Supporting Information for

Effect of Group Electronegativity on Electron Transfer in Bis(hydrazine) Radical Cations

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xyz coordinates for calculated structures

sBI4T DFT(50-50)/6-31G* S2
sBI4T^{+} DFT(50-50)/6-31G* S3
sBI4T^{+} DFT(50-50) at the TD-MPW1K/6-31G* level S5
sBI4T(X=PH$_2$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S7
sBI4T(X=SH) $^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S8
sBI4T(X= NH$_2$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S9
sBI4T(X=OH) $^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S10
sBI4T(X=Cl)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S10
sBI4T(X=F)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S11
sBI4T(X=NHCH$_3$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S12
sBI4T(X=N(CH$_3$)$_2$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S13
sBI4T(X=PHCH$_3$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S15
sBI4T(X=P(CH$_3$)$_2$)$^{+}$ DFT(50-50) at the TD-MPW1K/6-31G* level S16
The linear reaction coordinate energy profile S18

sBI4T DFT(50-50)/6-31G* Calculation -1161.13434571 Dipole Moment 0.2802 -0.7088 -0.3242

C	0.21438800	-0.37959500	0.78019000
H	0.40934000	0.52209900	1.34507600
C	-0.02465200	-0.00649700	-0.69134200
H	-0.20833500	1.05781400	-0.76552500
C	1.29854300	-0.26610800	-1.43799900
C	1.54453400	-1.14265700	0.88609700
H	1.68799600	-1.46566600	1.91069100
H	1.25279900	0.12433100	-2.44601300
N	2.58682700	-0.14397300	0.58417700
N	2.40053600	0.41749700	-0.73588900
C	1.66807700	-2.32182000	-0.08219800
H	0.86505400	-3.03346600	0.05287900
H	2.58002500	-2.86834300	0.12756000
C	1.68572600	-1.73980200	-1.50334200
H	1.02431700	-2.27666900	-2.17506400
H	2.67838600	-1.79862900	-1.93521800
C	2.47552000	1.90534300	-0.77354200
C	1.76358000	2.62453800	0.37397100
C	3.95287500	2.32077700	-0.72565300
C	1.93577000	2.41539700	-2.11106600
H	0.68420400	2.55008400	0.31080100
H	2.08228800	2.21654500	1.32643100
H	2.01696900	3.68206800	0.35319200
H	4.53696900	1.74072200	-1.43352000
H	4.05178200	3.37348500	-0.97979800
H	4.37970300	2.19394900	0.26250400
H	2.10714800	3.48593100	-2.17321700
H	2.45160300	1.94973600	-2.94707900
H	0.86927500	2.25404100	-2.22866400
C	3.98823400	-0.52266300	0.85142500
C	4.75221800	-1.28378900	-0.23086500
H	4.46814700	-2.32918800	-0.30348300
H	4.60644200	-0.81660800	-1.19760000
H	5.81474100	-1.25390800	0.00125500
C	4.11883300	-1.20882900	2.20373100
H	3.59058300	-0.65586800	2.97571100
H	3.74444900	-2.22921400	2.19206800
H	5.16817700	-1.25335100	2.48225600
H	4.50939300	0.42169100	0.95746000
C	-1.35152300	-0.63333800	-1.15012600
C	-1.11317200	-0.96049400	1.31184100
H	-1.08465900	-1.05665900	2.39422800
H	-1.48012500	-0.44746500	-2.20919000

N	-2.19677900	-0.00785100	0.99641100
N	-2.40514100	0.10882600	-0.42509800
C	-1.48260700	-2.29483800	0.68551500
H	-0.80936100	-3.07465200	1.02495000
H	-2.47181900	-2.56641000	1.03548900
C	-1.45886900	-2.13193100	-0.84223400
H	-0.64312800	-2.68119700	-1.29041800
H	-2.35931100	-2.53385000	-1.29011000
C	-3.82287100	-0.14262300	-0.83162500
C	-3.89792200	-0.31646700	-2.34935600
C	-4.64588700	1.10437400	-0.50522900
C	-4.51774900	-1.32205700	-0.14208800
H	-3.45099400	-1.24252600	-2.69605500
H	-3.41790700	0.51330100	-2.86189900
H	-4.94127300	-0.33087700	-2.65122200
H	-4.69665600	1.27916600	0.56279500
H	-5.66505700	0.97843100	-0.86220400
H	-4.22287000	1.98129900	-0.98385200
H	-5.57966300	-1.29829800	-0.37423100
H	-4.40444400	-1.24588400	0.93301400
H	-4.14343700	-2.28747700	-0.46261100
C	-2.06460600	1.24495800	1.78027800
C	-2.15534800	2.55433400	1.01151700
C	-3.05857800	1.21309600	2.93545600
H	-1.07733700	1.24239800	2.23703700
H	-1.58514100	2.52502500	0.09168800
H	-1.75934200	3.34981500	1.63809700
H	-3.17417200	2.81685600	0.75863100
H	-2.94855400	0.29851000	3.51222000
H	-4.08341400	1.25591800	2.57814500
H	-2.89797700	2.05565800	3.60547200

sBI4T^{+} DFT(50-50)/6-31G* Calculation -1160.92000407 Dipole Moment -8.1422 -0.9191 0.5411

C	0.24862100	-0.55407500	0.69573000
H	0.36018000	0.21731900	1.45070900
C	0.02199400	0.09611200	-0.67792200
H	-0.17722800	1.15342500	-0.55227300
C	1.36373200	0.00932400	-1.44776700
C	1.60483400	-1.27701300	0.68090500
H	1.74850900	-1.78159600	1.62837500
H	1.30846300	0.58156500	-2.36288900
N	2.60058100	-0.20151800	0.59503400
N	2.42038800	0.57883300	-0.61020300
C	1.76720200	-2.25097200	-0.48951000

H	0.98868000	-3.00260900	-0.50076200
H	2.69170500	-2.79964400	-0.36747600
C	1.78369500	-1.41785900	-1.77845000
H	1.15159900	-1.83808700	-2.55402700
H	2.78229300	-1.37011900	-2.19543600
C	2.48020300	2.05569200	-0.40084400
C	1.71186400	2.56489500	0.81969800
C	3.94640800	2.47343200	-0.22593300
C	1.97951000	2.77047800	-1.65633600
H	0.63576800	2.52924000	0.67794800
H	1.97137400	1.98639800	1.69917300
H	1.97086600	3.60304500	1.00826700
H	4.57192200	2.01141200	-0.98264700
H	4.03500500	3.55202200	-0.32226500
H	4.33265500	2.21449900	0.75271200
H	2.13989300	3.83739100	-1.54021300
H	2.52744800	2.45058800	-2.53850400
H	0.91749300	2.62801800	-1.83617800
C	4.01419400	-0.57771300	0.83429000
C	4.81840600	-1.11987300	-0.34367800
H	4.57817900	-2.14866000	-0.59381000
H	4.67591200	-0.50359800	-1.22344500
H	5.87423400	-1.09381300	-0.08701900
C	4.13833600	-1.47779400	2.05446800
H	3.57314200	-1.08434600	2.89523400
H	3.81303500	-2.49717700	1.86111700
H	5.18102200	-1.52869600	2.35243000
H	4.49237600	0.35241100	1.11089000
C	-1.28087500	-0.46174600	-1.27943900
C	-1.04206300	-1.31341300	1.04211200
H	-1.05805300	-1.62507700	2.07860200
H	-1.44923800	-0.02715900	-2.25028600
N	-2.13993000	-0.32035700	0.89170200
N	-2.36596200	0.03476000	-0.37963300
C	-1.41111900	-2.47993900	0.13589400
H	-0.73709600	-3.30946600	0.30354900
H	-2.39991500	-2.82632100	0.42087000
C	-1.39486100	-1.98780400	-1.31421900
H	-0.57198600	-2.40400400	-1.87523100
H	-2.29963800	-2.27919700	-1.83637700
C	-3.77058900	0.27694600	-0.92236100
C	-3.72120600	0.33122700	-2.44882200
C	-4.34301400	1.61191300	-0.45904000
C	-4.66994300	-0.88350300	-0.49982800
H	-3.38011700	-0.59264200	-2.90086400

H	-3.11768200	1.15687600	-2.81316800
H	-4.73439500	0.49791600	-2.79763300
H	-4.57604900	1.63647400	0.59453900
H	-5.27335100	1.78330400	-0.99062600
H	-3.67159000	2.43060000	-0.69609500
H	-5.67411500	-0.70032600	-0.86911300
H	-4.72647100	-0.98963500	0.57546400
H	-4.33039400	-1.82395500	-0.92127000
C	-2.46351600	0.47276900	2.12047600
C	-2.19248300	1.96338800	1.99454200
C	-3.80403600	0.12657800	2.75235700
H	-1.71289900	0.09823900	2.80594800
H	-1.21132300	2.14922700	1.57394500
H	-2.20405500	2.38434100	2.99560300
H	-2.92701600	2.49571900	1.41021000
H	-3.92759900	-0.94796700	2.84711400
H	-4.65499600	0.52664700	2.21630400
H	-3.82386200	0.54909800	3.75236500

sBI4T^{+} TD-MPW1K/6-31G* Calculation -1160.69631311 Dipole Moment -8.0075 -0.8900 0.5380 Excitation energy 1.7666 eV

C	0.24862100	-0.55407500	0.69573000
H	0.36018000	0.21731900	1.45070900
C	0.02199400	0.09611200	-0.67792200
H	-0.17722800	1.15342500	-0.55227300
C	1.36373200	0.00932400	-1.44776700
C	1.60483400	-1.27701300	0.68090500
H	1.74850900	-1.78159600	1.62837500
H	1.30846300	0.58156500	-2.36288900
N	2.60058100	-0.20151800	0.59503400
N	2.42038800	0.57883300	-0.61020300
C	1.76720200	-2.25097200	-0.48951000
H	0.98868000	-3.00260900	-0.50076200
H	2.69170500	-2.79964400	-0.36747600
C	1.78369500	-1.41785900	-1.77845000
H	1.15159900	-1.83808700	-2.55402700
H	2.78229300	-1.37011900	-2.19543600
C	2.48020300	2.05569200	-0.40084400
C	1.71186400	2.56489500	0.81969800
C	3.94640800	2.47343200	-0.22593300
C	1.97951000	2.77047800	-1.65633600
H	0.63576800	2.52924000	0.67794800
H	1.97137400	1.98639800	1.69917300
H	1.97086600	3.60304500	1.00826700
H	4.57192200	2.01141200	-0.98264700

H	4.03500500	3.55202200	-0.32226500
H	4.33265500	2.21449900	0.75271200
H	2.13989300	3.83739100	-1.54021300
H	2.52744800	2.45058800	-2.53850400
H	0.91749300	2.62801800	-1.83617800
C	4.01419400	-0.57771300	0.83429000
C	4.81840600	-1.11987300	-0.34367800
H	4.57817900	-2.14866000	-0.59381000
H	4.67591200	-0.50359800	-1.22344500
H	5.87423400	-1.09381300	-0.08701900
C	4.13833600	-1.47779400	2.05446800
H	3.57314200	-1.08434600	2.89523400
H	3.81303500	-2.49717700	1.86111700
H	5.18102200	-1.52869600	2.35243000
H	4.49237600	0.35241100	1.11089000
C	-1.28087500	-0.46174600	-1.27943900
C	-1.04206300	-1.31341300	1.04211200
H	-1.05805300	-1.62507700	2.07860200
H	-1.44923800	-0.02715900	-2.25028600
N	-2.13993000	-0.32035700	0.89170200
N	-2.36596200	0.03476000	-0.37963300
C	-1.41111900	-2.47993900	0.13589400
H	-0.73709600	-3.30946600	0.30354900
H	-2.39991500	-2.82632100	0.42087000
C	-1.39486100	-1.98780400	-1.31421900
H	-0.57198600	-2.40400400	-1.87523100
H	-2.29963800	-2.27919700	-1.83637700
C	-3.77058900	0.27694600	-0.92236100
C	-3.72120600	0.33122700	-2.44882200
C	-4.34301400	1.61191300	-0.45904000
C	-4.66994300	-0.88350300	-0.49982800
H	-3.38011700	-0.59264200	-2.90086400
H	-3.11768200	1.15687600	-2.81316800
H	-4.73439500	0.49791600	-2.79763300
H	-4.57604900	1.63647400	0.59453900
H	-5.27335100	1.78330400	-0.99062600
H	-3.67159000	2.43060000	-0.69609500
H	-5.67411500	-0.70032600	-0.86911300
H	-4.72647100	-0.98963500	0.57546400
H	-4.33039400	-1.82395500	-0.92127000
C	-2.46351600	0.47276900	2.12047600
C	-2.19248300	1.96338800	1.99454200
C	-3.80403600	0.12657800	2.75235700
H	-1.71289900	0.09823900	2.80594800
H	-1.21132300	2.14922700	1.57394500

H	-2.20405500	2.38434100	2.99560300
H	-2.92701600	2.49571900	1.41021000
H	-3.92759900	-0.94796700	2.84711400
H	-4.65499600	0.52664700	2.21630400
H	-3.82386200	0.54909800	3.75236500

sBI4T(X=PH_2)$^+$ TD-MPW1K/6-31G* Dipole Moment -7.6800 1.2475 1.3363 Excitation energy 1.9021 eV

C	-1.43134300	-1.05658000	-0.10694700
C	-1.24102800	1.44830600	-0.24200900
H	-1.26347000	2.53016600	-0.22688600
H	-1.61943100	-2.11391600	0.02735200
C	-0.01487700	0.89785000	0.50548500
H	-0.15785100	1.21697500	1.53451600
C	-0.06295500	-0.64498200	0.45844900
H	-0.02024900	-1.03164300	1.47298200
N	-2.38899700	0.98465300	0.57886600
N	-2.42936400	-0.34050400	0.72552700
C	1.22426700	-1.15928200	-0.20836400
C	1.42081300	1.33246100	0.13452800
H	1.56426600	2.39020300	0.33425500
H	1.19396200	-2.24172900	-0.29868100
N	2.33349600	0.59323700	1.00949400
N	2.27859200	-0.83351900	0.76047900
C	-1.71919200	-0.61924000	-1.53997800
H	-1.10890400	-1.18800000	-2.22886700
H	-2.75160800	-0.86412100	-1.76956600
C	1.82124400	0.99603400	-1.29502800
H	2.88054500	1.20922500	-1.39001800
H	1.31131500	1.63925400	-2.00498100
C	1.54491200	-0.49556900	-1.55275200
H	2.42435700	-0.97066000	-1.97494000
H	0.75671500	-0.64583300	-2.27911200
C	-1.47707700	0.89416600	-1.64893600
H	-2.33480700	1.39285200	-2.08909000
H	-0.62816400	1.12587600	-2.27684100
P	-3.71187600	2.00577700	1.20578700
H	-2.94277700	2.67472000	2.17529300
H	-3.52740900	2.98465300	0.21681800
P	-3.39219500	-1.06790100	2.03505800
H	-4.09731900	-1.96241700	1.21264100
H	-2.39699400	-1.99184100	2.39357500
P	2.13744900	0.83310200	2.75261200
H	3.36519300	0.25717500	3.11637100
H	2.63591300	2.15352700	2.77205100

P	3.91624900	-1.35482800	0.30537700
H	4.46375500	-1.19549900	1.59061100
H	3.66335300	-2.73269100	0.48685700

sBI4T(X=SH)$^{+}$ TD-MPW1K/6-31G* Dipole Moment -7.9881 1.2622 1.1574 Excitation energy 1.6419 eV

C	-1.36751500	-1.06949000	-0.13843800
C	-1.19396200	1.44882300	-0.20156000
H	-1.24060900	2.52807400	-0.14690300
H	-1.55515000	-2.12831300	-0.02352000
C	0.03899200	0.88343600	0.52115200
H	-0.07704800	1.19663400	1.55500500
C	-0.00661800	-0.65923400	0.44553400
H	0.02839700	-1.07141100	1.45019800
N	-2.32763400	0.94788200	0.62570300
N	-2.38535700	-0.38154000	0.70465100
C	1.28242500	-1.16196700	-0.22803000
C	1.46371600	1.32737200	0.12944100
H	1.61026700	2.37928500	0.34169600
H	1.26872200	-2.24229300	-0.31347300
N	2.38658300	0.58215400	0.99076700
N	2.32970500	-0.82672100	0.74885400
C	-1.65985600	-0.58714900	-1.55603700
H	-1.03912500	-1.12764100	-2.25770100
H	-2.68715400	-0.84033600	-1.79853000
C	1.86441100	0.99903800	-1.30218500
H	2.91877100	1.23456400	-1.39929400
H	1.34311500	1.63850800	-2.00658400
C	1.61372200	-0.49584700	-1.56497100
H	2.50404200	-0.96991700	-1.96476600
H	0.84151300	-0.65658900	-2.30649000
C	-1.43815100	0.93199600	-1.62072100
H	-2.30435000	1.43536000	-2.03816600
H	-0.59659300	1.19323900	-2.24696100
S	-3.69518800	1.91253100	1.01922100
H	-3.26194700	2.28840900	2.22785200
S	-3.12313700	-1.14391500	2.06077700
H	-4.25301300	-1.48361600	1.43103800
S	2.33534000	0.96878600	2.66964700
H	3.58611600	1.42698400	2.75915100
S	3.87999400	-1.50652700	0.40904600
H	3.98749600	-2.19186000	1.54997000

sBI4T(X=NH$_2$)$^{+}$ TD-MPW1K/6-31G* Dipole Moment -8.3094 1.4180 1.7579 Excitation energy 2.2369 eV

C	-1.40591100	-0.84833100	-0.21036400
C	-1.19303600	1.65053500	0.07272400
H	-1.21987900	2.71356600	0.28138100
H	-1.61673200	-1.90977600	-0.26592000
C	0.08550800	0.98237200	0.60215400
H	0.15688000	1.29080800	1.64163000
C	-0.10867900	-0.55234400	0.55657000
H	-0.25951600	-0.91172600	1.57248000
N	-2.25833800	1.03250900	0.89000400
N	-2.50848800	-0.26031700	0.59045500
C	1.22355000	-1.18126100	0.13221700
C	1.45570700	1.30472400	-0.03184700
H	1.63267100	2.37505700	-0.04820100
H	1.18683600	-2.25574400	0.27889200
N	2.49767400	0.71896800	0.81790500
N	2.16715700	-0.65761200	1.13477900
C	-1.53414100	-0.17797700	-1.57996900
H	-0.72215600	-0.48579800	-2.22223200
H	-2.45349400	-0.51187600	-2.04786000
C	1.68166300	0.70093700	-1.41526600
H	2.64705900	1.04863900	-1.76441000
H	0.94855500	1.04514500	-2.13433300
C	1.68173300	-0.83029400	-1.27881900
H	2.68542900	-1.21949200	-1.42066500
H	1.07534700	-1.32152100	-2.03257400
C	-1.55601800	1.34724700	-1.37886700
H	-2.54433100	1.75243600	-1.57213300
H	-0.87147200	1.86384800	-2.03890100
H	-3.90304100	1.17322400	1.90109500
H	-2.97520500	2.56206400	1.86092700
H	-3.83138200	-1.54912300	1.25162300
H	-2.47485600	-1.44147900	2.19644700
H	1.95998000	1.80394500	2.43906500
H	3.48329500	2.06675900	1.84527400
H	3.24480300	-2.11084900	1.89673700
H	3.71391100	-1.69763300	0.36106800
N	-3.30801200	1.76711600	1.33805700
N	-3.13595300	-0.92746200	1.62954400
N	2.76995400	1.37950200	2.00885800
N	3.36516900	-1.35616000	1.24570400

sBI4T(X=OH)$^{+}$ TD-MPW1K/6-31G* Dipole Moment -6.8609 0.7993 1.3914 Excitation energy 2.1380 eV

C	-1.33480700	-1.00538400	-0.32314000
C	-1.23828900	1.50088700	0.03933300

H	-1.33168800	2.54666300	0.30080400
H	-1.51363700	-2.07075000	-0.38865900
C	0.07004000	0.87338500	0.54345600
H	0.15355600	1.15695800	1.58632000
C	-0.04881200	-0.66633700	0.45131000
H	-0.18312600	-1.07406500	1.44930700
N	-2.25956600	0.79484900	0.84865200
N	-2.44050500	-0.46457000	0.50167500
C	1.28960300	-1.22843500	-0.04129200
C	1.42109800	1.27708000	-0.07557000
H	1.56613400	2.34924000	-0.02663000
H	1.30919600	-2.30619000	0.06370300
N	2.45305800	0.68518100	0.78189100
N	2.25002100	-0.70990200	0.94640700
C	-1.51116600	-0.28922800	-1.66817500
H	-0.69162900	-0.54805700	-2.32109200
H	-2.41748600	-0.64783300	-2.14367300
C	1.70489700	0.74421500	-1.47782500
H	2.67191100	1.12803100	-1.78278200
H	0.98419200	1.12432100	-2.19169400
C	1.72783500	-0.79267000	-1.43275300
H	2.73641300	-1.16202700	-1.57482300
H	1.12657100	-1.24992400	-2.21057700
C	-1.58800700	1.22828800	-1.42206900
H	-2.58795700	1.60546100	-1.61298900
H	-0.91778600	1.78513800	-2.06338600
O	-3.38761700	1.43669800	1.23493000
H	-3.31225400	1.58184200	2.18673100
O	-2.97307500	-1.22932000	1.49024300
H	-3.84924500	-1.49821900	1.18770000
O	2.33272600	1.27388300	2.05141900
H	3.22472800	1.56042700	2.25404000
O	3.47250500	-1.34252400	0.68664300
H	3.75038800	-1.66578900	1.54506900

sBI4T(X=Cl)$^{+}$ TD-MPW1K/6-31G* Dipole Moment -8.4839 1.4401 -1.9980 Excitation energy 1.9664 eV

C	-1.36000300	-1.07737900	-0.15714900
C	-1.18664400	1.45284600	-0.15320800
H	-1.24217500	2.52896800	-0.05518000
H	-1.56109400	-2.13629400	-0.06497300
C	0.04902200	0.86541200	0.54551900
H	-0.04696300	1.15747500	1.58543000
C	-0.00779900	-0.67578300	0.44893700
H	0.01692100	-1.09581300	1.45018900

N	-2.29455600	0.91209400	0.69449600
N	-2.39475500	-0.39706300	0.68091000
C	1.28373000	-1.17359000	-0.22310300
C	1.46342500	1.31395300	0.13070200
H	1.62417000	2.36135400	0.35270000
H	1.28659900	-2.25481700	-0.29147500
N	2.42597700	0.55848500	0.94739600
N	2.29962500	-0.81899500	0.78765800
C	-1.65951900	-0.55302800	-1.55910100
H	-1.02932800	-1.06351500	-2.27409200
H	-2.68182900	-0.81481900	-1.81037500
C	1.85587700	0.98689500	-1.30444300
H	2.90547100	1.23600300	-1.41330400
H	1.31753100	1.61874000	-2.00176500
C	1.62596000	-0.51185200	-1.55711200
H	2.52653600	-0.97447200	-1.94259100
H	0.85993600	-0.69062300	-2.29993400
C	-1.46101200	0.97195600	-1.57857900
H	-2.34430200	1.47381100	-1.95975600
H	-0.63829500	1.26655800	-2.21520500
Cl	-3.67433800	1.83502900	1.03281300
Cl	-3.06891600	-1.17624700	2.02994800
Cl	2.30095100	0.96591700	2.65621000
Cl	3.85900400	-1.51291400	0.38690600

sBI4T(X=F)$^{+}$ TD-MPW1K/6-31G* Dipole Moment -7.0849 1.2036 -3.7362 Excitation energy 2.1441 eV

C	-1.32967600	-1.01588200	-0.32386600
C	-1.23321500	1.50179300	0.05037300
H	-1.33668700	2.54231800	0.33054800
H	-1.52536100	-2.07882000	-0.38700200
C	0.07188800	0.86677100	0.55597500
H	0.15654000	1.14406000	1.59960400
C	-0.04720200	-0.67555500	0.45648000
H	-0.18099400	-1.08709900	1.45302600
N	-2.24112000	0.77327200	0.86377500
N	-2.43499200	-0.46051300	0.49518700
C	1.29141000	-1.23324500	-0.04337500
C	1.41935600	1.27731100	-0.06783000
H	1.57896500	2.34591500	-0.00348800
H	1.32730100	-2.30882300	0.07378200
N	2.45606400	0.65956400	0.76664100
N	2.23131100	-0.68990400	0.95363200
C	-1.51533300	-0.28800300	-1.66290900
H	-0.69553500	-0.54475800	-2.31634700
H	-2.42152700	-0.64658500	-2.13736100

C	1.70508000	0.74875200	-1.47254700
H	2.66938300	1.13724700	-1.77924800
H	0.98173700	1.13079300	-2.18163700
C	1.73292200	-0.78913900	-1.43045200
H	2.74298500	-1.15385500	-1.57129600
H	1.13680700	-1.24820000	-2.21022900
C	-1.59323800	1.22930300	-1.40957000
H	-2.59454500	1.60565700	-1.59406100
H	-0.92781700	1.79205500	-2.05051400
F	-3.36492300	1.41438200	1.20589000
F	-2.94038700	-1.23241100	1.46939400
F	2.31870700	1.23846800	2.03288000
F	3.44469100	-1.31556800	0.68713600

sBI4T(X=NHCH$_3$)$^+$ TD-MPW1K/6-31G* Dipole Moment -7.1990 1.4136 2.8374
Excitation energy 2.2585 eV

C	-1.20624100	-0.91528100	-0.06959100
C	-1.17854800	1.59339100	0.12943300
H	-1.26005500	2.65855700	0.31123700
H	-1.33668100	-1.99031300	-0.07783600
C	0.17201400	1.04737800	0.62290500
H	0.25033400	1.38111900	1.64762200
C	0.10549700	-0.49603800	0.61545100
H	0.03536400	-0.84349200	1.64094500
N	-2.17778200	0.94370800	1.01200800
N	-2.29214400	-0.36996600	0.77485600
C	1.45944800	-1.01995300	0.12970400
C	1.48437400	1.47629700	-0.07619200
H	1.57082700	2.55768600	-0.10447800
H	1.51784300	-2.09243000	0.28491300
N	2.63913600	0.97064600	0.67786700
N	2.40680500	-0.40583200	1.08392700
C	-1.45122700	-0.30384900	-1.45367000
H	-0.64862100	-0.57476300	-2.12436600
H	-2.36227700	-0.72164700	-1.86872300
C	1.67376000	0.87441600	-1.46820600
H	2.57943500	1.29806700	-1.88611300
H	0.86941600	1.13202700	-2.14571100
C	1.82416300	-0.64793600	-1.30464200
H	2.85320900	-0.94290400	-1.48492500
H	1.23567500	-1.20888500	-2.02341900
C	-1.57660900	1.22115900	-1.29799900
H	-2.60114000	1.54158200	-1.46523300
H	-0.96617100	1.76345700	-2.00723300
H	-3.31328600	2.51001400	1.00304900

H	-3.83400900	-1.52346000	1.05982100
H	3.87449300	2.28263600	1.42953100
H	3.96966000	-1.33676500	0.23858400
N	-3.29666800	1.61365600	1.46069200
N	-3.11553200	-1.08250900	1.60990600
N	3.13162400	1.69114300	1.74599400
N	3.64547400	-1.03777400	1.14758200
C	3.67314200	-2.09446100	2.12573300
H	2.95160300	-2.90016400	1.95290900
H	4.66686100	-2.53050800	2.12757300
H	3.48234300	-1.66928200	3.10439900
C	-2.44872700	-1.99640500	2.52615200
H	-1.83741700	-2.75272000	2.03657000
H	-1.83201900	-1.43007600	3.21500900
H	-3.22392000	-2.49535600	3.09554300
C	-3.37916500	1.75457200	2.91288700
H	-4.25529500	2.35752200	3.11910000
H	-3.52306300	0.77828700	3.35314100
H	-2.50297800	2.23395200	3.34468800
C	2.26766300	2.29278600	2.72581900
H	1.57017500	3.04455000	2.33951500
H	1.70438000	1.52164200	3.24428300
H	2.89774500	2.78134800	3.46165100

sBI4T(X=N(CH$_3$)$_2$)$^+$ TD-MPW1K/6-31G* Dipole Moment -6.7568 0.6048 2.9147 Excitation energy 2.2961 eV

C	-1.04147000	-0.96366500	-0.23644500
C	-0.91629700	1.47349100	0.38173100
H	-0.97824700	2.49905700	0.72394700
H	-1.21334700	-2.01446800	-0.43450500
C	0.35711000	0.77818100	0.89375900
H	0.35304300	0.94227700	1.96088000
C	0.21037100	-0.73884000	0.63474200
H	0.00818100	-1.23242800	1.57866200
N	-2.02486100	0.74513600	1.04849600
N	-2.17967300	-0.50388600	0.59797900
C	1.59150200	-1.26343000	0.21775900
C	1.74764300	1.22932700	0.38820300
H	1.88292500	2.29641500	0.53362300
H	1.59882500	-2.34867900	0.21540600
N	2.81370900	0.54871100	1.15241100
N	2.42311700	-0.83149800	1.36627200
C	-1.12516000	-0.12320400	-1.51501400
H	-0.28237300	-0.34001000	-2.15447700
H	-2.01626600	-0.40646400	-2.06549600

C	2.04206300	0.83104500	-1.05635400
H	3.00911500	1.24454500	-1.31753900
H	1.32853100	1.24697300	-1.75614900
C	2.08533200	-0.70596600	-1.11661000
H	3.09521000	-1.04590800	-1.29235900
H	1.49750800	-1.10794100	-1.93600200
C	-1.17626700	1.36236700	-1.11975500
H	-2.15185700	1.78540000	-1.33586900
H	-0.45816500	1.96029200	-1.66447000
C	-3.89257600	2.18714200	0.95066600
H	-3.38504000	3.09177600	0.61034800
H	-4.26196800	1.63476600	0.09453000
H	-4.74236900	2.47736100	1.55698000
C	-2.55139200	-2.18575000	2.21979300
H	-1.89572900	-2.95810800	1.81353700
H	-2.00690700	-1.59485900	2.94675000
H	-3.37799400	-2.66818400	2.72776600
C	3.21353300	-2.68222400	2.54750600
H	2.62790700	-2.30782700	3.37883700
H	2.65128600	-3.48715000	2.05650200
H	4.13000600	-3.11610000	2.93531700
C	2.28126300	1.45630200	3.35795100
H	1.65225000	0.59772500	3.56840500
H	2.81735800	1.69975500	4.26952500
H	1.65215900	2.32088500	3.10880100
C	-2.57721100	1.91787600	2.99670700
H	-2.02258800	1.18100500	3.56535400
H	-1.95371000	2.80156100	2.84487300
H	-3.44646300	2.20988100	3.57406700
C	-3.95968500	-1.97568300	0.22946000
H	-4.76672800	-2.45650300	0.76953900
H	-4.38961600	-1.23966600	-0.43944200
H	-3.43848700	-2.73620800	-0.35584200
C	4.26217400	2.10162300	2.11822000
H	5.00883800	1.69364600	1.44844300
H	3.87939300	3.03517700	1.68749400
H	4.73703100	2.34684000	3.06332500
C	4.48128400	-1.91469400	0.62666600
H	4.75553800	-1.01032900	0.09616100
H	5.37959000	-2.31418100	1.08614900
H	4.11580900	-2.66055600	-0.08806600
N	-3.11197900	-1.31188300	1.20201700
N	-3.04877500	1.32310200	1.75972500
N	3.24626900	1.10939000	2.34807100
N	3.54727400	-1.58976900	1.67615800

sBI4T(X=PHCH$_3$)$^+$ TD-MPW1K/6-31G* Dipole Moment -6.3867 1.3617 3.7809
Excitation energy 1.9594 eV

C	-1.32780400	-1.05436600	-0.09205000
C	-1.21382600	1.44739700	-0.30647000
H	-1.26238000	2.52843300	-0.32622700
H	-1.48398800	-2.11263100	0.07451500
C	0.02700900	0.95340900	0.45578200
H	-0.13347200	1.28542700	1.47788200
C	0.03443700	-0.58821100	0.44230700
H	0.10653200	-0.94733000	1.46450400
N	-2.35133800	0.97999900	0.52390300
N	-2.34214000	-0.34035500	0.71786200
C	1.32628800	-1.07462800	-0.23525200
C	1.45090300	1.42201100	0.08714100
H	1.56369400	2.48619400	0.27131800
H	1.32138300	-2.15734600	-0.31621100
N	2.37800000	0.71508900	0.97913600
N	2.39876100	-0.70797800	0.70261100
C	-1.63346600	-0.67257000	-1.53853300
H	-1.01019200	-1.24525300	-2.21282400
H	-2.65998900	-0.95232000	-1.75453000
C	1.86121300	1.08419700	-1.33920600
H	2.91609900	1.31711200	-1.43623300
H	1.33595300	1.71259700	-2.05173400
C	1.61326000	-0.41367800	-1.58883300
H	2.49715400	-0.87227000	-2.02059100
H	0.82084500	-0.58367400	-2.30607200
C	-1.43417600	0.84340700	-1.69633900
H	-2.30700500	1.30302900	-2.14949600
H	-0.59335100	1.08007300	-2.33345600
P	-3.80239000	1.95710700	0.94525500
H	-3.42077300	2.97671100	0.05785200
P	-3.41335700	-1.04483600	1.95037000
H	-3.90967400	-2.06365200	1.12082200
P	2.12716100	0.95972300	2.71912500
H	3.27178500	0.25433100	3.10999000
P	4.03604700	-1.17766000	0.19495200
H	3.64521400	-2.47909000	-0.19061400
C	-3.24299000	2.76858400	2.49615900
H	-2.22528100	3.14029700	2.45308900
H	-3.91157000	3.60753300	2.67593100
H	-3.34585100	2.08113300	3.32875900
C	-2.21567200	-2.03818300	2.92325100
H	-1.59608300	-2.70449400	2.33385100
H	-1.58491000	-1.38169300	3.51361200

H	-2.80208400	-2.64107700	3.61307400
C	2.83708400	2.65200400	2.88009400
H	3.06777000	2.83259000	3.92675800
H	3.74242500	2.76239500	2.29233300
H	2.11930600	3.40734300	2.57424000
C	4.78324600	-1.67267100	1.80274300
H	5.15285600	-0.80148000	2.33273000
H	4.08895100	-2.21485600	2.43565500
H	5.63943600	-2.30766800	1.58649400

sBI4T(X=PH(CH$_3$)$_2$)$^+$ TD-MPW1K/6-31G* Dipole Moment -6.7926 1.1911 3.1149
Excitation energy 2.1474 eV

C	-1.31831800	-1.05944600	-0.03402400
C	-1.08446600	1.42830300	-0.27058400
H	-1.07425000	2.50940500	-0.29945500
H	-1.52463900	-2.10889100	0.13037500
C	0.11722200	0.88096400	0.52160800
H	-0.06841800	1.21731700	1.53758200
C	0.06224700	-0.65741100	0.50764000
H	0.11469800	-1.01768400	1.52933900
N	-2.25638500	1.02121000	0.53873800
N	-2.29907500	-0.29359000	0.76844900
C	1.33232800	-1.19869500	-0.16650700
C	1.57518200	1.27818900	0.20477400
H	1.74087500	2.33067300	0.40066700
H	1.26054900	-2.27554800	-0.26793800
N	2.42666100	0.50446000	1.13199700
N	2.43510500	-0.90599000	0.77725800
C	-1.59092500	-0.67377800	-1.48680300
H	-0.99581700	-1.28897500	-2.14956800
H	-2.63022800	-0.89680400	-1.70797900
C	1.99434800	0.94169800	-1.21797600
H	3.06431900	1.10208300	-1.29429900
H	1.52338700	1.62223200	-1.92147900
C	1.64880400	-0.52625600	-1.50822400
H	2.49639300	-1.02169200	-1.96915600
H	0.83761000	-0.62628200	-2.21636000
C	-1.30445300	0.82611300	-1.66045600
H	-2.14006600	1.32575100	-2.13885700
H	-0.43792600	1.00901800	-2.28049000
P	-3.64557000	2.05142700	1.05220900
P	-3.29439200	-0.91098000	2.13839600
P	1.99575900	0.70103200	2.85451900
P	4.04489600	-1.35800600	0.11931400
C	-3.69835400	3.22650600	-0.35606600

H	-2.78386200	3.78270600	-0.53569000
H	-4.00404300	2.71921900	-1.26516700
H	-4.47958400	3.94402000	-0.11433400
C	-2.11867800	-2.11352000	2.87083800
H	-1.74721600	-2.86907800	2.18577000
H	-1.28477000	-1.59535700	3.33313200
H	-2.66472400	-2.62138800	3.66305500
C	3.67775900	-3.11967000	-0.30099000
H	3.12156600	-3.21699900	-1.22760700
H	4.63014300	-3.62180600	-0.44718100
H	3.14339500	-3.63105400	0.49644100
C	2.09928400	2.54250200	2.95272100
H	1.22225800	3.03044200	2.53844300
H	2.15127200	2.81435300	4.00342800
H	2.98739900	2.92514600	2.45589000
C	-2.80658900	3.07432700	2.32154600
H	-2.59835600	2.47266700	3.20012000
H	-1.88700900	3.53488700	1.97134100
H	-3.49261900	3.86438400	2.61708800
C	-4.40572500	-2.02958000	1.20446000
H	-4.98793800	-2.59852500	1.92506600
H	-5.10010600	-1.44579500	0.60908600
H	-3.87948500	-2.73134600	0.56338000
C	3.56805200	0.35188500	3.72382100
H	3.76429900	-0.71055500	3.76826900
H	4.41467200	0.86597800	3.27928000
H	3.44155300	0.70292000	4.74564000
C	5.01808800	-1.71666700	1.63204300
H	5.36308600	-0.80777400	2.10588400
H	4.47760500	-2.32681500	2.34986800
H	5.89990400	-2.26317600	1.30472700

The linear reaction coordinate energy profile:

