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Supporting Information

Differential Effects of Nitrogen Substitution in 5- and 6-Membered Aromatic Motifs

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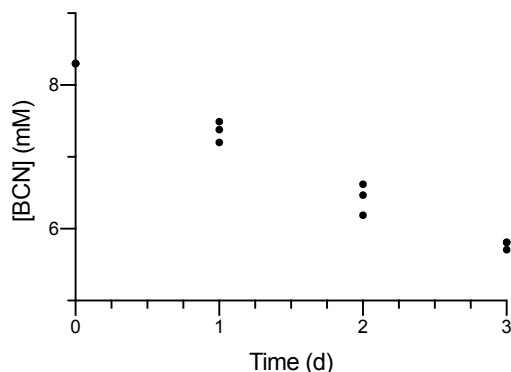
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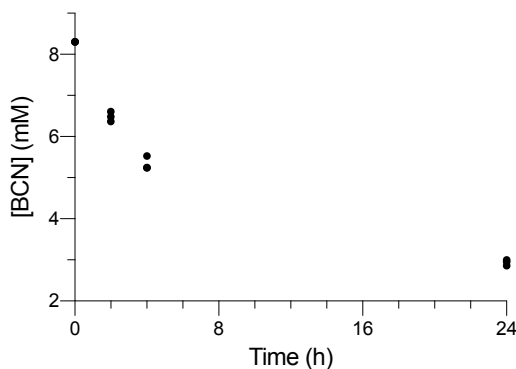
S1. Experimental Details

General. Chemicals and solvents were from commercial sources and used without further purification. NMR spectra were acquired on Bruker spectrometers operating at 500 MHz in the MIT Department of Chemistry Instrumentation Facility.

Reaction of 2,5-bis(trifluoromethyl)furan (1) with BCN. Stock solutions of 2,5-bis(trifluoromethyl)furan (16.6 mM) and BCN (166 mM) were prepared in deuterated MeOH. A 0.4-mL aliquot of the 2,5-bis(trifluoromethyl)furan stock solution was mixed with 0.4 mL of the BCN stock solution, and the mixture was added to an NMR tube. $^1\text{H-NMR}$ spectra were acquired in triplicate, and the NMR tubes were then placed in an oil bath at 60 °C. $^1\text{H-NMR}$ spectra were acquired again at 1, 2, and 3 days, and the integration of the peak for the protons adjacent to the alkyne on BCN was used to measure the disappearance of BCN over time. The disappearance of BCN is shown in the graph below. These data were used to calculate a second-order rate constant of $k = 1.8 \times 10^{-5} \text{ M}^{-1}\text{s}^{-1}$.



Reaction of 2,5-bis(trifluoromethyl)-1,3,4-oxadiazole (1N) with BCN. Stock solutions of 2,5-bis(trifluoromethyl)-1,3,4-oxadiazole (16.6 mM) and BCN (166 mM) were prepared in deuterated MeOH. A 0.4-mL aliquot of the 2,5-bis(trifluoromethyl)-1,3,4-oxadiazole stock solution was mixed with 0.4 mL of the BCN stock solution, and the mixture was added to an NMR tube. $^1\text{H-NMR}$ spectra were acquired in triplicate, and the NMR tubes were then placed in an oil bath at 60 °C. $^1\text{H-NMR}$ spectra were acquired again at 2, 4, and 24 h, and the integration of the peak for the protons adjacent to the alkyne on BCN was used to measure the disappearance of BCN over time. The disappearance of BCN is shown in the graph below. These data were used to calculate a second-order rate constant of $k = 1.3 \times 10^{-4} \text{ M}^{-1}\text{s}^{-1}$.



S2. M06-2X/6-311++G(d,p)// M06-2X/6-31G(d) Energetic Data

E, electronic energy
G, Gibbs free energy

Ethylene

E: -78.563592

G: -78.532718

1

E: -904.082614

G: -904.037259

1-TS

E: -982.620185

G: -982.521904

1-Adduct

E: -982.683706

G: -982.580609

1N

E: -936.143817

G: -936.122301

1N-TS

E: -1014.685583

G: -1014.610952

1N-Adduct

E: -1014.749406

G: -1014.670153

2

E: -884.235917

G: -884.177908

2-TS

E: -962.764324

G: -962.652996

2-Adduct

E: -962.817819

G: -962.701638

2N

E: -916.29739
G: -916.262967

2N-TS

E: -994.827393
G: -994.739858

2N-Adduct

E: -994.880396
G: -994.78823

3

E: -1227.063374
G: -1227.021731

3-TS

E: -1305.587136
G: -1305.493095

3-Adduct

E: -1305.658475
G: -1305.559096

3N

E: -1259.115948
G: -1259.098392

3N-TS

E: -1337.647885
G: -1337.577667

3N-Adduct

E: -1337.71838
G: -1337.642957

4

E: -868.167472
G: -868.099261

4-TS

E: -946.709669
G: -946.587902

4-Adduct

E: -946.790621

G: -946.662885

4N

E: -900.219087

G: -900.175184

4N-TS

E: -978.767044

G: -978.669436

4N-Adduct

E: -978.850259

G: -978.746522

5

E: -907.478979

G: -907.381222

5-TS

E: -986.013574

G: -985.863076

5-Adduct

E: -986.112237

G: -985.955649

5N

E: -939.526019

G: -939.452869

5N-TS

E: -1018.06685

G: -1017.940791

5N-Adduct

E: -1018.165882

G: -1018.033322

6

E: -906.301725

G: -906.225645

6-TS

E: -984.820493

G: -984.692178

6-Adduct

E: -984.877508

G: -984.74528

6N

E: -938.334742

G: -938.283983

6N-TS

E: -1016.872621

G: -1016.769216

6N-Adduct

E: -1016.936069

G: -1016.827895

6NN

E: -970.359459

G: -970.333897

6NN-TS

E: -1048.921656

G: -1048.843027

6NN-Adduct

E: -1048.989815

G: -1048.90517

S3. M06-2X/6-31G(d) Optimized Coordinates**Ethylene**

C	0.00000000	0.00000000	0.66360700
C	0.00000000	0.00000000	-0.66360700
H	0.00000000	0.92385400	1.23443400
H	0.00000000	-0.92385400	1.23443400
H	0.00000000	0.92385400	-1.23443400
H	0.00000000	-0.92385400	-1.23443400

1

C	-1.07840100	0.41329400	0.00003400
C	1.07840100	0.41329400	0.00003400
C	2.41397600	-0.24999300	0.00000400
C	-2.41397600	-0.24999300	0.00000400
F	-2.58087600	-1.02381800	-1.07636800
F	-2.58102500	-1.02367300	1.07643500
F	-3.36982400	0.68395400	-0.00011600
F	2.58087600	-1.02381700	-1.07636900
F	3.36982400	0.68395400	-0.00011600
F	2.58102500	-1.02367400	1.07643400
O	0.00000000	-0.39907900	0.00006000
C	-0.71555000	1.71990100	0.00000400
H	-1.38192700	2.56893600	-0.00003800
C	0.71555000	1.71990100	0.00000400
H	1.38192700	2.56893600	-0.00003700

1-TS

C	-1.06114600	0.01999200	0.33208300
C	-0.69390400	1.98575400	-0.49671900
C	0.69386600	1.98582300	-0.49634900
C	1.06119700	0.02036600	0.33193700
C	2.41392300	-0.39877800	-0.15202900
C	-2.41393100	-0.39878500	-0.15199800
F	-2.50845400	-0.32833000	-1.48176600
F	-2.71228900	-1.65315500	0.20556400
F	-3.33763900	0.40842400	0.38538500
F	2.50919500	-0.32683200	-1.48167300
F	3.33790500	0.40718800	0.38674500
F	2.71117900	-1.65378200	0.20417300
H	-1.24483800	2.58672500	0.21863600
H	-1.22590400	1.74912000	-1.41277700
H	1.24419400	2.58691600	0.21937900
H	1.22635700	1.74990300	-1.41230500
O	0.00004800	-0.49063400	-0.34334300
C	-0.68819300	0.26717700	1.66928100

H	-1.36389000	0.53888600	2.46765900
C	0.68829800	0.26724200	1.66924700
H	1.36397300	0.53914600	2.46757500

1-Adduct

C	1.05265900	0.28150500	0.11858800
C	0.77488100	1.56385900	-0.71955300
C	-0.77514000	1.56411100	-0.71894800
C	-1.05267500	0.28141700	0.11881000
C	-2.39721900	-0.36361300	-0.09705400
C	2.39721200	-0.36358600	-0.09709100
F	3.35765700	0.49504900	0.28449000
F	2.53293000	-1.47844900	0.62119800
F	2.59997400	-0.66671600	-1.38114200
F	-3.35772300	0.49498100	0.28445100
F	-2.59969700	-0.66656600	-1.38118100
F	-2.53315300	-1.47857500	0.62102600
H	1.17188900	1.43204700	-1.72810700
H	1.21823900	2.45428100	-0.27218700
H	-1.17301200	1.43381300	-1.72735200
H	-1.21799400	2.45417900	-0.27029300
O	-0.00001900	-0.57329700	-0.30970000
C	-0.66499900	0.58592100	1.55902500
H	-1.35505200	0.84994300	2.35017400
C	0.66538400	0.58607200	1.55889100
H	1.35558100	0.85048200	2.34977700

1N

C	-0.38099300	-0.00001200	1.04122600
C	-0.38099300	-0.00001200	-1.04122600
C	0.20361500	0.00001000	-2.42715500
C	0.20361500	0.00001000	2.42715500
F	0.96637500	-1.07889000	2.60237900
F	0.96671400	1.07868200	2.60218700
F	-0.76655100	0.00022300	3.32699100
F	0.96637500	-1.07889000	-2.60237900
F	-0.76655100	0.00022300	-3.32699100
F	0.96671400	1.07868200	-2.60218700
O	0.47323600	-0.00002200	0.00000000
N	-1.61821800	-0.00000500	0.69349800
N	-1.61821800	-0.00000500	-0.69349800

1N-TS

C	1.02805400	0.00539800	0.27932700
C	0.69287900	-2.00639900	-0.34271900
C	-0.69430900	-2.00610300	-0.34109900

C	-1.02772400	0.00527500	0.27918800
C	-2.42375200	0.38347000	-0.13147800
C	2.42397300	0.38322100	-0.13139000
F	2.56182900	0.26922400	-1.45476600
F	2.70719100	1.64069100	0.20556900
F	3.29637400	-0.42468200	0.46435000
F	-2.56163400	0.27004100	-1.45488500
F	-3.29628800	-0.42454400	0.46393500
F	-2.70675800	1.64083400	0.20600300
H	1.24444200	-2.51556500	0.43971800
H	1.22578700	-1.85325800	-1.27711800
H	-1.24405500	-2.51505000	0.44276100
H	-1.22923600	-1.85425100	-1.27457100
N	0.65382100	-0.17592100	1.55867500
N	-0.65372600	-0.17587400	1.55865700
O	0.00015400	0.48343000	-0.46186800

1N-Adduct

C	-1.02785600	0.25933100	-0.09731400
C	-0.77472300	1.69344200	0.42289900
C	0.77471800	1.69348000	0.42273600
C	1.02787800	0.25942400	-0.09769300
C	2.39213700	-0.34827400	0.11714700
C	-2.39216200	-0.34828900	0.11715700
F	-3.31385900	0.42889700	-0.45709100
F	-2.46981400	-1.56634000	-0.40867100
F	-2.66398500	-0.43021300	1.42252500
F	3.31408700	0.42892000	-0.45668100
F	2.66347800	-0.43037900	1.42257900
F	2.47004500	-1.56621500	-0.40881900
H	-1.18597400	1.78943700	1.42901800
H	-1.22169500	2.44416400	-0.22914600
H	1.18615200	1.78984000	1.42874700
H	1.22181100	2.44401100	-0.22947700
N	0.61710600	0.31700800	-1.54410700
N	-0.61713900	0.31716700	-1.54440500
O	0.00005400	-0.49292400	0.48578300

2

C	-1.10814600	-0.37826600	-0.02586400
C	1.10814600	-0.37826600	-0.02586400
C	2.46881100	0.21997200	0.00340600
C	-2.46881100	0.21997200	0.00340600

F	-3.37449900	-0.62587800	-0.49000100
F	-2.85973600	0.54930700	1.24313900
F	-2.50079200	1.35323900	-0.72143700
F	3.37449900	-0.62587800	-0.49000100
F	2.50079200	1.35323900	-0.72143700
F	2.85973600	0.54930700	1.24313900
N	0.00000000	0.41733800	-0.03096000
C	0.70825900	-1.69378200	0.00170800
H	1.36594500	-2.55018300	0.01141200
C	-0.70825900	-1.69378200	0.00170800
H	-1.36594500	-2.55018300	0.01141200
H	0.00000000	1.42387900	-0.12771600

2-TS

C	-1.08408500	-0.01223200	0.30664000
C	-0.69900500	1.92462100	-0.48414200
C	0.69907800	1.92464800	-0.48397300
C	1.08407700	-0.01236100	0.30671300
C	2.46576300	-0.37331400	-0.12894600
C	-2.46576900	-0.37329800	-0.12895400
F	-2.53706500	-0.43050200	-1.47100700
F	-2.86419900	-1.56264900	0.33661500
F	-3.34309000	0.54147700	0.29850400
F	2.53721700	-0.42966800	-1.47103500
F	3.34312500	0.54109200	0.29920500
F	2.86400200	-1.56301900	0.33588100
H	-1.24173100	2.53087500	0.23260500
H	-1.23063400	1.75155200	-1.41639300
H	1.24157300	2.53082900	0.23301300
H	1.23101500	1.75160600	-1.41604600
C	-0.68426800	0.24237600	1.65147800
H	-1.35392900	0.52011300	2.45367500
C	0.68421300	0.24232300	1.65151500
H	1.35386100	0.52000100	2.45374300
N	-0.00001400	-0.60243600	-0.32771200
H	0.00002100	-0.63507700	-1.34206200

2-Adduct

C	1.07472500	0.22576200	0.12913000
C	0.77492300	1.56175300	-0.63192300
C	-0.77492700	1.56176000	-0.63190500
C	-1.07472600	0.22576300	0.12913900
C	-2.45431700	-0.32992700	-0.09445500
C	2.45431800	-0.32992800	-0.09445600
F	3.38012000	0.58229600	0.24380300
F	2.68227400	-1.42789300	0.62532300

F	2.64007800	-0.63880100	-1.38841800
F	-3.38012400	0.58230200	0.24377400
F	-2.64005800	-0.63882000	-1.38841600
F	-2.68228600	-1.42788200	0.62533700
H	1.17940100	1.50950100	-1.64701900
H	1.21194400	2.42752200	-0.13194900
H	-1.17942700	1.50951300	-1.64699300
H	-1.21193500	2.42752900	-0.13191900
N	0.00000000	-0.67688400	-0.31583700
C	-0.66543200	0.45527200	1.57186300
H	-1.35149300	0.67803800	2.37941500
C	0.66543500	0.45527800	1.57185800
H	1.35150000	0.67808400	2.37939600
H	-0.00000400	-0.72719700	-1.33821200

2N

C	0.32380600	0.02344800	-1.06718100
C	0.32380600	0.02344800	1.06718100
C	-0.17033700	-0.00299400	2.48290800
C	-0.17033700	-0.00299400	-2.48290800
F	0.50613300	0.84014500	-3.25011700
F	-0.07591000	-1.22112100	-3.01281400
F	-1.46877400	0.34868400	-2.49422700
F	0.50613300	0.84014500	3.25011700
F	-1.46877400	0.34868400	2.49422700
F	-0.07591000	-1.22112100	3.01281400
N	-0.51585700	0.03120600	0.00000000
H	-1.52636500	0.08814900	0.00000000
N	1.57069000	0.00208800	-0.68141500
N	1.57069000	0.00208800	0.68141500

2N-TS

C	1.05048500	-0.03189600	-0.24078100
C	0.69854100	1.95230700	0.33113300
C	-0.69855400	1.95231700	0.33111800
C	-1.05048400	-0.03189800	-0.24078600
C	-2.47205000	-0.35901000	0.10667500
C	2.47205200	-0.35900700	0.10667500
F	2.60612300	-0.36093300	1.44585800
F	2.83677000	-1.56123500	-0.33592400
F	3.30284300	0.54689900	-0.39979700
F	-2.60605800	-0.36114100	1.44586400
F	-3.30283400	0.54700900	-0.39961200
F	-2.83683700	-1.56115000	-0.33610400
H	1.24114300	2.46166100	-0.45708900
H	1.23314400	1.86833500	1.27454900

H	-1.24113600	2.46166500	-0.45712200
H	-1.23318100	1.86836600	1.27452400
N	0.64691000	0.14956500	-1.53425900
N	-0.64690400	0.14956200	-1.53426300
N	-0.00000300	-0.58920600	0.46061300
H	0.00000300	-0.61139400	1.47374000

2N-Adduct

C	-1.04965200	0.20195200	-0.09967600
C	-0.77376100	1.66941000	0.34076700
C	0.77370700	1.66950300	0.34029500
C	1.04965400	0.20189500	-0.09975600
C	2.45062100	-0.31365400	0.10662900
C	-2.45060200	-0.31368500	0.10660700
F	-3.33986600	0.52921600	-0.42489100
F	-2.62618600	-1.51317500	-0.43456300
F	-2.70134100	-0.40533400	1.42417100
F	3.33986000	0.52910300	-0.42514100
F	2.70138800	-0.40490600	1.42421400
F	2.62621300	-1.51330500	-0.43418200
H	-1.19297800	1.83811300	1.33572900
H	-1.21545400	2.38525200	-0.35366600
H	1.19342600	1.83858900	1.33498000
H	1.21491500	2.38522000	-0.35457700
N	0.61866200	0.18189700	-1.52842200
N	-0.61872400	0.18264800	-1.52839200
N	0.00001400	-0.59837600	0.51050900
H	0.00001500	-0.49726500	1.52600700

3

C	-1.22118600	0.29043700	-0.00914100
C	1.22118600	0.29043700	-0.00914100
C	2.66757500	-0.08534200	0.00299600
C	-2.66757500	-0.08534200	0.00299600
F	-2.96971600	-0.91413700	-1.00457000
F	-3.00826700	-0.71076100	1.13708900
F	-3.43347200	1.00399300	-0.11104400
F	2.96971600	-0.91413700	-1.00457000
F	3.43347200	1.00399300	-0.11104500
F	3.00826700	-0.71076100	1.13708900
S	0.00000000	-0.92627800	-0.01406000
C	-0.71205000	1.55432700	-0.00617200
H	-1.33197100	2.44184200	-0.00688700
C	0.71205000	1.55432700	-0.00617300
H	1.33197100	2.44184200	-0.00688700

3-TS

C	-1.18584900	-0.04992000	0.25659300
C	-0.69607100	1.92230500	-0.55971700
C	0.69594500	1.92232800	-0.55977600
C	1.18587200	-0.04989500	0.25659000
C	2.64424300	-0.25427800	-0.01632300
C	-2.64422400	-0.25430000	-0.01632000
F	-2.91672200	-0.17296800	-1.32532600
F	-3.07933600	-1.44820600	0.40497100
F	-3.36208200	0.68302500	0.61729100
F	2.91670200	-0.17292800	-1.32533700
F	3.36212300	0.68302500	0.61729100
F	3.07935900	-1.44819100	0.40495500
H	-1.23908000	2.50039800	0.18019800
H	-1.23468300	1.73360400	-1.48268600
H	1.23901500	2.50043500	0.18008100
H	1.23447800	1.73363400	-1.48279600
C	-0.68669200	0.18345200	1.55836400
H	-1.32043400	0.50501100	2.37647100
C	0.68671100	0.18346000	1.55836200
H	1.32044800	0.50503100	2.37646900
S	0.00001500	-0.88817700	-0.72243700

3-Adduct

C	1.16274900	0.21792100	0.04300200
C	0.77453300	1.26244000	-1.04279000
C	-0.77457300	1.26247000	-1.04302400
C	-1.16342700	0.21885000	0.04324200
C	-2.61815900	-0.17066300	0.02930200
C	2.61787900	-0.17055600	0.02925300
F	3.37796900	0.91782500	0.23657300
F	2.90676300	-1.05287500	0.98981300
F	2.98040900	-0.70322300	-1.14281000
F	-3.37901200	0.91730100	0.23623000
F	-2.98001900	-0.70360000	-1.14279400
F	-2.90662400	-1.05311200	0.98985800
H	1.17351300	0.95319600	-2.01107500
H	1.19316000	2.23929500	-0.78736900
H	-1.17315600	0.95258100	-2.01126700
H	-1.19338900	2.23945700	-0.78839400
C	-0.66499700	0.77630500	1.36611700
H	-1.32780800	1.20076200	2.11148800
C	0.66496200	0.77597900	1.36604900
H	1.32803100	1.20007800	2.11136800
S	0.00065400	-1.17016900	-0.30459300

3N

C	1.16379800	-0.23600800	-0.01188800
C	-1.16458700	-0.23943600	-0.02745400
C	-2.65059900	0.02113000	0.00465100
C	2.65078500	0.02303900	0.00673300
F	2.87831900	1.33856300	-0.10598300
F	3.19188500	-0.39739400	1.14628100
F	3.25499200	-0.59764100	-0.99974800
F	-2.89378700	1.28218600	-0.37623200
F	-3.29599200	-0.80328600	-0.80860700
F	-3.13319700	-0.13504300	1.23631400
S	-0.00215400	1.03356700	-0.02554800
N	0.67931400	-1.43708200	-0.01388900
N	-0.67672900	-1.43947300	-0.02207100

3N-TS

C	-1.14014000	-0.06132000	0.20448900
C	-0.69441300	1.94797600	-0.49360000
C	0.69477000	1.94781500	-0.49364800
C	1.14009700	-0.06137400	0.20443400
C	2.62525100	-0.24876900	0.03658200
C	-2.62529600	-0.24870100	0.03658300
F	-2.94737000	-0.20920000	-1.26393800
F	-3.03012500	-1.42375100	0.51898400
F	-3.29030000	0.71691400	0.66475400
F	2.94733300	-0.20998500	-1.26395300
F	3.29009100	0.71731400	0.66420600
F	3.03020200	-1.42348800	0.51965500
H	-1.23745500	2.45891700	0.29372600
H	-1.23808200	1.79907900	-1.42191500
H	1.23797900	2.45866900	0.29362700
H	1.23834600	1.79881500	-1.42200400
N	-0.64662200	0.17719300	1.43830800
N	0.64664200	0.17716200	1.43828900
S	-0.00006400	-0.88499800	-0.83787700

3N-Adduct

C	-1.13013500	0.19411400	-0.02475800
C	-0.77338800	1.49133100	0.74038600
C	0.77335900	1.49140300	0.74048500
C	1.13036700	0.19444700	-0.02476200
C	2.59574200	-0.17224400	-0.04826600
C	-2.59563300	-0.17221000	-0.04832500
F	-3.31386000	0.84775300	-0.52471500
F	-2.82154400	-1.23952600	-0.81041800
F	-3.02739300	-0.44141700	1.19023400

F	3.31419100	0.84750600	-0.52481500
F	3.02753800	-0.44146600	1.19026800
F	2.82136500	-1.23962100	-0.81032400
H	-1.18796700	1.44488900	1.74842400
H	-1.19735100	2.35314400	0.21969900
H	1.18782700	1.44491800	1.74857800
H	1.19729400	2.35332700	0.21995800
N	0.61585600	0.45433100	-1.40541600
N	-0.61584600	0.45420800	-1.40540400
S	-0.00027700	-1.06976000	0.64615300

4

C	-0.28682500	-0.00001800	1.16247300
C	-0.28682500	-0.00001800	-1.16247300
C	0.17618800	0.00001000	-2.57536400
C	0.17618800	0.00001000	2.57536400
F	0.93387200	-1.07704900	2.83962400
F	0.93369500	1.07718800	2.83964100
F	-0.84854500	-0.00008000	3.43519200
F	0.93387200	-1.07704900	-2.83962400
F	-0.84854500	-0.00008000	-3.43519200
F	0.93369500	1.07718800	-2.83964100
C	-1.55951700	-0.00008900	0.73340600
H	-2.44201000	-0.00013800	1.36091400
C	-1.55951700	-0.00008900	-0.73340600
H	-2.44201000	-0.00013800	-1.36091400
C	0.65975400	0.00003600	0.00000000
H	1.31251800	-0.88263900	0.00000000
H	1.31241100	0.88279100	0.00000000

4-TS

C	-1.14128100	-0.16736000	0.23681200
C	-0.68802800	2.03757200	-0.03059800
C	0.68801100	2.03757600	-0.03063900
C	1.14128200	-0.16736600	0.23681200
C	2.56854700	-0.29571000	-0.17533100
C	-2.56854400	-0.29571200	-0.17533300
F	-2.79126700	0.24980500	-1.38260300
F	-2.95132800	-1.58112700	-0.25898500
F	-3.38026100	0.30763800	0.70404400
F	2.79125200	0.24974500	-1.38263200
F	3.38025500	0.30770800	0.70400800
F	2.95136300	-1.58112000	-0.25890900
H	-1.24419800	2.34895700	0.84646600
H	-1.23885500	2.06020600	-0.96544500
H	1.24423400	2.34897700	0.84638600

H	1.23877900	2.06019100	-0.96552300
C	-0.70241400	-0.33739600	1.54216000
H	-1.33906400	-0.32981600	2.41886400
C	0.70241500	-0.33739800	1.54215800
H	1.33906600	-0.32981800	2.41886200
C	0.00000000	-0.49973200	-0.68325400
H	-0.00000700	-1.58781000	-0.85395900
H	0.00000200	0.00842300	-1.64668900

4-Adduct

C	1.11256100	0.14986600	0.15023500
C	0.77613500	1.64387200	-0.14549400
C	-0.77613600	1.64387100	-0.14549500
C	-1.11256100	0.14986600	0.15023600
C	-2.52348400	-0.24389900	-0.17052800
C	2.52348400	-0.24389900	-0.17052800
F	3.40020400	0.46241600	0.56264200
F	2.74350500	-1.54207700	0.08202800
F	2.81442700	-0.03008200	-1.46323000
F	-3.40020400	0.46242100	0.56263700
F	-2.81442400	-0.03009000	-1.46323200
F	-2.74350800	-1.54207500	0.08203500
H	1.17641900	1.93028200	-1.12196000
H	1.20622900	2.30471300	0.60914600
H	-1.17642000	1.93028000	-1.12196200
H	-1.20623200	2.30471300	0.60914300
C	0.00000000	-0.56205600	-0.63965000
H	0.00000100	-1.64389800	-0.49187300
H	-0.00000100	-0.31245400	-1.70505200
C	0.66690800	-0.11856600	1.57731400
H	1.33658100	-0.17059800	2.42810600
C	-0.66690700	-0.11856500	1.57731400
H	-1.33657800	-0.17059300	2.42810800

4N

C	-1.11163200	-0.24832500	0.00501700
C	1.11163200	-0.24832500	-0.00501600
C	2.56606000	0.12668700	-0.00088000
C	-2.56606000	0.12668700	0.00088000
F	-2.82556300	0.93286500	1.04024500
F	-2.85252200	0.81050400	-1.11566200
F	-3.36233300	-0.92779800	0.07035200
F	2.85252100	0.81050700	1.11566000
F	3.36233300	-0.92779800	-0.07034900
F	2.82556300	0.93286200	-1.04024700
N	-0.71492800	-1.46324300	0.00316000

N	0.71492800	-1.46324300	-0.00316000
C	0.00000000	0.74707800	0.00000000
H	-0.00357800	1.39116200	-0.88743600
H	0.00357800	1.39116100	0.88743700

4N-TS

C	1.09549800	-0.16559000	-0.18714300
C	0.68703900	2.02234800	0.09259600
C	-0.68707300	2.02235000	0.09257000
C	-1.09549400	-0.16558300	-0.18714200
C	-2.55942300	-0.30490000	0.11423700
C	2.55942800	-0.30489500	0.11423700
F	2.81999200	0.14105800	1.35516300
F	2.94009200	-1.58652900	0.06747700
F	3.30440300	0.38702800	-0.74268500
F	-2.82001000	0.14114300	1.35512700
F	-3.30440800	0.38693400	-0.74274600
F	-2.94005100	-1.58655000	0.06757900
H	1.24173300	2.30787400	-0.79417200
H	1.24120700	2.03625000	1.02685100
H	-1.24173900	2.30787400	-0.79421600
H	-1.24126400	2.03626400	1.02681100
N	0.67028500	-0.24348600	-1.44001500
N	-0.67028100	-0.24348600	-1.44001700
C	0.00000100	-0.52994000	0.76430400
H	-0.00000300	-1.62438500	0.89626700
H	0.00000500	-0.04557900	1.73750400

4N-Adduct

C	-1.08378200	0.16224200	-0.07503300
C	-0.77481800	1.65924000	0.17845400
C	0.77481100	1.65924700	0.17835100
C	1.08378400	0.16222400	-0.07505800
C	2.51446500	-0.25771200	0.11671200
C	-2.51445900	-0.25772000	0.11671200
F	-3.33955000	0.46205900	-0.64746300
F	-2.68567100	-1.54859500	-0.18201100
F	-2.87899100	-0.08073600	1.39740700
F	3.33955500	0.46203800	-0.64749300
F	2.87898100	-0.08066000	1.39740200
F	2.68569500	-1.54860100	-0.18194200
H	-1.19083100	1.96553800	1.14093800
H	-1.20938500	2.28137000	-0.60567500
H	1.19092700	1.96561400	1.14076800
H	1.20927700	2.28134000	-0.60586200
N	0.61948800	-0.07138500	-1.47652000

N	-0.61951500	-0.07119600	-1.47654300
C	0.00000400	-0.55317700	0.72769200
H	0.00000700	-1.63594400	0.58305900
H	0.00001500	-0.29546500	1.78813100

5

C	1.40481900	-0.08813000	0.04448900
C	-1.40480300	-0.08808900	-0.04455600
C	-2.89793500	-0.04561000	0.01143600
C	2.89794600	-0.04561700	-0.01144200
F	3.32358800	0.70586800	-1.04116800
F	3.39580200	0.51417400	1.10449000
F	3.45063300	-1.25641500	-0.14128900
F	-3.39570600	0.51468300	-1.10429400
F	-3.45063700	-1.25647500	0.14068400
F	-3.32368900	0.70538300	1.04146100
C	0.73083100	-1.23826500	-0.05247900
H	1.25423800	-2.17834600	-0.18980000
C	-0.73084800	-1.23824000	0.05256900
H	-1.25427500	-2.17829900	0.18989300
C	0.70013000	1.22006900	0.30738000
H	1.28736300	2.05351000	-0.08869200
H	0.63803000	1.36354100	1.39519900
C	-0.70011600	1.22011200	-0.30729500
H	-0.63806300	1.36374900	-1.39508900
H	-1.28735000	2.05349700	0.08892900

5-TS

C	-1.35122100	-0.28933400	0.05685700
C	-0.68705400	1.89311900	-0.15589400
C	0.68683100	1.89302800	-0.15674800
C	1.35127200	-0.28946900	0.05693200
C	2.84390100	-0.13855900	0.07819700
C	-2.84387700	-0.13862900	0.07815800
F	-3.28203000	0.66528800	-0.90643400
F	-3.45581000	-1.32361800	-0.09734500
F	-3.28429500	0.37035400	1.23684100
F	3.28192800	0.66569300	-0.90617500
F	3.28431200	0.37015500	1.23700300
F	3.45597000	-1.32341900	-0.09770500
C	-0.77337600	-0.72431900	-1.27323500
H	-1.13800400	-1.74006300	-1.46370200
C	0.77347400	-0.72514500	-1.27293100
H	1.13711700	-1.74146700	-1.46218300
C	-0.70273600	-0.59460500	1.23190200
H	-1.24463700	-0.58328400	2.17229700

C	0.70273500	-0.59449000	1.23199600
H	1.24451700	-0.58292200	2.17245400
H	-1.17080700	-0.09893700	-2.07627000
H	1.17184900	-0.10100300	-2.07646000
H	-1.23945100	2.17564300	0.73387600
H	-1.23589700	1.96358300	-1.08889100
H	1.24041300	2.17564600	0.73225400
H	1.23454200	1.96314200	-1.09043600

5-Adduct

C	1.28166100	-0.00003200	-0.01112700
C	0.77288100	1.24495900	-0.77842500
C	-0.77294800	1.24486800	-0.77854200
C	-1.28162900	0.00004000	-0.01132100
C	-2.78888900	0.00036100	0.06607400
C	2.78888300	0.00051000	0.06614400
F	3.24824100	1.08471700	0.71200600
F	3.24791400	-1.07509300	0.72646800
F	3.35176000	-0.00794500	-1.15227900
F	-3.24807100	1.08471000	0.71193800
F	-3.35190400	-0.00788700	-1.15232000
F	-3.24787900	-1.07501100	0.72661700
H	1.16738800	1.21703200	-1.79885800
H	1.16291100	2.14547000	-0.29825200
H	-1.16742700	1.21695000	-1.79899000
H	-1.16295300	2.14545200	-0.29844800
C	0.77300500	-1.25624800	-0.76016000
H	1.16706700	-1.24294500	-1.78099500
C	-0.77301800	-1.25650100	-0.75947900
H	-1.16218100	-2.14945100	-0.26476700
C	0.66582000	0.01054700	1.36755700
H	1.27983100	0.01732700	2.26254100
C	-0.66583300	0.01053300	1.36762100
H	-1.27987500	0.01888200	2.26254500
H	-1.16784200	-1.24482600	-1.78007500
H	1.16292900	-2.14954300	-0.26661300

5N

C	1.31430400	-0.08319400	0.11929500
C	-1.31430200	-0.08316100	-0.11919200
C	-2.81867400	-0.09099800	0.01252900
C	2.81866500	-0.09100000	-0.01256600
F	3.18705300	0.72201800	-1.01625600
F	3.36267700	0.40032700	1.11189400
F	3.32143700	-1.29268600	-0.23846200
F	-3.36258000	0.40043700	-1.11194700

F	-3.32145200	-1.29271000	0.23829100
F	-3.18713700	0.72192800	1.01624900
C	0.64713500	1.23556100	0.40560600
H	1.30769000	2.05904600	0.12697900
H	0.43576400	1.32115800	1.47882100
C	-0.64711000	1.23557600	-0.40549200
H	-0.43572100	1.32114500	-1.47870400
H	-1.30766100	2.05906900	-0.12687400
N	-0.69581800	-1.17363200	0.10026200
N	0.69579600	-1.17364700	-0.10014900

5N-TS

C	1.27792100	-0.26309300	-0.05539800
C	0.68554600	1.88832100	0.33552500
C	-0.67611600	1.84853300	0.47656000
C	-1.28359700	-0.29154200	-0.06964800
C	-2.78569400	-0.12963000	-0.15214700
C	2.78402400	-0.14006300	-0.14814600
F	3.27525900	0.42098300	0.97390600
F	3.34702100	-1.35158500	-0.25498500
F	3.17640000	0.59766300	-1.17973200
F	-3.25185300	0.48652500	0.95055800
F	-3.17006200	0.57685800	-1.20789000
F	-3.37795700	-1.33153400	-0.20545500
C	0.75792600	-0.81286900	1.25651200
H	1.22880100	-1.79277600	1.39434700
C	-0.76584800	-0.95729600	1.18429300
H	-1.04799300	-2.01326900	1.10067300
H	1.08253800	-0.18839200	2.09090500
H	-1.26908700	-0.56219200	2.06828400
H	1.13304100	2.22654400	-0.59286600
H	1.33548300	1.88130900	1.20495200
H	-1.32251400	2.19578800	-0.32211700
H	-1.12912900	1.76865200	1.46020000
N	-0.66945000	-0.34058200	-1.22265700
N	0.67439500	-0.36799200	-1.21410100

5N-Adduct

C	-1.24019400	0.00014900	0.07081900
C	-0.77011200	1.26247700	0.81399700
C	0.77006900	1.26211700	0.81437700
C	1.24017200	-0.00003800	0.07084300
C	2.74238700	0.00002000	-0.12801600
C	-2.74239900	-0.00001900	-0.12806700
F	-3.15090000	1.08080900	-0.79828000
F	-3.15073100	-1.08100000	-0.79806900

F	-3.36495100	0.00006600	1.06409300
F	3.15073200	1.08069800	-0.79854500
F	3.36498000	0.00049800	1.06413200
F	3.15096300	-1.08099700	-0.79779400
H	-1.18069400	1.24815500	1.82694700
H	-1.16752900	2.14250600	0.30363300
H	1.18014000	1.24718500	1.82752200
H	1.16809700	2.14225900	0.30467700
C	-0.77016100	-1.26178700	0.81510200
H	-1.18010100	-1.24612900	1.82826800
C	0.77013100	-1.26221600	0.81451800
H	1.16738700	-2.14233800	0.30423200
H	1.18080200	-1.24747400	1.82741100
H	-1.16830800	-2.14208800	0.30579300
N	0.61941000	-0.00049000	-1.27215500
N	-0.61940800	-0.00050300	-1.27209600

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C	0.00613000	1.38168700	-0.04452600
C	-0.00613000	-1.38168700	-0.04452600
C	-0.00613000	-2.88488200	0.00959300
C	0.00613000	2.88488200	0.00959300
F	-1.04229900	3.40067500	-0.64632100
F	-0.06401600	3.32769300	1.27326300
F	1.11946200	3.40017500	-0.52845100
F	-1.11946200	-3.40017500	-0.52845100
F	1.04229900	-3.40067500	-0.64632100
F	0.06401600	-3.32769300	1.27326300
C	1.20771100	-0.69975700	-0.04689700
H	2.13963300	-1.25478300	-0.05992600
C	1.21416100	0.68984700	-0.04624700
H	2.15076100	1.23643100	-0.05803500
C	-1.21416100	-0.68984700	-0.04624700
H	-2.15076100	-1.23643100	-0.05803500
C	-1.20771100	0.69975700	-0.04689700
H	-2.13963300	1.25478300	-0.05992600

6-TS

C	-0.00033300	1.31497700	-0.24622900
C	0.00122700	0.69801600	1.80579200
C	-0.00122700	-0.69801600	1.80579200
C	0.00033300	-1.31497700	-0.24622900
C	0.00069700	-2.81522500	-0.15735900
C	-0.00069700	2.81522500	-0.15735900
F	1.08232500	3.26936700	0.49140700
F	-0.00069700	3.38384900	-1.37207100

F	-1.08409600	3.26889900	0.49112900
F	1.08409600	-3.26889900	0.49112900
F	-1.08232500	-3.26936700	0.49140700
F	0.00069700	-3.38384900	-1.37207100
C	1.22666600	0.67841800	-0.62420700
H	2.12879500	1.26664000	-0.75513000
C	1.22700900	-0.67782900	-0.62415500
H	2.12943900	-1.26559500	-0.75501600
H	-0.91169800	1.23216200	2.04732500
H	0.91663800	1.22867700	2.04557400
H	-0.91663800	-1.22867700	2.04557400
H	0.91169800	-1.23216200	2.04732500
C	-1.22700900	0.67782900	-0.62415500
H	-2.12943900	1.26559500	-0.75501600
C	-1.22666600	-0.67841800	-0.62420700
H	-2.12879500	-1.26664000	-0.75513000

6-Adduct

C	1.26926300	0.00006000	0.00020600
C	0.77116800	-0.15330600	-1.47869900
C	-0.77116700	-0.15317100	-1.47871200
C	-1.26926200	0.00004600	0.00020800
C	-2.77398700	0.00781300	0.07552300
C	2.77398700	0.00782300	0.07552200
F	3.29721400	1.02251600	-0.62975400
F	3.19821400	0.13989200	1.34083700
F	3.29711700	-1.13071800	-0.40499700
F	-3.29720000	1.02255700	-0.62968300
F	-3.29713100	-1.13069100	-0.40507600
F	-3.19821500	0.13979000	1.34084700
H	1.16762200	-1.08551900	-1.88775400
H	1.16786600	0.67495100	-2.07042900
H	-1.16784500	-1.08518700	-1.88798600
H	-1.16764300	0.67532400	-2.07026800
C	0.66435300	-1.16475700	0.76227200
H	1.29101000	-1.92679000	1.21273400
C	-0.66432800	-1.16476500	0.76225600
H	-1.29096600	-1.92681900	1.21271200
C	0.66432900	1.29636500	0.50717000
H	1.29094700	2.13457100	0.79189800
C	-0.66435500	1.29636000	0.50718800
H	-1.29099100	2.13454200	0.79193800

6N

C	-1.30862000	0.07720300	0.00016100
C	1.30862000	0.07720300	0.00016100

C	2.81624900	-0.06310700	-0.00004200
C	-2.81624900	-0.06310700	-0.00004200
F	-3.23648900	-0.72121900	-1.07897400
F	-3.23679300	-0.72234800	1.07800900
F	-3.39849000	1.14574700	0.00050500
F	3.23648900	-0.72121900	-1.07897400
F	3.39849000	1.14574700	0.00050500
F	3.23679300	-0.72234900	1.07800800
N	-0.65728400	-1.08358700	0.00031900
N	0.65728400	-1.08358700	0.00031900
C	0.69126000	1.32409200	0.00015800
H	1.27571400	2.23636800	0.00024900
C	-0.69126000	1.32409200	0.00015800
H	-1.27571400	2.23636800	0.00025000

6N-TS

C	-1.26352300	-0.25076700	-0.00164400
C	-0.69114700	1.81881400	-0.36255800
C	0.69142600	1.81875300	-0.36243600
C	1.26349500	-0.25088200	-0.00155100
C	2.76819300	-0.16057200	0.08733100
C	-2.76822900	-0.16053400	0.08730100
F	-3.27284700	0.22065700	-1.09884800
F	-3.30609600	-1.34670100	0.38667100
F	-3.16557700	0.71738100	1.00631000
F	3.27261600	0.22228600	-1.09837300
F	3.16551900	0.71614200	1.00746900
F	3.30627400	-1.34708900	0.38497700
C	-0.67922200	-0.88165700	-1.13342900
H	-1.29222400	-1.25640600	-1.94535600
C	0.67919600	-0.88174400	-1.13335400
H	1.29224300	-1.25655900	-1.94522200
H	-1.22972200	2.16498500	0.51329000
H	-1.23888400	1.85490500	-1.29882200
H	1.22985500	2.16479200	0.51356200
H	1.23937000	1.85478300	-1.29857500
N	-0.63826000	-0.31992000	1.22064500
N	0.63814900	-0.31994300	1.22068800

6N-Adduct

C	-1.23433600	0.00266600	0.07740600
C	-0.76844400	1.35767200	0.68262700
C	0.76843300	1.35788700	0.68222300
C	1.23434400	0.00270400	0.07744800
C	2.73501900	-0.07351200	-0.08680500
C	-2.73501800	-0.07349100	-0.08682700

F	-3.20534600	0.93814100	-0.81883600
F	-3.09954200	-1.21787300	-0.67042100
F	-3.32994600	-0.02223600	1.11698700
F	3.20536400	0.93812300	-0.81881300
F	3.32995700	-0.02226500	1.11700300
F	3.09947500	-1.21792300	-0.67037100
H	-1.18031900	1.44790700	1.68897400
H	-1.17076800	2.16655600	0.06866700
H	1.18098100	1.44909300	1.68820100
H	1.17006900	2.16640600	0.06732000
N	0.61340400	-0.00457100	-1.29784500
N	-0.61334900	-0.00463200	-1.29788400
C	-0.66601900	-1.12132200	0.88075900
H	-1.30309200	-1.85862600	1.35555000
C	0.66602500	-1.12123900	0.88086200
H	1.30306800	-1.85879800	1.35529200

6NN

C	0.04268500	-0.00005400	1.25374200
C	0.04268500	-0.00005400	-1.25374200
C	-0.00150000	0.00000400	-2.77433700
C	-0.00150000	0.00000400	2.77433700
F	1.21952100	-0.00009800	3.28963400
F	-0.65241500	1.08015000	3.20386800
F	-0.65267900	-1.07988700	3.20400100
F	1.21952100	-0.00009800	-3.28963400
F	-0.65267900	-1.07988700	-3.20400100
F	-0.65241500	1.08015000	-3.20386800
N	-1.15279000	-0.00009200	-0.65202900
N	-1.15279000	-0.00009200	0.65202900
N	1.22751200	-0.00007800	0.65925000
N	1.22751200	-0.00007800	-0.65925000

6NN-TS

C	-1.22097700	-0.28656200	0.00011200
C	-0.68301400	1.91008500	-0.00003200
C	0.68281600	1.91030600	-0.00036400
C	1.22104100	-0.28665900	0.00005600
C	2.73354500	-0.18545000	0.00000500
C	-2.73348700	-0.18546000	0.00000300
F	-3.15619000	0.47036000	-1.08193500
F	-3.28692100	-1.39595000	-0.00050600
F	-3.15646400	0.46962300	1.08225000
F	3.15630100	0.46992000	-1.08217500
F	3.15638000	0.47015300	1.08199900
F	3.28707400	-1.39589600	0.00010600

H	-1.23713100	2.04531100	0.92398800
H	-1.23769900	2.04547400	-0.92368300
H	1.23731400	2.04560500	0.92341600
H	1.23699300	2.04572200	-0.92431600
N	-0.64280700	-0.61519000	1.18406800
N	0.64280800	-0.61528300	1.18398700
N	0.64278100	-0.61571100	-1.18374900
N	-0.64287100	-0.61575400	-1.18369800

6NN-Adduct

C	-0.00000200	1.19970300	0.05960200
C	-0.00008200	0.76524400	1.54674000
C	0.00008200	-0.76524400	1.54674000
C	0.00000200	-1.19970300	0.05960200
C	-0.00000200	-2.70309900	-0.13743000
C	0.00000200	2.70309900	-0.13743000
F	1.08227700	3.24086500	0.43295900
F	-0.00056100	3.01765100	-1.42841300
F	-1.08176800	3.24106900	0.43388500
F	1.08176800	-3.24106900	0.43388500
F	-1.08227700	-3.24086500	0.43295900
F	0.00056100	-3.01765100	-1.42841300
H	-0.88832000	1.18457200	2.02218800
H	0.88796900	1.18475700	2.02238900
H	-0.88796900	-1.18475700	2.02238900
H	0.88832000	-1.18457200	2.02218800
N	-1.20318200	0.61760300	-0.55743800
N	-1.20324100	-0.61750500	-0.55740900
N	1.20318200	-0.61760300	-0.55743800
N	1.20324100	0.61750500	-0.55740900

S4. MP2/6-31G(d)//M06-2X/6-31G(d) NICS Calculations and Optimized Coordinates**Benzene**

NICS -11.5

C	-0.16819200	-1.38252200	0.00000000
C	0.16746300	1.38249400	0.00000000
H	0.29954400	2.46023600	0.00000000
H	-0.29749300	-2.46057900	0.00000000
C	-1.28154100	-0.54636900	0.00000000
H	-2.28054100	-0.97150200	0.00000000
C	-1.11349000	0.83700100	0.00000000
H	-1.98157300	1.48910100	0.00000000
C	1.11384500	-0.83643300	0.00000000
H	1.98155700	-1.48892400	0.00000000
C	1.28163700	0.54579500	0.00000000
H	2.28017100	0.97187000	0.00000000
Bq	-0.00004633	-0.00000566	0.00000000

Pyridine

NICS -9.6

C	-1.19711300	0.66820700	0.00000000
C	1.14048100	-0.71674800	0.00000000
H	2.05836000	-1.30070100	0.00000000
H	-2.15796700	1.17156700	0.00000000
C	-0.00438800	1.38224500	0.00000000
H	-0.00692500	2.46810800	0.00000000
C	1.19319900	0.67475300	0.00000000
H	2.15029800	1.18517000	0.00000000
N	0.00406700	-1.41703400	0.00000000
C	-1.13578100	-0.72385500	0.00000000
H	-2.05062100	-1.31252000	0.00000000
Bq	0.00007750	-0.02207200	0.00000000

1,2-Diazine

NICS -7.5

C	-1.31808200	-0.06924800	0.00000000
C	1.31808200	-0.06924800	0.00000000
H	2.40068400	-0.15620600	0.00000000
H	-2.40068400	-0.15620600	0.00000000
C	-0.68968400	1.17789900	0.00000000
H	-1.27034800	2.09422700	0.00000000
C	0.68968400	1.17789900	0.00000000
H	1.27034800	2.09422700	0.00000000
N	-0.66296200	-1.22713200	0.00000000
N	0.66296200	-1.22713200	0.00000000
Bq	0.00000000	-0.03949366	0.00000000

1,3-Diazine

NICS -7.5

C	1.35332300	0.00396100	0.00000000
H	2.43700200	0.00797900	0.00000000
C	0.62371000	-1.17888300	0.00000000
H	1.11984500	-2.14707100	0.00000000
C	0.61629500	1.18256800	0.00000000
H	1.10673700	2.15366000	0.00000000
N	-0.71772500	1.19260400	0.00000000
N	-0.71035600	-1.19667500	0.00000000
C	-1.30564300	-0.00415600	-0.00000100
H	-2.39313000	-0.00701300	0.00000300
Bq	-0.02339933	-0.00009683	-0.00000017

1,4-Diazine

NICS -7.6

C	1.12883200	0.69727800	0.00000000
H	2.06192800	1.25470700	0.00000100
N	-0.00045400	1.40553400	0.00000000
C	-1.12910600	0.69682200	0.00000000
H	-2.06282600	1.25329500	0.00000000
N	0.00039700	-1.40560900	0.00000000
C	1.12919500	-0.69662600	0.00000000
H	2.06258200	-1.25362300	0.00000100
C	-1.12882200	-0.69731900	0.00000000
H	-2.06187200	-1.25478700	0.00000000
Bq	0.00000700	0.00001333	0.00000000

1,2,3-Triazine

NICS -5.8

C	1.35161600	-0.00059900	0.00000000
H	2.43557700	-0.00082600	0.00000000
C	0.60264800	-1.16400600	0.00000000
H	1.05480500	-2.15140600	0.00000000
C	0.60361900	1.16346400	0.00000000
H	1.05645100	2.15059100	0.00000000
N	-0.73263300	1.14872900	0.00000000
N	-1.37579300	0.00047400	0.00000000
N	-0.73359300	-1.14799100	0.00000000
Bq	-0.04735600	0.00001183	0.00000000

1,2,4-Triazine

NICS -5.3

C	1.25195400	0.27043400	0.00000100
H	2.31766900	0.47928600	-0.00000100
N	0.42111200	1.32029500	0.00000000

C	-0.86134800	0.99669900	0.00000000
H	-1.58812200	1.80576800	0.00000000
N	-0.37067600	-1.33046100	0.00000000
C	-1.25826900	-0.34411400	0.00000000
H	-2.30330900	-0.63686600	0.00000000
N	0.91809900	-1.01644900	0.00000000
Bq	0.01681200	-0.01726600	0.00000017

1,3,5-Triazine

NICS -5.4

C	0.82730300	-0.98986900	0.00000000
H	1.52404400	-1.82515800	0.00000000
C	0.44393100	1.21131600	0.00000000
H	0.81858300	2.23246800	-0.00000100
N	-0.87891100	1.05222900	0.00000000
N	-0.47181800	-1.28696400	0.00000000
C	-1.27098600	-0.22162900	0.00000000
H	-2.34282300	-0.40716600	0.00000100
N	1.35054400	0.23487100	0.00000000
Bq	0.00001050	-0.00000766	0.00000000

1,2,3,4-Tetrazine

NICS -3.8

N	0.00000000	-0.65258100	-1.17692000
N	0.00000000	0.65258100	-1.17692000
N	0.00000000	1.35397100	-0.04964400
N	0.00000000	-1.35397100	-0.04964400
C	0.00000000	0.69584000	1.09673300
H	0.00000000	1.28997200	2.00554700
C	0.00000000	-0.69584000	1.09673300
H	0.00000000	-1.28997200	2.00554700
Bq	0.00000000	0.00000000	-0.04327700

1,2,3,5-Tetrazine

NICS -3.2

C	1.09933300	0.63395900	-0.00002300
H	2.05774700	1.14552800	0.00004900
N	-0.00620700	1.36875900	0.00000400
C	-1.10494800	0.62434100	0.00000300
H	-2.06832900	1.12659800	0.00000200
N	0.00627200	-1.35922800	0.00000000
N	1.14445600	-0.70128400	0.00000700
N	-1.13819500	-0.71138000	-0.00000200
Bq	0.00011850	-0.02413883	-0.00000183

1,2,4,5-Tetrazine

NICS -3.1

N	-0.65700200	1.19028900	0.00000000
C	-1.26063700	-0.00001600	-0.00000400
H	-2.34510700	-0.00001100	0.00001000
N	0.65701900	-1.19027300	0.00000000
N	-0.65701900	-1.19027300	0.00000000
N	0.65700200	1.19028900	0.00000000
C	1.26063700	-0.00001600	0.00000100
H	2.34510700	-0.00001100	-0.00000300
Bq	0.00000000	0.00000000	-0.00000050

1,2,3,4,5-Pentazine

NICS -0.7

N	-0.67785100	1.14872700	-0.00001400
N	0.63463300	-1.17679600	0.00000200
N	-0.67622000	-1.14963700	-0.00000400
N	0.63282000	1.17772300	0.00001200
C	1.25133300	0.00087400	-0.00001000
H	2.33664000	0.00163900	0.00001200
N	-1.31975900	-0.00100100	0.00001000
Bq	-0.02584066	-0.00001833	-0.00000067

Furan

NICS -13.9

C	-1.08886600	-0.34804500	0.00001000
H	-2.04352200	-0.85026400	0.00000700
C	1.08886500	-0.34804700	-0.00002600
H	2.04352100	-0.85026600	-0.00004600
O	-0.00000100	-1.15321200	0.00001200
C	0.71719500	0.95640800	0.00003000
H	1.37459700	1.81293500	0.00004300
C	-0.71719400	0.95640900	-0.00002100
H	-1.37459500	1.81293600	-0.00004900
Bq	-0.00000020	0.01270260	0.00000100

1-Azafuran

NICS -13.1

N	0.85303300	-0.84526600	-0.00057900
C	-1.10632600	0.18262100	-0.00023000
H	-2.18607100	0.16912000	-0.00008800
O	-0.50936500	-1.01462800	0.00046300
C	-0.17940600	1.17121300	-0.00012900
H	-0.33362600	2.23804600	0.00002600
C	1.04641200	0.44642900	0.00029400
H	2.05929800	0.82514000	0.00080000
Bq	0.02086960	-0.01192620	-0.00003620

2-Azafuran

NICS –12.5

C	1.09500600	-0.04293200	0.00005500
H	2.16738900	0.08432800	-0.00014500
C	-0.93469100	0.63693600	-0.00011300
H	-1.70815700	1.38680400	-0.00019000
N	0.41700000	-1.13926000	-0.00010300
O	0.35191600	1.08047900	0.00007200
C	-0.90487800	-0.71484700	0.00010900
H	-1.72618200	-1.41509300	0.00018200
Bq	0.00487060	-0.03592480	0.00000400

2,3-Diazafuran

NICS –13.3

N	-1.05365000	0.51638900	0.00007100
C	1.10212200	0.11592700	-0.00007100
H	2.14468800	0.39093500	-0.00013300
O	0.20903500	1.10313600	0.00002200
N	-0.91180500	-0.73001500	-0.00013200
C	0.42677700	-1.05637000	0.00010700
H	0.76782400	-2.07798300	0.00016900
Bq	-0.045504200	-0.01018660	-0.00000060

2,4-Diazafuran

NICS –11.9

N	-0.78828700	-0.88399800	0.00000300
C	-1.02380300	0.39507200	0.00000200
H	-2.03267500	0.78213400	-0.00001400
C	1.03227200	0.30454900	0.00000000
H	2.10302900	0.45206100	0.00000500
N	0.09531800	1.19416600	0.00000000
O	0.59120300	-0.95038700	-0.00000300
Bq	-0.01865940	0.01188040	0.00000040

3,4-Diazafuran

NICS –11.1

C	1.04805600	0.26854500	0.00004900
H	2.04262600	0.68614200	-0.00016100
C	-1.04805500	0.26854800	-0.00001800
H	-2.04262500	0.68614500	-0.00019500
N	0.69612400	-0.96785300	-0.00005000
N	-0.69612700	-0.96785100	0.00005000
O	0.00000100	1.11938600	0.00002200
Bq	-0.00000020	-0.05584500	0.00001060

2,5-Diazafuran

NICS –13.3

N	1.11985500	0.35710700	0.00014500
O	0.00056100	1.11398400	0.00008000
C	-0.71218300	-0.87666400	0.00027200
H	-1.41330800	-1.69721200	0.00046100
C	0.71099000	-0.87749500	-0.00024300
H	1.41105100	-1.69893200	-0.00033100
N	-1.11915200	0.35849700	-0.00027900
Bq	0.00001420	0.01508580	-0.00000500

2,3,4-Triazafuran

NICS –12.5

N	-0.98097000	-0.60684100	-0.00009500
O	0.33766100	-1.05222400	0.00008900
N	0.33498800	1.12444500	0.00001800
N	-0.95271900	0.64015500	0.00005200
C	1.05905500	0.05599100	-0.00008700
H	2.13528700	-0.02247400	-0.00002000
Bq	-0.04039700	0.03230520	-0.00000460

2,3,5-Triazafuran

NICS –13.7

N	-0.98097000	-0.60684100	-0.00009500
O	0.33766100	-1.05222400	0.00008900
N	0.33498800	1.12444500	0.00001800
N	-0.95271900	0.64015500	0.00005200
C	1.05905500	0.05599100	-0.00008700
H	2.13528700	-0.02247400	-0.00002000
Bq	-0.04039700	0.03230520	-0.00000460

2,3,4,5-Tetraazafuran

NICS –15.7

N	1.09086000	-0.27829300	-0.00000800
O	0.00314300	-1.08111600	-0.00019700
N	-1.08882500	-0.28449300	0.00038600
N	-0.69775400	0.89719000	-0.00038600
N	0.69212800	0.90115800	0.00023300
Bq	-0.00008960	0.03088920	0.00000560

Pyrrole

NICS –17.1

N	1.11772800	0.00493200	0.00014200
C	0.33592300	-1.11918000	-0.00003800
H	0.77695300	-2.10457100	-0.00022400
H	2.12511700	0.00924800	-0.00007200

C	-0.97723300	-0.71586200	0.00001700
H	-1.83771400	-1.36906400	0.00001200
C	-0.98383600	0.70710400	0.00007300
H	-1.85059400	1.35203600	-0.00003900
C	0.32568500	1.12238400	-0.00019900
H	0.75891400	2.11114600	0.00020900
Bq	-0.03634660	-0.00012440	-0.00000100

1,2-Diazole

NICS -16.4

N	0.06273300	-1.20058000	0.00014600
N	-1.00600800	-0.39510200	-0.00006000
H	-1.92549500	-0.80902000	0.00000300
C	0.68732900	0.98165400	0.00009800
H	1.30255000	1.86776500	0.00020100
C	1.09636600	-0.36982800	-0.00013100
H	2.10055500	-0.77002600	-0.00028500
C	-0.68816200	0.92043000	-0.00003300
H	-1.44788300	1.68752400	-0.00012600
Bq	0.03045160	-0.01268520	0.00000400

1,3-Diazole

NICS -15.5

N	-0.76293300	0.79473700	-0.00037900
C	0.59795900	0.98921100	0.00027000
H	1.03814300	1.97363400	0.00034800
H	-1.46959300	1.51426300	-0.00102200
C	1.13562900	-0.26914800	0.00011800
H	2.18035300	-0.54474200	0.00014700
C	-0.97724500	-0.54974600	0.00060500
H	-1.97124300	-0.97508500	0.00095500
N	0.14640200	-1.22187600	-0.00053400
Bq	0.02796240	-0.05136440	0.00001600

1,2,3-Triazole

NICS -16.0

N	0.50110600	-1.05978500	-0.00006800
N	1.05125900	0.15868900	0.00061400
H	2.05767900	0.24208300	-0.00114700
C	-1.06665700	0.43212700	0.00025600
H	-2.08243900	0.79475700	0.00055000
N	-0.78244500	-0.89956800	-0.00020800
C	0.11334100	1.13208000	-0.00061900
H	0.35521300	2.18256300	0.00040500
Bq	-0.03634660	-0.00012440	-0.00000100

1,2,4-Triazole

NICS -14.8

N	0.83952900	-0.65765900	-0.00010000
H	1.60500100	-1.31549100	-0.00003600
N	-0.42928500	-1.10561700	0.00005700
C	-1.11405900	0.02179900	0.00004000
H	-2.19445800	0.02709100	-0.00009100
C	0.86360800	0.68842800	0.00010500
H	1.77646300	1.26690100	0.00008400
N	-0.36514400	1.15758000	-0.00007500
Bq	-0.04107020	0.02090620	0.00000540

1,2,5-triazole

NICS -16.2

N	0.35606000	1.12381700	0.00027600
N	1.04347000	-0.00079200	-0.00008000
H	2.05314900	-0.00146400	-0.00012300
N	0.35424000	-1.12439500	-0.00012500
C	-0.90699700	-0.70144200	0.00022100
H	-1.72742000	-1.40214300	0.00033100
C	-0.90580500	0.70286800	-0.00025700
H	-1.72530300	1.40464900	-0.00048400
Bq	-0.01180640	0.00001120	0.00000700

1,3,4-Triazole

NICS -13.8

N	0.00053200	1.08645700	0.00016400
C	1.07788700	0.25050300	-0.00007500
H	2.10177400	0.59321600	-0.00006600
H	0.00161900	2.09524300	0.00005600
C	-1.07766100	0.25164000	-0.00020300
H	-2.10111900	0.59551900	-0.00024100
N	-0.68659800	-0.99266200	0.00017900
N	0.68554700	-0.99334300	-0.00006900
Bq	-0.00005860	-0.07948100	-0.00000080

1,2,3,4-Tetrazole

NICS -14.9

N	-0.62953200	-0.96528500	-0.00025600
N	-1.14958100	0.20693900	0.00017700
N	-0.19757200	1.16881700	-0.00001600
N	0.69795900	-0.78353900	0.00018000
C	0.94955000	0.53562400	-0.00011700
H	1.93375400	0.97689300	-0.00012900
H	1.32002400	-1.57916700	0.00023600
Bq	-0.06583520	0.03251120	-0.00000640

1,2,3,5-Tetrazole

NICS -15.5

N	0.65368500	0.94669400	-0.00014800
N	-0.64648900	0.98391100	0.00014500
N	0.97277700	-0.32969100	0.00007800
H	1.93447800	-0.64298400	0.00007300
N	-0.05014400	-1.16151500	-0.00000200
C	-1.05828400	-0.30448300	-0.00009000
H	-2.09357700	-0.60590300	-0.00004200
Bq	-0.02569100	0.02698320	-0.00000340

Pentazole

NICS -16.9

N	0.28398400	1.09454600	0.00002500
N	-0.93370500	0.67102700	-0.00006000
N	-0.93388900	-0.67078900	0.00007400
N	1.01087200	-0.00012600	0.00001600
H	2.02316700	-0.00015500	0.00002100
N	0.28371400	-1.09463600	-0.00005700
Bq	-0.05780480	0.00000440	-0.00000040

Thiophene

NICS -14.4

C	0.00850700	-1.23531600	-0.00000800
H	-0.28458200	-2.27573700	-0.00001300
C	0.00850700	1.23531600	0.00000700
H	-0.28458200	2.27573700	0.00001200
C	1.26792400	0.71472300	-0.00001200
H	2.16429200	1.32302400	-0.00001900
C	1.26792500	-0.71472300	0.00000900
H	2.16429300	-1.32302400	0.00001300
S	-1.19228800	0.00000000	0.00000200
Bq	0.27211500	0.00000000	-0.00000040

2-Azathiohpene

NICS -14.0

N	0.04783700	-1.25392000	-0.00020900
C	-0.02717700	1.23045900	0.00019400
H	0.24001000	2.27855300	0.00036400
C	-1.27211200	0.67158600	-0.00009400
H	-2.20376000	1.22179200	-0.00016900
C	-1.16247600	-0.75068900	-0.00002600
H	-2.00364600	-1.43706200	-0.00017900
S	1.15019500	-0.01212400	0.00006300
Bq	-0.25274660	-0.02293760	-0.00001440

3-Azathiophene

NICS –13.4

C	0.02610300	-1.19927100	-0.00002100
H	-0.25689700	-2.24486100	-0.00001500
C	0.07567700	1.21651100	0.00002200
H	-0.13705000	2.27533400	0.00005100
N	1.25232300	-0.78185400	0.00003400
C	1.28526000	0.59295600	-0.00010500
H	2.24354900	1.09721300	-0.00015000
S	-1.18363100	0.04275700	0.00003100
Bq	0.29114640	-0.02578020	-0.00000780

2,3-Diazathiophene

NICS –13.6

N	0.00483900	-1.24651900	0.00002000
C	0.05691300	1.20458300	-0.00006200
H	-0.14774300	2.26524900	-0.00008000
N	1.18805400	-0.78864500	0.00001400
C	1.27007700	0.58040000	0.00006300
H	2.24388500	1.04985300	0.00010100
S	-1.15052100	0.01382200	-0.00001600
Bq	0.27387240	-0.04727180	0.00000380

2,4-Diazathiophene

NICS –14.2

N	0.03392700	-1.23537200	-0.00000700
C	1.19111200	-0.62973100	0.00004400
H	2.10516700	-1.21244300	-0.00000700
C	0.03483900	1.19359300	0.00000300
H	-0.21939300	2.24689800	-0.00000300
N	1.25445300	0.74044300	-0.00001600
S	-1.14125900	-0.05957000	-0.00000700
Bq	0.27461440	0.00187260	0.00000340

2,5-Diazathiophene

NICS –13.6

N	-0.02971100	1.24346700	-0.00022700
C	1.17013100	-0.71520400	0.00015400
H	2.04550200	-1.35410700	0.00031000
C	1.17022700	0.71506100	-0.00011000
H	2.04569800	1.35382900	-0.00019500
N	-0.02990200	-1.24340300	0.00014400
S	-1.10725300	0.00004300	0.00001300
Bq	0.23469840	-0.00000720	-0.00000520

2,3-Diazathiophene

NICS –12.8

C	-0.08879600	1.17692200	-0.00000700
H	0.11013700	2.24047800	-0.00001400
C	-0.08879500	-1.17692200	0.00000600
H	0.11013800	-2.24047800	0.00001500
N	-1.28568000	0.68278800	-0.00002100
N	-1.28567900	-0.68278800	0.00000900
S	1.17779900	0.00000000	0.00000500
Bq	-0.31423020	0.00000000	-0.00000160

2,3,4-Triazathiophene

NICS –13.9

N	0.06789200	-1.21938900	0.00006700
N	1.27370600	0.65745600	0.00015100
N	1.21910300	-0.70175700	-0.00016600
C	0.07462700	1.16479800	-0.00002300
H	-0.10850700	2.23091600	-0.00002800
S	-1.14151000	-0.02336700	-0.00001300
Bq	0.29876360	-0.02445180	0.00000320

2,3,4-Triazathiophene

NICS –14.4

C	-1.18490500	-0.60928700	-0.00008500
H	-2.12247400	-1.14896700	-0.00003200
N	0.00752400	1.23069500	0.00003500
N	-1.18115900	0.76871400	-0.00002200
N	-0.02966500	-1.21821800	0.00012000
S	1.10343800	-0.04147800	-0.00002400
Bq	-0.25695340	0.02608520	0.00000480

2,3,4,5-Tetrazathiophene

NICS –15.8

N	0.04997700	-1.20004500	-0.00012800
N	0.05029000	1.20002800	0.00023600
N	1.20698900	0.69043800	0.00005800
N	1.20691300	-0.69061500	-0.00021000
S	-1.09994900	0.00008500	0.00001900
Bq	0.28284400	-0.00002180	-0.00000500

S5. LUMO Energies for Dienes 1–5, 1N–6N, and 6NN. LUMO energies (eV) were calculated at the M06-2X/6-311++G(d,p) basis set using the optimized geometries of the transition state.

