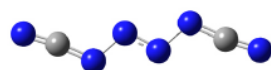
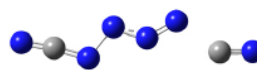


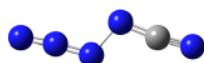
## S1:



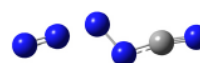
Im8 anion



Im8 anion TS1

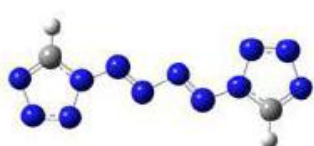


Im8 anion P1

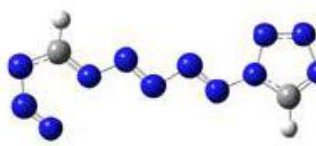


Im8 TS2

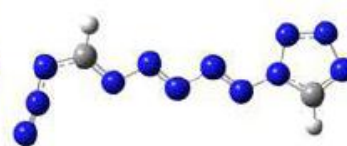
## S2:



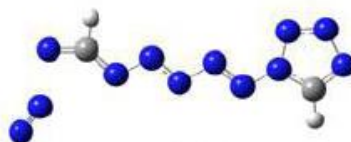
N<sub>12</sub>



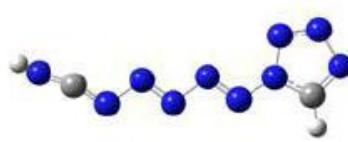
N<sub>12</sub>TS1



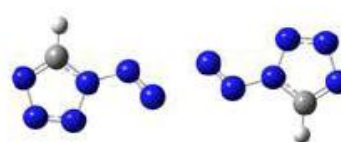
N<sub>12</sub>P1



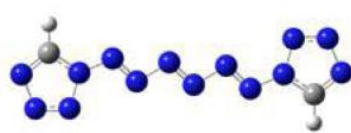
N<sub>12</sub>TS2



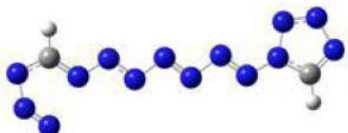
N<sub>12</sub>P2



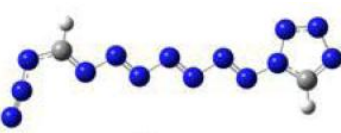
N<sub>12</sub>UTS1



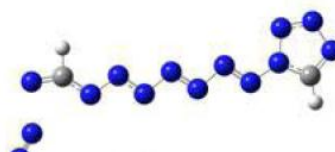
N<sub>14</sub>



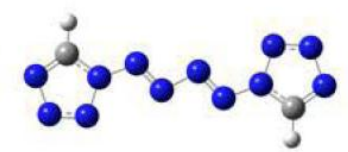
N<sub>14</sub>TS1



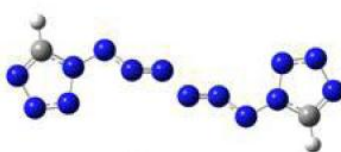
N<sub>14</sub>P1



N<sub>14</sub>TS2



N<sub>14</sub>P2



N<sub>14</sub>UTS1

## Corresponding to Fig. 1

### N10

```
1\1\GINC-ZHANG-X58A-UD3R\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ZHANG\31-Jul-2012\0\#n b3lyp/6-31+g(d,p) guess(read) freq(noraman) fchk=all\Title Card Required\0,1\C, 2.699143, -1.094473, 0.000024\N, 1.695452, -0.174673, 0.000054\H, 2.535151, -2.161107, 0.000035\N, 0.367428, -0.50271, 0.000235\N, -0.367452, 0.502709, -0.000025\N, -1.695475, 0.174673, 0.000096\C, -2.69916
```

6, 1.094474, 0.000059131\H, -2.535172, 2.161107, 0.000038\N, 2.250553, 1.077115, -0.000166\N, 3.519346, 0.885153, 0.000268\N, -2.250576, -1.077114, 0.00026\N, -3.51937, -0.885153, -0.000088\N, 3.840031, -0.456669, 0.000067\N, -3.840054, 0.456668, -0.000039\\Version=EM64L-G09RevB.01\State=1-A\HF=-624.7251735\RMSD=9.068e-09\RMSF=9.523e-05\ZeroPoint=0.081159\Thermal=0.0901685\Dipole=0., 0.0000014, 0.0000069\DipoleDeriv=1.11753, -0.0464961, 0.000169, -0.4190689, 0.2070882, 0.0000159, 0.0001732, -0.0000199, 0.1263248, -1.4447944, 0.0500639, -0.000132, -0.5968088, -0.0265816, -0.0000339, 0.0002964, -0.0000549, 0.0353908, 0.1212818, -0.0210064, 0.0000082, -0.0434803, 0.1369665, -0.0000058, -0.0000212, 0.0000104, 0.1715042, 1.0993094, -0.0973387, -0.000008, 0.580184, -0.0642522, 0.0000108, -0.000126, 0.0000493, 0.055583, 1.0993059, -0.097339, 0.0000395, 0.5801852, -0.0642528, -0.0000109, -0.0001562, 0.0000346, 0.0555827, -1.4447914, 0.050065, -0.0001282, -0.5968081, -0.0265793, -0.0000246, 0.0002006, -0.0000367, 0.0353916, 1.1175274, -0.0464975, 0.0000419, -0.419068, 0.207086, 0.0000039, 0.0001783, -0.0000238, 0.1263244, 0.1212815, -0.0210064, 0.0000022, -0.0434802, 0.1369673, -0.0000032, -0.0000167, 0.0000116, 0.1715046, 0.2648856, 0.3371379, 0.0000616, 0.791625, -0.1165201, -0.0000743, -0.0002601, 0.0000797, -0.0400357, -0.619596, -0.1414126, 0.0000924, 0.1315266, 0.2558259, 0.0001235, 0.0002414, -0.0000184, -0.1591064, 0.2648829, 0.3371359, 0.0000355, 0.7916225, -0.1165226, -0.0000192, -0.0001804, 0.0000627, -0.0400362, -0.6195927, -0.1414105, 0.0000574, 0.1315271, 0.2558258, 0.0000567, 0.0001191, -0.000031, -0.1591061, -0.5386155, -0.0809481, -0.0000582, -0.4439784, -0.3925264, -0.0000217, -0.000276, -0.0000434, -0.1896607, -0.5386145, -0.0809476, -0.0000291, -0.4439777, -0.3925246, -0.0000172, -0.0001726, -0.0000201, -0.1896609\Polar=177.457116, -4.4899762, 88.5571563, 0.004585, -0.0008785, 49.7373595\PG=C01 [X(C2H2N10)]\NImag=0\\

## Im2

1. 1\1\GINC-ZHANG-X58A-UD3R\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ZHANG\03-Aug-
2. 2012\0\\#N Geom=AllCheck Guess=TChech SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\\Title Card Required\\0, 1\C, 2.258566115, -0.9422363487, -0.0002541056\N, 1.4461180861, 0.0659602419, -0.0000545817\H, 1.9342223891, -1.9812205446, -0.000408595\N, 0.1430690799, -0.3877795557, -0.0000683503\N, -0.6388904603, 0.5871541051, 0.0001188839\N, -1.9611464005, 0.1923316333, 0.001163307\C, -2.9994266327, 1.0661130585, 0.0002965383\H, -2.8789764812, 2.1381359158, 0.0004542836\N, 4.6168226197, 1.3724056551, 0.0000207605\N, 4.062536833, 0.3883667632, -0.0001165474\N, -2.4637519674, -1.0771798775, -0.0000537631\N, -3.7438550482, -0.9396231524, 0.0000248533\N, 3.6283049117, -0.7948722105, -0.0002916797\N, -4.1177870443, 0.3833743164, 0.0002429725\\Version=EM64L-G09RevB.01\State=1-A\HF=-624.7249231\RMSD=3.375e-09\RMSF=4.781e-05\ZeroPoint=0.0800714\Thermal=0.0899406\Dipole=2.0186177, 0.5638013, -0.0000102\DipoleDeriv=2.5165669, 0.157024, -0.0000763, -0.5292988, 0.6397687, 0.0000958, -0.0001879, 0.0000652, 0.1922873, -1.8063568, 0.0246483, 0.0000719, 0.5853871, -0.3413163, -0.0000416, 0.0001664, -0.0000163, -0.2457

17. 55, 0.0740213, -0.035136, -0.0000022, -0.0226292, 0.0243869, -0.0000197, -0.0  
18. 000011, -0.0000191, 0.1516716, 1.0294497, -0.1112275, -0.0000608, 0.251346, -  
19. 0.0390624, -0.0000226, -0.0000082, -0.0000067, 0.0335817, 0.9078727, -0.0485  
20. 219, -0.0000493, 0.7551924, -0.0699327, -0.0000413, 0.0000781, -0.0000064, -0  
21. .0165136, -1.3600962, 0.0238277, 0.000067, -0.6608258, -0.0615589, 0.0000137  
22. , -0.0000383, -0.0000163, 0.0435019, 1.1432359, -0.0354186, -0.0000523, -0.37  
23. 76157, 0.19565, 0.0000295, -0.0001056, 0.0000138, 0.1123628, 0.122811, -0.022  
24. 2723, -0.0000011, -0.0459535, 0.1113336, -0.0000071, -0.000005, -0.0000077, 0  
25. .1708842, -0.5776316, -0.3277012, -0.0000306, -0.9797745, -0.511933, -0.0000  
26. 324, -0.0001377, -0.0000612, -0.052001, 0.9234749, 0.5929642, 0.0000675, 1.99  
27. 13633, 1.3733856, 0.0000983, 0.000296, 0.0001596, 0.2420965, 0.2566458, 0.317  
28. 2923, 0.0000346, 0.8340034, -0.1086661, -0.0000469, 0.0001143, -0.0000235, -0  
29. .0495174, -0.7220424, -0.1570123, 0.0000005, 0.0889423, 0.2088054, 0.0000543  
30. , 0.0000369, 0.0000652, -0.172952, -1.9254236, -0.3223182, 0.0000224, -1.4188  
31. 105, -1.0401386, -0.0000743, -0.0001542, -0.0001221, -0.2071952, -0.5825275,  
32. -0.0561485, 0.0000088, -0.4713262, -0.3807221, -0.0000057, -0.0000535, -0.00  
33. 00246, -0.202452\Polar=212.5375851, 6.0115244, 97.6892614, -0.0061859, 0.00  
34. 72356, 50.4203539\PG=C01 [X(C2H2N10)]\NImag=0\

### 3. Im3

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP/6-31+G(d,p)\C2H2N8\R00T\13-Sep-2012\0  
\#N Geom=AllCheck Guess=TChef SCRF=Check GenChk RB3LYP/6-31+G(d,p) F  
req\Title Card Required\0,1\C,2.2480967481,-1.2706478351,-0.12725919  
16\N,1.4356029769,-0.3245980677,-0.0708826985\H,3.6290866328,-2.505709  
6513,-0.7984370603\N,0.0898892441,-0.6513879301,-0.0770067675\N,-0.581  
3125951,0.397578841,0.011073537\N,-1.9358548107,0.1448282913,0.0076123  
251\C,-2.8755810996,1.1195722478,0.1041583166\H,-2.6424949476,2.169031  
7312,0.1943432992\N,-2.5696204725,-1.0609852961,-0.0914652555\N,-3.827  
35716,-0.7904708989,-0.0541482142\N,3.1555629747,-2.0662896531,-0.0172  
265444\N,-4.0591254912,0.559325221,0.0681042541\Version=EM64L-G09RevA  
.01\State=1-A\HF=-515.2584018\RMSD=9.726e-09\RMSF=2.786e-05\ZeroPoint=  
0.0688626\Thermal=0.0772385\Dipole=2.0389661,0.2850147,-0.5341384\Dipo  
leDeriv=2.0857121,-1.2458071,0.0009412,-2.2551666,1.667887,-0.0130512,  
0.2249955,-0.1311437,0.2409804,-2.0931077,0.8860234,0.0012274,1.033946  
9,-0.8595515,0.0192304,0.1292972,-0.0302628,-0.2345915,0.5459463,-0.10  
40758,-0.0349341,-0.1849004,0.4456543,-0.0059178,0.144568,-0.0884065,0  
.2515726,1.3405675,-0.4648521,-0.0190913,0.0324692,0.0253704,-0.008203  
1,-0.0150185,-0.0220624,0.0707418,0.8977926,-0.1824581,-0.0256067,0.62  
38851,-0.2044737,-0.0137978,0.0353908,-0.019073,-0.0025142,-1.2421263,  
0.2518797,0.025487,-0.4977495,0.014275,0.0014994,-0.0272845,-0.0008542  
,0.0384088,0.9981763,-0.1847018,-0.0174758,-0.4129262,0.2904174,0.0147  
151,-0.043185,0.0185132,0.1157247,0.1152521,-0.0228867,-0.0011568,-0.0  
402102,0.1264445,-0.0039807,-0.0029612,-0.003704,0.1715525,0.3079928,0  
.2369576,0.0236948,0.7065436,-0.2661738,-0.020558,0.0541207,-0.0211663

, -0.0458058, -0.6155016, -0.0061823, -0.0040534, 0.1376014, 0.1830579, 0.033  
9213, 0.0205999, 0.029731, -0.1687998, -1.7635573, 0.8297245, 0.0520214, 1.22  
52812, -1.1266664, 0.0071843, -0.4885027, 0.2767321, -0.2358308, -0.5771467,  
0.0063787, -0.0010538, -0.3687744, -0.2962412, -0.0110419, -0.0320201, -0.00  
83035, -0.2014385\Polar=161.6939741, -38.034661, 84.7823481, -2.107341, 2.4  
669226, 43.9225564\PG=C01 [X(C2H2N8)]\NImag=0\

#### 4. Im4

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ROOT\07-Sep-2012\  
0\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p)  
Freq\Title Card Required\0,1\C,-2.5447553665,0.9685134814,-0.0002272  
369\N,-1.7031008172,-0.0094570283,-0.0000815337\H,-2.2577363242,2.0184  
870907,-0.000326435\N,-0.405425518,0.4785397895,-0.0000711412\N,0.4046  
573135,-0.479753298,0.0000696822\N,1.7021982988,0.0084232665,0.0000816  
447\C,2.5437006027,-0.9696082923,0.000227415\H,2.2565883493,-2.0195584  
213,0.0003252152\N,-4.8317581144,-1.4204997373,-0.0000821698\N,-4.3133  
8007,-0.4151062427,-0.0001650454\N,4.8304994689,1.4192388716,0.0000841  
168\N,4.312576988,0.4136398476,0.0001661934\N,-3.9168971494,0.77710269  
12,-0.0002740073\N,3.9160323385,-0.7786070187,0.0002743019\Version=EM  
64L-G09RevA.01\State=1-A\HF=-624.7180819\RMSD=1.311e-09\RMSF=2.906e-05  
\ZeroPoint=0.0784472\Thermal=0.0893734\Dipole=-0.0000798,0.0002319,-0.  
0000001\DipoleDeriv=2.4432125,0.2051577,0.0000883,-0.370219,0.664616,-  
0.0000708,0.0001512,-0.000043,0.1710246,-1.664186,-0.0099607,-0.000068  
4,0.5704513,-0.3786517,0.0000438,-0.0001317,0.0000156,-0.2277525,0.067  
5772,-0.0398933,0.0000001,-0.0247789,-0.0054338,0.0000158,-0.0000017,0  
.0000151,0.1525149,0.7920149,-0.0902358,0.0000497,0.3085862,-0.0482599  
,0.0000155,0.0000074,-0.0000039,-0.045374,0.7921331,-0.0903435,0.00005  
07,0.3086671,-0.0483044,0.0000152,0.0000094,-0.0000042,-0.0453718,-1.6  
642643,-0.0099108,-0.0000687,0.5704651,-0.3785999,0.0000437,-0.0001316  
,0.0000156,-0.2276915,2.4433661,0.2052815,0.0000888,-0.3708587,0.66434  
18,-0.0000705,0.0001501,-0.0000423,0.1709966,0.0675294,-0.0399161,0,-  
0.0247737,-0.0054039,0.0000157,-0.0000013,0.0000147,0.1525029,-0.62031  
82,-0.3376792,0.0000096,-1.1279313,-0.5891036,0.0000009,0.0000945,0.00  
00392,-0.0710556,0.8799603,0.5804702,-0.0000312,2.1640746,1.4703766,-0  
.0000275,-0.0002013,-0.0001043,0.2367412,-0.6197755,-0.3374723,0.00000  
93,-1.1281189,-0.5891183,0.0000004,0.0000937,0.0000388,-0.0710162,0.87  
94485,0.5804475,-0.0000307,2.164227,1.4703429,-0.0000263,-0.0001997,-0  
.0001035,0.2367153,-1.898253,-0.3078191,-0.0000485,-1.5201483,-1.11352  
92,0.0000225,0.0000809,0.0000814,-0.2161045,-1.898445,-0.308126,-0.000  
0491,-1.5196425,-1.1132727,0.0000217,0.0000801,0.0000808,-0.2161296\Po  
lar=252.4725641,15.9084566,109.7060359,0.0080838,-0.0054822,51.1985791  
\PG=C01 [X(C2H2N10)]\NImag=0\

#### 5. Im5

```
1\1\GINC-ZHANGRUB-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N8\ROOT\14-Sep-2012\0
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\Title Card Required\0,1\C, 3. 610164534, -0. 1249632273, 0. 0234841315
\N, 2. 5351375494, -0. 7472031976, 0. 0308183771\H, 5. 3132125115, 0. 6128177405
, 0. 6363116568\N, 1. 350339706, -0. 0104048572, 0. 0300431956\N, 0. 3799500743,
-0. 8026055479, 0. 0187110514\N, -0. 8017336198, -0. 0778679133, 0. 0162263876\
C, -1. 8125308783, -0. 8792949636, -0. 0112165868\H, -1. 7283786693, -1. 9642968
553, -0. 0306037459\N, -3. 608834155, 1. 8970284893, 0. 0165314962\N, -3. 288490
4654, 0. 8125329825, 0. 001427116\N, 4. 7293234873, 0. 3286659904, -0. 143387521
5\N, -3. 1232400749, -0. 4330826403, -0. 0187015581\Version=EM64L-G09RevA. 0
1\State=1-A\HF=-515. 2530995\RMSD=6. 562e-09\RMSF=8. 826e-05\ZeroPoint=0.
0673433\Thermal=0. 0767495\Dipole=0. 0079311, -0. 056215, 0. 5657075\DipoleD
eriv=3. 2190853, 0. 7732934, -0. 1236115, 1. 8596277, 0. 641635, -0. 0822658, -0. 4
510419, -0. 0930301, 0. 2258862, -2. 6526369, -0. 331052, 0. 087928, -0. 5469458, -
0. 4286433, 0. 0434686, -0. 0388815, 0. 0314138, -0. 223806, 0. 587011, 0. 0330711,
0. 0166748, 0. 1006975, 0. 3535969, -0. 0299006, -0. 2038982, -0. 0508983, 0. 22073
26, 1. 2783366, 0. 026207, -0. 0214212, -0. 4942212, 0. 0022709, 0. 0017507, -0. 000
4234, -0. 0236487, 0. 0040487, 0. 6078338, -0. 0394569, 0. 0090124, -0. 5009996, 0.
0010506, 0. 0000825, -0. 0012226, -0. 0051383, -0. 0330571, -1. 5826243, 0. 138603
6, -0. 0046237, -0. 2786336, -0. 3586543, -0. 0025266, -0. 0159348, 0. 0031811, -0.
2310135, 2. 2997352, -0. 4145876, 0. 0078591, -0. 0083034, 0. 7353072, 0. 0080417,
0. 0234299, 0. 0066151, 0. 1742719, 0. 0758608, 0. 0254791, -0. 0009233, 0. 0066361
, -0. 0094346, -0. 0032263, 0. 0004138, -0. 0022808, 0. 1531122, -0. 3256301, 0. 272
2837, 0. 0037427, 0. 995729, -0. 779396, -0. 0088818, 0. 0152453, -0. 0097118, -0. 0
689687, 0. 3773644, -0. 3567454, -0. 0064548, -1. 8081996, 1. 8137969, 0. 0208396,
-0. 0307549, 0. 0236893, 0. 2386278, -2. 4430179, -0. 4198195, 0. 0320276, -0. 8336
832, -0. 5878629, 0. 0651707, 0. 6912221, 0. 1378017, -0. 2431542, -1. 441318, 0. 29
27236, -0. 00021, 1. 5082961, -1. 3836664, -0. 0125526, 0. 0118461, -0. 0179931, -0
. 2166799\Polar=208. 9484843, -2. 1855544, 83. 8162581, -1. 1518438, 0. 0078591,
44. 5622582\PG=C01 [X(C2H2N8)]\NImag=0\
```

## Im6

```
1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\Title Card Required\0,1\C, 3. 3932849283, 0. 2442096196, -0. 0799148958
\N, 2. 4393947872, -0. 5002457637, 0. 2016724264\H, 5. 0055512928, 1. 3262886037
, 0. 1382653227\N, 1. 1573808459, 0. 0381169361, 0. 1797585499\N, 0. 3254700346,
-0. 8457413003, 0. 4975470629\N, -0. 9853952427, -0. 4087523869, 0. 4985974016\
N, -1. 1685633209, 0. 8094569421, 0. 1705971215\N, -1. 5367095185, 1. 8477354767
, -0. 0923634662\N, 4. 4036441934, 0. 7943638728, -0. 482378523\Version=EM64L
-G09RevA. 01\State=1-A\HF=-421. 7876399\RMSD=6. 541e-09\RMSF=4. 531e-05\Ze
roPoint=0. 0446195\Thermal=0. 0521079\Dipole=0. 5994026, 0. 9158568, 0. 30935
07\DipoleDeriv=2. 3442296, 0. 7780974, -0. 4999721, 1. 7034109, 0. 759215, -0. 38
92777, -1. 0124, -0. 3120826, 0. 430725, -1. 9696924, -0. 2868804, 0. 3186253, -0. 7
```

521954, -0.4814727, 0.1893954, 0.3109019, 0.1227126, -0.2979543, 0.5081637, 0.034211, -0.0133163, 0.0604326, 0.3324022, -0.0586626, -0.2164375, -0.0907043, 0.2684964, 0.778748, 0.0997626, -0.1239403, -0.4163493, -0.0187368, 0.0465794, 0.0536296, -0.024764, 0.0218626, 1.1429538, -0.1797205, -0.0487657, -0.6419017, 0.1790024, 0.0175726, 0.0641886, -0.0348983, 0.0054749, -0.8799982, 0.0330992, 0.0530127, 1.2835078, -0.9212228, 0.0862337, -0.2878726, 0.2059662, -0.2254229, 0.2851247, -0.3198671, 0.0853222, -1.3570112, 1.4287666, -0.2057013, 0.3833029, -0.3086196, 0.2946098, -0.3299731, 0.2689779, -0.0494328, 0.8600562, -0.6774911, 0.0892422, -0.2215569, 0.1507787, -0.0829263, -1.8795561, -0.42768, 0.278467, -0.7399499, -0.6004628, 0.2246182, 0.9262441, 0.2916112, -0.4148652\Polar=128.8850504, 0.0437742, 65.9272668, -9.5888886, -9.2303158, 38.2440759\PG=C01 [X(C1H1N7)]\NImag=0\\

#### Im7

1\1\GINC-ZHANGRUBO-3\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\\Title Card Required\\0,1\N,2.0237914204, -0.2559139032, 0.0046107742\N,0.9684682313, -0.6724903339, 0.0406506689\N, -0.0996011494, -1.3285694835, 0.1216041638\N, -1.2214367588, -0.5059899322, 0.0383002151\C, -2.4945626363, -0.923999767, -0.1038511431\H, -2.7908935688, -1.9557199898, -0.2070366948\N, -1.2024434039, 0.8411845055, 0.1464557454\N, -2.4428170443, 1.2121014515, 0.0582084151\N, -3.2691260901, 0.1449774527, -0.0929941445\\Version=EM64L-G09RevA.01\HF=-421.8078323\RMSD=4.928e-09\RMSF=3.268e-05\ZeroPoint=0.0485485\Thermal=0.0547532\Dipole=0.7564482, -1.4314711, -0.0960581\DipoleDeriv=-1.0364779, -0.1170671, 0.037909, -0.346668, -0.0744967, 0.0112461, 0.0164138, 0.0051928, -0.0554599, 1.882118, 0.4531879, -0.0829502, 0.9472348, 0.2819762, -0.0121264, -0.0716544, -0.0220825, 0.2375115, -1.0044738, -0.1623563, 0.0100892, -0.8217061, -0.1504762, -0.014404, 0.0533867, 0.0189697, -0.1365526, 0.3202002, -0.1164673, 0.0414078, 0.3243284, -0.1097576, 0.0114511, 0.0348886, -0.0223833, 0.1066991, 0.6251503, -0.0708082, 0.0079461, -0.0367923, 0.1851194, -0.0027806, 0.0235937, -0.0003076, 0.107389, 0.1378286, 0.0172609, -0.003616, 0.02726, 0.0981081, -0.0045768, -0.0031071, -0.0060125, 0.1799298, -0.2939578, -0.2580225, -0.0449815, -0.4671373, 0.1159703, 0.0101921, -0.0699716, 0.0027445, -0.0663149, -0.2889773, 0.2590387, 0.0422103, 0.2153464, -0.0007234, 0.025513, -0.0057596, 0.0297294, -0.1624841, -0.3414104, -0.0047662, -0.0080148, 0.1581343, -0.34572, -0.0245145, 0.02221, -0.0058505, -0.2107179\Polar=99.8640644, 1.1587895, 56.7933236, 1.0808444, 0.9625869, 33.4222468\PG=C01 [X(C1H1N7)]\NImag=0\\

#### Im8

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N6\ROOT\10-Sep-2012\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\\Title Card Required\\0,1\C,3.7095275142, 0.2889019148, 0.034736029\N,2.7570046404, -0.5083186706, 0.0687270192\H,5.2434194574, 1.3457607481,



0.6273542769\N, 1.4676537985, 0.0123407897, -0.0149082873\N, 0.6511007687,  
-0.9347928849, 0.0373011329\N, -0.6383808075, -0.4138491773, -0.0454740374  
\C, -1.5911102567, -1.210885629, -0.0117481407\H, -3.125578444, -2.26839162  
85, -0.6024823375\N, 4.7405385247, 0.913920914, -0.1409660854\N, -2.6215281  
957, -1.8365343762, 0.1651554303\\Version=EM64L-G09RevA.01\State=1-A\HF=  
-405.787842\RMSD=2.188e-09\RMSF=4.923e-05\ZeroPoint=0.0562289\Thermal=  
0.0641587\Dipole=-0.0007543, 0.0001282, 0.0000479\DipoleDeriv=2.5313051,  
1.2611551, -0.1357537, 2.0037143, 1.2666555, -0.1237713, -0.4565671, -0.2291  
213, 0.2387397, -2.1977918, -0.8240266, 0.089821, -0.8455054, -0.6783624, 0.0  
645105, -0.0395003, 0.0356426, -0.2320813, 0.5448135, 0.0909838, 0.0241933, 0  
.1080445, 0.3857743, -0.0340649, -0.170572, -0.1011041, 0.2295029, 1.175817,  
0.2817361, -0.0081246, -0.3020118, -0.0807931, 0.0033816, 0.0643428, -0.0145  
41, 0.0187308, 1.1756707, 0.2814982, -0.0088009, -0.3022002, -0.0806822, 0.00  
2984, 0.0636085, -0.0147455, 0.0187099, -2.1983458, -0.8242252, 0.0904813, -0  
.8449225, -0.6784386, 0.0650511, -0.0390403, 0.0357822, -0.2320603, 2.530558  
6, 1.2609361, -0.1365142, 2.0039103, 1.2668903, -0.1244735, -0.4586614, -0.23  
00982, 0.2386497, 0.544619, 0.0907926, 0.0239348, 0.1080872, 0.3858629, -0.03  
4065, -0.1711617, -0.1012261, 0.229533, -2.0540435, -0.8098181, 0.0300603, -0  
.9642565, -0.8932591, 0.090124, 0.6023671, 0.3091448, -0.2548391, -2.0526027  
, -0.8090318, 0.0307028, -0.9648599, -0.8936477, 0.0903235, 0.6051845, 0.3102  
665, -0.2548854\Polar=166.514576, 52.5317182, 65.6601782, -2.8519853, -2.01  
21512, 38.0323892\PG=C01 [X(C2H2N6)]\NImag=0\\

#### Im9 (Im11)

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\N6\ROOT\17-Sep-2012\0\\#N  
Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\\  
Title Card Required\\0,1\N, 1.1300943314, -2.1494049633, -0.2431328922\N,  
0.2269230737, -1.5087126442, 0.0290173335\N, -0.7402808354, -0.8726310551,  
0.4927926429\N, -1.3417351044, -0.0891568181, -0.5590184216\N, -2.30901523  
12, 0.5468204217, -0.0952597893\N, -3.2124092342, 1.187225059, 0.1768291268  
\\Version=EM64L-G09RevA.01\State=1-A\HF=-328.3375994\RMSD=2.299e-09\RM  
SF=4.992e-05\ZeroPoint=0.0243004\Thermal=0.0297988\Dipole=0.0000215, 0.  
0000327, 0.0000042\DipoleDeriv=-0.8936579, 0.5739501, 0.1876518, 0.554087,  
-0.5060432, -0.1380314, 0.256976, -0.1931773, -0.1443424, 1.714116, -1.04198  
93, -0.4429399, -0.954075, 0.9028466, 0.3516623, -0.7473035, 0.5939999, 0.248  
8145, -0.8204643, 0.4680236, 0.2552934, 0.400005, -0.3967943, -0.2136172, 0.4  
903091, -0.4008569, -0.1044766, -0.8206199, 0.4679931, 0.2552848, 0.3999306,  
-0.3966668, -0.2135921, 0.4903679, -0.4007174, -0.1044489, 1.7144932, -1.042  
0812, -0.4430023, -0.9537552, 0.9024978, 0.3515363, -0.7472558, 0.5938925, 0.  
2487806, -0.8938672, 0.5741038, 0.1877123, 0.5538077, -0.5058402, -0.1379579  
, 0.2569062, -0.1931408, -0.1443271\Polar=76.17166, -39.3052184, 52.7894358  
, -9.6651268, 6.2662503, 28.2441821\PG=C01 [X(N6)]\NImag=0\\

#### Im10

```
1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\17-Sep-2012\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\Title Card Required\0,1\N,-3.4486803793,0.1952342478,-0.0000070474\N,-2.4249157849,-0.303903724,-0.0000000674\N,-1.3985166592,-1.0175891885,0.000008593\N,-0.2305979558,-0.2391809747,0.0000045469\C,0.826646126,-0.9684131048,0.0000108133\H,0.8247359325,-2.0558840652,0.0000172424\N,2.4377821954,1.9300135984,-0.0000139804\N,2.1983146361,0.8218166696,-0.0000054083\N,2.1107548892,-0.4258454586,0.0000044865\Version=EM64L-G09RevA.01\State=1-A\HF=-421.8067918\RMSD=5.188e-09\RMSF=6.533e-05\ZeroPoint=0.046838\Thermal=0.0540351\Dipole=0.3706893,-0.4326849,0.000035\DipoleDeriv=-1.380502,0.2688999,-0.0000046,0.6594773,-0.2009075,0.0000019,-0.0000088,0.0000016,-0.1115535,2.2961202,-0.69329,0.0000099,-1.584938,0.4392803,-0.0000048,0.000018,-0.0000038,0.2193941,-1.5831513,0.2512654,-0.0000043,0.5850904,-0.3129609,0.0000029,-0.0000084,0.000018,-0.1693199,0.1360301,0.0062067,0.0000014,0.6029145,-0.2755538,0.0000008,-0.0000011,0.0000017,-0.1549778,1.4375819,0.3312119,-0.0000035,0.3962034,0.7940434,-0.0000051,-0.0000083,-0.0000051,0.1294808,0.0666133,-0.0213234,0.0000002,-0.009759,-0.0217792,0.0000015,0.0000012,0.000008,0.1640443,-0.2297054,-0.2258479,0.0000018,-0.8675093,-0.9041034,0.0000062,0.0000065,0.0000064,-0.0908145,0.1743185,0.2385531,-0.0000017,1.4106335,1.9483862,-0.0000129,-0.0000103,-0.0000135,0.2357201,-0.9173052,-0.1556756,0.0000007,-1.1921128,-1.4664052,0.0000094,0.0000111,0.0000101,-0.2219736\Polar=122.859689,4.4440663,72.2594759,0.0000847,-0.0003363,33.0094802\PG=C01 [X(C1H1N7)]\NImag=0\
```

## Im12

```
1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C1H1N5\ROOT\17-Sep-2012\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\Title Card Required\0,1\N,1.0350051307,-0.9314011993,0.0002574056\N,-0.0585239726,-1.3001720906,0.0001267891\C,-1.2986783813,-1.676758706,-0.0000132306\H,-1.5309531464,-2.7284880314,-0.0000720839\N,-2.1076160872,1.5835915099,0.0000543003\N,-2.1678509423,0.4403735622,-0.0000157179\N,-2.3876686009,-0.7773280448,-0.0001184624\Version=EM64L-G09RevA.01\State=1-A\HF=-312.3267832\RMSD=2.365e-09\RMSF=6.558e-05\ZeroPoint=0.0360656\Thermal=0.0418896\Dipole=-0.1545763,-0.7797912,-0.0000421\DipoleDeriv=-1.3522567,0.3130896,-0.0001054,-0.4357591,0.0092211,-0.000036,-0.0001527,0.0000418,-0.1094845,1.7593092,-0.0662791,0.0001458,0.7048412,-0.2893965,0.0000533,0.0002001,-0.0000302,0.1326638,-0.1986415,-0.0173421,0.0000122,-0.6986664,0.5259652,-0.0000543,-0.0000149,0.0000338,-0.2149233,0.0688767,0.033049,-0.0000182,0.0580537,0.0902558,0.0000011,-0.0000198,-0.0000004,0.2466096,-0.0472071,-0.0406208,0.000008,0.5736807,-1.2348108,-0.0000036,0.0000372,-0.0000623,-0.1360729,-0.1287236,0.3025535,-0.0000231,-0.5581834,2.1220028,0.0000632,-0.0000646,0.0001531,0.2045733,-0.101357,-0.5244501,-0.0000193,0.3560333,-1.2232376
```



, -0.0000237, 0.0000146, -0.0001357, -0.1233659\Polar=66.946437, -5.7012477  
, 64.4103047, 0.0038957, 0.001378, 26.2846231\PG=C01 [X(C1H1N5)]\NImag=0\

### Im13

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C1H1N5\ROOT\17-Sep-2012\0  
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) F  
req\\Title Card Required\\0,1\C, 2.6391054509, -0.011992581, 0.0192314938  
\N, 1.6847756834, -0.8001973188, -0.0158150446\H, 4.1870832079, 0.923340114  
3, 0.6989390626\N, 0.377801603, -0.2579954113, 0.0492105939\N, -0.476435546  
9, -1.1725641778, 0.031406917\N, -1.3809221414, -1.8649611088, 0.0221789363  
\N, 3.667015743, 0.6392774834, -0.128725959\\Version=EM64L-G09RevA.01\Sta  
te=1-A\HF=-312.3375751\RMSD=2.199e-09\RMSF=6.874e-05\ZeroPoint=0.03587  
3\Thermal=0.0416156\Dipole=0.465865, 0.2794414, 0.6204783\DipoleDeriv=1.  
7876697, 1.0931676, -0.0623634, 1.4828267, 1.1405912, -0.0721955, -0.2076607  
, -0.1294384, 0.1771134, -0.5802981, -0.4350145, 0.0610553, -0.9038765, -0.72  
78648, 0.0504587, -0.0897001, 0.006037, -0.1528255, 0.4265961, 0.0539285, 0.0  
199069, 0.0648447, 0.3644449, -0.0167411, -0.1414512, -0.0746778, 0.1713896,  
-0.6315111, -0.5852937, -0.0301215, -0.7987935, -0.5663462, 0.0007261, -0.00  
58231, -0.0275684, -0.143344, 1.5134164, 1.1503827, 0.0163399, 1.576299, 1.20  
59667, -0.001114, 0.0470887, 0.0106155, 0.2354004, -0.9557889, -0.6028033, -0  
.0029497, -0.6865154, -0.5547612, 0.0008683, -0.0134316, -0.0034789, -0.1091  
786, -1.560084, -0.6743674, -0.0018675, -0.734785, -0.8620307, 0.0379974, 0.4  
109781, 0.2185111, -0.1785553\Polar=93.2749643, 36.9349522, 50.1653565, -0.  
3228674, -0.2006257, 26.72777\PG=C01 [X(C1H1N5)]\NImag=0\

### Im14

1\1\GINC-ZHANGRUBO-1\Freq\RB3LYP\6-31+G(d,p)\C1H1N9\ROOT\07-Sep-2012\0  
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) F  
req\\Title Card Required\\0,1\N, -1.5912597925, -0.2787907573, 0.21368575  
25\N, -0.2426107547, -0.5272634286, 0.1750212715\N, 0.4724595506, 0.4924009  
638, 0.0451700045\N, 1.81780238, 0.2016227628, 0.0107046538\C, 2.7882662744  
, 1.140955789, -0.1239352355\H, 2.5939863063, 2.1980299764, -0.2167621964\N  
, -1.9364036699, 0.9504117975, 0.1121415027\N, -2.437902901, 1.9607951609, 0  
.0379866117\N, 2.407845131, -1.0252497425, 0.101496077\N, 3.6735425885, -0.  
8017666096, 0.0223539335\N, 3.9507288872, 0.5361550875, -0.1187663753\\Ver  
sion=EM64L-G09RevA.01\State=1-A\HF=-531.2561286\RMSD=1.664e-09\RMSF=2.  
539e-05\ZeroPoint=0.057062\Thermal=0.065125\Dipole=-1.4707581, 1.466513  
3, -0.0734417\DipoleDeriv=-1.1584924, 0.1980503, 0.0256176, 1.367077, -0.85  
8219, 0.0017399, -0.0850523, 0.0549704, -0.1873765, 1.4221639, -0.1564982, -0  
.0477225, -0.3685821, 0.1148023, 0.0114921, -0.0279838, 0.0019667, 0.058701,  
0.5488543, 0.0772341, -0.032307, -0.7860658, -0.0353192, 0.0402347, 0.050134  
3, 0.000112, 0.0042991, -1.1020597, 0.0887243, 0.043765, 0.4841577, -0.038627  
3, -0.0143959, 0.0059515, 0.0041241, 0.0423121, 0.9637845, -0.0261557, -0.036  
4914, 0.3676728, 0.1302745, -0.0188506, -0.0738618, -0.0008354, 0.1137454, 0.

1115624, 0.0255954, 0.0003203, 0.0415626, 0.1076837, 0.0042991, -0.0012373, 0.0050556, 0.1719991, 0.4829188, -0.4883432, 0.0355442, -1.53369, 1.3946735, -0.0400197, 0.1355394, -0.0882377, 0.2425156, -0.4202913, 0.3215946, -0.0128216, 0.8762952, -0.5927888, 0.0130888, -0.0663914, 0.0392116, -0.0333392, 0.2712941, -0.372239, 0.0213627, -0.7003178, -0.051883, 0.0327822, 0.0527098, 0.0176225, -0.0486668, -0.5832243, 0.2176874, -0.0017812, -0.1007893, 0.2636389, -0.0368663, 0.0288771, -0.0513989, -0.1645428, -0.5365102, 0.11435, 0.004514, 0.3526797, -0.4342356, 0.0064956, -0.0186856, 0.0174089, -0.1996469\Polar=138.7950351, -17.3823154, 82.0037449, -2.8368015, -3.1629128, 41.1190912\PG=C01 [X(C1H1N9)]\NImag=0\

## Im15

1\1\GINC-ZHANGRUBO-1\Freq\RB3LYP\6-31+G(d,p)\N8\ROOT\11-Sep-2012\0\#N  
Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq\  
\Title Card Required\0,1\N,-2.4240212412,-0.9822117325,-0.382585357\N  
, -1.0535446944, -0.9687445482, -0.1716031977\N, -0.6000395697, 0.105966031  
5, 0.2917036293\N, 0.7706709717, 0.1194496866, 0.5026028072\N, -3.037079755  
4, 0.0897765175, -0.0808355531\N, -3.7416323657, 0.9517506984, 0.1295315707  
\N, 1.3833043176, -0.9526207085, 0.2006613237\N, 2.0857453371, -1.815940944  
8, -0.0110672232\Version=EM64L-G09RevA.01\State=1-A\HF=-437.787329\RMS  
D=7.289e-10\RMSF=6.202e-05\ZeroPoint=0.0329861\Thermal=0.0401633\Dipol  
e=-0.0002996, 0.0000132, -0.0000147\DipoleDeriv=-1.3025939, 0.351146, -0.0  
38651, 1.163718, -0.7295068, -0.0236541, 0.2602112, -0.146075, -0.2027787, 1.  
0674961, -0.0303191, 0.148046, -0.4436179, 0.0182972, -0.0634432, -0.0039489  
, -0.0012947, 0.0084074, 1.0684101, -0.030984, 0.1478311, -0.4432151, 0.01806  
28, -0.0634024, -0.0038235, -0.001424, 0.0081195, -1.3037954, 0.3523874, -0.0  
382527, 1.163371, -0.7302356, -0.0242998, 0.2600752, -0.1462469, -0.2029437,  
0.9577181, -0.7369944, -0.1618447, -1.5772668, 1.2204487, 0.1254581, -0.4703  
025, 0.2516511, 0.254961, -0.7223486, 0.4161673, 0.052526, 0.8571329, -0.5091  
434, -0.038337, 0.2140877, -0.1042843, -0.0604185, 0.9553927, -0.7365723, -0.  
1621143, -1.5785947, 1.2218721, 0.1260089, -0.4717486, 0.2526878, 0.2551555,  
-0.7202792, 0.4151692, 0.0524595, 0.8584726, -0.509795, -0.0383305, 0.215449  
4, -0.105014, -0.0605026\Polar=117.2352627, -32.0724021, 65.1190102, 1.1446  
669, 7.6202025, 34.2274\PG=C01 [X(N8)]\NImag=0\

## Corresponding to Fig 2

### TS1

1\1\GINC-ZHANGRUBO-1\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ROOT\07-Sep-2012\  
0\# opt=(calcall,ts,noeigentest) b3lyp/6-31+g(d,p) geom=connectivity\  
\Title Card Required\0,1\C,-3.1940549524,-1.2917341511,-0.0360668734\  
N,-1.6224260276,-0.1765431868,0.1539265318\H,-2.7565524116,-2.27380096  
38,0.0041553787\N,-0.3368231638,-0.4092239741,0.1083590436\N,0.4441433  
114,0.5725465452,0.0613073086\N,1.7699318571,0.1752066547,0.0181890707

```
\C, 2. 8114945424, 1. 0381615505, -0. 0523900929\H, 2. 7040153786, 2. 1109689016
, -0. 0856272954\N, -2. 1628641095, 1. 0625921863, 0. 0666709736\N, -3. 29068099
25, 1. 3252669736, -0. 037527703\N, 2. 2561847337, -1. 0950148279, 0. 0453340536
\N, 3. 5401071163, -0. 972633367, -0. 0096726078\N, -4. 1469725085, -0. 58249797
45, -0. 1246293701\N, 3. 9237842263, 0. 3404176333, -0. 071839418\Version=EM6
4L-G09RevA. 01\State=1-A\HF=-624. 6567929\RMSD=4. 034e-09\RMSF=2. 353e-06\
ZeroPoint=0. 0753517\Thermal=0. 0853816\Dipole=-1. 0199132, 0. 4846798, 0. 04
57555\DipoleDeriv=0. 6031613, -0. 0317748, 0. 0315158, 0. 4053428, 0. 2009769, 0
. 0226754, 0. 0253773, -0. 0150998, 0. 0844653, -0. 9570624, -0. 0205449, 0. 027896
6, 0. 8915124, 0. 0219645, 0. 0270799, 0. 0006338, 0. 0478477, -0. 1226493, 0. 16347
59, 0. 0070706, -0. 0042373, 0. 0076514, 0. 2256225, -0. 0054868, -0. 0011315, 0. 00
20336, 0. 2181047, 1. 1383527, 0. 2679838, -0. 0582318, -0. 0156264, -0. 0347363, -
0. 0022186, -0. 0447429, -0. 0092882, 0. 0965054, 0. 4941036, 0. 0063511, -0. 01715
07, -1. 1798465, -0. 0760006, 0. 019123, 0. 0156, -0. 0107518, -0. 0236803, -1. 0047
109, 0. 022029, 0. 01771, 0. 6450681, -0. 0501098, -0. 0125046, 0. 0178316, 0. 01152
, 0. 0425029, 1. 0372833, 0. 0141369, -0. 0191685, 0. 3310962, 0. 1719512, -0. 00477
75, -0. 0409536, -0. 0028826, 0. 1037446, 0. 1243011, 0. 0251662, 0. 0016187, 0. 048
2819, 0. 1081475, 0. 0013977, 0. 0003278, 0. 0014973, 0. 1731148, -0. 1100985, -1. 0
733149, -0. 0273072, -1. 0627716, -0. 0319151, -0. 0557448, -0. 0122338, -0. 10718
52, 0. 1229423, -0. 0293568, 0. 913617, 0. 0407676, 0. 7313845, 0. 2844756, 0. 03338
41, 0. 0139626, 0. 0909126, -0. 014549, 0. 1939034, -0. 3387292, 0. 0105789, -0. 779
8346, -0. 0871898, 0. 0158294, 0. 0152192, 0. 0124746, -0. 0484831, -0. 676917, 0. 1
853428, -0. 0046735, -0. 0300991, 0. 2007291, -0. 0166934, 0. 0255752, -0. 0198725
, -0. 1744106, -0. 4378243, -0. 0316216, -0. 0008963, -0. 3872671, -0. 5457579, -0.
0256272, -0. 0092737, -0. 004572, -0. 2571271, -0. 5386115, 0. 0542881, 0. 0015775
, 0. 395108, -0. 3881579, 0. 0035632, -0. 006192, 0. 0033662, -0. 2004807\Polar=19
9. 8343064, 1. 3256348, 97. 3615191, 0. 5302264, -0. 6771542, 51. 0083018\PG=C01
[X(C2H2N10)]\NImag=1\
```

## TS2

```
1\1\GINC-ZHANG-X58A-UD3R\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ZHANG\02-Aug-
2012\0\#n b3lyp/6-31+g(d,p) opt(ts,calcall,noeigentest) guess(read)\
Title Card Required\0,1\C,-2. 4301226193,-1. 1004165048, 0. 0003151636\N,
-1. 5665734428, -0. 1223292628, 0. 0001082351\H, -2. 1521190505, -2. 1498067399
, 0. 0004693863\N, -0. 2509509529, -0. 4618809977, 0. 0000891084\N, 0. 476113550
7, 0. 555984143, -0. 0001074852\N, 1. 8145593011, 0. 2341886497, -0. 0001332048\
C, 2. 8071756145, 1. 160467156, -0. 0003240745\H, 2. 6330830709, 2. 2251606049, -
0. 0004692514\N, -3. 0908599303, 1. 371358854, -0. 0000504116\N, -3. 849093605,
0. 4955364413, 0. 0001338769\N, 2. 3806917208, -1. 0086621604, 0. 0000156469\N,
3. 6516976427, -0. 8060454543, -0. 0000853081\N, -3. 7655228046, -0. 84087994, 0
. 0003475494\N, 3. 9578435048, 0. 5343622112, -0. 000297231\Version=EM64L-G0
9RevB. 01\State=1-A\HF=-624. 6952541\RMSD=3. 892e-09\RMSF=2. 120e-05\ZeroP
oint=0. 078617\Thermal=0. 0877364\Dipole=-1. 3611888, 0. 6456523, -0. 0000104
\DipoleDeriv=1. 4878988, 0. 0798252, -0. 0000862, 0. 6531611, 0. 3001092, -0. 000
```

0597, -0.0001765, -0.0000281, 0.1480201, -1.9506104, -0.1340441, 0.0001173, -  
0.5629813, -0.1332102, 0.0000248, 0.0001897, 0.0000022, -0.1708033, 0.145421  
, 0.0189028, -0.0000028, 0.0726832, 0.110168, 0.0000022, -0.0000126, 0.000004  
8, 0.1474411, 1.0983482, 0.1969774, -0.0000866, 0.2747719, -0.1728485, 0.0000  
232, -0.0001052, 0.0000255, 0.0600471, 1.0412282, 0.0487536, -0.0000659, -0.8  
545641, -0.0793157, 0.0000575, 0.0000744, 0.0000094, -0.0031899, -1.3347341,  
-0.0748147, 0.0000893, 0.6107809, -0.0388007, -0.0000224, -0.0000144, 0.0000  
149, 0.0421792, 1.116949, 0.0706476, -0.0000674, 0.4253864, 0.2091672, -0.000  
0379, -0.000121, -0.0000176, 0.1134637, 0.1191759, 0.0232139, -0.0000004, 0.0  
482164, 0.1185356, 0.0000051, -0.0000043, 0.0000061, 0.1713798, 1.8342185, -0  
.5496881, -0.0000091, 0.4311854, -0.475768, 0.0000593, -0.0001693, 0.0001124  
, 0.0309504, -1.792749, 0.3407447, 0.0000463, -1.1485237, 0.8507869, -0.00006  
62, 0.0002895, -0.0001467, 0.06258, 0.2999554, -0.3066704, 0.0000251, -0.8001  
794, -0.1514374, 0.0000612, 0.0000999, 0.0000334, -0.0434282, -0.7060774, 0.1  
223851, 0.0000121, -0.1463119, 0.2216327, -0.0000489, 0.0000487, -0.0000643,  
-0.1711613, -0.756087, 0.1073754, 0.0000134, 0.5450882, -0.3972102, 0.000004  
1, -0.0000581, 0.0000273, -0.1887556, -0.6029369, 0.0563916, 0.0000149, 0.451  
2868, -0.3618089, -0.0000023, -0.0000407, 0.0000207, -0.198723\Polar=206.95  
95782, 4.07208, 96.1853491, -0.0092888, -0.0073517, 50.2705979\PG=C01 [X(C2  
H2N10)]\NImag=1\

### TS3

1\1\GINC-ZHANG-X58A-UD3R\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ZHANG\02-Aug-  
2012\0\#n b3lyp/6-31+g(d,p) opt(ts,calcall,noeigentest)\Title Card R  
equired\0,1\C,-2.3727910841,-1.0775420506,-0.0001985028\N,-1.52050230  
98,-0.0605702339,-0.0004005442\H,-2.019124962,-2.1332073909,-0.0000405  
008\N,-0.2176633985,-0.3895499471,-0.0004034903\N,0.5233518476,0.62157  
71863,-0.0005977422\N,1.8613346429,0.2660806106,-0.0005989815\C,2.8732  
365289,1.1657577714,-0.0007854743\H,2.7263310449,2.2343138487,-0.00094  
74497\N,-3.5074390096,1.4844112303,-0.0005714843\N,-4.2402761228,0.642  
8920592,-0.0004019426\N,2.3935652567,-0.986327945,-0.0004252785\N,3.67  
37719329,-0.8173616024,-0.0005083088\N,-3.6262318837,-1.2710964018,-0.  
0001141651\N,4.0111135167,0.5101018653,-0.0007321349\Version=EM64L-G0  
9RevB.01\State=1-A\HF=-624.6737629\RMSD=5.483e-09\RMSF=1.606e-06\ZeroP  
oint=0.0736944\Thermal=0.084274\Dipole=-1.95949,0.4755073,0.000014\Dip  
oleDeriv=0.5092571,0.8795778,-0.0001586,0.8948297,0.3076024,-0.0000617  
, -0.0001597, -0.0000605, 0.1606187, -1.3748283, -0.5252786, 0.0001345, -1.03  
72691, -0.3046507, 0.0000561, 0.0002187, 0.0000348, -0.2275631, 0.178595, 0.0  
288614, -0.000004, 0.1489759, 0.3517389, -0.000032, -0.0000233, -0.0000269, 0  
.1949717, 1.2343982, 0.3742805, -0.0001097, 1.0090566, -0.0136808, -0.000024  
9, -0.0002148, 0.0000011, 0.0929542, 0.8212858, 0.0363123, -0.0000428, -1.163  
6829, -0.1852534, 0.0000731, 0.0001493, 0.0000223, -0.0394566, -0.9814677, -0  
.0848518, 0.0000583, 0.6172155, -0.0319808, -0.0000158, -0.0000521, 0.000014  
3, 0.0391155, 1.0181943, 0.0942273, -0.0000554, 0.3450795, 0.2175304, -0.0000

329, -0.0000957, -0.0000217, 0.1039577, 0.1219602, 0.0246531, -0.0000016, 0.04912, 0.1099291, 0.0000078, -0.0000057, 0.0000085, 0.1726462, 0.9196334, -0.0279526, -0.0000326, 0.2099669, 0.0194466, -0.0000054, -0.0000718, 0.0000048, 0.0420412, -0.7944419, 0.1447452, 0.0000118, -0.1409176, -0.2314681, 0.0000514, 0.0000592, 0.0000393, 0.0444581, 0.2121624, -0.2865563, 0.0000336, -0.7193917, -0.1798813, 0.0000521, 0.0001022, 0.000033, -0.0517759, -0.6828589, 0.1002222, 0.000006, -0.083228, 0.1777732, -0.0000528, 0.0000344, -0.0000607, -0.1790129, -0.5953274, -0.7776708, 0.0001465, -0.5078911, 0.0948321, -0.0000183, 0.0001015, -0.0000071, -0.1471773, -0.5865621, 0.0194303, 0.0000139, 0.3781364, -0.3319375, 0.0000031, -0.000042, 0.0000191, -0.2057774\Polar=218.2199338, 14.7781719, 98.2684819, -0.0095717, -0.0082431, 51.051286\PG=C01 [X(C2H2N10)]\NImag=1\

#### TS4

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\R00T\06-Sep-2012\0\#\freq b3lyp/6-31+g(d,p) geom=(connectivity,check) guess=read\Title Card Required\0,1\C,-2.3321392621,1.027923962,-0.0001927833\N,-1.5403463082,0.0078206412,-0.0000423206\H,-1.991904774,2.0618341422,-0.0002887934\N,-0.2224339441,0.4276217274,-0.0000235349\N,0.5363808841,-0.5726463772,0.0001243505\N,1.8498097551,-0.1888016836,0.0001458611\C,2.7405833322,-1.1314310393,0.0003007783\H,2.5031544051,-2.1906886794,0.0004100737\N,-4.7361915026,-1.2424356993,-0.0000643928\N,-4.1670114145,-0.2653052377,-0.000142618\N,3.3679114958,1.3706170361,0.0000395831\N,4.125478714,0.4944457147,0.0001844689\N,-3.7104304611,0.9060510941,-0.0002477271\N,4.0798310805,-0.8315336013,0.0003350546\Version=EM64L-G09RevA.01\State=1-A\HF=-624.6904603\RMSD=4.174e-09\RMSF=8.585e-06\ZeroPoint=0.0771692\Thermal=0.0872913\Dipole=-0.6359645,0.1606191,-0.0000468\DipoleDeriv=2.4568781,0.1277124,0.0000992,-0.4696805,0.6604764,-0.000765,0.0001643,-0.0000469,0.1728385,-1.5981207,0.0389321,-0.0000724,0.6320276,-0.391594,0.0000488,-0.0001374,0.0000194,-0.2295262,0.0636451,-0.043029,0.0000003,-0.0292388,0.0034728,0.0000148,-0.0000015,0.0000142,0.1526131,0.898583,-0.0778087,0.0000547,0.4457511,-0.024757,0.0000212,-0.0000032,-0.000004,-0.0305307,0.9372697,-0.1495805,0.0000625,-0.209803,-0.2212023,0.0000141,0.0000743,0.0000165,-0.0088761,-1.8842578,0.0858425,-0.0000942,0.6311245,-0.1500104,0.000029,-0.00016,0.0000023,-0.1654002,1.5593681,-0.0428802,0.0000761,-0.5995968,0.3133501,-0.0000501,0.0001421,-0.0000227,0.1287561,0.1408645,-0.0244066,0.0000025,-0.0810648,0.0755352,0.0000042,0.0000084,0.000007,0.1466107,-0.6827614,-0.3334193,0.0000058,-1.1096227,-0.5147997,-0.0000062,0.0000903,0.0000323,-0.0668417,1.0200868,0.6072918,-0.0000274,2.1760839,1.3404406,-0.0000121,-0.0001984,-0.00009,0.2384012,1.8624975,0.6131531,0.0000222,-0.487816,-0.5355247,0.0000393,0.0001565,0.0000979,0.0157505,-1.9589292,-0.4438212,-0.0000503,1.187252,0.9438529,-0.0000453,-0.000249,-0.0001276,0.0561967,-1.999854,-0.2837546,-0.0000576,-1.4752685,-1.0248569,0.0000151

, 0.0000729, 0.0000744, -0.213873, -0.8152698, -0.0742318, -0.0000214, -0.610148, -0.4743831, 0.0000036, 0.0000406, 0.0000273, -0.196119\Polar=248.2731505, 5.0619784, 106.9064796, 0.0092438, -0.0060319, 51.0713875\PG=C01 [X(C2H2N10)]\NImag=1\\

#### TS5

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ROOT\07-Sep-2012\0\#\# freq b3lyp/6-31+g(d,p) geom=(connectivity,check) guess=read\\Title Card Required\\0,1\C,2.3097359031,1.5999985006,0.0046702615\N,1.4317270218,0.6308402821,0.0009311031\H,2.0276808095,2.6856605772,0.0085406471\N,0.1371906855,1.0777696253,0.0021021697\N,-0.6630048404,0.1091708134,-0.0016560346\N,-1.9652087729,0.592406919,-0.0003529352\C,-2.8096263325,-0.3794087829,-0.0041785608\H,-2.5300257019,-1.4312239245,-0.0079054317\N,4.9547377322,-0.9048935791,-0.0053414728\N,4.1662896492,-0.129700007,-0.001582972\N,-5.090625713,2.0197197557,0.0036935608\N,-4.5788109656,1.0094941897,0.0002389905\N,3.5769452134,1.7638389188,0.0055615777\N,-4.1857966084,-0.1808842283,-0.0039342433\\Version=EM64L-G09RevA.01\State=1-A\HF=-624.6685214\RMSD=9.826e-09\RMSF=4.605e-06\ZeroPoint=0.0718821\Thermal=0.0838056\Dipole=0.5946231,-0.0715202,-0.0002631\DipoleDeriv=1.069617,0.9327685,0.0037667,1.6046387,0.5005672,0.0015959,0.0060519,0.0014345,0.1607127,-1.8757834,-0.4611105,-0.0021672,-1.0808642,-0.3911164,-0.0006928,-0.0045297,-0.0005562,-0.2568576,0.0678052,0.04569,0.0001633,0.0579229,0.2404372,0.0002584,0.0001232,0.0002018,0.1780177,1.7349792,0.3204354,0.0016619,0.4367649,-0.1251054,-0.0004492,0.0022618,-0.0004096,0.0136965,0.2031978,0.0000054,0.0000793,-0.6486463,-0.102839,-0.00028,-0.0022926,-0.0000885,-0.0785439,-1.1511081,0.0019747,-0.000277,-0.5186679,-0.4135369,-0.0008399,-0.0021863,-0.0006876,-0.2250112,2.2042252,-0.170966,0.000052,0.1428636,0.6804049,0.0019571,0.0012281,0.0018687,0.1498142,0.0585085,0.042952,0.0001215,0.0266175,-0.0163329,-0.000615,0.0000764,-0.0006091,0.1551285,-0.3487675,0.1079837,0.0002361,0.1192264,-0.0097374,0.0000023,0.0008609,-0.0002515,0.0244521,0.538946,-0.0222636,0.0000969,0.4768028,-0.2509127,-0.0014183,0.0013324,-0.0012306,0.1038214,-0.6449676,0.330506,0.0010181,1.1785276,-0.5953433,-0.0014817,0.0040459,-0.0017252,-0.0829131,0.8531163,-0.5675594,-0.0018571,-2.1728956,1.4492588,0.0037019,-0.0076291,0.004195,0.2317999,-0.9418372,-0.8113668,-0.0033086,-1.128668,0.1405911,0.0009742,-0.0042598,0.0009882,-0.1562349,-1.7679315,0.2509506,0.0004139,1.5063776,-1.1063351,-0.0027129,0.0049168,-0.00313,-0.2178823\Polar=261.3581636,-4.1256904,108.2391979,0.0357595,0.2101064,52.3340842\PG=C01 [X(C2H2N10)]\NImag=1\\

#### TS6

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N8\ROOT\13-Sep-2012\0\#\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Required\\0,1\C,3.1624859735,0.7718642956,0.1274708533\N,2.1515276963,-0



. 6177483207, 0. 0804175128\H, 5. 3224476861, 0. 7085972679, 0. 186937097\N, 0. 9  
614102155, -0. 4703227609, 0. 0511773827\N, -0. 0574792342, -1. 2181727603, 0. 0  
188658631\N, -1. 2274259986, -0. 4364971181, 0. 0058970182\C, -2. 4774743035, -  
0. 9276255693, -0. 0844644412\H, -2. 7137256637, -1. 9764644234, -0. 1668686513  
\N, -1. 2900446869, 0. 908459801, 0. 0971675611\N, -2. 5544147911, 1. 205065138,  
0. 0578139401\N, 4. 3351622222, 0. 8788542512, 0. 1613299219\N, -3. 3209941158,  
0. 088886199, -0. 0540590577\\Version=EM64L-G09RevA. 01\HF=-515. 1684655\RM  
SD=7. 105e-09\RMSF=8. 233e-07\ZeroPoint=0. 0646047\Thermal=0. 073736\Dipol  
e=3. 038104, -0. 941566, -0. 0073112\DipoleDeriv=2. 128566, 0. 7024103, 0. 06113  
39, -0. 4354606, -0. 2853578, -0. 0145086, 0. 0429656, 0. 0138667, 0. 1035015, -0. 2  
219936, 0. 4277601, 0. 0095597, -0. 3160055, -0. 1417716, -0. 0090607, -0. 0048393  
, 0. 0127687, -0. 1745447, 0. 6454134, 0. 0583768, 0. 007136, 0. 2505575, 0. 4943512  
, 0. 0074502, 0. 0111582, 0. 0030782, 0. 4008905, 0. 5556865, -0. 2840894, 0. 000500  
1, 1. 7382639, 0. 7085154, 0. 0530515, 0. 0357643, -0. 0042995, 0. 1875733, -0. 0361  
797, 0. 0788387, -0. 0028764, -1. 6571768, -0. 3151203, -0. 0481199, -0. 0290666, 0  
. 0017954, -0. 0904198, -0. 0778693, 0. 0169593, 0. 0048454, 0. 7406107, -0. 097434  
3, 0. 0117729, 0. 0250776, -0. 0116252, 0. 0472226, 0. 7692225, -0. 0019767, 0. 0173  
03, 0. 0054638, 0. 1914559, 0. 0043976, 0. 0236492, 0. 0074817, 0. 0871463, 0. 14116  
29, 0. 0174209, -0. 0012772, 0. 0297942, 0. 0845539, -0. 005504, 0. 0000297, -0. 005  
6318, 0. 177539, -0. 2116072, -0. 2651369, -0. 0281146, -0. 5772457, -0. 0072773, -  
0. 0085684, -0. 0463012, -0. 0046105, -0. 0658005, -0. 5092696, 0. 1892226, 0. 0142  
924, 0. 2310666, 0. 0115132, 0. 0227596, -0. 0007174, 0. 0205346, -0. 1817956, -2. 7  
429502, -0. 914811, -0. 0748976, -0. 2511708, -0. 3330234, -0. 007436, -0. 0701071  
, -0. 026207, -0. 2734474, -0. 4401817, -0. 0249748, -0. 0076047, 0. 2413026, -0. 31  
04048, -0. 0062343, 0. 0123871, -0. 0071511, -0. 2178651\Polar=188. 3130188, 25.  
4683351, 81. 4295569, 4. 1830433, 2. 2204111, 44. 1388266\PG=C01 [X(C2H2N8)]\N  
Imag=1\\

## TS7

1\1\GINC-ZHANGRUBO-3\Freq\RB3LYP\6-31+G(d,p)\C2H2N8\ROOT\13-Sep-2012\0  
\\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Re  
quired\\0, 1\C, 3. 3112592752, 0. 0879203018, -0. 0166041634\N, 2. 2761266884, -  
0. 5911582363, 0. 0773383074\H, 5. 0057455568, 0. 9252150297, 0. 4662918982\N, 1  
. 0540860484, 0. 079599666, 0. 1432517793\N, 0. 1249089866, -0. 761206002, 0. 247  
498652\N, -1. 1095129691, -0. 2927915705, 0. 3123403801\C, -2. 7809416511, -1. 1  
355558916, -0. 1197941329\H, -2. 5143653436, -2. 174002587, -0. 0285286977\N, -  
1. 4123984908, 1. 0020980442, 0. 122942415\N, -2. 4453889359, 1. 474657954, -0. 1  
204703829\N, 4. 3880197575, 0. 6016420719, -0. 271835343\N, -3. 6060659224, -0.  
3015247802, -0. 330745712\\Version=EM64L-G09RevA. 01\HF=-515. 1867633\RM  
SD=5. 194e-09\RMSF=2. 934e-06\ZeroPoint=0. 0629445\Thermal=0. 0723385\Dipole  
=1. 0799316, -0. 2745203, 0. 665043\DipoleDeriv=2. 8711609, 0. 8358547, -0. 2542  
829, 1. 8897631, 0. 736094, -0. 1804154, -0. 662648, -0. 1754429, 0. 254309, -2. 246  
1562, -0. 3776613, 0. 1667652, -0. 6464052, -0. 4828053, 0. 094152, 0. 1130863, 0. 0  
730637, -0. 2246564, 0. 5479975, 0. 0364731, 0. 0013422, 0. 0933912, 0. 3514838, -0

. 0347191, -0. 2169774, -0. 0626914, 0. 2257307, 0. 7987248, 0. 0065154, -0. 072565  
, -0. 7982403, 0. 0255678, 0. 01477, -0. 0259427, -0. 0446649, -0. 0035288, 0. 92934  
02, 0. 2252873, -0. 1035543, -0. 3864719, -0. 0791844, 0. 0245453, -0. 0348252, -0.  
0325111, 0. 0404988, -0. 7416758, -0. 0957216, 0. 0665983, 1. 0062194, -0. 0640639  
, 0. 0543397, -0. 0297292, 0. 1348076, -0. 1424118, 0. 6783296, 0. 0163644, 0. 08289  
23, 0. 3247552, 0. 1776784, 0. 0376184, 0. 0743786, -0. 0262552, 0. 083781, 0. 16260  
23, 0. 0172485, -0. 012349, 0. 0025567, 0. 1941906, -0. 008656, -0. 003586, 0. 00797  
47, 0. 2120323, -0. 3548718, -0. 9785245, -0. 0908543, -1. 0315622, 0. 211798, -0. 1  
176739, -0. 0196022, -0. 252769, 0. 118683, 0. 132911, 0. 8646869, 0. 1041117, 0. 75  
19469, 0. 0032221, 0. 0626441, 0. 0313953, 0. 199669, -0. 0127684, -2. 2203428, -0.  
4589697, 0. 1247949, -0. 869422, -0. 6280924, 0. 1087229, 0. 8129761, 0. 1978033, -  
0. 274698, -0. 5580196, -0. 0915532, -0. 012899, -0. 336531, -0. 4458887, -0. 05532  
8, -0. 0385258, -0. 0189838, -0. 2769713\Polar=198. 2539454, 11. 8673357, 79. 691  
3089, 0. 5400468, -2. 3747218, 46. 6497344\PG=C01 [X(C2H2N8)]\NImag=1\

## TS8

1\1\GINC-ZHANGRUBO-1\Freq\RB3LYP/6-31+G(d,p)\C2H2N8\ROOT\13-Sep-2012\0  
\# freq b3lyp/6-31+g(d,p) geom=check guess=read\Title Card Required\  
\0, 1\C, 3. 3802214061, 0. 0818161284, 0. 018978152\N, 2. 3508495453, -0. 6158631  
163, 0. 0281153224\H, 5. 0315486698, 0. 9394432768, 0. 6271828589\N, 1. 12219890  
58, 0. 036328545, 0. 0198227951\N, 0. 208494284, -0. 8222090245, 0. 0152542091\N  
, -1. 0187204317, -0. 2189696558, 0. 0063245839\C, -2. 059024602, -0. 9943998503  
, -0. 010507055\H, -2. 0071341046, -2. 0786052494, -0. 0199411368\N, -2. 2308163  
504, 1. 5717868627, 0. 0105528542\N, -3. 1364544265, 0. 8490138037, -0. 00452732  
09\N, 4. 464923157, 0. 6092412689, -0. 1469467247\N, -3. 3238810528, -0. 4663339  
891, -0. 0184325381\Version=EM64L-G09RevA. 01\State=1-A\HF=-515. 2249612\  
RMSD=3. 853e-09\RMSF=1. 297e-06\ZeroPoint=0. 0660698\Thermal=0. 0746642\Di  
pole=0. 6813174, 0. 0297654, 0. 5724128\DipoleDeriv=3. 0227504, 0. 9036772, -0.  
1186828, 2. 0021153, 0. 8090255, -0. 0909721, -0. 4506656, -0. 1206343, 0. 2310219  
, -2. 5103229, -0. 4515742, 0. 085205, -0. 6905043, -0. 4866267, 0. 0481755, -0. 042  
3038, 0. 0295571, -0. 2249379, 0. 5869514, 0. 0491854, 0. 019525, 0. 1194925, 0. 363  
9991, -0. 028254, -0. 1967268, -0. 0626985, 0. 2290857, 1. 3323206, 0. 0470835, -0.  
0211913, -0. 5756501, 0. 0387743, 0. 0000951, 0. 009493, -0. 0236531, 0. 0169478, 0  
. 8402844, -0. 01419, 0. 0084934, -0. 0547081, -0. 2598942, 0. 0023886, 0. 0042227,  
-0. 0059417, 0. 0054531, -1. 7803141, 0. 0760064, -0. 0039729, -0. 266469, -0. 1177  
308, 0. 0006246, -0. 0118784, 0. 0041834, -0. 1699223, 1. 4993374, -0. 0696343, 0. 0  
028795, 0. 3157292, 0. 2879066, 0. 0010956, 0. 0126635, 0. 001833, 0. 1316149, 0. 15  
51311, 0. 0131086, -0. 0002624, 0. 0603072, 0. 0703424, -0. 0005204, 0. 0010993, -0  
. 0004985, 0. 1473402, 1. 677736, -0. 9196651, -0. 0017437, 0. 0254855, -0. 4004404  
, -0. 0061804, 0. 0182901, -0. 0126621, 0. 0196659, -1. 872215, 0. 8332188, -0. 0002  
379, -0. 5439605, 0. 8722969, 0. 0113027, -0. 0267021, 0. 0142021, 0. 0548479, -2. 3  
420788, -0. 5194457, 0. 0273736, -0. 9465011, -0. 6613264, 0. 0674961, 0. 6786157,  
0. 1784411, -0. 2456239, -0. 6095807, 0. 0522294, 0. 0026145, 0. 5546634, -0. 51632  
63, -0. 0052512, 0. 0038923, -0. 0021284, -0. 1954933\Polar=204. 4426075, 10. 715

7046, 80. 6866408, -1. 0311081, -0. 3349799, 44. 4445703\PG=C01 [X(C2H2N8)]\NI  
mag=1\\

#### TS9

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N8\ROOT\07-Sep-2012\0  
\\# freq b3lyp/6-31+g(d,p) geom=(connectivity,check) guess=read\\Title  
Card Required\\0,1\C, 3. 6316941851, 0. 230496083, 0. 0175839997\N, 2. 619323  
8878, -0. 4839508044, 0. 0190670735\H, 5. 2453981934, 1. 1053724369, 0. 65865840  
04\N, 1. 3633434915, 0. 1348884123, 0. 0187546531\N, 0. 4805166267, -0. 75557087  
76, 0. 0117386334\N, -0. 765923419, -0. 1858296412, 0. 0086144164\C, -1. 7295104  
896, -1. 0680748005, -0. 0048753344\H, -1. 5537014343, -2. 1768730866, -0. 01347  
45099\N, -4. 1472191887, 1. 6657108266, -0. 0034446919\N, -3. 4336432837, 0. 821  
2388271, -0. 0019784775\N, 4. 70868212, 0. 7876364208, -0. 1429436779\N, -3. 006  
2816893, -1. 1181117965, -0. 0137064848\\Version=EM64L-G09RevA. 01\State=1-  
A\HF=-515. 2032972\RMSD=4. 645e-09\RMSF=1. 587e-06\ZeroPoint=0. 0608406\Th  
ermal=0. 0712364\Dipole=-0. 5249447, -0. 0245895, 0. 5870653\DipoleDeriv=2. 8  
019685, 1. 0497656, -0. 105601, 1. 9911628, 0. 9525047, -0. 0875857, -0. 3986566, -  
0. 1379755, 0. 19933, -2. 205359, -0. 5802903, 0. 0810933, -0. 8110761, -0. 5657448  
, 0. 0501692, -0. 04026, 0. 0282805, -0. 2221435, 0. 5314263, 0. 0526231, 0. 0197038  
, 0. 0982463, 0. 3612707, -0. 0284751, -0. 1934109, -0. 0761759, 0. 1958427, 0. 8263  
798, 0. 0582356, -0. 0201378, -0. 6416614, -0. 0816068, -0. 0012117, 0. 0015089, -0  
. 0249592, -0. 0307056, 1. 5614436, 0. 2360852, 0. 0072279, 0. 1176145, -0. 1758829  
, 0. 0030908, 0. 0022009, -0. 0067706, 0. 025373, -1. 7662811, -0. 483279, -0. 00361  
31, -0. 8367404, -0. 3153169, -0. 003936, -0. 0092173, -0. 0007649, -0. 2597877, 1.  
1443474, 0. 9820798, 0. 0061979, 1. 4246746, 0. 375799, 0. 0047168, 0. 0174614, 0. 0  
100587, 0. 1608277, 0. 0756983, 0. 0630972, -0. 000503, 0. 0427878, 0. 2410811, 0. 0  
003869, 0. 0005453, 0. 0019587, 0. 1794127, -0. 2878108, 0. 1162652, 0. 0002191, 0.  
1228964, -0. 0158712, -0. 0006969, -0. 0023001, 0. 0005495, 0. 026148, 0. 5095832,  
-0. 0632504, 0. 0004891, 0. 4260803, -0. 2965537, 0. 0001324, 0. 0079464, -0. 00321  
43, 0. 1036458, -2. 254684, -0. 6230007, 0. 0189964, -0. 9537847, -0. 7554814, 0. 06  
42387, 0. 6281951, 0. 2124858, -0. 2231444, -0. 9367124, -0. 8083313, -0. 0040726,  
-0. 9802001, 0. 2758023, -0. 0008294, -0. 0140131, -0. 003473, -0. 1547987\Polar=  
218. 4963539, 19. 1976527, 82. 0312729, -0. 6874725, -0. 3564332, 45. 743708\PG=C  
01 [X(C2H2N8)]\NI mag=1\\

#### TS10

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\C2H2N8\ROOT\23-Oct-2012\0  
\\# freq b3lyp/6-31+g(d,p) geom=check guess=read\\Title Card Required\\  
\0,1\C, -3. 5094375851, 1. 0688176808, 0. 0001488676\N, -2. 5591478471, -0. 2960  
954663, 0. 0002200061\H, -5. 527240629, 0. 5490850438, 0. 000316839\N, -1. 36420  
04019, -0. 2727182811, 0. 0001465428\N, -0. 3666349376, -1. 045233384, 0. 000159  
0847\N, 0. 8267510841, -0. 3115974417, 0. 0000190856\C, 1. 8508732118, -1. 08531  
9704, 0. 0000306494\H, 1. 7999454533, -2. 1723474693, 0. 0001361117\N, 3. 593207  
8976, 1. 7345065497, -0. 000342767\N, 3. 3047771742, 0. 6378022988, -0. 00022058

77\N, -4.7054090562, 1.1345053132, 0.000213609\N, 3.1614006359, -0.60436413  
99, -0.0000934413\\Version=EM64L-G09RevA.01\State=1-A\HF=-515.1598704\R  
MSD=2.799e-09\RMSF=1.066e-06\ZeroPoint=0.0631776\Thermal=0.0730304\Dip  
ole=-0.8704816, -0.5714412, 0.0001052\DipoleDeriv=2.7475963, -0.9931653, -  
0.0000679, 0.0737317, -0.2785598, 0.0000264, -0.0001667, 0.0000897, 0.051729  
9, -0.9961629, -0.2890723, 0.0000769, 0.7731896, -0.260157, -0.0000375, -0.00  
00229, 0.0000259, -0.1682409, 0.5909306, -0.0787666, -0.000005, -0.3390987, 0  
.4375786, 0.0000154, 0.0000194, -0.0000002, 0.3856803, 1.0724199, 0.2391736,  
-0.0000764, -2.2409004, 0.8663162, 0.0000694, 0.0001562, -0.0000788, 0.17646  
61, -0.6170205, -0.0513242, 0.000036, 1.5532071, -0.5284122, -0.0000525, -0.0  
001143, 0.0000433, -0.0967704, -0.3358125, -0.0704858, 0.0000144, 0.3101948,  
-0.3182955, -0.0000085, -0.0000218, 0.0000145, -0.209866, 1.8215794, 0.23528  
35, -0.0001247, 0.293995, 0.7783729, -0.0000802, -0.0001306, -0.0000763, 0.11  
75386, 0.0795594, -0.0345156, 0.000008, -0.0076913, -0.0361241, 0.0000189, 0.  
0000059, 0.0000203, 0.1592771, -0.3343239, -0.2443647, 0.0000377, -1.110238,  
-0.8060804, 0.0001346, 0.0001205, 0.0000828, -0.0948848, 0.2896173, 0.300106  
2, -0.0000323, 1.8651989, 1.7700508, -0.0002595, -0.0001813, -0.0001652, 0.22  
9775, -3.0906665, 1.1049296, 0.0000612, 0.3020001, -0.2893864, -0.0000221, 0.  
0001353, -0.0000695, -0.3329075, -1.2277164, -0.1177984, 0.000072, -1.473588  
9, -1.3353032, 0.0001955, 0.0002002, 0.0001134, -0.2177974\Polar=227.833964  
2, -26.4229216, 100.3651748, -0.0085242, -0.0037065, 44.5357885\PG=C01 [X(C  
2H2N8)]\NImag=1\\

#### TS11

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0  
\\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Re  
quired\\0, 1\C, 2.1701528729, 0.8665093442, 0.1076662633\N, 1.3035825591, -0  
.6106241557, 0.1430792636\H, 4.2934191756, 0.7676757841, 0.2887101493\N, 0.  
1100163049, -0.6359673769, -0.0048794299\N, -0.8430609351, -1.4594821744, -  
0.0482353059\N, -2.1466069283, -0.8513194398, -0.2541742384\N, -2.20269800  
1, 0.370711888, -0.0211186186\N, -2.3465134096, 1.4888962245, 0.1689524899\  
N, 3.3366113615, 1.0596959061, 0.1953804267\\Version=EM64L-G09RevA.01\HF=  
-421.687093\RMSD=2.289e-09\RMSF=3.118e-06\ZeroPoint=0.039816\Thermal=0  
.0481917\Dipole=1.7846256, 0.403302, 0.1248122\DipoleDeriv=2.1164522, 0.9  
081917, 0.0757287, -0.0345245, -0.2164118, 0.0178907, 0.1636256, 0.1147985, 0  
.0884535, -0.2471493, 0.5720155, 0.0045138, -0.4082829, -0.1256276, -0.02822  
42, 0.0029617, 0.0474936, -0.1763221, 0.5649783, 0.0582876, 0.0068772, 0.2810  
717, 0.4984813, 0.0121178, 0.0104355, -0.0034824, 0.3972449, 0.0327736, -0.46  
92408, -0.0092437, 1.4308212, 0.6962566, 0.0697542, -0.097618, -0.0914384, 0.  
1504812, 0.6908262, 0.0458847, 0.0269549, -1.6749563, -0.2159993, -0.1252709  
, 0.1761342, 0.0413463, -0.048242, -0.2891545, -0.0965937, 0.0321252, 1.21956  
87, -0.9923046, -0.0767555, 0.0694439, -0.1619666, -0.2041104, -0.2209102, -0  
.085768, -0.075733, -1.1515324, 1.6322802, 0.2563282, -0.3275726, 0.2545975,  
0.2215522, -0.0868928, 0.1181775, 0.0226151, 0.8299974, -0.8325648, -0.10145

79, 0.1771014, -0.118144, -0.1216989, -2.5609235, -1.0509546, -0.0838381, -0.4921629, -0.44411, -0.0243824, -0.1745118, -0.0832046, -0.3073583\Polar=135.7651115, 20.0495136, 82.3829284, 3.762736, 4.6318792, 35.4189182\PG=C01 [X(C1H1N7)]\NImag=1\\

## TS12

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0\\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Required\\0,1\C,2.4175902529,0.0965464586,0.0177218987\N,1.4651740626,-0.6941896628,-0.0032792113\H,3.9601458021,1.0724671904,0.6812043918\N,0.164820879,-0.1976735319,0.0077603578\N,-0.6802200629,-1.1327848702,0.0146897038\N,-1.9346295566,-0.8749507699,0.0139094757\N,-2.2128288138,0.568227804,-0.0037042474\N,-2.9502247336,1.4137136282,-0.0214980676\N,3.4450751704,0.7447407536,-0.1314213016\\Version=EM64L-G09RevA.01\HF=-421.7809053\RMSD=7.542e-09\RMSF=2.539e-06\ZeroPoint=0.0426048\Thermal=0.0501019\Dipole=0.1241103,0.8130457,0.6035099\DipoleDeriv=2.3755155,0.9017421,-0.0741572,1.9377662,0.942009,-0.07968,-0.3245587,-0.0995877,0.1895031,-1.6543773,-0.3865786,0.075863,-0.7587188,-0.6542656,0.0481703,-0.068222,0.0215663,-0.168856,0.4927239,0.0354356,0.0215117,0.1057399,0.354983,-0.0237882,-0.1718338,-0.0682183,0.1889232,0.4578543,-0.0815297,-0.0266402,-0.9239431,0.1164415,-0.0029921,0.0179466,-0.0264918,-0.0746081,0.9575307,0.7199025,-0.0023589,0.2818749,-0.1646768,0.0083107,-0.0032689,-0.0032815,0.0498316,-0.9182246,-0.6442536,0.0061698,0.4383778,0.1678682,-0.0031901,-0.0038044,0.0021597,-0.1703724,1.0943214,-0.5424763,0.0015447,-0.7957002,0.3584695,-0.0003215,0.0252057,-0.0092465,0.1895276,-0.8478951,0.511419,-0.0014884,0.7048752,-0.3720939,0.0006994,-0.0199502,0.0101153,0.0064972,-1.9574487,-0.5136609,-0.0004445,-0.9902719,-0.7487349,0.0527914,0.5484857,0.1729846,-0.2104462\Polar=149.3056871,1.5719788,66.0510868,-0.4423733,-0.6523147,35.1571678\PG=C01 [X(C1H1N7)]\NImag=1\\

## TS13

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0\\# freq b3lyp/6-31+g(d,p) geom=check guess=read\\Title Card Required\\0,1\N,-3.1047509554,0.6316610497,-0.0000151121\N,-2.1622797708,-0.0070225214,0.0000005806\N,-1.2528079836,-0.8667883376,0.0000242677\N,0.0128235901,-0.29571135,0.0000047098\C,1.0501276127,-1.0656566691,0.000008386\H,1.0133234378,-2.149308511,0.0000145792\N,1.0861130664,1.4445215885,-0.0000002481\N,2.0701983343,0.8085651273,-0.0000061995\N,2.3037186686,-0.4938233765,0.0000050362\\Version=EM64L-G09RevA.01\State=1-A\HF=-421.7744506\RMSD=5.416e-09\RMSF=5.366e-06\ZeroPoint=0.0456141\Thermal=0.0520304\Dipole=-0.3594293,-0.4729941,0.0000006\DipoleDeriv=-1.1165527,0.3606533,-0.000011,0.7076051,-0.3014343,0.000006,-0.0000164,0.0000044,-0.0963495,1.8060529,-0.7926072,0.0000239,-1.5604065,0.7268552,-0

. 0000134, 0. 0000416, -0. 0000115, 0. 229657, -1. 0109997, 0. 3543751, -0. 000008,  
0. 6176018, -0. 5448903, 0. 0000078, -0. 0000262, 0. 0000051, -0. 1157125, -0. 1883  
073, -0. 1071295, -0. 0000067, 0. 2902551, -0. 1650163, 0. 0000049, -0. 0000042, 0.  
0000056, -0. 1089789, 0. 8591794, 0. 0542699, 0. 0000052, -0. 0587373, 0. 2845081,  
-0. 0000035, 0. 0000029, -0. 0000026, 0. 1048683, 0. 1556151, -0. 010355, 0. 000000  
3, -0. 045182, 0. 0751784, 0. 0000005, 0. 0000042, 0. 0000017, 0. 1548016, 1. 338687  
1, 0. 9784165, -0. 0000086, 0. 2277403, -0. 3239438, 0. 0000012, -0. 0000139, -0. 00  
00092, 0. 0100716, -1. 4972666, -0. 8397839, 0. 0000073, 0. 1120453, 0. 7552383, 0.  
0000004, 0. 0000202, 0. 0000059, 0. 0164908, -0. 3464081, 0. 0021607, -0. 0000025,  
-0. 2909219, -0. 5064953, -0. 0000004, -0. 0000082, 0. 0000006, -0. 1948483\Polar=  
115. 0827118, -9. 1700298, 66. 9921576, 0. 0002418, -0. 0003508, 33. 1981197\PG=C  
01 [X(C1H1N7)]\NImag=1\

#### TS14

1\1\GINC-ZHANGRUBO-3\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\14-Sep-2012\0  
\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\Title Card Re  
quired\0, 1\N, 2. 0069300873, -1. 2047836118, -0. 4480180315\N, 1. 0537488946,  
-0. 833949063, 0. 0453832661\N, 0. 0634534677, -0. 5343930245, 0. 7691660374\N,  
-1. 0035082143, -0. 0483936095, -0. 0195625742\C, -2. 6426433809, -1. 034181660  
4, -0. 3539781918\H, -2. 2591164083, -2. 0086357487, -0. 6028820487\N, -1. 53252  
45272, 1. 0677231449, 0. 4296748164\N, -2. 6274697022, 1. 4672399342, 0. 4340667  
793\N, -3. 5874922167, -0. 3150453612, -0. 2479030532\Version=EM64L-G09RevA  
. 01\HF=-421. 7330598\RMSD=9. 113e-09\RMSF=1. 805e-06\ZeroPoint=0. 0424869\  
Thermal=0. 0496884\Dipole=0. 9632377, -0. 6989459, -0. 1747212\DipoleDeriv=-  
0. 9832959, 0. 254348, 0. 3194987, 0. 4379893, -0. 2031855, -0. 1320999, 0. 5311865  
, -0. 1522391, -0. 2104778, 1. 7722946, -0. 4443831, -0. 7428102, -0. 6341421, 0. 39  
88141, 0. 258227, -1. 2749059, 0. 3953561, 0. 5076979, -1. 2094031, 0. 3358502, 0. 3  
507934, 0. 1334995, -0. 2350044, -0. 1441381, 0. 4703871, -0. 1679271, -0. 2458599  
, 0. 3512935, 0. 0578479, 0. 265606, 0. 1123961, 0. 011004, -0. 0669771, 0. 5930095,  
-0. 1926085, -0. 0767921, 0. 5571168, -0. 001537, -0. 0231639, 0. 3123894, 0. 12704  
55, 0. 0400998, 0. 1111998, 0. 0762256, 0. 0527768, 0. 1476179, 0. 0305666, 0. 00707  
58, -0. 0229797, 0. 1532966, -0. 0136939, -0. 0031803, -0. 0209973, 0. 2009596, -0.  
2424918, -1. 2081382, -0. 5520177, -0. 5284635, 0. 1892058, 0. 1150342, -0. 575192  
1, 0. 0339855, 0. 0720725, 0. 1004052, 1. 0313079, 0. 3909573, 0. 4303278, -0. 02554  
, 0. 0175634, 0. 2382756, 0. 0635345, -0. 0098926, -0. 4935372, -0. 0558624, -0. 015  
9395, -0. 2410168, -0. 4156362, -0. 0740153, -0. 0907801, -0. 0353297, -0. 2904843  
\Polar=109. 9133682, -18. 169426, 65. 4317158, -7. 1479442, 10. 8625025, 42. 8132  
456\PG=C01 [X(C1H1N7)]\NImag=1\

#### TS15

1\1\GINC-ZHANGRUBO-3\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\17-Sep-2012\0  
\#n freq b3lyp/6-31+g(d,p) geom=check guess=read\opt ts\0, 1\N, 0. 001  
6763814, -0. 005244204, 0. 0011670374\C, 0. 0009774574, -0. 0013550902, 1. 29475  
52653\N, 1. 3008140654, 0. 0009294174, 1. 7681259219\N, 2. 1291849613, -0. 02135



04685, 0. 6329766493\N, 1. 3636170354, -0. 0276991674, -0. 3716157351\N, 1. 7387  
665933, 0. 0999722678, 2. 9984954351\N, 2. 1283329323, -1. 3832204617, 3. 597704  
3158\N, 2. 6078248886, -1. 9587446537, 4. 4245583569\H, -0. 8545307665, 0. 02031  
15143, 1. 9530696137\\Version=EM64L-G09RevA. 01\State=1-A\HF=-421. 7805066  
\RMSD=1. 986e-09\RMSF=1. 858e-05\ZeroPoint=0. 0450073\Thermal=0. 0513566\D  
ipole=-0. 5431387, -0. 4442022, 1. 3316638\DipoleDeriv=-0. 3313356, -0. 041172  
3, 0. 148374, 0. 014587, -0. 2132838, 0. 0266662, 0. 0810812, 0. 1077689, -0. 611431  
5, 0. 4027773, -0. 1531329, 0. 4769693, -0. 0059592, 0. 1761208, 0. 0087498, 0. 1165  
747, -0. 0641669, 0. 5413737, -0. 0843924, 0. 1265978, -0. 3364647, -0. 1747242, 0.  
2055094, -0. 4708784, -0. 4128027, 0. 2834973, -0. 9856897, -0. 3643607, 0. 077779  
, -0. 1877899, -0. 0043498, -0. 0636749, 0. 0363522, -0. 0802843, -0. 1342283, 0. 48  
7867, 0. 2200323, 0. 1058283, -0. 4045717, -0. 0001739, -0. 1437062, -0. 0135161, -  
0. 1281975, 0. 1043465, -0. 3324216, -0. 0415325, -0. 166945, 0. 4858511, -0. 11426  
75, 0. 0450024, -0. 2685166, 0. 576103, -0. 3624897, 1. 072482, 0. 1623874, -0. 2210  
747, 0. 0832158, 0. 2252627, 0. 0409298, 0. 5555483, 0. 0331839, -0. 4200408, 0. 160  
2591, -0. 0948098, 0. 2811366, -0. 2767163, 0. 0590198, -0. 2003989, 0. 1254401, -0  
. 2014636, 0. 4849426, -0. 4251756, 0. 1312341, -0. 0090167, 0. 0111325, 0. 0006051  
, 0. 1535016, 0. 0001544, 0. 0158052, 0. 0003703, 0. 0927364\Polar=60. 2901025, -9  
. 8992825, 50. 6827303, 16. 222233, -19. 5817117, 91. 0141776\PG=C01 [X(C1H1N7)  
]\NImag=1\\

#### TS16 (TS25)

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\N6\ROOT\16-Oct-2012\0\#\  
freq b3lyp/6-31+g(d,p) geom=check guess=read\\Title Card Required\\0, 1  
\N, -2. 7966990248, -0. 1027300241, 0. 2513071187\N, -1. 6708873452, -0. 0740316  
045, 0. 1563684958\N, -0. 4907227067, 0. 5426010234, -0. 3713136892\N, 0. 504457  
0181, -0. 2659460118, -0. 5898517271\N, 1. 6655606009, -0. 0328353151, 0. 214154  
1236\N, 2. 7882914577, -0. 0670580679, 0. 3393366782\\Version=EM64L-G09RevA.  
01\State=1-A\HF=-328. 3088297\RMSD=6. 072e-09\RMSF=2. 786e-05\ZeroPoint=0  
. 0192901\Thermal=0. 0253541\Dipole=-0. 0039594, -0. 0941931, 0. 3261155\Dipo  
leDeriv=-1. 3887418, -0. 2768587, 0. 3229372, 0. 1291171, -0. 0321329, -0. 035452  
6, -0. 1830298, 0. 0259207, -0. 024815, 1. 2075243, 0. 4716328, -0. 2948218, -0. 117  
5058, 0. 1390281, 0. 0861425, 0. 4877891, -0. 1062567, 0. 1667833, 0. 1801164, -0. 1  
150639, -0. 3003494, -0. 1508399, -0. 1123201, 0. 0998002, 0. 1673804, -0. 053463,  
-0. 1338735, 0. 1724678, -0. 2606126, 0. 2009481, -0. 0373639, -0. 0955399, -0. 079  
7249, -0. 2145214, 0. 0709883, -0. 1494933, 1. 2126866, 0. 2329376, 0. 5266704, 0. 1  
555473, 0. 1351343, -0. 1038954, -0. 4452113, 0. 0977175, 0. 1703029, -1. 3840533,  
-0. 0520352, -0. 4553845, 0. 0210452, -0. 0341696, 0. 0331301, 0. 1875931, -0. 0349  
068, -0. 0289044\Polar=117. 8182607, 1. 2165684, 27. 1554449, 1. 5737167, -0. 756  
3937, 29. 6465901\PG=C01 [X(N6)]\NImag=1\\

#### TS17

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C1H1N7\ROOT\17-Sep-2012\0\  
\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Req

```

uired\\0,1\\N, 3.5054220673, 0.870526591, 0.0000536513\\N, 2.4436278889, 0.51
13856379, -0.0001193953\\N, 1.4886873769, -0.7778363574, 0.0001659104\\N, 0.2
613063216, -0.4420963832, 0.0000391251\\C, -0.7543283161, -1.2292077607, -0.
0000085787\\H, -0.6920978915, -2.312070415, -0.0000138827\\N, -2.5425508232,
1.5725040653, 0.0000553162\\N, -2.2573133195, 0.4691247504, 0.0000172012\\N,
-2.0830563044, -0.7591991283, -0.0000283476\\Version=EM64L-G09RevA.01\\HF
=-421.7720804\\RMSD=3.583e-09\\RMSF=9.096e-05\\ZeroPoint=0.0432837\\Therma
l=0.050798\\Dipole=0.3395382, -0.2829931, -0.0000796\\DipoleDeriv=-1.33023
09, -0.5977386, 0.0001335, -0.3168055, -0.1248279, 0.0000436, -0.0003418, -0.
0001126, 0.0082137, 1.2415271, 0.5537535, -0.0001376, 0.338376, 0.0892268, -0
.0000105, 0.0005106, 0.0001402, 0.1151066, -0.5707089, 0.1437887, -0.0000342
, -0.2383037, -0.0737367, -0.0000556, -0.0000377, 0.0000058, -0.1684594, 0.32
93658, -0.0089855, 0.0000555, 0.4154799, -0.1330145, 0.0000573, -0.0003638, -
0.0000244, -0.0173243, 1.2350689, -0.0471259, -0.000005, -0.8524338, 0.68457
25, -0.000039, 0.0002873, -0.0000178, -0.0163444, 0.0080284, 0.0192857, -0.00
00102, 0.0059795, -0.044643, -0.0000056, -0.0000342, -0.0000119, 0.1834789, -
0.3428702, 0.2387113, 0.0000012, 1.0836555, -0.9050405, -0.0000151, 0.000048
, -0.0000411, -0.132124, 0.2145665, -0.3057739, -0.0000109, -1.6290134, 1.827
7581, 0.0000637, -0.0000668, 0.000084, 0.2266797, -0.7847466, 0.0040847, 0.00
00077, 1.1930655, -1.3202948, -0.0000388, -0.0000016, -0.0000222, -0.1992268
\\Polar=135.9337218, 7.5103519, 75.9726275, 0.0003066, 0.0002961, 33.9526936
\\PG=C01 [X(C1H1N7)]\\NImag=1\\

```

## TS18

```

1\\1\\GINC-ZHANGRUBO-3\\Freq\\RB3LYP\\6-31+G(d,p)\\C1H1N7\\ROOT\\17-Sep-2012\\0
\\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\\Title Card Re
quired\\0,1\\N, 3.4418786437, -0.979856641, 0.0000823232\\N, 2.5552175044, -0
.2584214429, 0.0000706513\\N, 1.7096492798, 0.6524703697, 0.0000586539\\N, 0.
3851161013, 0.1314710121, 0.0000481662\\C, -0.5077549557, 1.0613892363, 0.00
00494293\\H, -0.2906814548, 2.1704670148, 0.0000615542\\N, -3.3120850692, -1.
3606965342, 0.0000096248\\N, -2.4950728863, -0.6159383028, 0.0000189914\\N, -
1.7848031632, 1.2457462881, 0.0000396055\\Version=EM64L-G09RevA.01\\HF=-4
21.7481681\\RMSD=2.061e-09\\RMSF=1.231e-06\\ZeroPoint=0.0397962\\Thermal=0
.0482758\\Dipole=-0.7519084, 0.3779976, -0.0000023\\DipoleDeriv=-1.1070647
, 0.5459509, -0.0000102, 0.8337043, -0.5598424, 0.0000083, -0.0000118, 0.0000
068, -0.140012, 1.6049108, -1.0629932, 0.0000162, -1.730983, 1.140891, -0.000
0176, 0.0000224, -0.0000145, 0.2158257, -0.5993911, 0.4830262, -0.0000029, 0.
7620455, -0.668463, 0.0000088, -0.0000213, 0.0000079, -0.1275507, -0.2962244
, 0.2875671, -0.0000038, 0.9916164, -0.499865, 0.0000082, 0.0000101, 0.000000
9, -0.2249318, 0.8076393, -0.9756492, 0.0000012, -1.357797, 0.5579978, -0.000
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37376, 0.2062243, 0.0000013, 0.0000075, -0.0000013, 0.1733591, -0.2382172, -0
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. 0000051, 0. 000005, -0. 0000046, 0. 0950073, -0. 4468642, 0. 9031033, 0. 0000033,  
0. 8990452, 0. 0661042, 0. 0000096, -0. 0000075, 0. 0000128, -0. 1607583\Polar=12  
8. 2175948, -15. 0360589, 69. 7161793, 0. 0008558, -0. 0000169, 34. 4403006\PG=C0  
1 [X(C1H1N7)]\NImag=1\

#### TS19

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N6\ROOT\11-Sep-2012\0  
\# opt=(calcall, ts, noeigentest, cartesian, maxstep=1) b3lyp/6-31+g(d,p)  
nosymm geom=check guess=read\Title Card Required\0, 1\C, 2. 840085271,  
-0. 0511593501, 0. 0253684739\N, 1. 6530092185, -0. 3870993413, -0. 044947814\H  
, 4. 6095874482, 0. 1869540477, 0. 7642617048\N, 0. 6608481601, 0. 6309351319, 0.  
0115838941\N, -0. 4835992539, 0. 1138888646, -0. 054842947\N, -1. 6429376207, 0  
. 40937449, -0. 0636969244\C, -2. 872353899, -0. 7147466018, -0. 1803700539\H, -  
4. 7601603671, 0. 1910238175, -0. 1722761002\N, 4. 0470631407, 0. 1469885286, -0  
. 0824328718\N, -4. 0523315028, -0. 526226941, -0. 2013184627\Version=EM64L-  
G09RevA. 01\HF=-405. 6933582\RMSD=6. 115e-09\RMSF=4. 613e-07\ZeroPoint=0. 0  
521658\Thermal=0. 0605359\Dipole=-0. 8208521, 0. 3897989, 0. 6211129\DipoleD  
eriv=3. 3277919, 0. 5154604, 0. 0082257, 1. 1401066, 0. 3223876, -0. 0023983, -0. 1  
791546, -0. 0207368, 0. 1508608, -1. 8775781, -0. 2223633, 0. 0326711, -0. 2965876  
, -0. 2682333, 0. 0102277, -0. 1127445, 0. 0309323, -0. 2166749, 0. 5081527, 0. 0165  
369, 0. 020342, 0. 0307792, 0. 3314181, -0. 0141602, -0. 1739023, -0. 0106567, 0. 15  
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, -0. 1247369, -0. 0413814, -0. 062714, 1. 0602877, -0. 1239703, 0. 009593, 1. 85151  
43, 0. 5703556, 0. 0763726, 0. 1623209, 0. 0180839, 0. 2020001, -0. 6899083, 0. 2522  
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5, 0. 0133178, -0. 0144449, 0. 0611419, 0. 6666246, 0. 0511275, 0. 0109474, 0. 27989  
77, 0. 3835011, 0. 0073391, 0. 029863, 0. 0019932, 0. 3898532, -2. 460025, -0. 24178  
47, -0. 0498156, -0. 3834621, -0. 4847707, 0. 0116779, 0. 4910981, 0. 0328504, -0. 1  
689677, -3. 1587461, -0. 6182883, -0. 1192932, 0. 3379175, -0. 1235632, 0. 0232819  
, -0. 0575719, -0. 004106, -0. 3297647\Polar=219. 6271452, 25. 2191441, 51. 12296  
39, 5. 8848938, 1. 4387002, 38. 3606278\PG=C01 [X(C2H2N6)]\NImag=1\

#### TS20

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\C1H1N5\ROOT\17-Sep-2012\0  
\#n opt=(calcall, ts, noeigentest) b3lyp/6-31+G(d,p) nosymm\opt ts\0, 1  
\C, 0. 0517657426, 0. 000952333, 0. 0097260423\N, -0. 0340748692, 0. 044816319, 1  
. 2472919502\N, 0. 5369500023, 0. 0093422118, -1. 1166073374\N, 0. 5096266421, 0  
. 6584733503, -2. 2265466313\N, 1. 0006362607, -0. 2669411578, -3. 4487617478\N  
, 1. 29558683, -0. 2647282041, -4. 5307313821\H, -0. 9431766081, -0. 2050761428,  
1. 6354530255\Version=EM64L-G09RevA. 01\HF=-312. 3001897\RMSD=4. 464e-09\  
RMSF=9. 305e-05\ZeroPoint=0. 03231\Thermal=0. 038521\Dipole=-0. 5377779, -0  
. 4045554, -0. 1321881\DipoleDeriv=0. 1292881, -0. 1575822, -0. 2622193, -0. 079  
5573, 0. 2385375, 0. 1239965, -0. 6057178, 0. 1875274, 2. 5286541, -0. 0980901, 0. 1

220598, -0.2169766, 0.1377375, -0.4484182, -0.2565655, 0.5161075, 0.0200087,  
-2.1266822, -0.1197491, 0.1032392, 0.4906294, 0.0188918, -0.1340743, 0.54412  
65, 0.0363149, -0.2072837, -1.0130107, -0.1359234, -0.0069706, -0.1382171, -0  
.058739, -0.0013266, -0.2295275, 0.0649844, -0.0418354, 0.5487582, 0.2285048  
, -0.1220691, -0.3475319, 0.0944516, 0.0213375, -0.5388886, -0.3072142, 0.432  
518, 0.8889618, -0.1077264, 0.1198442, 0.3971712, -0.0477226, 0.0264307, 0.25  
05031, 0.3739852, -0.377289, -1.2869354, 0.1036961, -0.0585214, 0.0771444, -0  
.0650619, 0.2975134, 0.1063554, -0.07846, -0.0136461, 0.4602544\Polar=34.77  
62328, -1.299126, 30.4729325, -26.3997604, 4.4389857, 130.8848606\PG=C01 [X  
(C1H1N5)]\NImag=1\

## TS21

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C1H1N5\ROOT\17-Sep-2012\0\  
\# freq b3lyp/6-31+g(d,p) geom=check guess=read\Title Card Required\  
0, 1\N, -2.299817842, -0.962400921, 0.0389564045\N, -1.6643099464, -0.064284  
9244, -0.1779377504\C, -0.4545807872, 1.045716852, 0.4092446028\H, -0.90880  
4656, 1.9621982856, 0.0162697542\N, 2.2599136575, -0.9196524193, 0.07800357  
24\N, 1.4766243513, -0.1016397706, 0.0028014256\N, 0.7342962228, 0.87262189  
77, -0.2890050091\Version=EM64L-G09RevA.01\State=1-A\HF=-312.3006146\R  
MSD=7.053e-09\RMSF=2.315e-06\ZeroPoint=0.0333368\Thermal=0.0391336\Dip  
ole=-0.1285739, 0.1813089, -0.2593416\DipoleDeriv=-0.562351, -0.2807322, -  
0.2304684, -0.9780942, -0.4583636, -0.3560485, 0.4155509, 0.153545, 0.122558  
8, 0.1363339, 0.3842646, 0.3354838, 0.8259552, 0.4767792, 0.4459885, -0.58905  
77, -0.1483867, -0.0893882, 1.2946077, -0.2336573, -0.2184391, -0.3858548, 0.  
1683179, -0.0936229, -0.4346989, -0.3363408, -0.1117359, 0.0307519, 0.027621  
3, -0.0325512, 0.1046341, 0.0051231, 0.0742176, -0.0132961, 0.2398006, 0.1291  
485, -0.8434307, 0.4114026, -0.0972487, 0.8252982, -0.4652551, 0.0889039, -0.  
0096138, -0.0045099, -0.1023074, 1.2059387, -0.7596282, 0.2603328, -1.522220  
4, 1.0115082, -0.2415879, 0.3334999, -0.2206127, 0.2213491, -1.2618506, 0.450  
7292, -0.017109, 1.1302819, -0.7381097, 0.0821492, 0.2976157, 0.3165045, -0.1  
696249\Polar=85.4229484, -2.5867547, 56.6950155, 5.0434566, 1.5799713, 32.9  
66877\PG=C01 [X(C1H1N5)]\NImag=1\

## TS22

1\1\GINC-ZHANGRUB-0\Freq\RB3LYP\6-31+G(d,p)\C1H1N5\ROOT\17-Sep-2012\0\  
\# freq b3lyp/6-31+g(d,p) geom=check guess=read\Title Card Required\  
\0, 1\N, -2.6188784463, -0.7929030203, -0.21356997\N, -1.7529205564, -0.0846  
447036, -0.0255761182\C, -0.7068006001, 0.7655255461, 0.0528383397\H, -0.90  
57227142, 1.6475751616, 0.6592381029\N, 2.7327959937, -0.1639051592, 0.1971  
304978\N, 1.6133791919, -0.0349845292, 0.2290117548\N, 0.4029441314, 0.4314  
887046, -0.6135076068\Version=EM64L-G09RevA.01\State=1-A\HF=-312.30490  
53\RMSD=1.265e-09\RMSF=2.235e-05\ZeroPoint=0.0327085\Thermal=0.0385374  
\Dipole=-0.5546433, 0.3162139, 0.6305181\DipoleDeriv=-1.2709803, -0.40128  
48, -0.0000523, -0.9646052, -0.3780296, 0.0171076, -0.3878734, -0.0949436, -0

. 0560997, 1. 8096919, 0. 6967228, 0. 0978691, 1. 437134, 0. 5807658, -0. 063122, 0. 5880908, -0. 0164333, 0. 1291382, -0. 8765998, -0. 2557385, -0. 252065, -0. 427128 9, 0. 1198711, 0. 2297809, 0. 4859337, 0. 2895219, -0. 0137324, -0. 014233, 0. 04075 7, 0. 074453, 0. 0581325, 0. 0410999, -0. 1074972, 0. 0707091, -0. 1002806, 0. 12248 74, -1. 3492314, 0. 2654006, -0. 411918, -0. 0846328, -0. 0750741, 0. 027165, 0. 398 1167, -0. 0289636, -0. 0132491, 0. 6406273, -0. 4048255, 0. 5226451, 0. 5220013, 0. 2518233, -0. 0626441, -0. 9371067, -0. 0497468, 0. 0679086, 1. 0607253, 0. 0589684 , -0. 0309319, -0. 5409009, -0. 5404563, -0. 0407901, -0. 2178702, 0. 0008459, -0. 2 36453\Polar=117. 3039916, 6. 670981, 40. 9152069, 6. 1435166, 1. 0887712, 31. 627 4981\PG=C01 [X(C1H1N5)]\NImag=1\\

### TS23

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\C1H1N9\ROOT\10-Sep-2012\0 \\# freq b3lyp/6-31+g(d,p) geom=check guess=read\\Title Card Required\\ \0, 1\N, 2. 4398313798, -1. 0696054714, 0. 1465996368\N, 1. 0468221531, -1. 08641 86452, 0. 0326518849\N, 0. 5245299794, 0. 0444847704, -0. 1407598195\N, -0. 8035 439094, 0. 0933066327, -0. 2561919863\C, -2. 0640910797, 1. 5248844728, 0. 02369 72973\H, -1. 430209995, 2. 3889423865, -0. 0688595872\N, 2. 9867203766, 0. 06644 83965, 0. 0553796435\N, 3. 6179541497, 1. 0075757269, -0. 0090738029\N, -1. 5828 475364, -0. 9680947505, -0. 070482495\N, -2. 7338653831, -1. 0063366883, 0. 1027 71286\N, -3. 1489031349, 1. 0575981696, 0. 1846479426\\Version=EM64L-G09RevA . 01\State=1-A\HF=-531. 1844199\RMSD=2. 914e-09\RMSF=3. 435e-06\ZeroPoint= 0. 0513645\Thermal=0. 0604579\Dipole=0. 722113, 0. 7375413, -0. 1254275\Dipol eDeriv=-1. 3377785, -0. 155595, -0. 0110332, -1. 3726995, -0. 7018092, -0. 005548 1, 0. 0584382, 0. 0494356, -0. 1917459, 1. 2543528, -0. 0382096, 0. 0749988, 0. 6765 022, -0. 0299861, 0. 0271333, 0. 0380416, -0. 0021874, 0. 0048504, 0. 7371648, -0. 2 734033, 0. 101627, 0. 346741, -0. 0803795, -0. 0009861, -0. 0139181, -0. 0301486, 0 . 0404041, -1. 0795092, -0. 0330281, -0. 0206777, -0. 7828528, 0. 0511395, 0. 06025 83, 0. 1111887, 0. 0808154, -0. 1370597, 0. 5446369, -0. 044024, -0. 0493446, -0. 47 2256, 0. 2629361, 0. 0390408, -0. 0446078, -0. 01868, 0. 078025, 0. 1497273, -0. 009 9042, 0. 0059005, 0. 0138161, 0. 1890954, -0. 0096539, 0. 0036709, 0. 0050913, 0. 21 28145, 0. 8361282, 0. 6277974, -0. 0520161, 1. 8293138, 1. 161903, -0. 0342756, -0. 1606361, -0. 0603397, 0. 2301817, -0. 6970702, -0. 3233916, 0. 0097032, -1. 041947 6, -0. 4804622, 0. 0046411, 0. 0735879, 0. 0246502, -0. 0679123, 0. 4909392, 1. 1303 225, -0. 030872, 1. 0757008, -0. 3124651, -0. 1036972, -0. 1352411, -0. 1934844, 0. 1285914, -0. 490833, -0. 8818014, -0. 0231431, -0. 5647393, 0. 5262768, 0. 0513877 , 0. 0597334, 0. 1503126, -0. 0285113, -0. 4077584, 0. 0012372, -0. 005143, 0. 29242 12, -0. 5862486, -0. 0283003, 0. 0097424, -0. 005465, -0. 2696379\Polar=162. 6560 032, 6. 6154559, 87. 8220034, -1. 6880727, -1. 6177826, 42. 5417849\PG=C01 [X(C1 H1N9)]\NImag=1\\

### TS24

1\1\GINC-ZHANGRUB0-1\Freq\RB3LYP\6-31+G(d,p)\N8\ROOT\16-Oct-2012\0\\# freq b3lyp/6-31+g(d,p) geom=check guess=read\\Title Card Required\\0, 1

\N, -1.3670885559, -0.9356144832, -0.0007557675\N, -0.168091415, -0.4948048  
755, -0.0006323707\N, 0.1053952955, 0.7338119201, 0.0000575668\N, 1.4744332  
158, 1.0616651075, 0.0001711805\N, -2.3810461574, 0.1791523272, 0.000088835  
1\N, -3.4500472132, 0.5118423271, 0.000571187\N, 2.2682645085, 0.0879372963  
, 0.0002590094\N, 3.0943984218, -0.6948369195, 0.0002525394\\Version=EM64L  
-G09RevA.01\State=1-A\HF=-437.7768834\RMSD=6.615e-09\RMSF=6.777e-06\Ze  
roPoint=0.0306144\Thermal=0.0379866\Dipole=-0.5442535, 0.0298031, 0.0002  
31\DipoleDeriv=-0.6614109, -0.5172522, -0.0004596, 0.0370722, -0.13838, -0.  
0000388, 0.0001495, 0.0000955, -0.1541212, 0.2587489, 0.6300604, 0.0004543, 0  
.3931331, 0.1914591, 0.0000829, 0.0003, -0.00002, 0.0490294, 1.2619451, 0.175  
0514, 0.0001372, -0.8262298, -0.1610124, 0.0000428, -0.0006263, 0.0000149, -0  
.0618997, -1.3446277, 0.1514257, -0.000193, 1.2157293, -0.5013305, 0.0000735  
, 0.0003335, 0.0000227, -0.1754722, 1.3473382, -0.2837617, -0.0001622, -0.232  
7784, 0.1582019, -0.0000384, -0.0006368, 0.0000693, 0.1640543, -1.1944226, 0.  
2813165, 0.0002004, 0.2029416, -0.0349038, -0.0000322, 0.0005584, -0.0001238  
, 0.0288892, 1.311099, -0.7446858, 0.0001644, -1.6943158, 0.800393, -0.000254  
6, -0.000079, -0.0000748, 0.2390188, -0.9786699, 0.3078456, -0.0001414, 0.904  
4478, -0.3144271, 0.0001648, 0.0000008, 0.0000161, -0.0894987\Polar=140.574  
6839, -12.5066228, 55.6210797, -0.0005601, 0.0081743, 31.8142824\PG=C01 [X(  
N8)]\NImag=1\\

**The coordinates corresponding to Table 3**

**N12**

1\1\GINC-ZHANGRUBO-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N12\R00T\05-Oct-2012\  
0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p)  
Freq\\Title Card Required\\0,1\C, -2.5977538541, -1.0373605012, -0.000163  
1281\N, -1.57117791, -0.138123302, 0.0000329842\H, -2.4532775264, -2.106901  
4484, -0.0002863101\N, -0.2579677244, -0.4967404851, 0.0001349656\N, 0.5168  
434511, 0.4835732626, 0.0002475263\N, 1.82271276, -0.0424682065, 0.00023281  
4\N, -2.105977848, 1.1286315954, -0.0003051937\N, -3.374557709, 0.960604669  
7, 0.0004162883\N, -3.7239981348, -0.3795721101, -0.0002922808\N, 2.5976343  
76, 0.9376095849, 0.0003629767\N, 3.9109044869, 0.5784836039, 0.0002672362\  
C, 4.9376867696, 1.4773205437, 0.0002423692\H, 4.7938078723, 2.5469399288, 0  
.0003533058\N, 4.4451985713, -0.688409422, -0.0000049319\N, 5.7139123286, -  
0.5207883491, 0.0001349992\N, 6.0637767611, 0.8191956354, 0.000340949\\Ver  
sion=EM64L-G09RevA.01\State=1-A\HF=-734.1667066\RMSD=9.988e-09\RMSF=5.  
481e-05\ZeroPoint=0.0900333\Thermal=0.1009415\Dipole=-0.0009218, 0.0001  
889, -0.0000642\DipoleDeriv=1.319611, 0.0836511, 0.0001037, 0.5012651, 0.23  
67572, 0.0000605, -0.0000528, 0.000033, 0.1327542, -1.9297674, -0.1245787, 0.  
0000306, 0.7052388, -0.0362886, -0.0000697, -0.0003308, 0.0000293, 0.0565541  
, 0.124133, 0.0211094, -0.0000199, 0.0481296, 0.138336, -0.0000095, 0.0000402  
, -0.0000153, 0.1691459, 1.7869931, 0.1587814, 0.0001315, -0.1515217, -0.0289  
398, 0.0000024, -0.0002986, -0.0000805, 0.0281658, -0.3088991, -0.0031498, -0



. 0000576, -0. 52723, -0. 0619186, -0. 0000307, 0. 0002508, 0. 0000155, -0. 0069997  
, -0. 3075304, -0. 0027655, 0. 0000386, -0. 5269751, -0. 0619759, -0. 0000076, -0. 0  
000292, 0. 0000224, -0. 0068893, 0. 3676859, -0. 309769, -0. 0001245, -0. 9473733,  
-0. 1241386, -0. 0002475, 0. 0003868, 0. 0000849, -0. 0357981, -0. 755919, 0. 11071  
59, -0. 0002073, -0. 2116777, 0. 2464253, 0. 0003072, -0. 0006657, 0. 0000389, -0. 1  
552138, -0. 6042307, 0. 0631689, 0. 0001371, 0. 5834073, -0. 3700659, 0. 0000006, 0  
. 0006834, -0. 0001234, -0. 1885561, 1. 785879, 0. 1582098, 0. 0000003, -0. 1526947  
, -0. 0288738, -0. 0000139, -0. 0001298, -0. 0000119, 0. 0281602, -1. 9286076, -0. 1  
241007, -0. 0000743, 0. 7056625, -0. 0363432, -0. 0000258, 0. 0003416, -0. 0000292  
, 0. 0564927, 1. 3193579, 0. 0833635, 0. 0000061, 0. 5009081, 0. 2365946, -0. 000031  
, 0. 0000193, 0. 0000718, 0. 1327054, 0. 1241543, 0. 0211085, 0. 0000051, 0. 0481459  
, 0. 1382558, 0. 0000042, -0. 0000129, -0. 0000395, 0. 1691562, 0. 3666399, -0. 3097  
597, -0. 0000268, -0. 9473825, -0. 1239473, 0. 0000403, -0. 0001995, -0. 0000384, -  
0. 0358289, -0. 7556191, 0. 1108624, 0. 0000275, -0. 2110535, 0. 2462593, 0. 000030  
9, -0. 0000749, 0. 0000712, -0. 1552742, -0. 6038806, 0. 0631525, 0. 0000298, 0. 583  
1513, -0. 3701364, -0. 0000105, 0. 0000719, -0. 0000289, -0. 1885743\Polar=254. 4  
63163, 15. 7295738, 101. 0670803, 0. 0062677, 0. 004793, 57. 6427837\PG=C01 [X(C  
2H2N12)]\NImag=0\

#### N12TS1

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N12\R00T\08-Oct-2012\  
0\#\# freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\Title Card R  
equired\0, 1\C, -3. 6382574702, 0. 9966563032, 0. 0003106218\N, -2. 6747534525  
, 0. 1124608923, 0. 0001044618\H, -3. 4697040154, 2. 0693847579, 0. 000517918\N,  
-1. 4106054219, 0. 5899664623, 0. 0001601031\N, -0. 5649338997, -0. 3422796981,  
-0. 0000444385\N, 0. 6973597222, 0. 2640204514, 0. 0000327825\N, -4. 0718866267  
, -1. 5440831866, -0. 0001739798\N, -4. 8937322776, -0. 7327225249, 0. 000006661  
6\N, -4. 9391910066, 0. 6080234811, 0. 0002747641\N, 1. 5447093477, -0. 65450779  
25, -0. 0001558752\N, 2. 831815932, -0. 1874999655, -0. 0001084539\C, 3. 9224508  
039, -1. 0021332759, -0. 0002736912\H, 3. 8622505137, -2. 0794374704, -0. 000451  
8926\N, 3. 2637064479, 1. 1134806946, 0. 0000968002\N, 4. 544949772, 1. 04696302  
94, 0. 0000515935\N, 4. 9966366312, -0. 2579971583, -0. 0001773755\Version=EM  
64L-G09RevA. 01\HF=-734. 1371518\RMSD=3. 448e-09\RMSF=4. 679e-06\ZeroPoint  
=0. 0874385\Thermal=0. 0985213\Dipole=-1. 5501024, -0. 753264, -0. 0000674\Di  
poleDeriv=1. 8825405, -0. 0224295, -0. 0000559, -0. 7118436, 0. 2805948, 0. 00004  
5, -0. 0001902, 0. 0000248, 0. 1586388, -2. 6021944, 0. 0593611, 0. 0000822, 0. 4629  
763, -0. 1053102, -0. 0000055, 0. 0001681, 0. 0000066, -0. 1523056, 0. 1569605, -0.  
0154738, -0. 0000032, -0. 076175, 0. 1024557, -0. 0000064, -0. 0000178, -0. 000007  
6, 0. 1455994, 1. 9936174, -0. 1363994, -0. 0000816, -0. 6461109, -0. 1993836, -0. 0  
000276, -0. 0001821, -0. 0000426, 0. 0336692, -0. 7336226, 0. 0712941, 0. 0000305,  
0. 6593112, -0. 0148864, -0. 0000078, 0. 0001489, 0. 0000091, -0. 0744742, 0. 16247  
54, -0. 0501756, -0. 0000117, 0. 4754982, -0. 0624264, -0. 0000269, 0. 0000737, -0.  
0000098, 0. 0060971, 1. 9498898, 0. 7133112, 0. 0000847, -0. 3058969, -0. 4182403,  
-0. 0000821, -0. 0001143, -0. 0001082, 0. 0369602, -1. 9834792, -0. 5579955, -0. 00

00492, 1. 1496645, 0. 8488666, 0. 0001189, 0. 0002826, 0. 000166, 0. 0764839, -0. 87  
53739, -0. 0990203, 0. 0000002, -0. 7268628, -0. 409318, -0. 0000209, -0. 0001222,  
-0. 0000402, -0. 188947, 1. 4875925, -0. 004891, -0. 0000444, 0. 5421999, -0. 02035  
48, -0. 0000194, 0. 0000627, -0. 0000066, 0. 0164636, -1. 7952389, -0. 0093913, 0. 0  
000532, -0. 8580232, -0. 091412, 0. 0000008, -0. 0001029, -0. 000022, 0. 0484593, 1  
. 3831225, -0. 005682, -0. 0000379, -0. 419704, 0. 1943044, 0. 0000244, -0. 0001091  
, 0. 0000114, 0. 1230106, 0. 1314941, -0. 022111, -0. 0000027, -0. 0519063, 0. 12006  
05, -0. 0000068, -0. 0000077, -0. 0000074, 0. 1693939, 0. 2848165, 0. 3266028, 0. 00  
00443, 1. 0105095, -0. 0425965, -0. 0000303, 0. 0001659, -0. 0000098, -0. 0392193,  
-0. 8388574, -0. 1823323, -0. 0000103, 0. 1196785, 0. 2222548, 0. 0000601, 0. 00003  
27, 0. 0000693, -0. 1640272, -0. 6037428, -0. 0646674, 0. 0000017, -0. 6233154, -0.  
4046087, -0. 0000155, -0. 0000883, -0. 0000329, -0. 1958026\Polar=296. 6434486,  
-2. 0045295, 108. 2598182, -0. 0072773, 0. 0092851, 58. 2199811\PG=C01 [X(C2H2N  
12)]\NImag=1\

### N12p1

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N12\R00T\12-Oct-2012\  
0\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p)  
Freq\Title Card Required\0, 1\C, -3. 5189910666, 0. 8515966648, 0. 00027169  
63\N, -2. 6213944288, -0. 0860199249, 0. 0000714662\H, -3. 2833292308, 1. 914414  
7846, 0. 0004677227\N, -1. 368893262, 0. 4758475655, 0. 0001468189\N, -0. 491496  
8802, -0. 4244317394, -0. 0000462127\N, 0. 7525320069, 0. 2263194192, 0. 0000355  
96\N, -5. 6634782515, -1. 658864633, -0. 00015129\N, -5. 1953883977, -0. 6319482  
323, 0. 000032209\N, -4. 867481382, 0. 5873791925, 0. 0002556888\N, 1. 629830004  
3, -0. 662637957, -0. 0001530304\N, 2. 9020875236, -0. 1511446983, -0. 000100595  
6\C, 4. 018634776, -0. 9286855306, -0. 0002708317\H, 3. 9942054237, -2. 00734709  
03, -0. 0004580581\N, 3. 2899537003, 1. 1627301187, 0. 0001151868\N, 4. 57330141  
87, 1. 1394189813, 0. 0000725103\N, 5. 0680144362, -0. 1491837908, -0. 000166586  
4\Version=EM64L-G09RevA. 01\State=1-A\HF=-734. 1657802\RMSD=6. 416e-09\R  
MSF=2. 291e-05\ZeroPoint=0. 0888709\Thermal=0. 100726\Dipole=-2. 2019855, -  
0. 6831727, -0. 0000483\DipoleDeriv=2. 9311917, 0. 2711677, -0. 0000198, -0. 586  
6698, 0. 6625475, 0. 0001026, -0. 0001801, 0. 0000798, 0. 2063523, -2. 499366, -0. 0  
404095, 0. 000053, 0. 5477606, -0. 3427251, -0. 0000371, 0. 0001631, -0. 000021, -0  
. 223771, 0. 0826642, -0. 0301463, -0. 0000041, -0. 0188543, 0. 0214818, -0. 000023  
6, -0. 0000018, -0. 0000234, 0. 1489682, 1. 940349, -0. 0644258, -0. 0000622, -0. 09  
46822, -0. 0014568, 0. 0000012, -0. 0000666, -0. 0000008, 0. 002939, -0. 871856, 0.  
0016459, 0. 0000189, 0. 4831017, -0. 0383484, -0. 0000042, 0. 0001107, 0. 0000097,  
-0. 0861859, 0. 1425682, -0. 0504873, -0. 0000109, 0. 4706787, -0. 0594075, -0. 000  
0261, 0. 0000799, -0. 0000102, 0. 0074342, -0. 4998486, -0. 3096651, -0. 0000468, -  
1. 0685859, -0. 5722147, -0. 0000718, -0. 0001917, -0. 0000924, -0. 045144, 0. 7867  
848, 0. 5135857, 0. 000083, 2. 1677377, 1. 5085234, 0. 0001822, 0. 0003982, 0. 00022  
66, 0. 2466255, -2. 0363982, -0. 3397603, -0. 0000159, -1. 6367279, -1. 1429014, -0  
. 0001345, -0. 0002644, -0. 0001689, -0. 2078594, 1. 4313753, 0. 0396912, -0. 00003  
7, 0. 6021104, -0. 0032467, -0. 0000205, 0. 0000666, -0. 0000061, 0. 0179779, -1. 74

01264, -0.0508439, 0.0000453, -0.9076761, -0.1165483, -0.000001, -0.000106, -  
0.0000251, 0.0462088, 1.3823801, 0.0245163, -0.0000342, -0.3747092, 0.185423  
2, 0.0000224, -0.0001074, 0.0000097, 0.121102, 0.1339244, -0.0214922, -0.0000  
025, -0.050533, 0.1158578, -0.0000079, -0.000008, -0.0000084, 0.1694905, 0.23  
43277, 0.3298676, 0.0000493, 1.0118262, -0.0092629, -0.0000255, 0.0001701, -0  
.0000048, -0.0410354, -0.8336125, -0.208503, -0.0000167, 0.0749302, 0.211810  
5, 0.0000636, 0.0000307, 0.0000718, -0.1655195, -0.5843576, -0.064741, 0.0000  
007, -0.6197071, -0.4195323, -0.0000197, -0.0000934, -0.0000366, -0.1975832\  
Polar=301.753527, 8.0145758, 110.722842, -0.0053666, 0.0094343, 58.3218446\  
PG=C01 [X(C2H2N12)]\NImag=0\

## N12TS2

1\1\GINC-ZHANGRUB0-0\Freq\RB3LYP\6-31+G(d,p)\C2H2N12\R00T\15-Oct-2012\  
0\# freq b3lyp/6-31+g(d,p) geom=check guess=read\Title Card Required  
\0, 1\C, -3.3713641708, -1.1074099702, -0.0002332259\N, -2.4763621788, -0.1  
33550599, -0.0000780612\H, -3.0943488845, -2.1930817548, -0.0003789409\N, -  
1.2071455806, -0.577445481, -0.0001119576\N, -0.3881864683, 0.3868501376, 0  
.0000411378\N, 0.8845205506, -0.1813852729, -0.0000092677\N, -5.9125299647  
, 1.5157876975, 0.0000842866\N, -5.1628986009, 0.7036150281, -0.0000170896\  
N, -4.6305091947, -1.2448441488, -0.0002789613\N, 1.7178966403, 0.749526377  
3, 0.0001418714\N, 3.0160909121, 0.2923317553, 0.0001087016\C, 4.0948002187  
, 1.1176841481, 0.0002465052\H, 4.0227467481, 2.1940593334, 0.0003906183\N,  
3.4603818753, -1.0004543701, -0.0000551543\N, 4.7440509145, -0.9213656111,  
-0.0000136386\N, 5.1797051837, 0.3849497305, 0.0001731762\Version=EM64L-  
G09RevA.01\State=1-A\HF=-734.1205294\RMSD=5.936e-09\RMSF=1.323e-05\Zer  
oPoint=0.0823757\Thermal=0.0951925\Dipole=-2.8043231, 0.4939014, 0.\Dipo  
leDeriv=1.0607464, 0.9462121, 0.0001525, 1.5419663, 0.4549208, 0.0000712, 0.  
0002341, 0.0000571, 0.1885654, -2.1536018, -0.5486666, -0.0001204, -1.060678  
9, -0.3522642, -0.00004, -0.0001911, -0.000029, -0.229038, 0.0951888, 0.04215  
51, 0.0000039, 0.0976071, 0.3050101, 0.0000183, 0.0000116, 0.0000169, 0.18964  
2, 2.4887735, 0.4564745, 0.0001187, 1.0489353, -0.0152926, 0.0000139, 0.00020  
14, 0.000001, 0.0498155, -1.331397, -0.216274, -0.0000579, -0.7222527, -0.127  
2143, -0.0000173, -0.0001285, -0.0000052, -0.1205839, 0.7525244, 0.1525049, 0  
.0000383, -0.3456144, -0.1118101, -0.0000252, -0.0000301, -0.000014, 0.01117  
07, -0.2581773, 0.0588856, 0.0000016, 0.054426, 0.0385624, 0.0000027, 0.00000  
3, 0.000002, 0.03153, 0.4726446, 0.0265178, 0.0000121, 0.6158199, -0.3144855,  
-0.0000464, 0.0000922, -0.0000581, 0.1060359, -0.8945713, -0.8249642, -0.000  
133, -1.1948295, 0.2046002, 0.0000223, -0.0001829, 0.0000307, -0.1378536, 1.0  
788455, 0.0199891, 0.0000286, -0.8222143, -0.07558, -0.0000292, -0.0000901, -  
0.0000111, 0.0007925, -1.5568472, -0.0656985, -0.0000476, 0.8139337, -0.0588  
262, 0.0000054, 0.0000738, -0.0000137, 0.043802, 1.3094023, 0.0639991, 0.0000  
376, 0.3977935, 0.214815, 0.000023, 0.0000852, 0.0000149, 0.1145087, 0.131629  
1, 0.0233349, 0.0000022, 0.0517419, 0.1136437, -0.0000064, 0.0000063, -0.0000  
068, 0.1700121, 0.2766791, -0.2962531, -0.0000323, -0.9685793, -0.1082281, -0

. 0000321, -0. 000125, -0. 0000163, -0. 0446997, -0. 8488617, 0. 1300891, 0. 000001  
8, -0. 0887307, 0. 1890972, 0. 0000467, -0. 0000262, 0. 000052, -0. 1713994, -0. 622  
9772, 0. 0316942, -0. 0000061, 0. 5806762, -0. 3569484, -0. 0000068, 0. 0000663, -0  
. 0000204, -0. 2023002\Polar=313. 6013635, 15. 6119663, 109. 996206, 0. 0079474,  
0. 007401, 59. 2778305\PG=C01 [X(C2H2N12)]\NImag=1\

## N12P2

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C2H2N10\ROOT\16-Oct-2012\0  
\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) F  
req\Title Card Required\0,1\C,-3.3105000907,-1.1863784822,-0.0741134  
029\N,-2.4101047711,-0.3187349389,-0.0831029179\H,-4.823379913,-2.3347  
599359,-0.6389582939\N,-1.1064340467,-0.761434682,-0.0689351246\N,-0.3  
304826453,0.2254005522,-0.0512318922\N,0.9727589455,-0.2968884786,-0.0  
403942666\N,-4.2893681862,-1.8771742221,0.089752398\N,1.7537972144,0.6  
76694208,-0.0056063755\N,3.0706849102,0.299247779,0.0047204893\C,4.101  
8399851,1.1867165028,0.0466970059\H,3.9670991721,2.2568414053,0.076772  
1884\N,3.5913740521,-0.9680231801,-0.0254318003\N,4.864906201,-0.81371  
143,-0.0019142625\N,5.2249821727,0.5186199025,0.0437682548\Version=EM  
64L-G09RevA.01\State=1-A\HF=-624.7000087\RMSD=5.241e-09\RMSF=2.847e-05  
\ZeroPoint=0.0776227\Thermal=0.0879883\Dipole=-2.186494,0.310467,-0.52  
98299\DipoleDeriv=2.7847253,1.3012446,-0.0914198,2.4686947,1.4678586,-  
0.0959632,-0.4775065,-0.2258795,0.2790372,-2.8519617,-0.9515547,0.0575  
226,-1.0114507,-0.7303235,0.0523961,-0.0772253,0.0067903,-0.217759,0.6  
369128,0.1154074,0.025888,0.208949,0.4374579,-0.0211288,-0.1968213,-0.  
0970138,0.2753845,2.1266688,0.5489835,-0.0083679,0.3266788,0.099068,0.  
001218,0.03082,-0.013281,0.0476173,-0.6796152,-0.1965504,0.0073179,-0.  
5747564,-0.1447128,-0.0021999,-0.003625,-0.0032735,-0.0741335,0.112479  
4,0.1098645,-0.0054322,-0.4023648,-0.1383665,-0.0023514,-0.0082316,0.0  
023714,0.0099994,-2.2070391,-0.8573231,0.0090393,-1.2895619,-0.9968055  
,0.0643587,0.7223099,0.3303503,-0.277603,1.4527311,0.1602027,0.0194043  
, -0.4040272,-0.070567,-0.0056934,0.0136809,0.0008588,0.0186383,-1.7192  
266,-0.2028332,-0.0181653,0.7024522,-0.012479,0.0049202,-0.0099381,-0.  
006179,0.046292,1.2608236,0.1420975,0.0119192,0.4534158,0.262373,0.005  
9879,0.0283683,0.0060519,0.1234692,0.1247512,0.0234127,-0.0002773,0.04  
67252,0.1285541,-0.000959,0.0009959,-0.000763,0.1698049,0.3293711,-0.2  
695695,-0.0076849,-0.9098485,-0.1812866,-0.0101873,-0.0188628,-0.00807  
15,-0.0402711,-0.7608011,0.0588665,0.0011681,-0.1580312,0.2018966,0.01  
20134,-0.0159868,0.0112904,-0.1637229,-0.6098195,0.0177514,-0.0009121,  
0.543125,-0.3226674,-0.0024112,0.0120225,-0.003252,-0.1967533\Polar=24  
6.5836552,47.6466309,93.9973002,0.3096978,0.101757,51.6345283\PG=C01 [X  
(C2H2N10)]\NImag=0\

## N12UTS1

1\1\GINC-ZHANGRUB0-1\Freq\UB3LYP\6-31+G(d,p)\C2H2N12\ROOT\17-Oct-2012\

```
0\\# freq ub3lyp/6-31+g(d,p) geom=check guess=(mix,read) scf=qc\\Title
Card Required\\0,1\\C,-4.0947521852,-1.0963285945,-0.0002260784\\N,-3.1
15757838,-0.1559138138,-0.0001069453\\H,-3.9115267199,-2.1598301825,-0.
00031729\\N,-1.7316554808,-0.4261695703,-0.0000857796\\N,-0.9745446656,0
.4929444588,0.0000229451\\N,0.9745310301,-0.4929376827,-0.000000802\\N,-
3.689432858,1.0838905143,-0.0000128037\\N,-4.9541801832,0.8694584674,-0
.000075028\\N,-5.2483749835,-0.4787978477,-0.0002083613\\N,1.7316424787,
0.4261758484,0.0001079502\\N,3.1157446544,0.1559190834,0.0001304871\\C,4
.0947396971,1.09633314,0.0002498123\\H,3.9115150199,2.1598348639,0.0003
402101\\N,3.689418754,-1.0838856651,0.0000375774\\N,4.9541662398,-0.8694
545588,0.000100692\\N,5.2483620401,0.4788015391,0.0002334141\\Version=E
M64L-G09RevA.01\\State=1-A\\HF=-734.1251862\\S2=0.587984\\S2-1=0.\\S2A=0.02
7954\\RMSD=0.000e+00\\RMSF=4.581e-06\\ZeroPoint=0.0854035\\Thermal=0.09715
07\\Dipole=0.0000008,0.0000006,-0.0000014\\DipoleDeriv=1.0535238,0.02740
55,0.0000333,0.5580067,0.1969295,0.0000235,0.0000818,0.0000056,0.14360
72,-1.4923614,-0.0098074,-0.0000535,0.996107,0.0249935,0.0000282,0.000
0378,-0.0000055,0.0834673,0.1216834,0.0216827,0.0000004,0.0497431,0.13
29503,-0.0000019,0.0000029,-0.0000027,0.171675,1.4242354,-0.0475813,0.
0000424,-1.5823668,-0.185823,-0.0000717,-0.0000971,-0.0000202,0.017057
5,0.0154292,0.1229989,0.0000127,0.7234517,0.1048922,0.0000363,0.000066
9,0.0000159,-0.0249593,0.0154302,0.1229992,0.0000124,0.7234511,0.10489
23,0.000036,0.0000665,0.0000159,-0.0249593,0.2436456,-0.3400195,-0.000
0218,-1.0098811,-0.117024,-0.0000414,-0.0000826,-0.0000189,-0.0363912,
-0.7485342,0.1470183,-0.0000061,-0.0874342,0.2406357,0.0000337,-0.0000
279,0.0000414,-0.1581091,-0.617622,0.0783027,-0.0000071,0.3523738,-0.3
975544,-0.0000066,0.0000182,-0.0000157,-0.1963475,1.4242342,-0.047582,
0.0000432,-1.5823677,-0.1858228,-0.0000717,-0.0000948,-0.0000201,0.017
0575,-1.4923608,-0.0098068,-0.0000542,0.9961081,0.0249932,0.0000286,0.
0000359,-0.0000055,0.0834673,1.0535243,0.0274052,0.0000337,0.5580061,0
.1969293,0.0000236,0.0000821,0.0000056,0.1436072,0.1216835,0.0216828,0
.,0.0497431,0.1329504,-0.0000019,0.0000029,-0.0000026,0.1716751,0.2436
446,-0.3400197,-0.0000215,-1.0098813,-0.1170234,-0.0000417,-0.0000818,
-0.0000191,-0.0363912,-0.7485341,0.1470187,-0.0000065,-0.0874335,0.240
6356,0.0000335,-0.0000283,0.0000413,-0.158109,-0.6176217,0.0783027,-0.
0000073,0.3523739,-0.3975546,-0.0000064,0.0000176,-0.0000155,-0.196347
5\\Polar=271.0545401,5.2695942,102.2888243,0.0076567,0.0041794,58.36932
65\\PG=C01 [X(C2H2N12)]\\NImag=1\\
```

#### N14

```
1\\1\\GINC-ZHANGRUB-2\\Freq\\RB3LYP\\6-31+G(d,p)\\C2H2N14\\ROOT\\05-Oct-2012\\0
\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) F
req\\Title Card Required\\0,1\\C,-2.6500327489,-0.9161643563,0.00004302
3\\N,-1.5610648451,-0.0915210573,-0.0007124058\\H,-2.5812252571,-1.99326
07658,-0.0003229242\\N,-0.2792888446,-0.5426122009,-0.0012558131\\N,0.56
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#### N14TS1

1\1\GINC-ZHANGRUBO-3\Freq\RB3LYP\6-31+G(d,p)\C2H2N14\R00T\09-Oct-2012\0\#\freq b3lyp/6-31+g(d,p) nosymm geom=check guess=read\Title Card Required\0, 1\C, -2.4613824761, -0.8658844761, -0.0033871435\N, -1.4848200641, 0.0066177272, -0.000514959\H, -2.3060735879, -1.9406922598, -0.0064500343\N, -0.2308406326, -0.4876766339, -0.001864533\N, 0.6312700325, 0.433471071, 0.001030184\N, 1.8785408743, -0.1965676034, -0.0009666304\N, -2.8678852



535, 1. 6838759057, 0. 0039266296\N, -3. 6954405231, 0. 8798742572, 0. 001296930  
7\N, -3. 755742188, -0. 4624183148, -0. 0026065311\N, 2. 7571191478, 0. 69634431  
34, 0. 0110363827\N, 4. 0055648338, 0. 0446443978, 0. 0088350845\N, 4. 873021372  
8, 0. 9443992769, 0. 0023320058\N, 6. 1477482225, 0. 4563966895, 0. 0016257577\C  
, 7. 2542059872, 1. 2527786349, -0. 0041379586\H, 7. 2120243976, 2. 3310484754, -  
0. 0069454373\N, 6. 5585776815, -0. 8541195599, 0. 003558445\N, 7. 8386419431, -  
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. 000808, 0. 0025111, 0. 0001173, 0. 1612972, -2. 9799004, -0. 0991099, -0. 0014705  
, -0. 4797812, -0. 106252, -0. 0001258, 0. 001177, -0. 0008851, -0. 1486908, 0. 1625  
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01814, 0. 145247, 2. 4555781, 0. 1599612, 0. 0016019, 0. 8333795, -0. 1838223, 0. 00  
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. 724164, -0. 0482807, 0. 0000886, -0. 0101954, 0. 0026822, -0. 065934, 1. 1108998,  
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416, -0. 0177948, 2. 0741106, -0. 7060677, -0. 0014453, 0. 3234618, -0. 3939932, -0  
. 0010816, 0. 0013654, -0. 001515, 0. 0402301, -2. 1050644, 0. 5571402, 0. 0009574,  
-1. 2942958, 0. 8106706, 0. 0015657, -0. 0044852, 0. 0023103, 0. 0815315, -0. 98475  
31, 0. 081962, -0. 0000872, 0. 8369351, -0. 382016, -0. 0002264, 0. 0021334, -0. 000  
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-0. 0003381, 0. 0059225, -0. 0056004, -0. 0433895, -0. 4088403, 0. 0403277, -0. 001  
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, 0. 0058761, 0. 0279848, -2. 0807522, -0. 0005024, 0. 002028, 0. 9697321, -0. 09265  
69, -0. 0010004, 0. 0097555, -0. 0053352, 0. 0514463, 1. 5261589, 0. 0098831, -0. 00  
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. 1358419, 0. 0223724, 0. 0001168, 0. 0561687, 0. 1254795, 0. 0001068, -0. 0000391,  
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#### N14p1

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C2H2N14\R00T\12-Oct-2012\0  
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755093, -0. 003512401\N, -0. 1931606365, -0. 3676899653, -0. 0019680956\N, 0. 69  
10347745, 0. 5299265324, -0. 0000244089\N, 1. 9258982535, -0. 1315796923, -0. 00  
22584315\N, -4. 4762782397, 1. 7796242628, 0. 0024507286\N, -4. 0107376968, 0. 7

520110974, 0.0007895062\N, -3.6878149232, -0.4698965239, -0.0011356631\N, 2  
.8250821063, 0.7397915095, 0.0100438006\N, 4.058727302, 0.0575583588, 0.007  
4930919\N, 4.9474243578, 0.9356301015, 0.0026564788\N, 6.2109493252, 0.4158  
352336, 0.0014210669\C, 7.3357351359, 1.1851867249, -0.0027659668\H, 7.3194  
306434, 2.2641275084, -0.0039048063\N, 6.5897519894, -0.9035852963, 0.00144  
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\RMSD=5.188e-09\RMSF=2.021e-05\ZeroPoint=0.0973511\Thermal=0.1114478\D  
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, -0.0000142, 0.7333495, 0.6813548, 0.0011569, 0.0007989, 0.0006013, 0.210268  
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8, 0.0010306, 0.2708721, 0.024159, 0.0008724, 0.0030113, 0.002575, 0.0120161,  
-1.5735143, -0.0287207, -0.0014164, -0.5401547, -0.0775949, 0.0000258, -0.00  
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.0409654, -0.0010545, 0.0011589, -0.004114, -0.0166941, -0.5218797, 0.300639  
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, 0.0009718, -0.2788348, 0.0020302, -0.0005136, 0.0055678, -0.0049429, -0.041  
9972, -0.363107, 0.0496498, -0.0010316, -0.5510062, -0.0647023, -0.0002472, -  
0.00198, 0.0040749, 0.0031207, 1.8357319, -0.0321001, -0.0013319, -0.4682111  
, -0.0001236, 0.0016434, -0.0086559, 0.0051816, 0.026633, -2.0232626, 0.03704  
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741, 1.5222777, -0.015662, -0.0017012, 0.4232484, 0.1943676, -0.0001654, -0.0  
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223442, 0.0000492, 0.0000362, -0.000186, 0.1689193, 0.271933, -0.3277957, 0.0  
003245, -1.117509, -0.0046868, 0.0013751, 0.0010056, 0.0011066, -0.0374058, -  
0.9087167, 0.1998177, -0.0001683, -0.1135737, 0.2206789, -0.0006933, 0.00053  
62, -0.000653, -0.1604842, -0.6092117, 0.0628022, 0.0002576, 0.7064786, -0.41  
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#### N14TS2

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C2H2N14\R00T\15-Oct-2012\0  
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254813603, -0.6637680494, 0.0000339956\N, -1.4705394117, 0.2759120368, 0.00  
00415473\N, -0.227416132, -0.3365091223, 0.0000398103\N, -6.8996363854, 1.6  
33704627, 0.0000363243\N, -6.1930439089, 0.7838401016, 0.0000344025\N, -5.7

696103967, -1.2042519886, 0.0000241328\N, 0.6560182024, 0.5558699822, 0.000  
0529872\N, 1.8982012741, -0.1011775542, 0.0000510713\N, 2.7765727934, 0.787  
1727028, 0.0000504845\N, 4.0481303756, 0.2765226994, 0.0000501784\C, 5.1638  
529996, 1.0558904214, 0.0000506413\H, 5.1372904588, 2.1345105904, 0.0000526  
248\N, 4.4384099079, -1.0372258255, 0.0000472175\N, 5.7212998754, -1.011621  
4898, 0.0000463853\N, 6.214313787, 0.2784104335, 0.0000485438\\Version=EM6  
4L-G09RevA.01\State=1-A\HF=-843.5605621\RMSD=4.317e-09\RMSF=2.926e-06\  
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06, 0.0000375, 0.0000078, 0.0318539, 0.54886, -0.0004603, 0.0000027, 0.623254  
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00024, -0.0000649, -0.000022, -0.0611423, 0.1210778, 0.0830817, -0.0000024, -  
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, -0.000099, 0.0488098, 1.503105, 0.0294732, 0.0000046, 0.426071, 0.2083887, 0  
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3094032, 0.0000019, -1.1104777, -0.0523421, -0.0000025, 0.000026, 0.0000065,  
-0.0401731, -0.9362492, 0.1620765, -0.0000013, -0.1058381, 0.2015827, 0.0000  
023, 0.0000715, 0.0000167, -0.1649658, -0.6363505, 0.0430251, -0.0000048, 0.7  
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(C2H2N14)]\NImag=1\\

## N14p2

1\1\GINC-ZHANGRUB-2\Freq\RB3LYP\6-31+G(d,p)\C2H2N12\ROOT\16-Oct-2012\0  
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req\\Title Card Required\\0,1\C, 4.4603935537, -1.1806646579, -0.04675133  
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5636, -0.5679353549\N, 2.2401192411, -0.8582280599, -0.0644055903\N, 1.4162  
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#### N14UTS1

1\1\GINC-ZHANGRUB0-3\Freq\UB3LYP\6-31+G(d,p)\C2H2N14\R00T\23-Oct-2012\0\\# freq ub3lyp/6-31+g(d,p) guess=(mix,read) geom=check\\Title Card Required\\0,1\C, 5.0391400841, -0.9411196463, 0.1379846442\N, 3.8126823893, -0.4247648606, -0.1183963444\H, 5.2333367748, -1.9898791811, 0.299396321\N, 2.657466693, -1.154559701, -0.2929456883\N, 1.6191539906, -0.4300452334, -0.1651258702\N, 0.4644882358, -0.5249201654, -0.4884064527\N, 3.9282138927, 0.9200064035, -0.2786938483\N, 5.1789647127, 1.1838064314, -0.1036068382\N, 5.9015146144, 0.0500293771, 0.1542904092\N, -0.4643301514, 0.5248121697, 0.4871753122\N, -1.6189195634, 0.4300610916, 0.1638910524\N, -2.6572809005, 1.154642708, 0.2915979346\N, -3.8125317685, 0.4248366275, 0.1175650369\C, -5.0390200546, 0.9411552372, -0.1387402406\H, -5.2331608195, 1.9898484295, -0.3008241677\N, -3.9281607968, -0.9198249196, 0.2788100693\N, -5.17900722

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**Electronic energies of important species at various methods  
combined with aug-cc-PVTZ basis set**

	M06-2X	MP2
N <sub>10</sub>	-624.703880090	-623.67571298
IM8 <sup>0</sup>	-405.76487384	-405.07037126
N <sub>2</sub>	-109.53368511	-109.36461377
HCN	-93.42341236	-93.25954770
HNC	-93.40301335	-93.23129470
N <sub>12</sub>	-734.14130927	
N <sub>14</sub>	-843.57597218	