-0.00003100
C	2.38194300	1.01194500	-0.00004800
C	2.93136600	-0.30015600	-0.00004400
H	2.84832400	1.98408300	-0.00006300
O	4.21361700	-0.64092300	-0.00004600
H	4.80094000	0.12588900	-0.00004500
O	-4.21361800	-0.64092200	0.00003400
H	-4.80094100	0.12589000	0.00008500

F5.H-

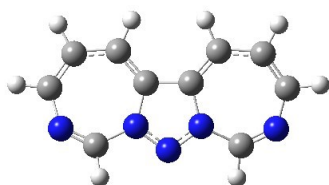
0 1			
C	-0.71986000	-0.49676300	0.16209900
N	-0.00059100	1.73796700	-0.01833900
N	1.08672100	0.82428600	0.07222100
N	-1.08800700	0.82563000	0.08882200
C	0.71940400	-0.49701500	0.15565700
C	-1.87529000	-1.25695300	0.08393400
C	-2.44954500	0.96328000	-0.08794000
C	-2.94528900	-0.33434300	-0.05902800
H	-2.93411400	1.92053400	-0.17442200
H	-1.95778200	-2.33030900	0.10710000
C	1.87595900	-1.25685700	0.08632200
H	1.95924300	-2.32998700	0.11598400
C	2.44899000	0.96319700	-0.09360400
C	2.94563700	-0.33428200	-0.05718600
H	2.93212900	1.92021900	-0.18986300
O	4.24958300	-0.73380200	-0.13771100
H	4.80598300	0.03386800	-0.29894400
O	-4.24883100	-0.73446800	-0.14219100
H	-4.80472800	0.03234400	-0.30922800
H	0.00635500	2.28272100	0.84814700

F5.NHC

l 1			
C	-0.61585500	1.75877600	-0.07727300
N	0.04649700	-0.39931300	-0.73470200
N	-1.24515900	-0.41962800	-0.09936300
N	0.33964200	1.01098700	-0.73770200
C	-1.71195900	0.86709800	0.18195600
C	-0.08068700	3.00888500	0.15354600
C	1.54368700	1.69695800	-0.82811200
C	1.25947700	2.96524100	-0.32877400
H	2.37335700	1.34108400	-1.41600700
H	-0.57207900	3.86844400	0.57796000
C	-3.07673600	0.79872500	0.31794500
H	-3.75409600	1.60198900	0.55557400
C	-2.32255600	-1.27926000	-0.32178000
C	-3.44614800	-0.54893000	0.02126900
H	-2.19419200	-2.33146100	-0.51202300
O	-4.72713900	-0.96400000	0.12309500
H	-4.82217700	-1.86166800	-0.21226100
O	2.05209800	4.05864800	-0.31593400
H	2.89925700	3.87244800	-0.73401000
C	0.99469700	-1.16357700	-0.02472700

N	1.64307800	-2.19089100	-0.60466300
N	1.41958000	-1.05965900	1.24982200
C	2.49501600	-2.75166500	0.32026900
C	1.47587000	-2.64687200	-1.99440200
C	2.35474600	-2.04360200	1.47508000
C	0.98416500	-0.05566600	2.23784600
H	3.12141500	-3.59510800	0.08598100
H	2.43312100	-2.57732700	-2.50997700
H	1.12843800	-3.67950700	-1.99231600
H	0.74368200	-2.00698400	-2.47902900
H	2.83992200	-2.15960200	2.42921800
H	1.48829800	-0.27409400	3.17612300
H	1.26155200	0.93913000	1.89098300
H	-0.09393500	-0.12165500	2.37169200

F6-Singlet



l 1			
N	0.00000000	1.61037800	-0.00000300
N	1.05142400	0.84295200	0.01012000
N	-1.05142400	0.84295200	-0.01012100
C	-2.34296100	1.46174800	-0.28516500
C	2.34296100	1.46174700	0.28516900
H	-2.20794700	2.49462400	-0.59388700
H	2.20794700	2.49462300	0.59389300
C	-0.72845700	-0.54545700	0.01605900
C	0.72845700	-0.54545700	-0.01605700
C	1.61776300	-1.56616200	-0.09677800
C	-1.61776200	-1.56616200	0.09678100
H	-1.19162900	-2.56154500	0.13817500
H	1.19163000	-2.56154500	-0.13816900
C	3.83372600	-0.37740200	-0.12767000
C	-3.83372700	-0.37740300	0.12766700
H	-4.89964100	-0.48217200	0.28661400
H	4.89964000	-0.48217000	-0.28662200
C	-3.05067700	-1.47984100	0.20217000
C	3.05067700	-1.47984100	-0.20217100
H	-3.56219400	-2.41775200	0.38627600
H	3.56219400	-2.41775100	-0.38627900
N	-3.47113300	0.92465000	-0.21389400
N	3.47113200	0.92464900	0.21389500

F6-Triplet

l 3			
N	0.00000000	1.64388100	0.00000000
N	1.04713000	0.85218200	0.00001900
N	-1.04713000	0.85218200	-0.00001900
C	-2.34827900	1.48897500	0.00002800
C	2.34827900	1.48897500	-0.00002800
H	-2.24091900	2.56776300	0.00026500

H	2.24091900	2.56776300	-0.00026500
C	-0.69843300	-0.49266300	-0.00003500
C	0.69843300	-0.49266300	0.00003500
C	1.61223300	-1.59229900	-0.00013300
C	-1.61223300	-1.59229900	0.00013300
H	-1.15153700	-2.57150200	0.00025200
H	1.15153700	-2.57150200	-0.00025200
C	3.82467700	-0.39276800	0.00011300
C	-3.82467700	-0.39276800	-0.00011200
H	-4.89440800	-0.56458800	-0.00044700
H	4.89440800	-0.56458800	0.00044700
C	-2.98665300	-1.52710900	0.00020400
C	2.98665300	-1.52710900	-0.00020400
H	-3.50845400	-2.47839200	0.00043900
H	3.50845400	-2.47839200	-0.00043900
N	-3.48376900	0.91757700	-0.00011100
N	3.48376900	0.91757700	0.00011100

F6.H⁻

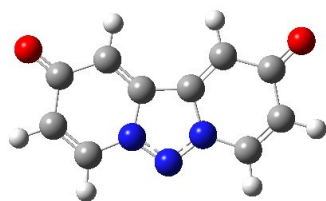
0 1			
N	-0.00002000	-1.45759900	1.06564500
N	1.16265100	-0.71368900	0.66064500
N	-1.16271200	-0.71369500	0.66060300
C	-1.90436800	-1.34562000	-0.38939600
C	1.90445900	-1.34566000	-0.38920300
H	-1.43302100	-2.22726000	-0.82080200
H	1.43320000	-2.22738400	-0.82053800
C	-0.72788400	0.60835500	0.28685100
C	0.72785100	0.60835700	0.28687000
C	1.60868600	1.59067600	-0.00212700
C	-1.60873500	1.59067700	-0.00210600
H	-1.22047000	2.57748000	-0.22836400
H	1.22039800	2.57745300	-0.22845800
C	3.64770800	0.20943300	-0.30920300
C	-3.64768800	0.20937200	-0.30937100
H	-4.73161500	0.16001900	-0.31813900
H	4.73163600	0.16010000	-0.31789200
C	-3.03771500	1.38688800	-0.02950100
C	3.03768600	1.38693900	-0.02943800
H	-3.67082900	2.25614700	0.11972600
H	3.67075200	2.25623100	0.11979900
N	-3.03929000	-0.95088900	-0.78399200
N	3.03937300	-0.95089200	-0.78377400
H	-0.00005700	-1.42194700	2.08052100

F6.NHC

l 1			
N	0.34104800	-0.31266300	0.63197300
N	-1.06886700	-0.48270800	0.47994900
N	0.73484400	0.99197900	0.14473500
C	1.02051600	1.94400200	1.20362800
C	-1.79275900	-0.45354800	1.74052500
H	0.75669100	1.64057400	2.21517000
H	-1.21251300	-0.16199900	2.61335700
C	-0.39498900	1.47706200	-0.62239300
C	-1.51787900	0.58262300	-0.39380000
C	-2.79041900	0.60615000	-0.85243700
C	-0.27913300	2.60142400	-1.36699400

H	-1.12321600	2.90256200	-1.97741200
H	-3.06736000	1.39143300	-1.54677700
C	-3.82621900	-1.01059900	0.72543500
C	1.75566100	3.55636100	-0.31843900
H	2.59289500	4.24100900	-0.39199200
H	-4.64600800	-1.68598500	0.94236800
C	0.89704500	3.42801400	-1.36655500
C	-3.79705500	-0.34658200	-0.46070200
H	1.05634700	4.07405800	-2.22310500
H	-4.64518300	-0.47636900	-1.12461300
N	1.54888600	3.06222400	0.96026000
N	-3.01182900	-0.75497400	1.81936100
C	1.08655400	-1.32904800	0.02732700
N	0.76625600	-2.18612900	-0.96490200
N	2.33560500	-1.61715900	0.44254500
C	1.84564800	-3.02812100	-1.17337200
C	-0.48127000	-2.26160800	-1.74549600
C	2.82586000	-2.66508200	-0.31064100
C	3.06924900	-0.91183700	1.49935400
H	1.81602700	-3.80992200	-1.91203700
H	-0.34553500	-3.03612800	-2.49676700
H	-1.31503700	-2.50709400	-1.09284700
H	-0.67287400	-1.31015700	-2.23767800
H	3.81515400	-3.06144700	-0.16231600
H	3.84742700	-1.57328000	1.87396700
H	3.51581500	0.00071300	1.10465000
H	2.38089300	-0.66722100	2.30593600

F7-Singlet



1 1			
N	0.00000000	1.81252700	-0.00000100
N	1.04882600	1.03629200	0.00000100
N	-1.04882600	1.03629200	-0.00000100
C	-2.36179400	1.52282300	-0.00000200
C	-3.36486800	0.63228600	-0.00000200
C	-3.12878100	-0.83173600	-0.00000200
C	2.36179400	1.52282300	0.00000100
C	3.12878100	-0.83173600	0.00000500
C	3.36486800	0.63228600	0.00000200
C	-0.72706200	-0.34384800	0.00000000
C	0.72706200	-0.34384800	0.00000100
C	1.70915500	-1.26575400	0.00000200
C	-1.70915500	-1.26575400	-0.00000100
H	1.50300700	-2.32879500	0.00000200
H	-1.50300700	-2.32879500	0.00000000
H	-4.39433900	0.96633400	-0.00000300
H	-2.45321200	2.60036700	-0.00000200
H	2.45321200	2.60036700	-0.00000100
O	4.03442000	-1.63980300	0.00000000
O	-4.03442000	-1.63980300	-0.00000200
H	4.39433900	0.96633400	0.00000100

F7-Triplet

1 3			
N	0.00000000	1.88778200	-0.00000300
N	1.05227600	1.04868400	-0.00000300
N	-1.05227600	1.04868400	-0.00000300
C	-2.36054300	1.50864900	-0.00000200
C	-3.35909000	0.59756400	0.00000000
C	-3.09112100	-0.84329300	-0.00000100
C	2.36054300	1.50864900	0.00000100
C	3.09112100	-0.84329300	-0.00001000
C	3.35909000	0.59756400	0.00000300
C	-0.71352500	-0.28615900	-0.00000200
C	0.71352500	-0.28615900	-0.00000200
C	1.70762100	-1.25820400	-0.00000100
C	-1.70762100	-1.25820400	0.00000000
H	1.47416100	-2.31503200	0.00000300
H	-1.47416100	-2.31503200	0.00000200
H	-4.39322700	0.91676400	0.00000100
H	-2.47392000	2.58376000	-0.00000200
H	2.47392000	2.58376000	0.00000500
O	4.01112300	-1.68060800	0.00001100
O	-4.01112300	-1.68060800	0.00000300
H	4.39322700	0.91676400	0.00001000

F7.H-

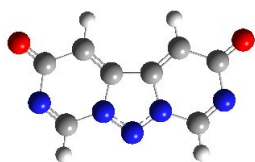
0 1			
N	-0.00000100	1.96631400	0.13564700
N	1.09860600	1.06724400	0.02320800
N	-1.09860600	1.06724300	0.02319700
C	-2.39878600	1.46822400	-0.10817900
C	-3.37741700	0.53200100	-0.12411400
C	-3.09703000	-0.91064500	-0.01908500
C	2.39878500	1.46822400	-0.10817900
C	3.09703400	-0.91064000	-0.01901200
C	3.37741700	0.53200100	-0.12411000
C	-0.73128000	-0.26299800	0.08215500
C	0.73128000	-0.26299800	0.08216400
C	1.66792300	-1.24262500	0.05285000
C	-1.66792100	-1.24262600	0.05283400
H	1.38104300	-2.28567600	0.06388000
H	-1.38104100	-2.28567700	0.06388400
H	-4.41091200	0.83243100	-0.23270300
H	-2.56082100	2.53464700	-0.19567700
H	2.56081900	2.53464600	-0.19569800
O	3.98047900	-1.76090800	-0.01602900
O	-3.98048100	-1.76090600	-0.01598100
H	4.41090900	0.83242900	-0.23272900
H	-0.00000400	2.29860600	1.10682400

F7.NHC

1 1			
N	-0.63600400	-0.00036400	-0.78882200
N	0.23110100	-1.11155100	-0.54239600
N	0.22971000	1.11190500	-0.54228200
C	-0.06895300	2.41233300	-0.88940700

C	0.83107200	3.38063500	-0.61749300
C	2.13922900	3.09638800	0.01192800
C	-0.06590100	-2.41229900	-0.88977200
C	2.14311000	-3.09370000	0.01153500
C	0.83535400	-3.37950100	-0.61801900
C	1.47597900	0.73120300	-0.06194800
C	1.47690700	-0.72934000	-0.06205700
C	2.41917300	-1.65897700	0.21408000
C	2.41706300	1.66198900	0.21435200
H	3.40201400	-1.36896400	0.56168000
H	3.40024900	1.37316400	0.56196800
H	0.61498800	4.40862500	-0.87619600
H	-1.02804200	2.58004700	-1.36171600
H	-1.02476800	-2.58113500	-1.36213400
O	2.93724100	-3.96847800	0.31012800
O	2.93215600	3.97213700	0.31087300
H	0.62060000	-4.40771800	-0.87693000
C	-1.77973800	-0.00112800	0.04969900
C	-3.21930100	-0.00241500	1.72429000
C	-3.93098000	-0.00230500	0.56306000
H	-3.55326600	-0.00297500	2.74817900
H	-4.99407500	-0.00272200	0.39234500
C	-0.77904500	-0.00151000	2.37532100
H	-0.17030000	-0.89507900	2.24873000
H	-0.17065700	0.89232200	2.24887700
H	-1.21963800	-0.00166400	3.36915400
C	-3.37516800	-0.00108000	-1.90152300
H	-3.96022200	0.89099400	-2.12273600
H	-2.45959800	-0.00099500	-2.48595700
H	-3.96032400	-0.89298200	-2.12314500
N	-3.02231900	-0.00147100	-0.47004000
N	-1.88319200	-0.00165400	1.39577000

F8-Singlet



1 1			
N	0.00000000	1.78093800	0.00001900
N	1.04151500	1.00222500	0.00003400
N	-1.04151500	1.00222500	0.00000900
C	-2.39363500	1.46233400	0.00000800
C	-3.13977400	-0.77385000	-0.00010000
C	2.39363500	1.46233400	-0.00002000
C	3.13977400	-0.77385100	0.00022200
C	-0.72770200	-0.37822400	0.00000200
C	0.72770200	-0.37822400	0.00004500
C	1.73762700	-1.26788200	0.00005500
C	-1.73762700	-1.26788200	-0.00002400
H	1.57709800	-2.33855000	0.00000600
H	-1.57709800	-2.33855000	-0.00000900
H	-2.50129000	2.54392100	0.00003900
H	2.50129000	2.54392100	-0.00011100
O	4.07207500	-1.52985600	-0.00018800
O	-4.07207500	-1.52985700	0.00001500

N	-3.35608200	0.64719500	-0.00002200
N	3.35608200	0.64719500	0.00000700

F8-Triplet

1 3			
N	0.00000000	1.86336000	-0.00002200
N	-1.04504300	1.02066500	-0.00003100
N	1.04504300	1.02066500	-0.00002300
C	2.39620800	1.44483900	0.00001300
C	3.10441000	-0.78866800	-0.00004700
C	-2.39620800	1.44483900	0.00002200
C	-3.10441000	-0.78866800	-0.00013700
C	0.71047600	-0.30951200	-0.00002700
C	-0.71047600	-0.30951200	-0.00003700
C	-1.73450900	-1.26154800	-0.00001400
C	1.73450900	-1.26154800	-0.00000400
H	-1.53863100	-2.32593200	0.00003400
H	1.53863100	-2.32593200	0.00001900
H	2.53429700	2.52196500	0.00003900
H	-2.53429700	2.52196500	0.00007700
O	-4.04331800	-1.57854100	0.00011700
O	4.04331800	-1.57854100	0.00008100
N	3.35037600	0.60788700	0.00001700
N	-3.35037600	0.60788700	0.00000800

F8.H-

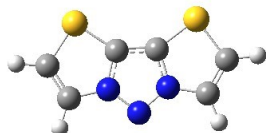
0 1			
N	0.00000100	1.93897900	0.19153600
N	-1.10100400	1.03604700	0.08968700
N	1.10100000	1.03604400	0.08962700
C	2.39989100	1.39719900	-0.15138200
C	3.10087300	-0.84668900	-0.04043000
C	-2.39988300	1.39719800	-0.15141200
C	-3.10088300	-0.84666700	-0.04024500
C	0.73053300	-0.30092300	0.12201100
C	-0.73053500	-0.30092200	0.12204200
C	-1.68482300	-1.25062000	0.04185700
C	1.68481700	-1.25062500	0.04183400
H	-1.44294000	-2.30430000	0.02835900
H	1.44293200	-2.30430600	0.02841700
H	2.57147200	2.46338900	-0.28136900
H	-2.57144800	2.46337900	-0.28148500
O	-4.01098300	-1.64463000	0.00658300
O	4.01098100	-1.64462800	0.00667300
N	3.35692300	0.54652000	-0.21565100
N	-3.35691400	0.54651900	-0.21567500
H	0.00002400	2.27942900	1.15770900

F8.NHC

1 1			
N	0.60933100	-0.00108600	-0.71855000
N	-0.24008700	1.12230900	-0.42068800
N	-0.24312700	-1.12208200	-0.42000100
C	-0.06743500	-2.39435700	-0.94701200
C	-2.10736800	-3.08825700	-0.00524100
C	-0.06083400	2.39394100	-0.94799100

C	-2.09830200	3.09398300	-0.00549400
C	-1.51154200	-0.72680500	0.01926600
C	-1.50949500	0.73080700	0.01904200
C	-2.44969600	1.67418400	0.21533600
C	-2.45450600	-1.66741400	0.21554800
H	-3.45472800	1.42717800	0.52935200
H	-3.45887700	-1.41741600	0.52931300
H	0.84877800	-2.54998400	-1.51343400
H	0.85563000	2.54677500	-1.51476400
O	-2.77679900	4.00910400	0.38340500
O	-2.78896300	-4.00131200	0.38309300
N	-0.91114500	-3.32832100	-0.75929700
N	-0.90175300	3.33040000	-0.76015300
C	1.79183900	-0.00248300	0.05677600
N	3.00831500	-0.00407100	-0.52143500
N	1.95830700	-0.00233900	1.39642700
C	3.96400400	-0.00502700	0.46769800
C	3.29633500	-0.00484800	-1.96782500
C	3.30820100	-0.00391300	1.66167400
C	0.90050100	-0.00074500	2.42467600
H	5.01796000	-0.00646600	0.24712100
H	3.87180300	0.88662500	-2.21497700
H	3.86930700	-0.89806200	-2.21449700
H	2.35635100	-0.00369400	-2.51188400
H	3.69055000	-0.00417600	2.66852800
H	0.28610200	-0.89392500	2.32566400
H	1.38444000	-0.00227200	3.39812400
H	0.28967800	0.89500300	2.32663100

F9-Singlet



1 1			
C	0.00000000	0.69569700	-0.34698100
N	0.00000000	0.00000000	1.83156100
N	0.00000000	-1.03221100	0.98593800
N	0.00000000	1.03221100	0.98593800
C	0.00000000	-0.69569700	-0.34698100
C	0.00000000	2.39848700	1.24613900
C	0.00000000	3.09851400	0.09272600
H	0.00000000	4.17269800	-0.01085300
H	0.00000000	2.75382600	2.26429500
C	0.00000000	-2.39848700	1.24613900
C	0.00000000	-3.09851400	0.09272600
H	0.00000000	-4.17269800	-0.01085300
H	0.00000000	-2.75382600	2.26429500
S	0.00000000	-2.10188800	-1.34479900
S	0.00000000	2.10188800	-1.34479900

F9-Triplet

1 3			
C	0.00000000	0.69348100	-0.34809400
N	0.00000000	0.00000000	1.89242500

N	0.00000000	-1.07198000	0.99425500
N	0.00000000	1.07198000	0.99425500
C	0.00000000	-0.69348100	-0.34809400
C	0.00000000	2.42206000	1.23409600
C	0.00000000	3.13332300	0.08241600
H	0.00000000	4.20281800	-0.04604900
H	0.00000000	2.79401900	2.24779800
C	0.00000000	-2.42206000	1.23409600
C	0.00000000	-3.13332300	0.08241600
H	0.00000000	-4.20281800	-0.04604900
H	0.00000000	-2.79401900	2.24779800
S	0.00000000	-2.08101800	-1.34972100
S	0.00000000	2.08101800	-1.34972100

F9.H-

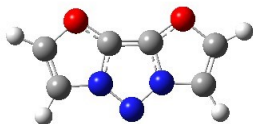
0 1			
C	-0.67065000	-0.33865200	-0.26595500
N	0.00012800	1.83852000	0.10979700
N	1.09214900	1.03706900	-0.41798300
N	-1.09205500	1.03697900	-0.41707700
C	0.67072200	-0.33876700	-0.26657800
C	-2.38219600	1.20648700	0.09605600
C	-3.03320100	0.06056200	0.33791600
H	-4.07516300	-0.05885500	0.58897800
H	-2.78924600	2.20518800	0.16131200
C	2.38216900	1.20643200	0.09586800
C	3.03296300	0.06051800	0.33821100
H	4.07481400	-0.05884700	0.58980100
H	2.78937000	2.20508400	0.16099300
S	2.04241900	-1.38976500	0.01332700
S	-2.04246500	-1.38968700	0.01318600
H	0.00057300	1.65122100	1.13844000

F9.NHC

1 1			
C	-1.61601500	0.67005700	-0.41742300
N	0.51527400	-0.00006000	-1.08398700
N	-0.44236900	-1.10702100	-1.13641000
N	-0.44228600	1.10699000	-1.13645800
C	-1.61606300	-0.66997100	-0.41739600
C	-0.08442900	2.41375800	-0.76348900
C	-1.03154000	3.04373500	-0.05485500
H	-1.06315400	4.09371800	0.19218300
H	0.80236200	2.86344700	-1.18620300
C	-0.08462200	-2.41380900	-0.76341400
C	-1.03179000	-3.04369200	-0.05477300
H	-1.06349400	-4.09366600	0.19229200
H	0.80214000	-2.86357600	-1.18610600
S	-2.45172900	-2.03065000	0.30159100
S	-2.45155700	2.03082100	0.30155300
C	1.46980900	-0.00006900	-0.00842400
N	2.78127600	-0.00007700	-0.34366600
N	1.40364300	-0.00001200	1.34684200
C	3.54454100	-0.00002900	0.79697000
C	3.32990900	-0.00016500	-1.71059400
C	2.68416300	0.00001500	1.85081600
C	0.20512600	0.00001500	2.20478300
H	4.62074400	-0.00003200	0.77015400

H	3.94095400	0.89156400	-1.84834600
H	3.94064800	-0.89210300	-1.84836500
H	2.50149000	-0.00002100	-2.41221700
H	2.87900600	0.00006100	2.90967900
H	-0.38869300	-0.89107800	2.01565700
H	0.54587200	-0.00005600	3.23776000
H	-0.38859500	0.89119100	2.01574300

F10-Singlet



1 1			
C	0.00000000	0.68956000	-0.57765100
N	0.00000000	0.00000000	1.60669200
N	0.00000000	-1.02327800	0.74646400
N	0.00000000	1.02327800	0.74646400
C	0.00000000	-0.68956000	-0.57765100
C	0.00000000	2.41870300	0.83914100
C	0.00000000	2.84458400	-0.44134400
H	0.00000000	3.82662700	-0.88217500
H	0.00000000	2.95077700	1.77478100
C	0.00000000	-2.41870300	0.83914100
C	0.00000000	-2.84458400	-0.44134400
H	0.00000000	-3.82662700	-0.88217500
H	0.00000000	-2.95077700	1.77478100
O	0.00000000	1.78248800	-1.33276900
O	0.00000000	-1.78248800	-1.33276900

F10-Triplet

1 3			
C	-0.54251900	0.24848500	0.69098100
N	1.63226900	-0.11336200	0.00000000
N	0.78680600	0.27965100	-1.08964500
N	0.78680600	0.27965100	1.08964500
C	-0.54251900	0.24848500	-0.69098100
C	0.80630900	-0.15151000	2.42428200
C	-0.47736300	-0.24839700	2.80633300
H	-0.97091800	-0.42831400	3.74481100
H	1.71606800	-0.25467200	2.99188000
C	0.80630900	-0.15151000	-2.42428200
C	-0.47736300	-0.24839700	-2.80633300
H	-0.97091800	-0.42831400	-3.74481100
H	1.71606800	-0.25467200	-2.99188000
O	-1.33553700	0.00384000	1.70961900
O	-1.33553700	0.00384000	-1.70961900

F10.H-

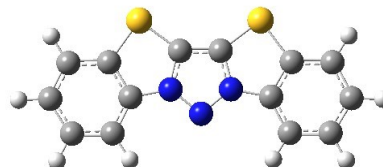
0 1			
C	-0.66466900	-0.56584200	-0.31395100
N	0.00000200	1.59797000	0.13665900
N	1.09675300	0.80844000	-0.44470200
N	-1.09674600	0.80843600	-0.44466900

C	0.66467500	-0.56584900	-0.31398800
C	-2.36917000	0.78666800	0.17477600
C	-2.72891700	-0.48991000	0.35264400
H	-3.65946200	-0.94746200	0.64099100
H	-2.95734000	1.68027700	0.30085100
C	2.36916200	0.78666700	0.17477600
C	2.72890400	-0.48991000	0.35266300
H	3.65944200	-0.94745700	0.64104000
H	2.95733700	1.68027400	0.30084900
O	-1.71724300	-1.38011400	-0.02054300
O	1.71724700	-1.38011700	-0.02054400
H	0.00001900	1.34134700	1.15243500

F10.NHC

1 1			
C	-1.91220500	0.66457400	-0.33035300
N	0.18783900	0.00042700	-1.09619500
N	-0.80237600	-1.11706200	-1.13128600
N	-0.80246700	1.11778400	-1.13064200
C	-1.91213000	-0.66441900	-0.33071600
C	-0.53271700	2.41044600	-0.60801200
C	-1.54547200	2.74218300	0.20323100
H	-1.82628700	3.67521600	0.66230500
H	0.23554700	3.04660100	-1.01557600
C	-0.53252300	-2.41002000	-0.60945100
C	-1.54521500	-2.74230600	0.20164700
H	-1.82594200	-3.67563400	0.66017500
H	0.23577500	-3.04587400	-1.01742200
O	-2.44685200	1.69546100	0.38069300
O	-2.44665600	-1.69575500	0.37978400
C	1.17418700	0.00014200	-0.05678800
N	1.15712400	-0.00063700	1.30290300
N	2.47478200	0.00029400	-0.43501500
C	2.45416900	-0.00091500	1.76095400
C	-0.00613900	-0.00104500	2.20774300
C	3.27708500	-0.00033100	0.67705000
C	2.97268800	0.00123400	-1.82153100
H	2.68733300	-0.00151600	2.81207000
H	-0.60604500	-0.89291000	2.04785700
H	0.37506700	-0.00119200	3.22654200
H	-0.60634300	0.89068400	2.04823800
H	4.35178600	-0.00030800	0.61329300
H	3.57647600	0.89422200	-1.98106300
H	3.57886500	-0.89007300	-1.98133700
H	2.11714800	0.00024600	-2.48989500

F11-Singlet



1 1			
C	-0.92875900	-0.00003300	0.69361400
N	1.24201500	-0.00010700	0.00000000

N	0.40174400	-0.00004600	-1.03138400
N	0.40174400	-0.00004600	1.03138400
C	-0.92875900	-0.00003300	-0.69361400
C	0.66781000	-0.00001600	2.40720400
C	-0.53745500	0.00002700	3.12552300
C	0.66781000	-0.00001600	-2.40720400
C	-0.53745500	0.00002700	-3.12552300
S	-1.97124300	-0.00001800	-2.07634100
S	-1.97124300	-0.00001800	2.07634100
C	-0.51817000	0.00007500	-4.51793900
C	1.90941500	-0.00002200	-3.03469500
C	1.91707900	0.00002700	-4.42253300
C	0.71929800	0.00007500	-5.15224600
C	1.90941500	-0.00002200	3.03469500
C	1.91707900	0.00002700	4.42253300
C	-0.51817000	0.00007500	4.51793900
C	0.71929800	0.00007500	5.15224600
H	-1.43643700	0.00010600	-5.09120800
H	0.75563900	0.00010500	-6.23455400
H	2.86319700	0.00002700	-4.94854500
H	2.82293700	-0.00005700	-2.45474200
H	2.82293700	-0.00005700	2.45474200
H	2.86319700	0.00002700	4.94854500
H	-1.43643700	0.00010600	5.09120800
H	0.75563900	0.00010500	6.23455400

F11-Triplet

1 3

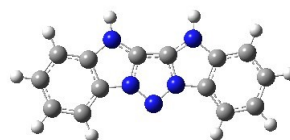
C	0.90833000	-0.00002500	-0.69088300
N	-1.32369400	-0.00002200	0.00000000
N	-0.43300400	-0.00003600	1.06933300
N	-0.43300400	-0.00003600	-1.06933300
C	0.90833000	-0.00002500	0.69088300
C	-0.68095500	-0.00001000	-2.42831200
C	0.53765400	0.00000800	-3.14501700
C	-0.68095500	-0.00001000	2.42831200
C	0.53765400	0.00000800	3.14501700
S	1.94314200	-0.00000100	2.05608200
S	1.94314200	-0.00000100	-2.05608200
C	0.56056100	0.00002800	4.53349800
C	-1.89849500	-0.00000600	3.09709200
C	-1.86678700	0.00001600	4.49241300
C	-0.66223700	0.00003200	5.20353800
C	-1.89849500	-0.00000600	-3.09709200
C	-1.86678700	0.00001600	-4.49241300
C	0.56056100	0.00002800	-4.53349800
C	-0.66223700	0.00003200	-5.20353800
H	1.49528700	0.00004100	5.08012900
H	-0.67537100	0.00004800	6.28569400
H	-2.80373700	0.00002000	5.03576300
H	-2.83092900	-0.00002000	2.54861100
H	-2.83092900	-0.00002000	-2.54861100
H	-2.80373700	0.00002000	-5.03576300
H	1.49528700	0.00004100	-5.08012900
H	-0.67537100	0.00004800	-6.28569400

F11.H-

0 1

C	0.66836500	-1.19212200	0.72464200
N	0.00014000	0.83524500	1.65105600
N	-1.15567500	0.04236200	1.26146000
N	1.15634400	0.04253700	1.26289800
C	-0.66717800	-1.19164300	0.72328000
C	2.16315500	0.54907800	0.41029500
C	2.74908200	-0.45634700	-0.37306600
C	-2.16332900	0.54865100	0.41006700
C	-2.74890900	-0.45687700	-0.37348800
S	-1.92571200	-2.04000100	-0.15536100
S	1.92753300	-2.04017100	-0.15336000
C	-3.84562800	-0.18508100	-1.17632700
C	-2.65160000	1.84753900	0.37234600
C	-3.73953400	2.12668300	-0.45693500
C	-4.33860100	1.12229900	-1.21562500
C	2.65029200	1.84834700	0.37159900
C	3.73743800	2.12803900	-0.45853300
C	3.84506400	-0.18402000	-1.17674700
C	4.33687300	1.12376100	-1.21707400
H	-4.29746800	-0.96340200	-1.77996700
H	-5.18675200	1.35351000	-1.84885600
H	-4.12199600	3.13944800	-0.50707200
H	-2.18057400	2.61871800	0.96908100
H	2.17898600	2.61939500	0.96828500
H	4.11899100	3.14110800	-0.50944700
H	4.29720700	-0.96227500	-1.78024600
H	5.18440700	1.35536500	-1.85099100
H	-0.00052300	0.77003400	2.66423400

F12-Singlet



1 1

C	-0.69361400	-0.96181500	-0.00017800
N	0.00000700	1.22897000	-0.00022700
N	1.02754100	0.37294900	-0.00050300
N	-1.02753800	0.37295300	-0.00011600
C	0.69361000	-0.96181800	-0.00046100
C	-2.41903000	0.51188900	0.00019300
C	-2.92306200	-0.80473300	0.00023200
C	2.41903300	0.51188100	-0.00019200
C	2.92305900	-0.80474500	0.00003700
C	4.29609300	-1.03379900	0.00051900
C	3.24358400	1.63091400	-0.00029900
C	4.61092700	1.39184800	0.00028200
C	5.12370100	0.08311000	0.00078400
C	-3.24358900	1.63091700	0.00019400
C	-4.61093000	1.39184200	-0.00003700
C	-4.29608900	-1.03380200	0.00002600
C	-5.12370400	0.08310400	-0.00021700
H	4.70422100	-2.03662500	0.00062000
H	6.19702100	-0.06115900	0.00122400
H	5.29606600	2.22985200	0.00031000
H	2.83294000	2.63173100	-0.00070500
H	-2.83295500	2.63173800	0.00033700

H	-5.29607100	2.22984400	-0.00008200
H	-4.70421300	-2.03662900	0.00013000
H	-6.19702300	-0.06116400	-0.00041800
N	-1.84417100	-1.69693900	0.00131500
N	1.84417500	-1.69694200	-0.00138200
H	1.90801200	-2.70164500	0.00646200
H	-1.90803700	-2.70163800	-0.00678100

F12-Triplet

1 3			
C	-0.68985000	-0.94448900	-0.01050600
N	-0.00000200	1.30012800	0.00007100
N	1.06300600	0.40448100	0.01531800
N	-1.06300300	0.40448400	-0.01506100
C	0.68985200	-0.94448900	0.01069200
C	-2.44247300	0.53229100	-0.00438800
C	-2.94049500	-0.79506700	-0.00264100
C	2.44247100	0.53229100	0.00445500
C	2.94049500	-0.79506800	0.00262100
C	4.29812200	-1.06298200	-0.00118100
C	3.29598300	1.62117000	0.00111500
C	4.67018700	1.34390400	-0.00396500
C	5.16264000	0.03765500	-0.00479100
C	-3.29598500	1.62116900	-0.00111400
C	-4.67019000	1.34390200	0.00381100
C	-4.29812000	-1.06298400	0.00101400
C	-5.16264200	0.03765300	0.00455800
H	4.67802900	-2.07704600	-0.00238100
H	6.23156400	-0.13082900	-0.00845300
H	5.36788600	2.17204400	-0.00705600
H	2.91868600	2.63451400	0.00229500
H	-2.91868900	2.63451400	-0.00223000
H	-5.36789000	2.17204100	0.00684100
H	-4.67802700	-2.07704800	0.00214400
H	-6.23156600	-0.13083400	0.00810200
N	-1.83375500	-1.67098600	-0.00591100
N	1.83375900	-1.67098600	0.00595900
H	1.89358300	-2.67846600	0.00453800
H	-1.89357800	-2.67846600	-0.00450300

F12.H-

0 1			
C	-0.66688900	0.99912800	-0.50830700
N	-0.00000200	-1.22184400	-0.40336000
N	1.09055400	-0.35492400	-0.81533000
N	-1.09055400	-0.35492400	-0.81533300
C	0.66688800	0.99912700	-0.50829800
C	-2.37480900	-0.48192300	-0.25495800
C	-2.83509200	0.81171400	0.06552600
C	2.37480800	-0.48192300	-0.25495700
C	2.83509200	0.81171400	0.06552600
C	4.11395300	1.00885500	0.55874600
C	3.17518800	-1.59581500	-0.06991200
C	4.46243400	-1.39824600	0.44870300
C	4.92312200	-0.11985600	0.75193300
C	-3.17518700	-1.59581500	-0.06991200
C	-4.46243300	-1.39824700	0.44870400
C	-4.11395200	1.00885500	0.55874800

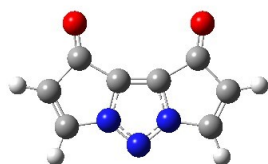
C	-4.92312000	-0.11985600	0.75193500
H	4.47528400	2.00116200	0.80348900
H	5.92367600	0.01028200	1.14737900
H	5.10667100	-2.25413700	0.61084700
H	2.80982600	-2.58440200	-0.31831900
H	-2.80982600	-2.58440100	-0.31832100
H	-5.10667000	-2.25413800	0.61084800
H	-4.47528300	2.00116200	0.80349100
H	-5.92367400	0.01028200	1.14738200
N	-1.82030100	1.74745900	-0.24055800
N	1.82030000	1.74746100	-0.24055600
H	1.75503800	2.60379600	0.28818200
H	-1.75504100	2.60380500	0.28816000
H	-0.00000200	-1.18227800	0.64195800

F12.NHC

1 1			
C	0.91903000	-1.80418700	-0.01908500
N	0.15057000	0.33904100	-0.59829800
N	-0.86787200	-0.60768200	-0.44319900
N	1.25429200	-0.50262700	-0.40743800
C	-0.43149500	-1.86314600	0.00175300
C	2.61276400	-0.28643200	-0.31080500
C	3.15902800	-1.53519700	0.07489000
C	-2.25283300	-0.56510400	-0.52290900
C	-2.68689000	-1.84683700	-0.10729800
C	-4.03719800	-2.15167800	-0.07067700
C	-3.14541800	0.42413500	-0.89895500
C	-4.50549100	0.10540500	-0.86181600
C	-4.93936600	-1.15619500	-0.45729700
C	3.40876600	0.83062200	-0.50909200
C	4.78264800	0.67670000	-0.30140800
C	4.52121900	-1.68054600	0.26346200
C	5.32584600	-0.55150400	0.07200100
H	-4.38362100	-3.12307900	0.25174800
H	-5.99763100	-1.37143600	-0.43608700
H	-5.23086600	0.85025400	-1.15407200
H	-2.80600700	1.40049500	-1.21088700
H	2.98536700	1.77693500	-0.81494000
H	5.43399000	1.52603400	-0.44586000
H	4.94827200	-2.62957300	0.55418300
H	6.39327900	-0.63901200	0.21171300
N	2.11026200	-2.45658700	0.20584800
N	-1.56768900	-2.61538000	0.23363700
H	-1.58988400	-3.56430000	0.55892500
H	2.20941800	-3.41463100	0.48747000
C	0.07810100	1.56760200	0.35606900
C	-1.46886000	2.81642300	1.43226900
C	-0.96308300	3.56597100	0.41261100
H	-2.19361400	3.06058700	2.18586500
H	-1.16723300	4.58275800	0.13503700
N	-0.83968400	1.58035400	1.36456900
N	-0.03583400	2.78749800	-0.26052700
C	-1.03422900	0.48346900	2.30320300
H	-2.02503100	0.05045200	2.17438200
H	-0.28270200	-0.27752500	2.11990600
H	-0.92375200	0.84110400	3.32384500
C	0.73020700	3.19802300	-1.42777400
H	0.17524600	3.94829500	-1.98114200
H	1.69303000	3.61115500	-1.13329100

H	0.89693500	2.33401900	-2.06378400
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F13-Singlet



1 1			
C	0.68276400	0.24604500	0.00001800
N	0.00000000	-1.91432800	0.00004600
N	-1.01897900	-1.08634400	0.00003600
N	1.01897900	-1.08634400	0.00001300
C	-0.68276500	0.24604500	0.00004700
C	2.43858600	-1.29958500	-0.00003600
C	3.03441800	-0.10250800	-0.00004900
H	4.09726800	0.08689000	-0.00007300
H	2.82099900	-2.30883400	-0.00004300
C	-2.43858600	-1.29958500	0.00000600
C	-3.03441800	-0.10250800	-0.00001800
H	-4.09726800	0.08689000	-0.00007500
H	-2.82099900	-2.30883500	-0.00002500
O	-2.16461900	2.18259600	-0.00004000
O	2.16461900	2.18259600	-0.00004600
C	-2.00749100	1.00033700	0.00009200
C	2.00749100	1.00033700	-0.00002000

F13-Triplet

1 3			
C	-0.69376400	0.25097900	-0.00008300
N	0.00000000	-1.91727900	-0.00000500
N	1.02265300	-1.10002500	0.00008300
N	-1.02265300	-1.10002500	-0.00007000
C	0.69376400	0.25097900	0.00012400
C	-2.42692800	-1.30239400	-0.00007800
C	-3.00183800	-0.08428400	0.00001900
H	-4.05691300	0.14119400	0.00015900
H	-2.83807300	-2.29947700	-0.00001700
C	2.42692700	-1.30239400	0.00009300
C	3.00183800	-0.08428400	-0.00015900
H	4.05691300	0.14119300	-0.00043200
H	2.83807300	-2.29947700	0.00001100
O	2.09646100	2.19465100	0.00014700
O	-2.09646100	2.19465200	-0.00011000
C	1.94194000	0.97098500	0.00032300
C	-1.94194000	0.97098500	-0.00025100

F13.H-

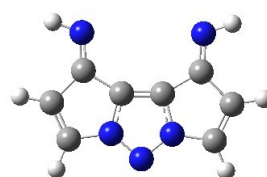
0 1			
C	0.67242200	0.14340800	-0.50334200
N	-0.00004400	-2.09312700	-0.23863100
N	-1.13166200	-1.18690600	-0.38906000
N	1.13161700	-1.18689300	-0.38896900

C	-0.67247100	0.14341800	-0.50347700
C	2.25888400	-1.16941200	0.43780500
C	2.72251400	0.09152400	0.60212700
H	3.65069600	0.38109500	1.06885800
H	2.67275800	-2.10561500	0.78310900
C	-2.25888500	-1.16938300	0.43779800
C	-2.72241800	0.09156400	0.60224200
H	-3.65044800	0.38120000	1.06923200
H	-2.67269300	-2.10557700	0.78320700
O	-1.84000100	2.25085100	-0.10504500
O	1.84009400	2.25081800	-0.10517600
C	-1.78117800	1.04494500	-0.01992000
C	1.78105700	1.04495200	-0.01962800
H	0.00001200	-2.62208100	-1.10764400

F13.NHC

1 1			
C	1.51172600	-0.66856800	0.33747800
N	-0.53361000	0.00015800	-0.57396300
N	0.24780800	1.16013500	-0.08983000
N	0.24785000	-1.16005000	-0.09051500
C	1.51169900	0.66844400	0.33786400
C	0.52033100	-2.27485100	-0.93053800
C	1.78672500	-2.70087800	-0.77994100
H	2.21390400	-3.60594900	-1.18395000
H	-0.28669400	-2.71885100	-1.49500700
C	0.52024800	2.27544100	-0.92919300
C	1.78662600	2.70142700	-0.77834400
H	2.21376800	3.60675500	-1.18181600
H	-0.28679100	2.71974600	-1.49340100
O	3.66694200	1.79559600	0.48292100
O	3.66701000	-1.79572700	0.48185600
C	2.53084500	1.75615000	0.09090300
C	2.53091000	-1.75608800	0.08986700
C	-1.80512100	-0.00005300	0.02158600
C	-3.52546300	-0.00073800	1.40936500
C	-4.01665800	-0.00002000	0.14045300
H	-4.03674700	-0.00124900	2.35686700
H	-5.03108600	0.00022800	-0.21960000
N	-2.15112700	-0.00073000	1.32429100
N	-2.93490100	0.00038000	-0.71255800
C	-1.23371700	-0.00142000	2.47668800
H	-0.61267800	-0.89425200	2.44540600
H	-0.61192500	0.89090100	2.44586300
H	-1.83567000	-0.00137600	3.38206400
C	-3.02002000	0.00134500	-2.18164500
H	-3.55243500	0.89398500	-2.50861600
H	-2.01167300	0.00040400	-2.58565400
H	-3.55452000	-0.88967700	-2.50959900

F14-Singlet



1 1			
C	0.68536300	-0.22038200	-0.00001000
N	0.00000000	1.94805800	-0.00018100
N	-1.01864900	1.11441500	-0.00006700
N	1.01864900	1.11441500	-0.00014200
C	-0.68536300	-0.22038200	0.00004900
C	2.43157000	1.31363800	-0.00022700
C	3.00756500	0.10283500	-0.00016500
H	4.07077800	-0.08548900	-0.00021500
H	2.83190600	2.31506100	-0.00033900
C	-2.43157000	1.31363800	-0.00003900
C	-3.00756500	0.10283500	0.00013900
H	-4.07077800	-0.08548900	0.00021600
H	-2.83190600	2.31506100	-0.00013500
C	-1.96531400	-0.96894700	0.00019700
C	1.96531400	-0.96894700	0.00000700
N	2.03177800	-2.23394300	0.00011800
H	2.99676700	-2.57394300	0.00009400
N	-2.03177800	-2.23394300	0.00031500
H	-2.99676700	-2.57394300	0.00037100

F14-Triplet

1 3			
C	-0.69503700	-0.23799700	0.00001600
N	-0.00000300	1.97934700	0.00002900
N	1.02403800	1.13394300	-0.00001000
N	-1.02404000	1.13394000	0.00004300
C	0.69504000	-0.23799600	-0.00002100
C	-2.37438100	1.34560600	0.00008500
C	-2.95834400	0.07641200	0.00009900
H	-4.02489800	-0.10216300	0.00014000
H	-2.79901000	2.33701600	0.00009900
C	2.37437600	1.34561200	-0.00004700
C	2.95834200	0.07641700	-0.00009700
H	4.02489600	-0.10215600	-0.00014500
H	2.79900200	2.33702300	-0.00003300
C	1.94204900	-0.96243300	-0.00007300
C	-1.94204600	-0.96243600	0.00004800
N	2.05690500	-2.26807200	-0.00012400
H	3.03843400	-2.55320500	-0.00013500
N	-2.05689800	-2.26807300	0.00005700
H	-3.03842700	-2.55320700	0.00006500

F14.H⁻

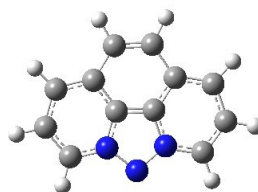
0 1			
C	0.67394200	0.13750700	-0.48926100
N	0.00000000	-2.10532500	-0.26492900
N	-1.13359300	-1.20112800	-0.39236300
N	1.13359200	-1.20112700	-0.39236000
C	-0.67394300	0.13750700	-0.48926500
C	2.25435300	-1.19267500	0.44587200
C	2.70525000	0.06969900	0.61836300
H	3.63813300	0.35277700	1.08277400
H	2.67839000	-2.12963000	0.77543700
C	-2.25435500	-1.19267500	0.44586800
C	-2.70524100	0.06970000	0.61837700

H	-3.63811300	0.35278100	1.08280700
H	-2.67839100	-2.12963100	0.77543500
C	-1.76721000	1.01544400	-0.02273400
C	1.76720500	1.01544600	-0.02272200
H	0.00000000	-2.61016600	-1.14753300
N	1.79225700	2.28664200	-0.17209100
H	2.62424400	2.67211500	0.28049100
N	-1.79226000	2.28664100	-0.17209800
H	-2.62423900	2.67211400	0.28049900

F14.NHC

1 1			
C	1.50392600	-0.66985300	0.29782300
N	-0.55035900	0.00009700	-0.59594200
N	0.23011800	1.16227100	-0.12565000
N	0.23015100	-1.16220000	-0.12606900
C	1.50390900	0.66980200	0.29806000
C	0.50404400	-2.27264900	-0.97385300
C	1.77160900	-2.68666300	-0.81178300
H	2.19426000	-3.59696400	-1.21121400
H	-0.30122000	-2.72816300	-1.53082300
C	0.50398300	2.27302200	-0.97304400
C	1.77154000	2.68700800	-0.81083600
H	2.19416600	3.59746200	-1.20994600
H	-0.30129200	2.72872000	-1.52984700
C	2.49295700	1.74771600	0.08146900
C	2.49299900	-1.74766800	0.08085800
C	-1.80782600	-0.00003800	0.02860600
C	-3.49524100	-0.00044500	1.45685300
C	-4.01671900	-0.00001000	0.20060000
H	-3.98307900	-0.00075000	2.41652700
H	-5.03918200	0.00014400	-0.13557600
N	-2.12290900	-0.00045200	1.33847000
N	-2.95460700	0.00023500	-0.67799000
C	-1.17638700	-0.00087200	2.46654600
H	-0.55524400	-0.89274400	2.41717500
H	-0.55468600	0.89061900	2.41736200
H	-1.75496900	-0.00077200	3.38712100
C	-3.07147700	0.00077600	-2.14394900
H	-3.61099500	0.89304900	-2.46034200
H	-2.07126200	0.00042200	-2.56792100
H	-3.61187700	-0.89076200	-2.46090200
N	3.66518800	1.75366000	0.57769100
H	4.19586200	2.56579300	0.25600500
N	3.66522900	-1.75376000	0.57708300
H	4.19592300	-2.56576600	0.25511100

F15-Singlet



1 1			
C	-0.02500800	-0.00054600	0.67926100

N	2.13804900	-0.00007700	0.00000000
N	1.28193400	-0.00020900	-1.06325700
N	1.28193400	-0.00020900	1.06325700
C	-0.02500800	-0.00054600	-0.67926100
C	-1.16472800	-0.00016700	1.47681800
C	1.55105400	0.00015100	2.40010600
C	0.46214100	0.00033600	3.26447700
H	0.68381000	0.00063100	4.32401700
C	-0.88770800	0.00025600	2.84836300
H	-1.67551800	0.00057900	3.59094300
C	1.55105400	0.00015100	-2.40010600
C	-1.16472800	-0.00016700	-1.47681800
C	-0.88770800	0.00025600	-2.84836300
H	-1.67551800	0.00057900	-3.59094300
C	0.46214100	0.00033600	-3.26447700
H	0.68381000	0.00063100	-4.32401700
H	2.58675200	0.00034400	2.70603900
H	2.58675200	0.00034400	-2.70603900
C	-2.38803400	-0.00002900	0.68834400
H	-3.33805300	0.00016000	1.20912400
C	-2.38803400	-0.00002900	-0.68834400
H	-3.33805300	0.00016000	-1.20912400

F15-Triplet

I 3			
C	0.00018400	-0.03785000	0.67989300
N	0.00004800	2.10192400	0.00000000
N	0.00011400	1.26485300	-1.05694700
N	0.00011400	1.26485300	1.05694700
C	0.00018400	-0.03785000	-0.67989300
C	0.00002500	-1.18510600	1.47451400
C	-0.00000100	1.56697100	2.42658500
C	-0.00009000	0.47520500	3.28888700
H	-0.00018300	0.70151500	4.34790500
C	-0.00009000	-0.87308100	2.88996300
H	-0.00019200	-1.65517900	3.63739400
C	-0.00000100	1.56697100	-2.42658500
C	0.00002500	-1.18510600	-1.47451400
C	-0.00009000	-0.87308100	-2.88996300
H	-0.00019200	-1.65517900	-3.63739400
C	-0.00009000	0.47520500	-3.28888700
H	-0.00018300	0.70151500	-4.34790500
H	-0.00001800	2.60737500	2.71064800
H	-0.00001800	2.60737500	-2.71064800
C	-0.00009000	-2.36892700	0.72224300
H	-0.00021100	-3.32769600	1.22577000
C	-0.00009000	-2.36892700	-0.72224300
H	-0.00021100	-3.32769600	-1.22577000

F15.H-

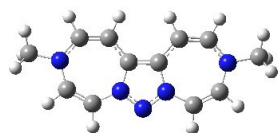
O 1			
C	0.69472900	0.04147300	0.06085900
N	-0.00201800	-2.10756700	-0.05558600
N	-1.12321000	-1.22543300	-0.05084700
N	1.12563300	-1.23297600	0.08427000
C	-0.69130000	0.04432700	-0.00294700
C	1.47244200	1.20976700	0.02517400
C	2.47344400	-1.54341600	-0.03602100
C	3.32027200	-0.41550300	-0.05282500

H	4.38335300	-0.62421000	-0.10007600
C	2.90587600	0.90233400	-0.01300800
H	3.63609800	1.70005300	-0.04367600
C	-2.46840000	-1.54549600	-0.03283100
C	-1.47115100	1.21289300	-0.00302200
C	-2.90677000	0.90060600	0.00664700
H	-3.63858300	1.69740200	0.03087100
C	-3.32122500	-0.41361900	-0.00683700
H	-4.38495200	-0.62387800	-0.00899000
H	2.77532500	-2.57554000	-0.00636200
H	-2.76328300	-2.56753800	-0.19475700
C	0.72095300	2.38403700	0.00145900
C	-0.72108900	2.38511000	0.00739000
H	1.23145000	3.33939900	-0.02993500
H	-1.23010900	3.34195000	0.01184400
H	-0.05881300	-2.70088100	0.77198900

F15.NHC

I 1			
C	1.47080700	-0.67848200	-0.24381900
N	0.54825300	-0.00060000	-2.19348100
N	0.91567200	1.06066500	-1.42392500
N	0.91591100	-1.06136900	-1.42335800
C	1.47065600	0.67853300	-0.24418100
C	1.97058500	-1.47565600	0.77940600
C	0.79212600	-2.39616000	-1.66213600
C	1.26116200	-3.26224700	-0.68199700
H	1.16195500	-4.32154700	-0.88085600
C	1.85031400	-2.84660900	0.53221900
H	2.19488500	-3.58893700	1.24085700
C	0.79159700	2.39530100	-1.66342100
C	1.97026000	1.47636700	0.77861500
C	1.84968500	2.84716000	0.53069300
H	2.19409400	3.58994500	1.23893100
C	1.26043800	3.26201700	-0.68374400
H	1.16099300	4.32118800	-0.88317000
H	0.34319300	-2.70277600	-2.59471400
H	0.34259800	2.70131800	-2.59616400
C	2.50657800	-0.68760500	1.87921100
H	2.92654300	-1.20821200	2.73164200
C	2.50642900	0.68902500	1.87884100
H	2.92627800	1.21018300	2.73099200
C	-1.90388900	-0.00021100	0.22353000
C	-3.79213900	0.00045900	1.52915800
C	-4.19878900	-0.00010600	0.23920000
H	-4.36026300	0.00090800	2.44436200
H	-5.18925300	-0.00024900	-0.18433100
C	-3.05886100	-0.00117100	-1.98851700
H	-3.57043300	0.88657900	-2.36849000
H	-2.02955200	-0.00114000	-2.33919300
H	-3.57006100	-0.88950700	-2.36762700
C	-1.57751000	0.00086800	2.69382100
H	-1.77220800	-0.88767200	3.29948500
H	-0.53550300	0.00071000	2.38355000
H	-1.77216400	0.88992300	3.29874400
N	-2.40324500	0.00038600	1.49649100
N	-3.04342100	-0.00045600	-0.53219500

F16-Singlet



1 1			
N	0.00000000	1.79381200	-0.00372600
N	-1.04566600	1.00241000	-0.01420100
N	1.04566600	1.00241000	-0.01420300
C	2.33252300	1.59726600	-0.00946400
C	3.51770900	0.96807900	-0.00507700
C	-2.33252400	1.59726600	-0.00947000
C	-3.51770900	0.96807700	-0.00508500
H	-4.37448100	1.62908200	0.00375100
H	-2.28626000	2.67430800	-0.01321300
C	0.69185100	-0.33786100	-0.03091200
C	-0.69185000	-0.33786100	-0.03091100
N	-3.86393400	-0.37009600	-0.02016800
N	3.86393400	-0.37009400	-0.02016900
C	-1.62004200	-1.43720900	-0.04516600
C	2.97121800	-1.42243800	-0.03164700
C	1.62004300	-1.43720800	-0.04517700
C	5.29786100	-0.68502500	0.11539000
H	5.49149500	-1.67215200	-0.30047900
H	5.88631700	0.03877300	-0.44775800
H	5.61039500	-0.66924900	1.16295400
C	-2.97121700	-1.42243900	-0.03163700
H	-3.46607800	-2.38489500	-0.03844900
H	-1.16492800	-2.41729100	-0.07186900
C	-5.29786200	-0.68502300	0.11538900
H	-5.61040900	-0.66919900	1.16294800
H	-5.88631300	0.03874900	-0.44780000
H	-5.49148900	-1.67216900	-0.30043700
H	1.16493000	-2.41729000	-0.07189100
H	3.46608000	-2.38489300	-0.03846900
H	2.28625900	2.67430900	-0.01319800
H	4.37448000	1.62908400	0.00376800

F16-Triplet

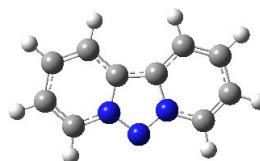
1 3			
N	0.00000000	1.90966500	0.00100400
N	-1.07562300	1.04262500	-0.00545100
N	1.07562200	1.04262400	-0.00545100
C	2.32144400	1.58078500	-0.00401700
C	3.53769600	0.94619800	-0.00682800
C	-2.32144400	1.58078400	-0.00401400
C	-3.53769600	0.94619600	-0.00682700
H	-4.39941500	1.59721100	-0.00026700
H	-2.31379500	2.66134400	-0.00148300
C	0.68413800	-0.30530600	-0.01418600
C	-0.68413800	-0.30530600	-0.01418600
N	-3.84513300	-0.38943400	-0.02109600
N	3.84513400	-0.38943100	-0.02109600
C	-1.58543300	-1.41553500	-0.02325100
C	2.94525800	-1.43301600	-0.02214700
C	1.58543400	-1.41553400	-0.02325000
C	5.27581100	-0.74409500	0.06913400
H	5.45034000	-1.68222900	-0.45458300

H	5.87246900	0.03230500	-0.40583100
H	5.58020300	-0.84831100	1.11355800
C	-2.94525700	-1.43301800	-0.02214800
H	-3.42647800	-2.40129800	-0.02631500
H	-1.11566600	-2.38939400	-0.03499600
C	-5.27581200	-0.74409200	0.06913200
H	-5.58022300	-0.84823500	1.11355800
H	-5.87246200	0.03227400	-0.40590000
H	-5.45033100	-1.68226300	-0.45452100
H	1.11566800	-2.38939400	-0.03499600
H	3.42648000	-2.40129600	-0.02631400
H	2.31379300	2.66134500	-0.00148700
H	4.39941400	1.59721400	-0.00027000

F16.H-

0 1			
N	0.00000000	1.85804000	0.18168800
N	-1.09668600	1.04718800	-0.25926000
N	1.09668600	1.04718800	-0.25925900
C	2.36201800	1.57526100	-0.09196600
C	3.54526000	0.94301500	0.04121400
C	-2.36201800	1.57526100	-0.09196900
C	-3.54526000	0.94301500	0.04121300
H	-4.42495100	1.56992500	0.08182700
H	-2.36858900	2.65618300	-0.13754500
C	0.68726600	-0.30373800	-0.19168500
C	-0.68726600	-0.30373700	-0.19168600
N	-3.84386700	-0.42682900	0.05076100
N	3.84386800	-0.42682900	0.05075900
C	-1.57733900	-1.42062400	-0.19332400
C	2.93337600	-1.44843500	-0.07106400
C	1.57733900	-1.42062400	-0.19332100
C	5.22105600	-0.77194900	0.38645700
H	5.42536500	-1.79940800	0.08561700
H	5.91170300	-0.11849500	-0.15251900
H	5.41973700	-0.67654000	1.46131700
C	-2.93337600	-1.44843500	-0.07106500
H	-3.40431400	-2.42394900	-0.07874600
H	-1.10856400	-2.38726500	-0.32164500
C	-5.22105600	-0.77194800	0.38645900
H	-5.41973900	-0.67652800	1.46131700
H	-5.91170300	-0.11850300	-0.15252600
H	-5.42536100	-1.79941200	0.08563100
H	1.10856400	-2.38726500	-0.32163900
H	3.40431400	-2.42394900	-0.07874400
H	2.36858900	2.65618300	-0.13754100
H	4.42495000	1.56992600	0.08182900
H	-0.00000200	1.78541200	1.21495400

F17-Singlet



I 1			
C	0.00000000	0.70793600	-0.54438100
N	0.00000000	0.00000000	1.63214000
N	0.00000000	-1.04778200	0.79640100
N	0.00000000	1.04778200	0.79640100
C	0.00000000	-0.70793600	-0.54438100
C	0.00000000	1.72037900	-1.51430700
C	0.00000000	2.34802800	1.22933900
C	0.00000000	3.33786500	0.28710900
H	0.00000000	4.36740000	0.61966200
C	0.00000000	3.03069500	-1.09490800
H	0.00000000	3.83349700	-1.82057200
C	0.00000000	-2.34802800	1.22933900
C	0.00000000	-1.72037900	-1.51430700
C	0.00000000	-3.03069500	-1.09490800
H	0.00000000	-3.83349700	-1.82057200
C	0.00000000	-3.33786500	0.28710900
H	0.00000000	-4.36740000	0.61966200
H	0.00000000	1.45702600	-2.56362900
H	0.00000000	2.49034000	2.30012500
H	0.00000000	-1.45702600	-2.56362900
H	0.00000000	-2.49034000	2.30012500

F17-Triplet

I 3			
C	0.00000000	0.70033700	-0.56538200
N	0.00000000	0.00000000	1.66778200
N	0.00000000	-1.08511400	0.78796600
N	0.00000000	1.08511400	0.78796600
C	0.00000000	-0.70033700	-0.56538200
C	0.00000000	1.72894800	-1.51937700
C	0.00000000	2.36637300	1.22515500
C	0.00000000	3.37884900	0.29732200
H	0.00000000	4.40740500	0.62565000
C	0.00000000	3.04359700	-1.08488400
H	0.00000000	3.83927900	-1.81984400
C	0.00000000	-2.36637300	1.22515500
C	0.00000000	-1.72894800	-1.51937700
C	0.00000000	-3.04359700	-1.08488400
H	0.00000000	-3.83927900	-1.81984400
C	0.00000000	-3.37884900	0.29732200
H	0.00000000	-4.40740500	0.62565000
H	0.00000000	1.48885900	-2.57414200
H	0.00000000	2.50358500	2.29832900
H	0.00000000	-1.48885900	-2.57414200
H	0.00000000	-2.50358500	2.29832900

F17.H-

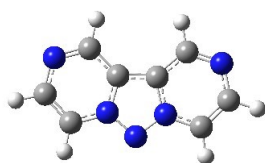
O 1			
C	0.68475200	0.57238400	-0.07814900
N	-0.00004400	-1.62768200	0.21743500
N	-1.07807700	-0.80561300	-0.24360700
N	1.07809800	-0.80556700	-0.24317100
C	-0.68476700	0.57238200	-0.07829500
C	1.72732700	1.53712000	0.01129100
C	2.37787700	-1.20556200	-0.04029800
C	3.36102400	-0.27850500	0.05651400
H	4.39220000	-0.59731700	0.12212900

C	3.02577600	1.12923800	0.05464500
H	3.82146800	1.86064500	0.12457100
C	-2.37788400	-1.20555400	-0.04031800
C	-1.72730900	1.53712800	0.01121000
C	-3.02576300	1.12927800	0.05465400
H	-3.82145500	1.86067800	0.12462000
C	-3.36097700	-0.27848800	0.05664600
H	-4.39214100	-0.59729600	0.12251200
H	1.46670900	2.58679700	0.07524000
H	2.54072500	-2.27537400	-0.03529400
H	-1.46665800	2.58679900	0.07515700
H	-2.54076800	-2.27536100	-0.03525700
H	-0.00024900	-1.53407100	1.26432500

F17.NHC

I 1			
C	2.30148100	-1.15284800	-0.03338100
N	1.14421400	0.82156700	0.03147000
N	2.46269800	1.04781600	0.04071600
N	1.06961300	-0.51949300	-0.01310200
C	3.24083500	-0.09583600	0.00290500
C	2.35986300	-2.55202100	-0.08212800
C	-0.12250000	-1.19688600	-0.03799700
C	-0.06000100	-2.56418200	-0.08594500
H	-0.99493500	-3.10951700	-0.10720500
C	1.17534900	-3.25272400	-0.10826600
H	1.18703000	-4.33449100	-0.14632900
C	3.00440400	2.30705400	0.08463700
C	4.63889400	0.01891300	0.00906200
C	5.19631500	1.27557300	0.05272900
H	6.27190600	1.39406000	0.05834600
C	4.36563400	2.42221200	0.09067200
H	4.79989600	3.41252500	0.12509900
H	3.32070700	-3.04903200	-0.09800400
H	-1.05948400	-0.61384200	-0.01933000
H	5.24821300	-0.87466500	-0.02068900
H	2.29727000	3.12322700	0.11109500
C	-3.13475200	0.08732500	0.00153700
N	-3.89978100	0.48467100	-1.05562900
N	-3.95378200	0.32019000	1.06737800
C	-5.14847000	0.94861100	-0.66198900
C	-3.46198700	0.43037800	-2.44369400
C	-5.18281000	0.84328200	0.68684900
C	-3.58750500	0.04865300	2.45042100
H	-5.88987000	1.30408100	-1.35788300
H	-4.13161700	-0.19943700	-3.03404800
H	-3.43786400	1.43176000	-2.88016000
H	-2.46059100	0.00609200	-2.46829600
H	-5.95962600	1.09131100	1.39071300
H	-3.60938700	0.96651000	3.04252000
H	-4.27186900	-0.67804900	2.89445900
H	-2.57900500	-0.35881500	2.46141300

F18-Singlet



1 1			
N	-0.00001900	1.63073100	0.00000000
N	-0.00000500	0.79685500	1.04549500
N	-0.00000500	0.79685500	-1.04549500
C	-0.00000200	1.20275100	-2.35174700
C	0.00000900	0.21172700	-3.29971600
H	0.00001000	0.47938200	-4.34946900
C	-0.00000200	1.20275100	2.35174700
C	0.00000900	0.21172700	3.29971600
H	0.00001000	0.47938200	4.34946900
H	-0.00000500	2.26683000	-2.53847500
H	-0.00000500	2.26683000	2.53847500
C	-0.00000200	-0.54200800	-0.70661900
C	-0.00000200	-0.54200800	0.70661900
N	0.00000900	-1.11428600	3.01169500
N	0.00000900	-1.11428600	-3.01169500
C	-0.00000100	-1.48632700	-1.75278300
H	0.00001300	-2.54860800	-1.53072600
C	-0.00000100	-1.48632700	1.75278300
H	0.00001300	-2.54860800	1.53072600

F18-Triplet

1 3			
N	1.69517300	-0.00012000	0.00000000
N	0.79244800	-0.00146600	1.08716300
N	0.79244800	-0.00146600	-1.08716300
C	1.19634900	0.00048600	-2.37975800
C	0.20603000	0.00135700	-3.33938500
H	0.45985800	0.00242200	-4.39048400
C	1.19634900	0.00048600	2.37975800
C	0.20603000	0.00135700	3.33938500
H	0.45985800	0.00242200	4.39048400
H	2.26098200	0.00082100	-2.57178800
H	2.26098200	0.00082100	2.57178800
C	-0.55185100	-0.00129700	-0.70123400
C	-0.55185100	-0.00129700	0.70123400
N	-1.11769200	0.00088800	3.01783100
N	-1.11769200	0.00088800	-3.01783100
C	-1.48806600	-0.00029300	-1.75120300
H	-2.55201300	-0.00028900	-1.53791200
C	-1.48806600	-0.00029300	1.75120300
H	-2.55201300	-0.00028900	1.53791200

F18.H-

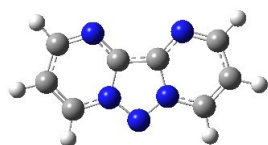
0 1			
N	-0.00008600	-1.64614700	0.20463700
N	-1.07581500	-0.81942500	-0.26954300
N	1.07584600	-0.81934000	-0.26878600
C	2.38613000	-1.16941700	-0.02710700
C	3.30955500	-0.18472400	0.08968500
H	4.35964900	-0.42719100	0.18336500

C	-2.38614600	-1.16939000	-0.02725000
C	-3.30946700	-0.18469200	0.08986800
H	-4.35953300	-0.42715900	0.18391700
H	2.61245800	-2.22697900	-0.01891600
H	-2.61256600	-2.22693400	-0.01909900
C	0.68676200	0.54922600	-0.11898000
C	-0.68679800	0.54922300	-0.11922800
N	-2.99405500	1.17099100	0.08831500
N	2.99408500	1.17090600	0.08818700
C	1.73743200	1.50030600	0.00540200
H	1.48688300	2.55678000	0.06648500
C	-1.73738800	1.50031300	0.00539500
H	-1.48677200	2.55677500	0.06648800
H	-0.00042600	-1.54926500	1.25138000

F18.NHC

1 1			
N	-0.54788400	1.27211600	-0.78035600
N	-0.69798700	-0.87634100	-1.01650100
C	-0.40861100	-2.21652100	-1.20619500
C	-1.29846200	-3.12651000	-0.74362200
H	-1.16216300	-4.17830100	-0.95740500
C	-0.03838300	2.54717600	-0.59651500
C	-0.78978400	3.44047600	0.08958900
H	-0.47208500	4.47165300	0.16908000
H	0.46181500	-2.45852900	-1.80072500
H	0.87793500	2.79792200	-1.11170300
C	-1.82084800	-0.48642800	-0.22712500
C	-1.71793800	0.87135200	-0.06662000
N	-1.99799000	3.12727300	0.69717700
N	-2.43314900	-2.79562900	-0.01024600
C	-2.66928300	-1.53841900	0.22448500
H	-3.54542800	-1.28908000	0.81806300
C	-2.42527100	1.90204500	0.61818700
H	-3.35545600	1.65467800	1.12359700
C	3.50706100	-0.33522400	0.63031100
C	2.73220100	-0.78595700	1.65215300
H	4.57798600	-0.28378200	0.53253000
H	3.00762800	-1.20804600	2.60361800
C	1.37760000	-0.06688500	0.04514300
N	1.41471500	-0.61847600	1.28235500
N	2.65750500	0.08796900	-0.36411400
N	0.31582700	0.13593700	-0.95569500
C	0.28314300	-0.99256600	2.14620400
H	-0.45571800	-0.19479600	2.14640600
H	-0.16651300	-1.91998000	1.79350000
H	0.66891100	-1.13389300	3.15333200
C	3.09711800	0.63892100	-1.65544300
H	2.27443300	0.56731800	-2.36160300
H	3.39468100	1.68059200	-1.53098100
H	3.94547500	0.05555100	-2.00935400

F19-Singlet



I 1			
N	0.00000000	1.65232400	0.00000000
N	1.04319000	0.81120700	0.00000100
N	-1.04319000	0.81120700	-0.00000100
C	-2.35562700	1.20319900	-0.00000300
C	-3.29143700	0.20908500	-0.00000400
H	-4.34308300	0.46261300	-0.00000600
C	-2.87482400	-1.15022000	-0.00000100
H	-3.61039700	-1.94713600	-0.00000300
C	2.35562700	1.20319900	0.00000200
C	2.87482400	-1.15022000	0.00000200
H	3.61039700	-1.94713600	0.00000600
C	3.29143700	0.20908500	0.00000300
H	4.34308300	0.46261300	0.00000600
H	-2.54583800	2.26761700	-0.00000400
H	2.54583800	2.26761700	0.00000200
N	-1.60657000	-1.51382000	0.00000000
N	1.60657000	-1.51382000	0.00000200
C	-0.70939500	-0.53672000	0.00000000
C	0.70939500	-0.53672000	0.00000100

F19-Triplet

I 3			
N	0.00000000	1.68651700	0.00000100
N	-1.08252000	0.81130000	-0.00000100
N	1.08252000	0.81130000	0.00000200
C	2.36880100	1.20173300	0.00000300
C	3.32846900	0.20760800	0.00000400
H	4.37879300	0.45698500	0.00000500
C	2.88795700	-1.13946600	0.00000200
H	3.61738600	-1.94352400	0.00000300
C	-2.36880100	1.20173300	-0.00000200
C	-2.88795700	-1.13946600	-0.00000300
H	-3.61738600	-1.94352400	-0.00000500
C	-3.32846900	0.20760800	-0.00000400
H	-4.37879300	0.45698500	-0.00000500
H	2.56136900	2.26726800	0.00000400
H	-2.56136900	2.26726800	-0.00000200
N	1.61314800	-1.52313000	0.00000100
N	-1.61314800	-1.52313000	-0.00000200
C	0.70303300	-0.55332900	0.00000000
C	-0.70303300	-0.55332900	-0.00000100

F19.H⁻

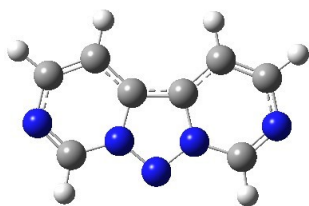
O 1			
N	-0.00003800	-1.64714300	0.23508200
N	1.07348700	-0.82172600	-0.22734600
N	-1.07347000	-0.82177100	-0.22773100
C	-2.37681100	-1.18127800	-0.04923500
C	-3.31457900	-0.20279000	0.01900100
H	-4.36660300	-0.44375600	0.06998700
C	-2.86819200	1.17629400	0.03921600

H	-3.61009600	1.96777400	0.10937500
C	2.37680200	-1.18128700	-0.04927700
C	2.86820700	1.17625300	0.03927200
H	3.61011500	1.96773000	0.10945500
C	3.31461500	-0.20279900	0.01884200
H	4.36664800	-0.44377100	0.06956200
H	-2.58385800	-2.24423000	-0.02472700
H	2.58382500	-2.24424600	-0.02487900
N	-1.62111100	1.54796900	0.03492800
N	1.62113000	1.54796200	0.03507200
C	-0.68290100	0.57061700	-0.05383400
C	0.68289000	0.57061800	-0.05370600
H	-0.00020200	-1.55030600	1.27952600

F19.NHC

I 1			
N	0.32975100	0.09603500	-0.95393100
N	-0.48330100	1.26135600	-0.77771500
N	-0.71644600	-0.87037800	-0.97273600
C	-0.54572600	-2.19494000	-1.28261800
C	-1.48864200	-3.06809300	-0.85474500
H	-1.44775000	-4.10822400	-1.14431500
C	-2.55605900	-2.57863000	0.00153500
H	-3.27888600	-3.28584700	0.39742000
C	0.02773700	2.53504200	-0.72966800
C	-1.88047800	3.08586400	0.64320700
H	-2.43265000	3.83516200	1.20241400
C	-0.68625100	3.48365700	-0.07990600
H	-0.37198300	4.51730300	-0.09610100
H	0.30394300	-2.45249400	-1.90281000
H	0.93712700	2.72526300	-1.28519000
N	-2.69620300	-1.33670400	0.36362100
N	-2.32405100	1.86470200	0.70764500
C	-1.81188600	-0.43429600	-0.12600900
C	-1.65210600	0.91213800	0.01889300
C	1.37746200	-0.13313100	0.04421000
N	2.66477700	-0.03922000	-0.35906700
N	1.38337100	-0.61727900	1.31022100
C	3.49122800	-0.44111400	0.66406600
C	3.13494000	0.43183000	-1.67107900
C	2.69212500	-0.81029400	1.69941900
C	0.23635600	-0.91622600	2.18807000
H	4.56396400	-0.43303500	0.57390200
H	3.49752000	1.45679200	-1.58708700
H	3.94425200	-0.21672600	-2.00265700
H	2.30791200	0.38507700	-2.37392600
H	2.94459600	-1.19087500	2.67439800
H	-0.24234200	-1.84271800	1.87445400
H	0.62010200	-1.02760400	3.19963200
H	-0.48329800	-0.10250300	2.15135600

F20-Singlet



1 1			
N	0.00000000	0.00000000	1.62102600
N	0.00000000	1.04153700	0.78231200
N	0.00000000	-1.04153700	0.78231200
C	0.00000000	-2.36566900	1.18556500
C	0.00000000	-3.03063700	-1.01630900
H	0.00000000	-3.88437600	-1.68254300
C	0.00000000	2.36566900	1.18556500
C	0.00000000	3.03063700	-1.01630900
H	0.00000000	3.88437600	-1.68254300
H	0.00000000	-2.54026200	2.25502600
H	0.00000000	2.54026200	2.25502600
C	0.00000000	-0.70749700	-0.55965300
C	0.00000000	0.70749700	-0.55965300
C	0.00000000	-1.74367700	-1.50338800
H	0.00000000	-1.53134500	-2.56397900
C	0.00000000	1.74367700	-1.50338800
H	0.00000000	1.53134500	-2.56397900
N	0.00000000	-3.31916800	0.31491900
N	0.00000000	3.31916800	0.31491900

F20-Triplet

1 3			
N	0.00000000	0.00000000	1.64786200
N	0.00000000	1.08004600	0.77348700
N	0.00000000	-1.08004600	0.77348700
C	0.00000000	-2.37181200	1.18012300
C	0.00000000	-3.04337500	-1.00074100
H	0.00000000	-3.88968300	-1.67860000
C	0.00000000	2.37181200	1.18012300
C	0.00000000	3.04337500	-1.00074100
H	0.00000000	3.88968300	-1.67860000
H	0.00000000	-2.54240000	2.25163900
H	0.00000000	2.54240000	2.25163900
C	0.00000000	-0.69873600	-0.58331200
C	0.00000000	0.69873600	-0.58331200
C	0.00000000	-1.75200000	-1.50767600
H	0.00000000	-1.56673400	-2.57312800
C	0.00000000	1.75200000	-1.50767600
H	0.00000000	1.56673400	-2.57312800
N	0.00000000	-3.36235200	0.32682900
N	0.00000000	3.36235200	0.32682900

F20.H-

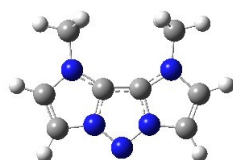
0 1			
N	-0.00000800	-1.65198800	0.50751700
N	-1.10648100	-0.77887000	0.26883000
N	1.10651800	-0.77889600	0.26899800
C	2.28831600	-1.14065100	-0.29641700

C	2.97246600	1.04289900	-0.21599500
H	3.81778900	1.70931800	-0.33841000
C	-2.28836700	-1.14063900	-0.29634300
C	-2.97244800	1.04293000	-0.21602200
H	-3.81774700	1.70937800	-0.33845400
H	2.41231300	-2.20147400	-0.49591400
H	-2.41243500	-2.20147800	-0.49570700
C	0.67721800	0.59473000	0.30749700
C	-0.67718000	0.59473700	0.30739900
C	1.76483100	1.52368400	0.16915100
H	1.60597300	2.58261600	0.32788200
C	-1.76477700	1.52370400	0.16903300
H	-1.60588500	2.58263900	0.32770000
N	3.23833900	-0.29659600	-0.52827100
N	-3.23840700	-0.29657600	-0.52814600
H	-0.00008200	-1.80887700	1.52057700

F20.NHC

1 1			
N	0.34498300	-0.00003500	-0.62790400
N	-0.45675800	-1.15343000	-0.25561500
N	-0.45679000	1.15337800	-0.25574800
C	-0.59630500	2.24161700	-1.12781900
C	-2.45106900	2.90903600	0.04854500
H	-3.11923800	3.73988700	0.23178000
C	-0.59621900	-2.24179300	-1.12753300
C	-2.45097500	-2.90912000	0.04889400
H	-3.11912200	-3.73996700	0.23222700
H	0.15716200	2.33296400	-1.90533700
H	0.15726200	-2.33322000	-1.90502700
C	-1.66791400	0.67552900	0.36906200
C	-1.66789500	-0.67554600	0.36913700
C	-2.60312300	1.72017100	0.67906000
H	-3.44027400	1.52997800	1.33820000
C	-2.60307400	-1.72018000	0.67925500
H	-3.44023800	-1.52992900	1.33836100
N	-1.50115500	3.12455200	-0.95858700
N	-1.50103900	-3.12474000	-0.95819400
C	1.57694800	0.00003200	0.04982900
N	1.84550100	0.00021600	1.37066000
N	2.74919300	-0.00007200	-0.61470900
C	3.21259900	0.00022900	1.53801400
C	0.86475500	0.00040100	2.46801800
C	3.77800700	0.00005000	0.30106200
C	2.92784300	-0.00032100	-2.07524300
H	3.66618400	0.00036700	2.51433600
H	0.24607000	-0.89245000	2.40312000
H	1.41537300	0.00040300	3.40553800
H	0.24626400	0.89338000	2.40299300
H	4.81197200	-0.00000200	0.00180400
H	3.48083600	0.89182900	-2.36758600
H	3.48035800	-0.89284400	-2.36735800
H	1.94837900	-0.00012100	-2.54405500

F21-Singlet



1 1			
C	-0.69829300	-0.07857400	-0.00000800
N	0.00000000	2.11714900	-0.00002000
N	1.03011700	1.25552100	0.00000800
N	-1.03011700	1.25552100	-0.00000300
C	0.69829300	-0.07857500	0.00000700
C	-2.40897600	1.39223300	-0.00001600
C	-2.89801500	0.11933700	-0.00004300
H	-3.92365900	-0.20962400	-0.00006300
H	-2.90007500	2.34866100	-0.00003100
C	2.40897600	1.39223300	0.00001900
C	2.89801500	0.11933700	-0.00000500
H	3.92365900	-0.20962400	-0.00001500
H	2.90007500	2.34866100	0.00003500
N	1.85708400	-0.79538500	-0.00000300
N	-1.85708300	-0.79538500	-0.00007800
C	1.97918700	-2.25211100	-0.00002100
H	1.51790500	-2.67411500	0.89482800
H	1.51833100	-2.67407200	-0.89511200
H	3.03675700	-2.50714000	0.00023200
C	-1.97918700	-2.25211100	0.00012200
H	-1.51769500	-2.67423600	-0.89456100
H	-1.51854100	-2.67395100	0.89537900
H	-3.03675700	-2.50714000	-0.00035700

F21-Triplet

1 3			
C	-0.69374100	0.06225200	-0.26304300
N	-0.00004400	-2.13590000	0.10362900
N	1.07639400	-1.28958000	-0.24020600
N	-1.07643800	-1.28958600	-0.24041000
C	0.69373100	0.06223200	-0.26290600
C	-2.41030300	-1.36607200	0.16153600
C	-2.87248200	-0.09835000	0.21306900
H	-3.87345600	0.26878400	0.36302200
H	-2.92203200	-2.30615500	0.27720400
C	2.41028300	-1.36611400	0.16158400
C	2.87250200	-0.09839700	0.21304000
H	3.87349200	0.26871900	0.36292000
H	2.92198500	-2.30621100	0.27725700
N	1.81378300	0.79901000	-0.06891800
N	-1.81377200	0.79904700	-0.06893200
C	1.89221000	2.25106700	0.04697000
H	1.32967600	2.71604000	-0.76307600
H	1.50539500	2.58723300	1.01325600
H	2.93472800	2.55052200	-0.04072300
C	-1.89214600	2.25109400	0.04709400
H	-1.50520700	2.58716400	1.01336400
H	-1.32969700	2.71612500	-0.76297700
H	-2.93466600	2.55058600	-0.04044600

F21.H-

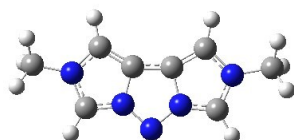
0 1			
C	0.67270500	0.05675500	-0.40073400
N	0.00001900	-2.05021600	0.27949900
N	-1.08852100	-1.33465000	-0.37488400
N	1.08854900	-1.33465400	-0.37490900
C	-0.67268800	0.05674200	-0.40069100
C	2.37474800	-1.31379300	0.20901300
C	2.80956700	-0.04058000	0.23818900
H	3.79795800	0.33436700	0.45476100
H	2.92420200	-2.22474100	0.38046600
C	-2.37474400	-1.31381100	0.20896600
C	-2.80959000	-0.04060500	0.23809000
H	-3.79800400	0.33432800	0.45458100
H	-2.92418700	-2.22476600	0.38041800
N	-1.82032000	0.83949500	-0.25223800
N	1.82032200	0.83951100	-0.25218500
C	-1.76465600	2.22828200	0.15293600
H	-1.29116300	2.35931100	1.13864700
H	-1.20478500	2.80715300	-0.58477000
H	-2.77917300	2.62667600	0.19320600
C	1.76462300	2.22829900	0.15297600
H	1.20481200	2.80716700	-0.58477700
H	1.29104700	2.35932800	1.13864900
H	2.77913500	2.62669400	0.19333200
H	0.00003000	-1.68964900	1.26603500

F21.NHC

1 1			
C	-1.99816300	0.74830800	-0.04723600
N	-0.84823000	-1.23899400	0.13369700
N	-2.17848200	-1.41870800	0.14757100
N	-0.78694900	0.09936000	0.01403300
C	-2.93882200	-0.27871200	0.04359000
C	0.25317500	1.01440700	-0.06855400
C	-0.36441700	2.22503400	-0.18187000
H	0.07998700	3.20175900	-0.27328300
H	1.31296700	0.71765800	-0.03714700
C	-3.00970600	-2.52370400	0.24726200
C	-4.27921500	-2.02862200	0.20132100
H	-5.21415100	-2.56093600	0.24896800
H	-2.63601900	-3.52722500	0.33980600
N	-4.25107100	-0.64895800	0.07637500
N	-1.74782200	2.07898300	-0.17015200
C	-5.40592200	0.24131000	-0.00521400
H	-5.40373100	0.94806100	0.82683600
H	-5.40694800	0.78126300	-0.95405200
H	-6.30936600	-0.36194800	0.05305000
C	-2.73833400	3.14623500	-0.26795300
H	-3.36732700	3.00824800	-1.14980600
H	-3.35792600	3.18088100	0.63056300
H	-2.21218000	4.09372100	-0.36291700
C	3.38999900	0.01760700	0.01502700
N	4.55685100	0.69881200	0.20282800
N	3.82153900	-1.25763800	-0.20439000
C	5.67301900	-0.12152500	0.10072400
C	4.62914000	2.12633100	0.47828700
C	5.20561100	-1.36462900	-0.15851600
C	2.93576900	-2.38286200	-0.47068000
H	6.68086200	0.23852200	0.22217800
H	5.16183800	2.31039400	1.41389700

H	5.13940100	2.65255000	-0.33203200
H	3.61366300	2.50554500	0.56834700
H	5.72886000	-2.29432500	-0.30695100
H	3.06498400	-2.74313600	-1.49437100
H	3.14351400	-3.20101000	0.22250500
H	1.90792800	-2.05509400	-0.33246000

F22-Singlet



I 1			
C	-0.71124500	-0.52457700	-0.00192100
N	0.00000000	1.72198400	0.00118500
N	1.03794000	0.83942500	0.00214000
N	-1.03794000	0.83942500	0.00213900
C	0.71124500	-0.52457700	-0.00192000
C	-1.90540500	-1.21152100	-0.01433100
C	-2.36856200	0.98409600	-0.00651700
H	-2.91092400	1.91162200	-0.00784500
H	-2.11799700	-2.26556100	-0.01978100
C	1.90540500	-1.21152100	-0.01432700
H	2.11799700	-2.26556100	-0.01977500
C	2.36856200	0.98409600	-0.00651500
H	2.91092400	1.91162200	-0.00784300
N	2.89779800	-0.26565400	-0.01979700
N	-2.89779800	-0.26565400	-0.01979800
C	-4.33680200	-0.55180800	0.03013700
H	-4.53601400	-1.46024800	-0.53530800
H	-4.65965000	-0.68000700	1.06389400
H	-4.88029000	0.27371500	-0.42572200
C	4.33680200	-0.55180800	0.03013400
H	4.65965200	-0.68000600	1.06389100
H	4.53601300	-1.46024900	-0.53531000
H	4.88029000	0.27371500	-0.42572700

F22-Triplet

I 3			
C	0.70552000	-0.51077700	-0.28178900
N	-0.04309300	1.70075500	0.04997900
N	-1.05335000	0.90424800	-0.48905600
N	1.01377700	0.82534300	0.02067300
C	-0.71005100	-0.49965600	-0.45643200
C	1.89447900	-1.18381700	-0.23358700
C	2.32525300	0.96438200	0.25375400
H	2.83434100	1.87955900	0.50204200
H	2.13667100	-2.21797000	-0.40217700
C	-1.83666800	-1.17937900	-0.09725600
H	-1.97430100	-2.23828300	0.05605500
C	-2.40260800	1.02882200	-0.01315300
H	-3.04990500	1.79155100	-0.42966700
N	-2.85744300	-0.29287500	0.10460200
N	2.87469800	-0.24967000	0.10683600

C	4.30395300	-0.55430400	0.24734200
H	4.43920000	-1.31082200	1.02019600
H	4.69550200	-0.91765100	-0.70297200
H	4.83255200	0.35245200	0.53372000
C	-4.23258200	-0.63073400	0.45489700
H	-4.32961000	-1.71325800	0.51553500
H	-4.49006000	-0.19125900	1.42050800
H	-4.92029200	-0.25613900	-0.30713400

F22.H-

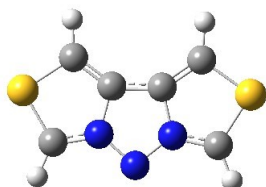
O 1			
C	-0.69507300	-0.41178300	-0.55225700
N	-0.00000100	1.69408600	0.24050400
N	1.10028000	0.98139600	-0.44984200
N	-1.10025600	0.98137300	-0.44985900
C	0.69509800	-0.41179000	-0.55228900
C	-1.80742800	-1.18377400	-0.25217300
C	-2.35607100	0.96995700	0.16895700
H	-3.06895100	1.77062700	0.02078300
H	-1.92494900	-2.25269200	-0.19206200
C	1.80741600	-1.18378200	-0.25204600
H	1.92493200	-2.25270500	-0.19197000
C	2.35601600	0.96995900	0.16917500
H	3.06896000	1.77057000	0.02095700
N	2.78719300	-0.33588600	0.15927300
N	-2.78727000	-0.33585100	0.15899900
C	-4.14887000	-0.73044500	0.47748600
H	-4.18428800	-1.80765500	0.63614900
H	-4.46621800	-0.22471500	1.39116200
H	-4.83251800	-0.46577700	-0.33431400
C	4.14893300	-0.73041900	0.47722000
H	4.46796000	-0.22131000	1.38840700
H	4.18365000	-1.80701200	0.64029100
H	4.83165700	-0.46965200	-0.33662100
H	0.00000800	1.33696100	1.23926100

F22.NHC

I 1			
N	-0.74241600	-1.45016100	0.63492500
N	1.04290600	0.62239200	-1.04112000
N	0.01782200	1.34731300	-0.45306100
C	-1.24341800	0.87458600	-0.06301900
C	-1.58489100	-0.53265800	0.04740000
C	-0.02675600	2.68334700	-0.50546000
H	0.79037600	3.30456300	-0.82795200
C	-1.38898300	-2.59157900	0.58352100
H	-1.02815400	-3.53719100	0.95881200
C	1.90166000	-0.00516100	-0.24103300
N	2.83905200	-0.81622200	-0.81411500
N	2.15587400	-0.01144200	1.10423200
C	3.67163400	-1.33647500	0.17073600
C	2.92638800	-1.05672200	-2.24780500
C	3.24661500	-0.85371200	1.35264700
C	1.37877400	0.62086500	2.16467400
H	4.48637800	-1.99735500	-0.06647800
H	3.64976500	-1.85169300	-2.42070100
H	1.95105400	-1.35681300	-2.63096000
H	3.24473400	-0.15381100	-2.77265700

H	3.60997100	-1.01784700	2.35142900
H	1.92713900	0.49809500	3.09722500
H	1.26404200	1.68946400	1.98232000
H	0.40480100	0.14038100	2.25842200
N	-2.61287200	-2.46580000	-0.00818100
N	-1.24934000	3.09809200	-0.14535500
C	-2.74987100	-1.14753000	-0.35893000
H	-3.62065700	-0.77737500	-0.87432800
C	-2.01417100	1.98835400	0.14631100
H	-3.03045400	2.07109400	0.49125000
C	-1.69040400	4.49238900	-0.05629300
H	-2.56983500	4.63796600	-0.68347000
H	-1.92854000	4.74262000	0.97779800
H	-0.88975700	5.14002400	-0.40803200
C	-3.58409500	-3.53197800	-0.24074700
H	-4.52351500	-3.30653800	0.26574000
H	-3.76550700	-3.65429800	-1.30949500
H	-3.18391900	-4.46284500	0.15779800

F23-Singlet



1 1			
C	0.00000000	0.71546900	-0.55451300
N	0.00000000	0.00000000	1.68054100
N	0.00000000	-1.04752100	0.81428900
N	0.00000000	1.04752100	0.81428900
C	0.00000000	-0.71546900	-0.55451300
C	0.00000000	2.35526700	1.06650800
H	0.00000000	2.77351800	2.05974700
C	0.00000000	-2.35526700	1.06650800
H	0.00000000	-2.77351800	2.05974700
H	0.00000000	1.88367700	-2.42615500
H	0.00000000	-1.88367700	-2.42615500
C	0.00000000	1.82539600	-1.34972100
C	0.00000000	-1.82539600	-1.34972100
S	0.00000000	-3.24494600	-0.38682200
S	0.00000000	3.24494600	-0.38682200

F23-Triplet

1 3			
C	0.00000000	0.71062600	-0.58582200
N	0.00000000	0.00000000	1.63472900
N	0.00000000	-1.04298000	0.77118700
N	0.00000000	1.04298000	0.77118700
C	0.00000000	-0.71062600	-0.58582200
C	0.00000000	2.35548900	1.07612100
H	0.00000000	2.72089200	2.09070400
C	0.00000000	-2.35548900	1.07612100
H	0.00000000	-2.72089200	2.09070400
H	0.00000000	1.93921000	-2.44584300

H	0.00000000	-1.93921000	-2.44584300
C	0.00000000	1.84535400	-1.37453600
C	0.00000000	-1.84535400	-1.37453600
S	0.00000000	-3.29675000	-0.34120600
S	0.00000000	3.29675000	-0.34120600

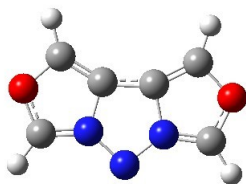
F23.H-

0 1			
C	-0.71272200	-0.46722000	-0.45657700
N	-0.00002200	1.69321400	0.17976800
N	1.11566000	0.90216100	-0.43918300
N	-1.11567800	0.90218100	-0.43931800
C	0.71271400	-0.46722800	-0.45653900
C	-2.37323900	1.04604300	0.11740900
H	-2.97159800	1.92345000	-0.07846600
C	2.37323800	1.04601700	0.11739200
H	2.97147200	1.92357800	-0.07813700
H	-1.65067000	-2.41240300	-0.07006600
H	1.65077200	-2.41240900	-0.07020400
C	-1.71205000	-1.33903500	-0.15451500
C	1.71208400	-1.33903200	-0.15457200
S	3.13784400	-0.49493800	0.30939700
S	-3.13782800	-0.49496900	0.30942000
H	-0.00008900	1.45614900	1.21135400

F23.NHC

1 1			
N	-1.45058700	-1.17366500	0.88776300
N	0.77084100	-0.01137900	-0.88617100
N	0.09199000	1.10247300	-0.44741200
C	-1.28008900	1.03774500	-0.15093400
C	-1.95757100	-0.25386300	-0.00173400
C	0.56358800	2.34878100	-0.48544300
H	1.58096200	2.57212100	-0.76360300
C	-2.20359500	-2.23174600	0.92390900
H	-2.01526200	-3.08927600	1.55531700
C	1.87519900	-0.35536100	-0.22117800
N	2.83376600	-1.11425000	-0.82251900
N	2.27550800	-0.16822000	1.07417200
C	3.82675800	-1.42083700	0.10243300
C	2.77510500	-1.56969100	-2.20806900
C	3.49266500	-0.82963400	1.26603700
C	1.46684500	0.39506300	2.15558800
H	4.68123400	-2.01906700	-0.16072900
H	3.78959900	-1.65933200	-2.59418400
H	2.26946900	-2.53498200	-2.27738000
H	2.22033800	-0.83882500	-2.79328700
H	3.99862800	-0.80969300	2.21517100
H	1.92275500	0.10682000	3.10077300
H	1.43511000	1.48570400	2.10650100
H	0.45888500	-0.01936700	2.11168200
C	-3.10928300	-0.62132400	-0.64479300
H	-3.66922600	-0.07897300	-1.39030400
C	-1.80884200	2.27882300	0.02487000
H	-2.82147900	2.52128700	0.30361400
S	-3.58502300	-2.18730700	-0.12590200
S	-0.62412200	3.51550300	-0.16275500

F24-Singlet



1 1			
C	0.00000000	0.71422400	-0.66357900
N	0.00000000	0.00000000	1.59816000
N	0.00000000	-1.04074500	0.71582700
N	0.00000000	1.04074500	0.71582700
C	0.00000000	-0.71422400	-0.66357900
C	0.00000000	2.35501100	0.83674100
H	0.00000000	2.96259200	1.72382300
C	0.00000000	-2.35501100	0.83674100
H	0.00000000	-2.96259200	1.72382300
H	0.00000000	2.19809700	-2.35357800
H	0.00000000	-2.19809700	-2.35357800
C	0.00000000	1.90294800	-1.31945300
C	0.00000000	-1.90294800	-1.31945300
O	0.00000000	2.89179200	-0.38710600
O	0.00000000	-2.89179200	-0.38710600

F24-Triplet

1 3			
C	0.00000000	0.70342600	-0.69236000
N	0.00000000	0.00000000	1.55343400
N	0.00000000	-1.03375900	0.68079600
N	0.00000000	1.03375900	0.68079600
C	0.00000000	-0.70342600	-0.69236000
C	0.00000000	2.35918400	0.85313400
H	0.00000000	2.90434200	1.78330000
C	0.00000000	-2.35918400	0.85313400
H	0.00000000	-2.90434200	1.78330000
H	0.00000000	2.28169400	-2.35629000
H	0.00000000	-2.28169400	-2.35629000
C	0.00000000	1.92742200	-1.34550000
C	0.00000000	-1.92742200	-1.34550000
O	0.00000000	2.94080200	-0.31515600
O	0.00000000	-2.94080200	-0.31515600

F24.H-

0 1			
C	0.70805900	0.60972900	-0.39382300
N	-0.00103200	-1.57186200	0.20986900

N	-1.11061400	-0.77533000	-0.42318700
N	1.11017700	-0.77525700	-0.42051000
C	-0.70793100	0.60979900	-0.39473000
C	2.34861600	-0.80386900	0.17992600
H	3.11337000	-1.53162200	-0.04449300
C	-2.34874700	-0.80413800	0.18033500
H	-3.11532900	-1.52792000	-0.05144100
H	1.94553900	2.37685500	0.19348200
H	-1.94288400	2.37708200	0.19616300
C	1.78292700	1.32720500	0.02144500
C	-1.78187800	1.32734200	0.02278100
O	2.79624000	0.49239100	0.32504000
O	-2.79550400	0.49370600	0.32592600
H	-0.00257800	-1.32243700	1.23975700

F24.NHC

1 1			
C	-1.60993300	-0.91264600	-0.36553200
N	0.44190800	0.35691600	-0.27097100
N	-2.46994800	1.42805400	-0.53682600
N	-0.19809700	-0.81895900	-0.49353900
C	-2.45702500	0.18093000	0.08216400
C	0.23405100	-1.99065300	-0.93849600
H	1.23494600	-2.27248500	-1.21007400
C	-3.37522200	2.08499900	0.10185700
H	-3.71364400	3.09609300	-0.05610200
H	-2.84476500	-2.70864600	-0.83413800
H	-3.70397300	-0.55213600	1.81133000
C	-1.91624300	-2.17369300	-0.74394300
C	-3.38013100	0.16926600	1.08113700
O	-0.77760300	-2.84319600	-1.08460400
O	-3.97618000	1.38663800	1.10216200
C	1.75049300	0.31922000	0.00708900
N	2.48195400	-0.49196700	0.83535900
N	2.59510600	1.28916200	-0.43428600
C	3.78939600	-0.00888900	0.89618000
C	1.92649600	-1.50327600	1.73012400
C	3.85192400	1.09477000	0.12146200
C	2.21430500	2.37727200	-1.33653800
H	4.54490800	-0.49608000	1.48761600
H	2.59211500	-1.61416700	2.58379000
H	0.95145100	-1.17329300	2.09047000
H	1.82510100	-2.47257400	1.23564500
H	4.67594900	1.75274900	-0.09302700
H	1.19075700	2.20372500	-1.66011300
H	2.26814200	3.33128900	-0.81037600
H	2.88413900	2.39174300	-2.19667400

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