

Supplementary Information for

The Effect of Nitro Groups on N₂ Extrusion from Aromatic Azide-Based Energetic

Materials

Ashley L. Shoaf and Craig A. Bayse*

Department of Chemistry and Biochemistry, Old Dominion University

Norfolk, Virginia 23529, United States

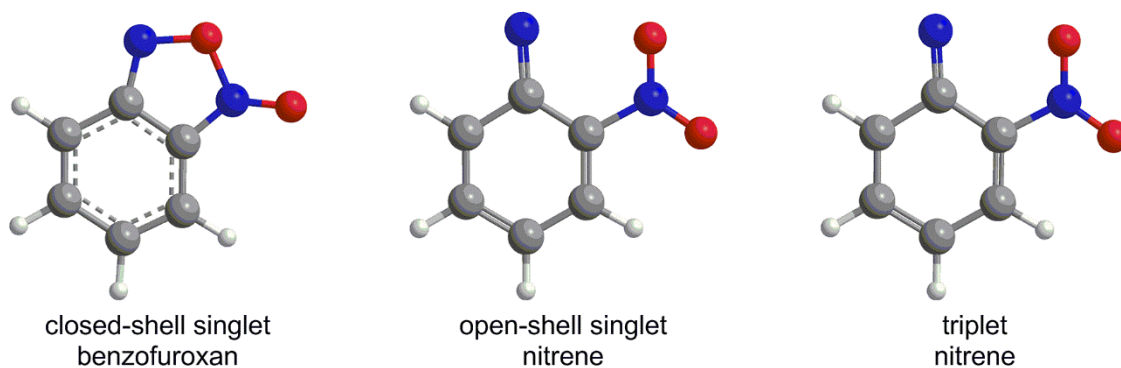


Figure S1. DFT(M06-2X)/TZVP structures of *o*-NAzB from nitrene optimization.

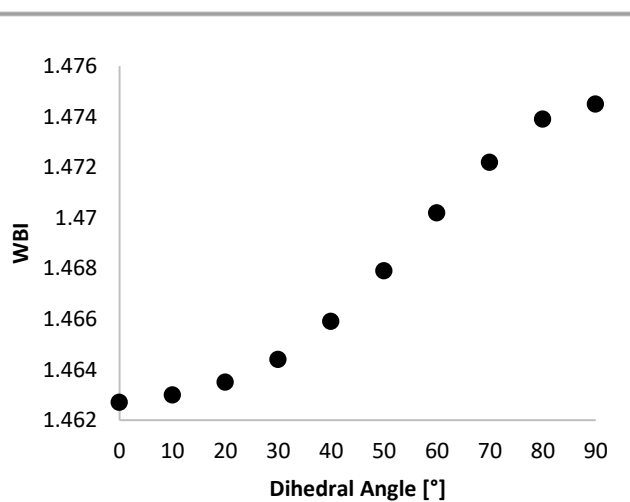


Figure S2. N-N₂ bond deactivation represented by increasing WBIs at larger dihedral angles in AzB.

Cartesian coordinates for the structures (i.e., reactants, transition states and products) for the simple azides and aromatic azide-based energetic materials in the gas phase.

NB

```
1\1\GINC-COREV2-25-011\Freq\RM062X\TZVP\C6H5N1O2\ASHOA001\02-Dec-2016\
0\#N Geom=AllCheck Guess=TChech SCRF=Check Test GenChk RM062X/TZVP Fr
eq\CSD ENTRY NITRBE01\0,1\N,1.3658186328,4.7721528071,2.4640381262\O
,1.6370847874,4.5300818444,3.6198033243\O,1.5925253092,5.8228662761,1.
9049620696\C,0.7084241305,3.7043786284,1.6761096097\C,0.3904587047,3.9
581432737,0.3533868182\H,0.6242042155,4.9205919031,-0.0787152544\C,-0.
2249308441,2.9527453678,-0.3772845228\H,-0.4839179913,3.1257870941,-1.
4134015206\C,-0.5074597737,1.7294295639,0.2187129086\H,-0.9879810412,0
.9490152215,-0.3571622095\C,-0.1771161635,1.5015905476,1.5493247391\H,
-0.3989314388,0.5477910603,2.0091644696\C,0.4387368667,2.4960535903,2.
2944382686\H,0.709084606,2.3523728217,3.3306231734\Version=AM64L-G09R
evB.01\State=1-A\HF=-436.7149739\
```

AzB

```
1\1\GINC-COREV2-25-001\Freq\RM062X\TZVP\C6H5N3\ASHOA001\02-May-2017\0\
\#N Geom=AllCheck Guess=TChech SCRF=Check Test GenChk RM062X/TZVP Freq
\test\0,1\C,-2.1184594373,-1.3923101536,0.\C,-2.3615249345,-0.022990
895,0.\C,-1.309510439,0.8772350289,0.\C,0.0001158275,0.4064111168,0.\C
,0.2535855117,-0.9628810826,0.\C,-0.8099986284,-1.8547265571,0.\H,-2.9
433890721,-2.0922670051,0.\H,-3.3787402695,0.3472433716,0.\H,-1.479089
5349,1.9457231909,0.\H,1.2711088855,-1.3360133247,0.\H,-0.6098251339,-
2.9186183284,0.\N,1.0183568241,1.3969762476,0.\N,2.1774351699,0.990210
7729,0.\N,3.2636982308,0.7206526179,0.\Version=AM64L-G09RevB.01\State
=1-A\HF=-395.798574\
```

AzB closed-shell singlet nitrene

```
1\1\GINC-COREV3-23-015\Freq\RM062X\TZVP\C6H5N1\ASHOA001\27-Jun-2018\0\
\#N Geom=AllCheck Guess=TChech SCRF=Check Test GenChk RM062X/TZVP Freq
\Title Card Required\0,1\C,0.,0.,-1.7624796449\C,0.,-1.1889810652,-1
.0478051253\C,0.,-1.2301089383,0.3313744903\C,0.,0.,1.0592382068\C,0.,
1.2301089383,0.3313744903\C,0.,1.1889810652,-1.0478051253\H,0.,0.,-2.8
42121629\H,0.,-2.1375211578,-1.571696497\H,0.,-2.161726374,0.873961317
\H,0.,2.161726374,0.873961317\H,0.,2.1375211578,-1.571696497\N,0.,0.,2
.3553054673\Version=ES64L-G09RevD.01\State=1-A1\HF=-286.1942649\
```

AzB open-shell singlet nitrene

```
1\1\GINC-COREV2-22-018\Freq\UM062X\TZVP\C6H5N1\ASHOA001\27-Jun-2018\0\
\#N Geom=AllCheck Guess=TChech SCRF=Check Test GenChk UM062X/TZVP Freq
\Title Card Required\0,1\C,0.,0.,-1.7437916583\C,0.,-1.216099493,-1.
0459174209\C,0.,-1.2380053105,0.3230196595\C,0.,0.,1.0679571907\C,0.,1
```

.2380053105,0.3230196595\C,0.,1.216099493,-1.0459174209\H,0.,0.,-2.825
2664044\H,0.,-2.1478632856,-1.5967654552\H,0.,-2.1643601929,0.88108105
64\H,0.,2.1643601929,0.8810810564\H,0.,2.1478632856,-1.5967654552\N,0.
,0.,2.3598759586\\Version=ES64L-G09RevD.01\State=1-A2\HF=-286.2491474\
S2=1.031207\S2-1=0.\S2A=0.249497\

AzB triplet nitrene

1\1\GINC-COREV4-21-016\Freq\UM062X\TZVP\C6H5N1(3)\ASHOA001\27-Jun-2018
\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP F
req\\Title Card Required\\0,3\C,0.,0.,-1.745844939\C,0.,-1.2098076091,
-1.0509531616\C,0.,-1.2238440112,0.3271647473\C,0.,0.,1.0476162407\C,0
,1.2238440112,0.3271647473\C,0.,1.2098076091,-1.0509531616\H,0.,0.,-2
.8279233582\H,0.,-2.1442707217,-1.5973653016\H,0.,-2.1517666164,0.8840
102057\H,0.,2.1517666164,0.8840102057\H,0.,2.1442707217,-1.5973653016\
N,0.,0.,2.382049847\\Version=ES64L-G09RevD.01\State=3-A2\HF=-286.26810
11\S2=2.045423\S2-1=0.\S2A=2.000842\

AzB closed-shell singlet product

1\1\GINC-COREV4-21-010\Freq\RM062X\TZVP\C6H5N3\ASHOA001\22-Aug-2017\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq
\test\\0,1\C,-2.5756033722,-0.6775896959,0.\C,-2.4189503916,0.7059100
413,0.\C,-1.1871044258,1.3193371232,0.\C,-0.004609109,0.4900896864,0.\
C,-0.1652951205,-0.9082507634,0.\C,-1.4356724207,-1.4606510634,0.\H,-3
.5599714357,-1.1220408744,0.\H,-3.2895526841,1.3514259324,0.\H,-1.0927
883039,2.3942717724,0.\H,0.7206649077,-1.5239746754,0.\H,-1.5187411372
, -2.5407841726,0.\N,1.070888196,1.2320393049,0.\N,2.8958427607,-0.2236
450776,0.\N,3.9748575363,-0.354018538,0.\\Version=AM64L-G09RevB.01\Sta
te=1-A\HF=-395.7266919\

AzB open-shell singlet transition state

1\1\GINC-COREV2-22-028\Freq\UM062X\TZVP\C6H5N3\ASHOA001\29-Jun-2018\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Freq
\test\\0,1\C,2.5825396663,0.4210938804,-0.1468945359\C,2.2396898832,-
0.9197879712,-0.1718277404\C,0.9040976212,-1.2979711834,-0.0914252608\
C,-0.0906465834,-0.3345263816,0.1727171688\C,0.2797125003,1.0320972635
,0.2100089722\C,1.5902719884,1.3972302246,0.0121609404\H,3.6161099081,
0.7200782047,-0.2649475209\H,3.0028308846,-1.6739857812,-0.317137747\H
,0.601620817,-2.3330299859,-0.1765512283\H,-0.4900341143,1.7767992067,
0.3732452909\H,1.8637582399,2.4451099033,0.0110648613\N,-1.2775698819,
-0.8572516183,0.5608258414\N,-2.6475689888,0.110945029,-0.2441364672\N
, -3.7074619406,0.3697592103,-0.2304575746\\Version=AM64L-G09RevB.01\St
ate=1-A\HF=-395.7329506\S2=0.\S2-1=0.\S2A=0.\

AzB open-shell singlet product

1\1\GINC-COREV2-25-006\Freq\UM062X\TZVP\C6H5N3\ASHOA001\29-Jun-2018\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Freq

\\test\0,1\C,2.5350338612,0.5349651682,-0.295999592\C,2.343727367,-0.8489805589,-0.2857381498\C,1.1059600202,-1.3518385403,0.0478698586\C,0.0576619844,-0.485889569,0.5109546102\C,0.3284329864,0.9246766392,0.5409775276\C,1.52657358,1.4248867862,0.0830348796\H,3.4950283248,0.9301748603,-0.6086351605\H,3.1498094205,-1.5049245494,-0.5884364786\H,0.8854677993,-2.4118536508,0.0170716804\H,-0.468435036,1.5663033048,0.8968084434\H,1.7146411948,2.4906157069,0.0606814549\N,-1.1006812252,-0.9651289528,0.8937955822\N,-3.102869374,0.7010785357,-0.768710421\N,-3.9406849034,0.0140898199,-0.6794342349\\Version=AM64L-G09RevB.01\State=1-A\HF=-395.747436\S2=0.\S2-1=0.\S2A=0.\

AzB triplet product

1\1\GINC-COREV1-22-001\Freq\UM062X\TZVP\C6H5N3(3)\ASHOA001\27-Jul-2018\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Freq\\test\0,3\C,-2.2068796664,-1.4605354599,0.\C,-2.6155215893,-0.1263201949,0.\C,-1.6840731198,0.8893691441,0.\C,-0.2980634709,0.5788970078,0.\C,0.103924117,-0.78327592,0.\C,-0.8486834801,-1.7793126883,0.\H,-2.9465901836,-2.2504978789,0.\H,-3.6710568385,0.1141949867,0.\H,-1.981409535,1.9299741877,0.\H,1.1618268955,-1.0094607134,0.\H,-0.5395023687,-2.8168531664,0.\N,0.6127866228,1.554663078,0.\N,4.2695538258,1.0655147587,0.\N,3.6178987911,0.1955568586,0.\\Version=AM64L-G09RevB.01\State=3-A\HF=-395.7986259\S2=2.045229\S2-1=0.\S2A=2.000831\

o-NAzB

1\1\GINC-COREV4-21-001\Freq\RM062X\TZVP\C6H4N4O2\ASHOA001\07-May-2018\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq\\Title Card Required\0,1\C,2.034865022,-0.0381139185,-1.4610997199\C,2.4309150162,0.8963110912,-0.5125514991\C,1.8730775631,0.8552109784,0.7542705872\C,0.9508747675,-0.1277030153,1.0628117258\C,0.5260265838,-1.0663274949,0.1213653911\C,1.0881074007,-1.0012884493,-1.154684122\H,2.4601213949,-0.0143335074,-2.4560384111\H,3.1644318168,1.651762636,-0.7573605016\H,2.1414647639,1.5716241938,1.5186962434\H,0.77371786,-1.7065724764,-1.9144633847\N,0.4334118803,-0.1516427974,2.4434135177\O,0.3042381531,-1.2257397479,2.9805863456\O,0.2081258564,0.9240497703,2.9588046027\N,-0.476948621,-1.9787023969,0.4871014892\N,-0.8137274825,-2.7937006609,-0.3716634463\N,-1.1980762352,-3.5775131248,-1.068390718\Version=AM64L-G09RevB.01\State=1-A\HF=-600.285918\

o-NAzB closed-shell singlet transition state

1\1\GINC-COREV2-22-034\Freq\RM062X\TZVP\C6H4N4O2\ASHOA001\12-Dec-2017\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq\\test\0,1\C,2.4639448038,-1.5271832031,-0.0764370297\C,2.8456501312,-0.2154934657,-0.2931728331\C,1.8931455531,0.8044831033,-0.2620299477\C,0.5801933413,0.5038162948,0.0006586291\C,0.1317632113,-0.83511107358,0.2087297254\C,1.1222982711,-1.8373075551,0.1089347783\H,3.1983809643,-2.321658424,-0.1101237998\H,3.8805053934,0.0290904353,-0.4931464114

\H,2.1728592279,1.8382457925,-0.4143138802\H,0.7910523962,-2.859407316
1,0.2308163237\N,-0.3536581355,1.6319713126,0.0793466971\O,-1.49317222
21,1.4466709203,-0.2874478202\O,0.0787568514,2.6812464996,0.5058126821
\N,-0.9974127748,-1.2881997994,0.7958217672\N,-2.5312911595,-0.9283286
141,-0.2750127935\N,-3.6103638531,-0.986448245,-0.4088130874\\Version=
AM64L-G09RevB.01\State=1-A\HF=-600.2239628\

o-NAzB closed-shell singlet product

1\1\GINC-COREV2-25-049\Freq\RM062X\TZVP\C6H4N4O2\ASHOA001\13-Dec-2017\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\\test\0,1\C,2.5390765121,-1.137924527,0.1523927752\C,1.7175279659,
-1.6231868137,-0.8197777292\C,0.2873862626,-1.4316196751,-0.808245703\
C,-0.2947394162,-0.5704856895,0.0535108543\C,0.6513056412,0.200402705,
0.7912091992\C,2.0168059338,-0.2399077928,1.1657790498\H,3.5498726792,
-1.5218496855,0.2335890127\H,2.1151616282,-2.3009467853,-1.5631695445\
H,-0.344200647,-2.0131879429,-1.4688717719\H,2.3497240675,-0.297410430
9,2.1927520905\N,-1.7295407375,-0.4360810441,0.2264017278\O,-2.1002130
033,0.2716603609,1.1384489999\O,-2.4481975782,-1.0310213812,-0.5469322
037\N,1.4683765694,1.1353624128,0.7255252266\N,-0.8705714321,2.2662049
517,-0.9283825945\N,-0.8453314455,3.3222083377,-1.1843533892\\Version=
AM64L-G09RevB.01\State=1-A\HF=-600.2719525\

o-NAzB closed-shell singlet benzofuroxan

1\1\GINC-COREV2-22-003\Freq\RM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\\Title Card Required\0,1\C,0.1478831717,2.504285591,0.0607003547\C
,-1.2891967969,2.3906284601,-0.003725916\C,-1.9102129862,1.1849684666,
-0.0297017057\C,-1.0594767317,0.0537224223,0.0104195198\C,0.3544495708
,0.1378832647,0.0738520102\C,0.9708224414,1.4278247255,0.0995269948\H,
0.5762127367,3.4982407767,0.0784496978\H,-1.8768041001,3.2984215741,-0
.0315586653\H,-2.983540192,1.0650361575,-0.0772364051\H,2.046885962,1.
5164279442,0.1481551433\N,-1.3503274598,-1.2454329641,-0.0009472159\O,
-0.1404536995,-1.9328595363,0.0545083941\O,-2.3861238749,-1.8796801025
, -0.0470628447\N,0.8989519584,-1.0537267798,0.1002576381\\Version=ES64
L-G09RevD.01\State=1-A\HF=-490.7935269\

o-NAzB open-shell singlet nitrene

1\1\GINC-COREV3-23-030\Freq\UM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fr
eq\\Title Card Required\0,1\C,0.1217570109,2.5710412172,0.0493112985\
C,-1.263335159,2.3488363461,-0.0006966393\C,-1.7688247507,1.0471150924
, -0.0139765434\C,-0.9130168022,-0.0206534574,0.0218288718\C,0.52344772
82,0.14789819,0.0735587211\C,0.9946004745,1.5206099366,0.0857173371\H,
0.5019502715,3.5842080537,0.0593071549\H,-1.9473242003,3.1857135224,-0
.029274966\H,-2.8325246641,0.8566434723,-0.0520912662\H,2.0654951676,1
.6674055338,0.1244851311\N,-1.481444793,-1.372914059,0.0067373059\O,-0

.7094757534,-2.3041324872,0.0383243756\O,-2.6925717511,-1.4701840648,-
0.036534604\N,1.4003372212,-0.7958472962,0.108940823\Version=ES64L-G0
9RevD.01\State=1-A\HF=-490.7381452\S2=1.030153\S2-1=0.\S2A=0.241467\

o-NAzB triplet nitrene

1\1\GINC-COREV2-22-003\Freq\UM062X\TZVP\C6H4N2O2(3)\ASHOA001\27-Jun-20
18\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP
Freq\Title Card Required\0,3\C,0.1113670685,2.5683235956,0.04981119
49\C,-1.2661461111,2.353130773,0.0002890364\C,-1.7705047144,1.05744128
74,-0.0135875923\C,-0.9030171259,-0.0108097343,0.0218056686\C,0.506546
2171,0.1634484922,0.0726352794\C,0.9836336366,1.5037977282,0.085333257
5\H,0.4996454152,3.5783634027,0.0604445642\H,-1.9480439584,3.192029143
3,-0.0275034675\H,-2.8330401201,0.8625954696,-0.0517185167\H,2.0548731
02,1.6516670946,0.1239041405\N,-1.4714873207,-1.3695625204,0.005793498
8\O,-0.6977214969,-2.2989756551,0.0379312397\O,-2.6802859231,-1.468848
2272,-0.0386439529\N,1.4132513313,-0.8168608497,0.1091426495\Version=
ES64L-G09RevD.01\State=3-A\HF=-490.757267\S2=2.047376\S2-1=0.\S2A=2.00
0886\

m-NAzB

1\1\GINC-COREV2-25-055\Freq\RM062X\TZVP\C6H4N4O2\ASHOA001\22-Jun-2018\
0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\Title Card Required\0,1\C,0.1619935954,2.2587710481,-0.7380351285
\C,-1.2064808478,2.0408497802,-0.7744450877\C,-1.7206190061,1.04767980
14,0.0415309484\C,-0.9424014352,0.2753748506,0.8781339926\C,0.42820171
16,0.5106372631,0.8990624836\C,0.9802949515,1.5031052724,0.0902667356\
H,0.599813018,3.0265334005,-1.3618407454\H,-1.8654654743,2.6142013289,
-1.4094912653\H,2.0477443765,1.6895089797,0.1036859989\N,1.1773160584,
-0.3094732005,1.7741520149\N,2.3925281183,-0.1121393242,1.8039853923\N
,3.5010641489,-0.0165045424,1.9077484447\H,-1.3828091374,-0.4905307311
,1.4999422995\N,-3.1824676533,0.7968934572,0.0190628749\O,-3.612198472
5,-0.0753891471,0.7398526592\O,-3.8533308319,1.4821055534,-0.720180047
8\Version=AM64L-G09RevB.01\State=1-A\HF=-600.2952538\

m-NAzB closed-shell nitrene

1\1\GINC-COREV2-25-002\Freq\RM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\Title Card Required\0,1\C,-0.1283542343,2.0078426008,0.0000309583
\C,1.1580035702,1.4824506622,-0.0000792227\C,1.2614541982,0.1081230199
,-0.0000037504\C,0.1944194908,-0.7649498247,0.0001612546\C,-1.10708754
88,-0.20762599,0.0002682669\C,-1.2568038389,1.2177061722,0.0001964525\
H,-0.2703442875,3.0814387092,-0.0000234273\H,2.0405766831,2.1021842344
,-0.0002242653\H,-2.2469996411,1.6458225432,0.0002739255\N,-2.18439305
78,-0.9371786024,0.0004286529\H,0.3458470218,-1.831824853,0.0002180282
\N,2.6211477383,-0.4974542035,-0.0001070474\O,2.6982347139,-1.70551959
08,0.0000299281\O,3.5643841921,0.2593311225,-0.0002667539\Version=ES6

4L-G09RevD.01\State=1-A\HF=-490.6898601\

m-NAzB open-shell nitrene

1\1\GINC-COREV2-22-018\Freq\UM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fr
eq\Title Card Required\0,1\C,-0.1398448433,2.0317355832,0.0000126218
\C,1.1434517794,1.4736841806,-0.0000492259\C,1.2642139439,0.0834028129
,0.0000510098\C,0.1968329464,-0.7679802277,0.000208775\C,-1.1273635131
, -0.2016394538,0.0002779442\C,-1.2553779361,1.2351241218,0.0001717185\
H,-0.2478140177,3.1083687926,-0.0000673061\H,2.0330501401,2.0862525279
, -0.0001718964\H,-2.2529558239,1.6529721226,0.0002187184\N,-2.17158310
87,-0.9678824539,0.0004294023\H,0.3295936201,-1.8403065344,0.000275992
1\N,2.631395571,-0.5003939749,-0.0000206431\O,2.7240343887,-1.70582268
9,-0.0002190217\O,3.5624518534,0.2728311922,-0.0002150889\Version=ES6
4L-G09RevD.01\State=1-A\HF=-490.7432788\S2=1.033429\S2-1=0.\S2A=0.2671
75\

m-NAzB triplet nitrene

1\1\GINC-COREV2-25-043\Freq\UM062X\TZVP\C6H4N2O2(3)\ASHOA001\27-Jun-20
18\0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP
Freq\Title Card Required\0,3\C,-0.1323430985,2.0301241144,0.0000157
684\C,1.1454129841,1.4761528826,-0.0000924039\C,1.2660805434,0.0923050
294,-0.0000162529\C,0.1878768081,-0.758801851,0.0001630669\C,-1.109685
3403,-0.1910395358,0.0002740882\C,-1.2494507553,1.2209378235,0.0001962
455\H,-0.2465663475,3.1059509006,-0.0000438598\H,2.0348614105,2.089591
395,-0.0002352377\H,-2.2471773236,1.6399826657,0.0002807021\N,-2.18933
48117,-0.9827963473,0.0004555915\H,0.3228252989,-1.8313010073,0.000215
4034\N,2.6284784112,-0.4969659174,-0.0001340688\O,2.7139914796,-1.7036
187215,-0.0000476476\O,3.5651157411,0.269824569,-0.0001283954\Version
=ES64L-G09RevD.01\State=3-A\HF=-490.7631045\S2=2.045216\S2-1=0.\S2A=2.
000851\

p-NAzB

1\1\GINC-COREV4-21-023\Freq\RM062X\TZVP\C6H4N4O2\ASHOA001\22-Jun-2018\
0\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\Title Card Required\0,1\C,0.1842591543,2.2658605285,-0.7460616445
\C,-1.1787423252,2.0278487669,-0.751574666\C,-1.7617191739,1.054685895
1,0.0458338451\C,-0.9530946221,0.2999734559,0.871620901\C,0.4239551444
,0.5233304847,0.8930627327\C,0.9921448226,1.5076361242,0.0827348221\H,
0.5964356745,3.0346366434,-1.3841074655\H,2.060370416,1.6859229133,0.0
94412026\N,1.1643041374,-0.297886355,1.768304833\N,2.3830669528,-0.110
6596641,1.7980300773\N,3.4915439958,-0.0251525877,1.902780831\H,-1.367
2613016,-0.468787176,1.5092200041\H,-2.8309413006,0.9024589962,0.00971
40875\N,-2.037936088,2.8362226019,-1.6347416932\O,-3.2281709389,2.6077
544825,-1.6217286859\O,-1.5023135976,3.6805028203,-2.3204361147\Versi
on=AM64L-G09RevB.01\State=1-A\HF=-600.2973483\

p-NAzB closed-shell singlet nitrene

```
1\1\GINC-COREV4-21-016\Freq\RM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\Title Card Required\0,1\C,-0.4854230446,-1.0658820925,0.000422964
\C,-1.3634046181,0.0067236662,0.0000518612\C,-0.8879490081,1.308738591
5,-0.0002099634\C,0.4571189972,1.5744181305,-0.000104683\C,1.382861074
5,0.4722434066,0.0002785278\C,0.8720490667,-0.8735154551,0.0005586055\
H,-0.8782514832,-2.0744478174,0.000644053\H,1.5664050413,-1.69749357,0
.0008628827\N,2.6455376633,0.6861158511,0.000447807\H,0.8411601115,2.5
811881561,-0.0002798088\H,-1.591168679,2.1315262546,-0.0004926845\N,-2
.7979661792,-0.2365579089,-0.0000692913\O,-3.5359280601,0.7292798621,-
0.0004836145\O,-3.1759788822,-1.391776075,0.0002093442\Version=ES64L-
G09RevD.01\State=1-A\HF=-490.6970247\
```

p-NAzB open-shell singlet nitrene

```
1\1\GINC-COREV2-22-027\Freq\UM062X\TZVP\C6H4N2O2\ASHOA001\27-Jun-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fr
eq\Title Card Required\0,1\C,-0.4829514638,-1.0916195553,0.000558447
\C,-1.3461118811,0.0094012416,0.0001188905\C,-0.8940725746,1.333556172
,-0.000226407\C,0.4495435212,1.5757889639,-0.0001842495\C,1.3887940009
,0.4736442344,0.0002896532\C,0.8653998253,-0.8767975793,0.0006469048\H
,-0.9000583366,-2.0886267997,0.0007806956\H,1.570849703,-1.6961395107,
0.0010047358\N,2.6582175121,0.6879170383,0.0003623433\H,0.8450608757,2
.5820231006,-0.0004622486\H,-1.6167129492,2.1371662939,-0.0005217544\N
,-2.7948372826,-0.2361819224,0.0000399591\O,-3.5269331555,0.7313952775
,0.0000177673\O,-3.1671257948,-1.3909659549,-0.0005887372\Version=ES6
4L-G09RevD.01\State=1-A\HF=-490.7455592\S2=1.031347\S2-1=0.\S2A=0.2506
99\
```

p-NAzB triplet nitrene

```
1\1\GINC-COREV4-21-023\Freq\UM062X\TZVP\C6H4N2O2(3)\ASHOA001\27-Jun-20
18\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP
Freq\Title Card Required\0,3\C,-0.4881159278,-1.0847014667,0.000379
3772\C,-1.3463405024,0.0093368713,-0.0000998733\C,-0.8969733844,1.3254
721453,-0.0003460033\C,0.4579037155,1.5611381137,-0.0001348464\C,1.369
693943,0.4702287719,0.0003634244\C,0.868928448,-0.8601596767,0.0006111
397\H,-0.8994357938,-2.0839579378,0.0005394341\H,1.5726811076,-1.68153
49279,0.0009856853\N,2.6842176249,0.6925650989,0.0005661814\H,0.851345
3424,2.5686737953,-0.0003317185\H,-1.6151338937,2.1329273788,-0.000694
693\N,-2.8022141151,-0.2374594286,-0.0003348721\O,-3.5335112446,0.7288
879903,0.0002054831\O,-3.1739833194,-1.3908557279,0.0001272813\Version=
ES64L-G09RevD.01\State=3-A\HF=-490.7644139\S2=2.049405\S2-1=0.\S2A=2
.000948\RMSD=2.672e-09\
```

AzTNB

1\1\GINC-COREV1-22-003\Freq\RM062X\TZVP\C6H2N6O6\ROOT\23-Jul-2018\0\#\#
N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq\|
CSD ENTRY d:so18a\0,1\C,4.5268959038,8.5304610945,4.4085573785\C,3.45
52418465,9.3546643165,4.1140903221\H,2.854161444,9.1734980086,3.233000
5177\C,3.19608525,10.4225539577,4.9422419152\C,3.966259435,10.68079332
77,6.0623139926\H,3.7654977201,11.5334533425,6.6977208693\C,4.98417930
23,9.8069013824,6.3545078144\C,5.3229795162,8.700902711,5.5555085483\N
,4.8383758167,7.5088331861,3.3887611424\N,2.0744277759,11.3271851636,4
.618152867\N,5.7201231067,10.053946375,7.6160842029\N,6.423894763,7.97
91252285,5.9708764304\N,6.5465623271,6.7787433191,5.6894356398\N,6.789
2050802,5.7034578066,5.5546997919\O,6.0067176828,7.2219148327,3.234958
6724\O,3.9158267832,7.0629650365,2.7516421255\O,1.4342040929,11.078234
658,3.6232992024\O,1.8787866453,12.2507925509,5.3737210341\O,6.1216820
16,11.1816140733,7.7883417645\O,5.8188934922,9.1329596289,8.3880857687
\Version=AM64L-G09RevB.01\State=1-A\HF=-1009.2566241\

AzTNB closed-shell singlet transition state

1\1\GINC-COREV2-22-017\Freq\UM062X\TZVP\C6H2N6O6\ASHOA001\03-Jul-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fr
eq\test\0,1\O,-1.4567862867,-2.9458634372,-0.2309208016\O,-2.3205339
673,-1.6473577211,1.2530914143\O,4.1283815354,-0.2050785532,-0.1569125
046\O,3.3538240393,-2.214505105,-0.1927774745\O,1.0079256159,3.5354844
386,0.0583893271\O,-1.0897555403,3.0362120672,0.2036400651\N,-1.519079
5579,-1.9056787756,0.3817389714\N,3.2255068164,-1.0113340399,-0.141259
2907\N,0.0987586538,2.7445130615,0.1145059638\N,-2.0012389388,1.129389
8399,-0.0452850482\N,-3.1785428003,-0.0706850247,-0.5782429508\N,-4.19
17208568,-0.2436702057,-0.9403882086\C,-0.8064533987,0.5024657422,0.04
5563281\C,-0.4909860671,-0.8875955222,0.0943873375\C,0.790624079,-1.36
91566888,-0.0052765532\C,1.8578333548,-0.4857295934,-0.0576193896\C,1.
6517736484,0.873130501,0.0116763442\C,0.355623766,1.3286673272,0.07585
73476\H,0.9639738096,-2.437698151,-0.0042802112\H,2.4733250952,1.57858
68401,0.0064783811\Version=AM64L-G09RevB.01\State=1-A\HF=-1009.207426
1\

AzTNB closed-shell singlet product

1\1\GINC-COREV3-23-011\Freq\RM062X\TZVP\C6H2N6O6\ASHOA001\30-Jun-2018\
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fr
eq\test\0,1\O,1.3701092416,-2.8727179474,-0.6931406219\O,2.567427268
1,-1.1955899896,-1.3290757191\O,-4.0682596122,-0.2167318855,0.56009662
4\O,-3.2597443349,-2.1742049013,0.1727761305\O,-0.4694185322,3.7726050
07,0.1570728572\O,1.394190107,2.6574325301,-0.3813150709\N,1.561176578
9,-1.6930343337,-0.8837201339\N,-3.1682390567,-0.972749097,0.274992753
5\N,0.0473828717,2.7101899433,-0.0779266753\N,1.7896058626,1.368774932
3,-0.6169059754\N,2.6201214159,-0.9139226286,1.7340402193\N,3.48787087
55,-0.9297724412,2.3882663718\C,0.7148218821,0.6422618229,-0.456640695
1\C,0.4697957541,-0.768262119,-0.5525821927\C,-0.7640636854,-1.2577085

219,-0.300113798\C,-1.8387275272,-0.3768088869,0.0266176233\C,-1.70269
45944,0.9690841499,0.1301187521\C,-0.4075087123,1.4494809454,-0.123063
9926\H,-0.9421568196,-2.3240698519,-0.3475568402\H,-2.5280779827,1.620
511273,0.3856773835\\Version=AM64L-G09RevB.01\State=1-A\HF=-1009.29904
88\

AzPNB

1\1\GINC-COREV2-25-018\Freq\RM062X\TZVP\C6N8O10\ASHOA001\24-Mar-2017\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\|0,1\O,-2.9522519355,-1.7080973941,-1.1821173127\O,-2.25758903
35,-2.6650694915,0.626640645\O,3.2539641923,-0.2331242534,1.0039927057
\O,2.930989492,-1.547729021,-0.6834156671\O,-0.3404232235,3.5522075072
, -0.9001055495\O,-1.3835408296,3.3257665329,0.9806495668\N,-2.21641628
68,-1.8210261118,-0.2314892003\N,2.5895833113,-0.7325064658,0.13345268
71\N,-0.7533344293,2.9223066993,0.0421381634\N,-2.7618394415,1.1368483
314,-0.1503024632\N,-3.7832226838,0.475481995,0.109241314\N,-4.7798453
851,0.0378598781,0.3244345609\C,-1.5111471087,0.5641648637,-0.06418461
7\C,-1.1617748024,-0.7904533142,-0.101974112\C,0.1548849653,-1.2041361
36,-0.0144321037\C,1.1781659596,-0.2873157487,0.0616226822\C,0.8650663
639,1.0606880605,0.0687441867\C,-0.4435410845,1.4705013968,0.029331286
3\N,0.4684990256,-2.6592649829,-0.0186569086\O,1.1076872293,-3.0594220
989,0.917196162\O,0.0461483521,-3.2848889728,-0.955250886\N,1.95088799
97,2.0765576186,0.0922453021\O,1.8741894115,2.9129920452,0.9530059408\
O,2.7902508217,1.9613756622,-0.761200123\\Version=AM64L-G09RevB.01\Sta
te=1-A\HF=-1418.1813634\

AzPNB closed-shell singlet transition state

1\1\GINC-COREV1-22-016\Freq\RM062X\TZVP\C6N8O10\ASHOA001\04-May-2018\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\|0,1\O,3.1618888021,-0.4908007057,1.2526390936\O,3.0529869278,
-1.438390291,-0.6844190862\O,-3.1252440222,-1.6608432137,-0.7916442753
\O,-1.9856853193,-2.8617193383,0.5960095257\O,-1.8438106752,3.21668146
42,0.4646520507\O,0.2661995799,3.5564938664,0.1590760702\N,2.604436860
8,-0.7843855503,0.2252508805\N,-2.1720754297,-1.8877106114,-0.09038239
49\N,-0.724625968,2.8391922482,0.2442187629\N,1.8146527224,2.168372599
1,-0.0663889877\N,3.4019022091,1.542704898,-0.4312694131\N,4.425581114
8,1.8023410165,-0.7011783939\C,0.9569845333,1.1206959854,0.0183079421\
C,1.2225626334,-0.2775603195,0.0681226058\C,0.2234385515,-1.2101455647
, -0.010364851\C,-1.1183477431,-0.8551727097,-0.0526077937\C,-1.4317892
683,0.4830362204,-0.0098661806\C,-0.4324513304,1.4332644945,0.09353193
06\N,0.6022416508,-2.6525511657,-0.055543953\O,0.2842543513,-3.2375333
962,-1.0551910604\O,1.2004822601,-3.0736021882,0.8983841605\N,-2.87006
36899,0.8878265738,-0.0391643703\O,-3.2568713496,1.3610056088,-1.06933
33429\O,-3.4867164014,0.6734380791,0.9697930801\\Version=AM64L-G09RevB
.01\State=1-A\HF=-1418.127574\

AzPNB closed-shell singlet product

```
1\1\GINC-COREV2-25-059\Freq\RM062X\TZVP\C6N8O10\ASHOA001\06-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\test\0,1\O,-2.709408,2.532567,-0.96559\O,-3.287157,1.214157,0.6495
9\O,0.944123,-3.121935,0.321415\O,-0.573478,-3.060861,-1.218661\O,3.34
6866,1.952873,-0.307836\O,1.476413,3.18879,-0.290327\N,-2.53807,1.6163
84,-0.205831\N,0.170002,-2.562888,-0.411587\N,2.149286,1.96705,-0.2901
33\N,0.132156,3.000149,-0.319869\N,-0.048216,0.156653,2.608419\N,-0.10
4318,-0.10797,3.661259\C,-0.037806,1.707223,-0.327604\C,-1.236093,0.92
6616,-0.314716\C,-1.132833,-0.416456,-0.340409\C,0.135107,-1.085571,-0
.333782\C,1.289581,-0.384039,-0.29832\C,1.200318,1.019547,-0.275332\N,
-2.358214,-1.252435,-0.226732\O,-2.375961,-1.999007,0.718127\O,-3.1987
1,-1.09419,-1.068022\N,2.622698,-1.031986,-0.236192\O,3.234363,-0.8438
49,0.780378\O,2.957087,-1.655873,-1.208369\Version=AM64L-G09RevB.01\S
tate=1-A\HF=-1418.2215161\
```

TAzTNB

```
1\1\GINC-CR-054\Freq\RM062X\TZVP\C6N12O6\ASHOA001\09-Sep-2016\0\#N Ge
om=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq\test
\0,1\O,-2.3365588442,-2.4793070296,-1.0410623465\O,-2.8498761533,-1.8
93178832,0.9700300015\O,3.3610988459,-0.2862940202,0.812441317\O,2.939
9906205,-1.4829874231,-0.9284577496\O,-0.7817675625,3.4601740883,-0.84
12293506\O,-0.9146525583,3.3539616994,1.3104387391\N,-2.1870582438,-1.
8219876134,-0.042983012\N,2.6195056838,-0.722780396,-0.0406292354\N,-0
.7296761321,2.8828370039,0.2178427735\N,-2.7251213912,1.1043644169,0.1
489728335\N,-3.7085527432,0.456074776,-0.2476576414\N,-4.6755168243,0.
0117980766,-0.5667409052\N,0.338160181,-2.636968964,-0.1286307711\N,1.
3632851117,-3.1787798717,0.3114560167\N,2.2004751813,-3.8124463548,0.6
758534934\N,1.8187913296,2.1422253662,0.2079719818\N,2.9377593041,2.05
7961334,-0.3196478413\N,3.9595495689,2.1420118814,-0.7486247898\C,-1.4
59493069,0.5392589848,0.0837701516\C,-1.1192007998,-0.804312087,-0.047
2621806\C,0.2020569785,-1.253681708,-0.0772226733\C,1.2174473398,-0.29
20382932,0.0012536293\C,0.9280493765,1.0768011707,0.1226585419\C,-0.40
64181999,1.4422737949,0.1631290174\Version=AM64L-G09RevB.01\State=1-A
\HF=-1336.3872345\
```

TAzTNB, N_A-N_B closed-shell singlet transition state

```
1\1\GINC-COREV2-22-030\Freq\UM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fre
q\test\0,1\O,-2.6275045589,-2.1184895292,-1.0067783624\O,-2.72172205
62,-1.8287207694,1.1257282248\O,3.3486176299,-0.6076956597,0.797434337
5\O,2.8076936471,-1.6964533935,-0.9798615082\O,0.2896530438,3.78853445
38,-0.1616989389\O,-1.6515417011,3.2171894877,0.5728310441\N,-2.261570
1448,-1.6164809496,0.027715636\N,2.5681431576,-0.9256378391,-0.0741843
413\N,-0.5097520932,2.959831594,0.1891199683\N,-2.5994177953,1.3963067
223,0.2081631528\N,-3.8559220099,0.3222989864,-0.301416792\N,-4.922801
```

1642,0.2326448545,-0.5087595061\N,0.1161266322,-2.5827301479,-0.181929
695\N,1.0749911543,-3.2276471119,0.2697431961\N,1.8374474779,-3.945024
173,0.6417632872\N,2.0960577753,1.9576782993,0.2612844339\N,3.18801668
14,1.7727340542,-0.2887419441\N,4.2063027991,1.7678850526,-0.736524584
5\C,-1.406517319,0.7397910612,0.1007147509\C,-1.1577354832,-0.63814631
59,-0.0447793522\C,0.1096982093,-1.1935537697,-0.1048673229\C,1.225634
8033,-0.3426575112,-0.0336252059\C,1.0713053981,1.0386990311,0.1080715
313\C,-0.2335700836,1.5461135731,0.1417859906\\Version=AM64L-G09RevB.0
1\State=1-A\HF=-1336.3323785\

TAzTNB, N_A-N_B closed-shell singlet product

1\1\GINC-COREV3-23-013\Freq\UM062X\TZVP\C6N12O6\ASHOA001\07-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fre
q\test\0,1\O,2.7027458681,-2.4245709382,0.6182051201\O,3.3022196323,
-1.6106558064,-1.2879494368\O,-3.1733886139,-0.4453911986,-0.695838422
4\O,-2.4401595848,-1.4734667534,1.0504880369\O,0.6170731216,3.84662437
22,-0.6986030917\O,2.4659311632,2.5930904872,-0.6729594743\N,2.5723571
54,-1.6854650402,-0.3270064115\N,-2.2931403172,-0.7707953985,0.0749271
028\N,1.0810872935,2.7409450666,-0.6268704284\N,2.8093376173,1.2766666
856,-0.5648742098\N,0.585035756,0.3917635808,2.5783670326\N,0.78753331
59,-0.0265522075,3.5612479947\N,-0.0069327075,-2.5955923976,-0.0971970
441\N,-1.047600225,-3.1268120769,-0.5097288832\N,-1.9039365052,-3.7549
28819,-0.8414987349\N,-1.6833980483,2.1315173068,-0.3152179135\N,-2.82
2241367,1.9821861669,0.1644265296\N,-3.8530569489,2.0346001237,0.57181
06124\C,1.6810195929,0.6287856079,-0.4678609886\C,1.4315874671,-0.7615
515098,-0.3086989979\C,0.151139158,-1.2164548185,-0.1909295602\C,-0.94
55084155,-0.2626571151,-0.1924633167\C,-0.7781188304,1.0959208758,-0.3
439846486\C,0.573166424,1.5076628062,-0.5181168662\\Version=AM64L-G09R
evB.01\State=1-A\HF=-1336.4291424\

TAzTNB, N_D-N_E closed-shell singlet transition state

1\1\GINC-COREV2-22-004\Freq\UM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fre
q\test\0,1\O,-1.3397778461,-3.2026162906,-0.2622602767\O,-3.04058696
06,-2.0990010174,0.4756942822\O,3.3677048562,0.0469491795,0.6175513328
\O,2.9683072815,-0.8547699723,-1.2962887527\O,-1.4494249026,3.23523357
18,-0.7035139263\O,-1.2365310932,3.2057248482,1.4428285911\N,-1.896670
8147,-2.1616524716,0.0746170594\N,2.6211492591,-0.3435120306,-0.256733
2846\N,-1.1611428651,2.7119392196,0.3467741384\N,-2.9072757596,0.71627
72275,0.2240703342\N,-3.7781015333,0.1409117549,-0.4466851099\N,-4.661
4417972,-0.2414021992,-0.999329022\N,0.6601691574,-2.6148338944,-0.088
4791285\N,2.296723676,-2.7581242895,0.4570668756\N,3.0820292015,-3.446
8393342,0.7709979625\N,1.4439086927,2.3117558823,0.220742495\N,2.55908
8562,2.3979355595,-0.3174081511\N,3.5494492499,2.643909954,-0.75667384
85\C,-1.5838691029,0.3048582758,0.1514356703\C,-1.0743036405,-1.000575
3228,0.0046563674\C,0.3205241676,-1.2888055873,-0.0540184008\C,1.18059

57245,-0.165271469,-0.0380781519\C,0.7128710058,1.1328312427,0.1619810
217\C,-0.6625625185,1.323988163,0.2748969225\\Version=AM64L-G09RevB.01
\State=1-A\HF=-1336.3349683\

TAzTNB, N_D-N_E closed-shell singlet product

1\1\GINC-COREV2-22-029\Freq\UM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fre
q\test\0,1\O,1.5870009553,2.696041595,-0.9513138586\O,3.4597718324,1
.5800817902,-0.443302173\O,-3.3126945721,0.7693990869,0.1800379708\O,-
2.4260202736,2.1547783786,-1.2100386033\O,0.4217507943,-3.6079206561,-
0.2045166076\O,0.3321661271,-3.0185472439,1.8694103699\N,2.2518984582,
1.5534451968,-0.5610635009\N,-2.3868842468,1.1808032568,-0.4984107086\
N,0.3527056908,-2.7957668907,0.6864907334\N,2.6440227963,-1.4066952294
,0.3866196948\N,3.6896087886,-1.1453653713,-0.2407343442\N,4.693781966
1,-1.0610750773,-0.704081551\N,0.2402976232,2.4746598961,-0.9836946433
\N,-1.4859061188,2.7673922511,1.7801428245\N,-1.7011447021,3.599132062
7,2.446023534\N,-1.9941237407,-1.7624092387,0.3096370255\N,-3.11319707
55,-1.6957390275,-0.2298528809\N,-4.1338654309,-1.8067568022,-0.646972
3635\C,1.4759828483,-0.7339788674,0.0786707183\C,1.3340845277,0.606124
3741,-0.3903154525\C,0.0753116818,1.2255297519,-0.6285740579\C,-1.1260
023149,0.4718071474,-0.4128809374\C,-1.0163540951,-0.8287037336,0.0398
963387\C,0.2936204805,-1.3770466492,0.2738874728\\Version=AM64L-G09Rev
B.01\State=1-A\HF=-1336.4358574\

TAzTNB, N_G-N_H closed-shell singlet transition state

1\1\GINC-COREV4-21-010\Freq\UM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Fre
q\test\0,1\O,-2.3138341493,-2.4933725996,-1.0834123262\O,-2.80337004
81,-1.9735426152,0.9504681802\O,3.1736210052,-0.4118266991,1.127610011
1\O,3.0066216539,-1.2735754478,-0.8383492999\O,-1.8113583206,3.3909464
98,-0.1356546823\O,0.2038950322,3.5648902662,0.6067371036\N,-2.1727052
709,-1.8443167718,-0.0776620282\N,2.5649755969,-0.6632718182,0.1136505
019\N,-0.7632792167,2.9105052036,0.2132499858\N,-2.8308433724,1.002405
7641,0.2316370227\N,-3.7783005606,0.3306991277,-0.2027761353\N,-4.7263
145384,-0.1343742485,-0.5511142099\N,0.3577905297,-2.5600058754,-0.160
9229595\N,1.3970480952,-3.0935769157,0.2580325966\N,2.2443834867,-3.72
5034212,0.6013118263\N,1.7505719357,2.2253167052,0.1705284624\N,3.2347
279775,1.7031378513,-0.5254551521\N,4.2170744114,2.0140428991,-0.88412
03321\C,-1.5351240695,0.5439536008,0.0777999109\C,-1.1543657463,-0.778
8407311,-0.0928883032\C,0.1865175373,-1.1828183318,-0.100086577\C,1.17
05042884,-0.2085772585,0.0280154018\C,0.874098758,1.1723481954,0.12324
2386\C,-0.5059430153,1.4973984134,0.1534066165\\Version=AM64L-G09RevB.
01\State=1-A\HF=-1336.3314243\

TAzTNB, N_G-N_H closed-shell singlet product

1\1\GINC-COREV2-22-003\Freq\UM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0

\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/TZVP Freq
q\\test\\0,1\\O,-2.6631390633,1.502102187,1.5173575223\\O,-3.3521685,1.1
737839792,-0.4988472662\\O,3.2860558899,0.8177273686,-0.9432972621\\O,2.
4722274825,2.1956795514,0.4983867125\\O,-0.453841672,-3.839291085,-0.92
92267923\\O,1.5458501896,-2.8622499754,-1.122873584\\N,-2.5341395669,1.0
885305752,0.393354283\\N,2.3828743837,1.254677605,-0.2727001569\\N,0.182
534224,-2.8205734669,-0.8585217069\\N,-2.4245688866,-1.8317562908,-0.17
18572363\\N,-3.5002606613,-1.4657802374,0.3421518379\\N,-4.5116869273,-1
.3053318535,0.7698371302\\N,-0.3668921548,2.5054382598,0.2185380432\\N,0
.3843917365,3.3992861793,-0.2097306206\\N,0.9180684626,4.3103157857,-0.
547356162\\N,2.0980762381,-1.6192404618,-0.9923728492\\N,3.0685854339,-
.522262035,1.9159873401\\N,3.8766107818,-0.8056448229,2.5855619976\\C,-1
.3524556279,-0.9687408851,-0.2021698806\\C,-1.2868728657,0.3705777871,0
.067919093\\C,-0.0905347492,1.174452538,-0.01983705\\C,1.1055987537,0.57
37894762,-0.3534159077\\C,1.1131922206,-0.8280591753,-0.6578705609\\C,-0
.1067411219,-1.5479720035,-0.5748299241\\Version=AM64L-G09RevB.01\\Stat
e=1-A\\HF=-1336.4353986\\

TAzTNB-1

1\\1\\GINC-COREV2-25-074\\Freq\\RM062X\\TZVP\\C6N12O6\\ASHOA001\\29-Mar-2017\\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq
q\\test\\0,1\\O,-2.3310935769,-2.5079853324,-0.9914608261\\O,-2.90034135
64,-1.8432886724,0.9792874488\\O,3.2776732379,-0.5205448705,0.999791439
1\\O,2.9595175161,-1.2662288625,-0.9983085422\\O,-1.335552921,3.39557151
53,-0.713349646\\O,-0.3847668903,3.4610966396,1.2203392212\\N,-2.2094441
45,-1.8106010931,-0.0169018527\\N,2.5997279318,-0.7233541743,0.02515416
96\\N,-0.74835963,2.8939156128,0.2121172475\\N,-2.7363444027,1.101681266
3,0.0987297577\\N,-3.7123702399,0.4549340167,-0.3113771216\\N,-4.6732812
378,0.0094015711,-0.6483514751\\N,0.3281040961,-2.6403035335,-0.0500632
117\\N,1.4086887793,-3.1613428532,0.2723977097\\N,2.295604044,-3.7761178
287,0.536879911\\N,2.0526340417,1.8804633391,0.1743908243\\N,1.962911329
2,3.0863130606,-0.1085230549\\N,2.054558484,4.1682401875,-0.3445459906\\
C,-1.4645025633,0.5478577984,0.0333709156\\C,-1.1362890178,-0.798965160
2,-0.0318173937\\C,0.1857269318,-1.2601596392,-0.014216087\\C,1.18755830
83,-0.3027566466,0.0735862402\\C,0.9248670796,1.0711947557,0.1422710066
\\C,-0.4078177387,1.4633977035,0.1123184503\\Version=AM64L-G09RevB.01\\S
tate=1-A\\HF=-1336.3873905\\

TAzTNB-1 closed-shell singlet transition state

1\\1\\GINC-COREV1-22-011\\Freq\\RM062X\\TZVP\\C6N12O6\\ASHOA001\\04-May-2018\\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Freq
q\\test\\0,1\\O,-3.0570605178,0.818334892,1.4405674639\\O,-3.1369821918,
1.510415981,-0.597487671\\O,2.9217332017,1.9072921141,-0.9838750054\\O,2
.3275214015,2.3960369669,1.029551837\\O,-0.5190878133,-3.4856905558,-0.
0481469562\\O,1.4934111917,-3.2566934251,-0.7888907306\\N,-2.5963417023,
0.9601468153,0.331564471\\N,2.2135249585,1.7910122898,-0.0163183187\\N,0

.4671389188,-2.8077845775,-0.321346123\N,-1.9857127037,-2.0083167282,0
.0305650191\N,-3.5611172639,-1.3102138171,-0.2221444551\N,-4.61647667,
-1.5301416746,-0.38527598\N,-0.6128259987,2.6386528863,0.1742190576\N,
0.1385658008,3.5504792425,-0.2069358826\N,0.6876701406,4.4688980635,-0
.505870892\N,2.7416417314,-0.8021128058,-0.1257842\N,3.1621222828,-1.8
253773849,0.4371110132\N,3.7024814981,-2.6673677414,0.91759561\C,-1.06
12456431,-1.001270729,0.0300946641\C,-1.2557830046,0.3896614883,0.0978
289518\C,-0.2213844957,1.3150578773,0.0297274106\C,1.0868270737,0.8450
717491,-0.1054547852\C,1.3854831969,-0.5101144874,-0.118325821\C,0.303
9186084,-1.4091464395,-0.1030636771\\Version=AM64L-G09RevB.01\State=1-
A\HF=-1336.3354359\

TAzTNB-1 closed-shell singlet product

1\1\GINC-COREV1-22-012\Freq\RM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\|test\|0,1\O,-1.7318532051,-2.535363575,-2.3523738589\O,-1.097642467
2,-3.4454809931,-0.5024437604\O,2.7185262263,0.5379550053,1.7239196294
\O,3.3578603285,0.0375132446,-0.2743023222\O,-3.0397162022,1.326181060
7,-0.9792665029\O,-2.1023796069,3.1528557467,-0.0920283183\N,-1.186167
6504,-2.5196360013,-1.2740464855\N,2.5159588315,0.254982384,0.56971686
74\N,-1.962839387,1.9991514012,-0.4390394795\N,-2.7031661905,0.0324132
701,-1.2514625196\N,-1.2792798203,-0.6647489184,2.2376491735\N,-1.3494
152376,-1.3042457332,3.1141344974\N,1.423274051,-2.2879931357,-0.36768
78523\N,2.3311344653,-2.4486175386,0.4611933014\N,3.1669808974,-2.7473
738116,1.1313489868\N,0.9557622396,2.4579733565,0.5907249895\N,0.58343
5141,3.561013729,0.1424216558\N,0.4039158574,4.6151858517,-0.152180618
2\C,-1.4461080844,-0.0829197079,-0.9104822932\C,-0.6154992141,-1.23462
9813,-0.8581886799\C,0.6438131799,-1.1403694562,-0.3348527598\C,1.1115
73048,0.1430498227,0.1319567794\C,0.3774074058,1.2981288526,0.11283301
31\C,-0.9367036063,1.149184959,-0.4216814429\\Version=AM64L-G09RevB.01
\State=1-A\HF=-1336.4297164\

TAzTNB-2

1\1\GINC-COREV1-22-002\Freq\RM062X\TZVP\C6N12O6\ASHOA001\06-Dec-2017\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\|test\|0,1\O,0.2632382135,-3.5933042712,-0.1567958621\O,-1.792356161
7,-3.1092818412,-0.5888913201\O,0.8652352594,2.0346321753,2.2918684225
\O,2.3848974402,0.51319009,2.1427369809\O,0.0048434583,1.6684712215,-3
.5205961275\O,-1.8872543333,2.1233881694,-2.5858390585\N,-0.6319414498
,-2.817913886,-0.3998817568\N,1.374098424,1.0648255917,1.774446828\N,-
0.8086530654,1.5915827579,-2.6318971701\N,-1.44469395,-0.987504954,-2.
6670518448\N,-1.4079374983,-2.1693825405,-3.0465365759\N,-1.4640559759
,-3.1736982042,-3.5176029394\N,0.6757661114,-1.6263813732,1.745375472\N,
1.7593442969,-2.2253835291,1.8147946094\N,2.6824444814,-2.810936463,
2.0084637736\N,0.4693042289,2.7169392282,-0.5927175058\N,1.4045010387,
3.2759563769,0.0031903962\N,2.195808864,3.9134976521,0.4515892017\C,-0

.7347547028,-0.603347837,-1.5389902107\C,-0.2880170248,-1.3923629845,-
0.4710051356\C,0.4433821809,-0.8566038723,0.5849892401\C,0.6958013718,
0.5120223807,0.5954986437\C,0.275145787,1.35156191,-0.4442406573\C,-0.
4321553643,0.7499860523,-1.4761840236\\Version=ES64L-G09RevD.01\State=
1-A\HF=-1336.3897534\

TAzTNB-2 N_A-N_B closed-shell singlet transition state

1\1\GINC-COREV1-22-001\Freq\RM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\|0,1\O,2.6820360896,2.0666636418,-0.4357887966\O,3.148743889,0
.9595022942,1.3580753985\O,-3.1490190927,0.9582736921,1.3582220536\O,-
2.6827720537,2.065759498,-0.4355607855\O,0.000591969,-3.3337575977,-1.
3955941814\O,0.0006932283,-3.6926615587,0.7355337608\N,2.4495536919,1.
2431440006,0.412092682\N,-2.4499647239,1.2422443061,0.4122372431\N,0.0
00550707,-2.9897971339,-0.2400996554\N,2.3400466536,-1.7471453026,0.00
98998582\N,3.4521415292,-1.2689450125,-0.2717293862\N,4.4999318038,-0.
9950190804,-0.5190687854\N,-0.0003988397,2.4972316167,0.8236389219\N,-
0.0007805926,3.5969361544,-0.8261302859\N,-0.0010925835,4.5582074031,-
1.3350997149\N,-2.3393843332,-1.7479884021,0.0099365788\N,-3.451651239
3,-1.2701792378,-0.2716771207\N,-4.4995380848,-0.9966138955,-0.5190059
757\C,1.2405145786,-0.9007861418,0.095313061\C,1.1995505187,0.47819838
01,0.2740961892\C,-0.0001979456,1.2027428172,0.3818869636\C,-1.1996921
625,0.4777622481,0.2741394786\C,-1.2401566157,-0.9012317945,0.09533514
85\C,0.0002926086,-1.5303648949,-0.00032265\\Version=AM64L-G09RevB.01\
State=1-A\HF=-1336.3265524\

TAzTNB-2 N_A-N_B closed-shell singlet product

1\1\GINC-COREV4-21-010\Freq\RM062X\TZVP\C6N12O6\ASHOA001\06-May-2018\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\|0,1\O,2.1171178931,-3.1639772952,-0.1456299802\O,3.4829179442
, -1.5953125279,-0.7096587857\O,-3.3153011656,-0.8866886706,-1.18550078
91\O,-1.8003693909,-2.5308893193,-1.0871591561\O,0.570857354,2.9021230
824,1.4180858235\O,0.9639057795,3.3533061154,-0.6551594241\N,2.3870911
758,-2.0098452803,-0.3720884153\N,-2.1618292259,-1.2038725536,-0.97822
10215\N,0.6728556768,2.6142337745,0.2495485266\N,2.67936014,0.97375801
85,0.3021405061\N,3.633276767,0.3859976123,0.8423175823\N,4.5503054436
,0.0291345835,1.3524954476\N,-0.472052004,-2.6836254666,-0.8196152781\
N,-2.7149290845,-0.1634624694,1.9417887796\N,-2.9988059596,-0.46899739
12,2.9455235021\N,-1.8018370685,1.8936610602,-0.4615131471\N,-3.024967
2829,1.693374401,-0.3383956761\N,-4.1296310129,1.7224983152,-0.2462317
09\C,1.5205421185,0.3002973341,-0.0232590787\C,1.311341576,-1.04151794
12,-0.2680123961\C,-0.0218328628,-1.4840336896,-0.5532604506\C,-1.0691
906413,-0.525056939,-0.6466340392\C,-0.883966328,0.8682006572,-0.39209
22528\C,0.4039071585,1.2030365898,-0.1006505681\\Version=AM64L-G09RevB
.01\State=1-A\HF=-1336.4364011\

TAzTNB-2 N_D-N_E closed-shell singlet transition state

```
1\1\GINC-COREV1-22-028\Freq\RM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\0,1\O,2.6992401511,2.0107501768,-0.4660716293\O,3.0104468026,
1.0465727082,1.4354732238\O,-3.2282482317,0.9095479189,1.196556845\O,-
2.5515378547,2.2962684368,-0.3047943182\O,-0.8954085521,-3.6597301996,
-0.5932760836\O,1.0972316305,-3.4937878079,0.2056790864\N,2.399107025,
1.2325505057,0.4106801479\N,-2.4349347703,1.2935204563,0.365016829\N,0
.0087369057,-3.0205189094,-0.1219348318\N,2.3024385013,-1.7946181445,0
.0747529922\N,3.6640775003,-0.8371099033,-0.3852111385\N,4.7153161505,
-0.8513236752,-0.6757469897\N,0.0906631642,2.5433744798,0.4830178173\N
,-0.076609408,3.3357166738,-0.456001447\N,-0.1837322556,4.1540825369,-
1.1983556987\N,-2.4297421463,-1.6736661546,0.1269631565\N,-3.495343750
5,-1.2127347212,-0.3035178671\N,-4.5114160076,-0.9596493006,-0.6768695
83\C,1.2145060727,-0.9713648783,0.1222562144\C,1.173659745,0.439493553
,0.2135209287\C,0.0016836745,1.1655566994,0.1929978608\C,-1.2264309287
,0.4934785141,0.1668479693\C,-1.2847495505,-0.9013432708,0.1037268649\
C,-0.0629968674,-1.5905426941,0.0585236505\\Version=AM64L-G09RevB.01\
tate=1-A\HF=-1336.3338122\
```

TAzTNB-2 N_D-N_E closed-shell singlet product

```
1\1\GINC-COREV2-22-001\Freq\RM062X\TZVP\C6N12O6\ASHOA001\04-May-2018\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/TZVP Fre
q\\test\0,1\O,-2.273595559,2.5183495423,-0.2400100137\O,-3.1592471791
,0.8743990242,-1.3102217569\O,3.4696971838,0.7697378431,-0.7804446895\
O,2.7183095582,1.6336745858,1.0459136007\O,0.1665120177,-3.9680689923,
-0.4188477521\O,-1.784390806,-2.8937078555,-0.5968082152\N,-2.26263492
58,1.3881421121,-0.6863900568\N,2.6071110927,0.9586123532,0.0508161332
\N,-0.3996862158,-2.9086666431,-0.4637938751\N,-2.2499830796,-1.612438
8699,-0.6194865015\N,-3.3773909914,0.2099075758,1.7333996526\N,-4.2941
608804,-0.0594546703,2.2515310234\N,0.4880083674,2.4864550687,-0.36989
31868\N,0.0650491441,3.286778916,0.4758386238\N,-0.2020974866,4.110206
9894,1.1694024544\N,2.2974260645,-2.0253347141,-0.1245604558\N,3.42438
66219,-1.6924813174,0.2927864634\N,4.4643170263,-1.5765101382,0.661315
1837\C,-1.1957947838,-0.8501362439,-0.502759463\C,-1.0765233771,0.5788
109702,-0.456742282\C,0.1639345967,1.1300849431,-0.2662206747\C,1.3228
293873,0.2766398468,-0.1649921032\C,1.2927256155,-1.0933300624,-0.2321
226761\C,-0.0126153915,-1.6293922636,-0.4234514327\\Version=AM64L-G09R
evB.01\State=1-A\HF=-1336.4338606\
```