

**Supporting Information**  
**for**  
**Scaling Approach for Intramolecular Magnetic Coupling**  
**Constants of Organic Diradicals**

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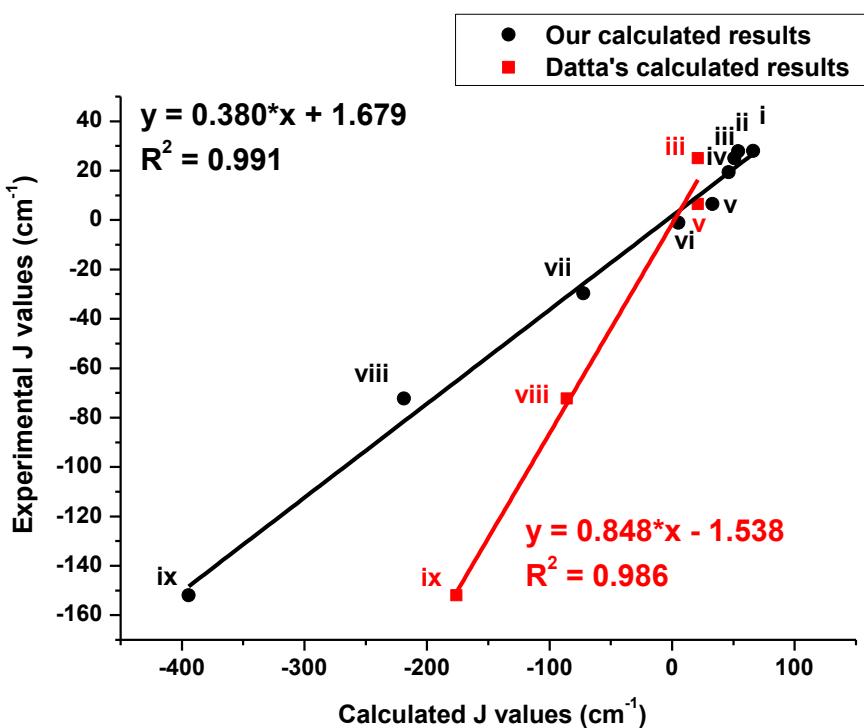
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## 1. Calculated intramolecular magnetic coupling constants of diradicals (i–xiii)

**Table S1.** Calculated absolute energies in atomic unit (a.u.), the  $\langle S^2 \rangle$  value and intramolecular magnetic exchange coupling constants ( $J$  in  $\text{cm}^{-1}$ ) using UB3LYP/6-311++G(d, p) for diradicals (i–xiii).

Diradical	$E_T$ in au ( $\langle S^2 \rangle$ )	$E_{BS}$ in au ( $\langle S^2 \rangle$ )	$J$ ( $\text{cm}^{-1}$ )
2,4-thiophene based <b>NN</b> diradical (i)	-1619.79833644 (2.127578)	-1619.7980298 (1.110525)	66.2
3,5-pyridine based <b>NN</b> diradical (ii)	-1315.0650742 (2.122624)	-1315.06482439 (1.108671)	54.1
1,3-phenylene based <b>NN</b> diradical (iii)	1299.02637548 (2.120136)	-1299.02614091 (1.106967)	50.8
1,3-phenylene based <b>OVER</b> diradical (iv)	-1131.79403604 (2.049175)	-1131.79382485 (1.04301)	46.1
2,6-pyridine based <b>NN</b> diradical (v)	-1315.0575241 (2.11934)	-1315.05737224 (1.110697)	33.0
1,2,4-triazole based <b>NN</b> diradical (vi)	-1309.03000419 (2.109469)	-1309.02998017 (1.108146)	5.3
1,4-phenylene based <b>OVER</b> diradical (vii)	-1131.79437842 (2.041718)	-1131.79470467 (1.052755)	-72.4
1,4-phenylene based <b>NN</b> diradical (viii)	-1299.02726918 (2.103744)	-1299.02822813 (1.141702)	-218.8
2,5-thiophene based <b>NN</b> diradical (ix)	-1619.79926274 (2.101517)	-1619.80093782 (1.16955)	-394.5
1,3-phenylene based <b>DTDA</b> diradical (x)	-2119.18783234 (2.038235)	-2119.18768073 (1.033255)	33.1
2,4-thiophene based <b>DTDA</b> diradical (xi)	-2439.95024916 (2.039691)	-2439.95011558 (1.034594)	29.2
1,4-phenylene based <b>DTDA</b> diradical (xii)	-2119.18821589 (2.032037)	-2119.18848437 (1.041462)	-59.5
2,5-thiophene based <b>DTDA</b> diradical (xiii)	-2439.94930754 (2.032925)	-2439.94968391 (1.048519)	-83.9

2. Calculated intramolecular magnetic coupling constants of four diradicals (iii, v, vii and ix) studied by Datta et al..



**Figure S1.** Comparison of our calculated results and Datta's calculated results.

Diradical	Datta's calculated $J$ value <sup>a</sup> ( $\text{cm}^{-1}$ )	Experimental $J$ value ( $\text{cm}^{-1}$ )
1,3-phenylene based NN diradical (iii)	21	25
2,6-pyridine based NN diradical (v)	21	6.5
1,4-phenylene based NN diradical (viii)	-86	-72.3
2,5-thiophene based NN diradical (ix)	-176	-152

<sup>a</sup>The calculated  $J$  values were obtained by using Yamaguchi's formalism (eq 3) with DFT calculations in ref 7a [B3LYP/6-311+G(d,p)]

### **3. Comparison between our calculation method with Datta's one.**

It was found that Datta et. al. used totally different calculation procedure from our one. Thus, it is not surprising that the discrepancies between our calculated results and Datta's ones were found. To obtain the fully optimized geometries of triplet state, Datta et al. used ROHF methodology. Then, single-point calculations performed to calculate the  $J$  values on the optimized geometry at the UB3LYP with 6-311G(d,p) and 6-311+G(d,p) level. Moreover, to obtain the BS states, single-point UB3LYP calculations were carried out using the initial guess values of molecular orbitals, which are in turn retrieved from the ROHF calculations. And the structure of BS calculation is taken from the triplet calculation. And both spin states have exactly the same geometry.

On the other hand, our calculations were performed at UB3LYP/6-311++G(d,p) level. And especially the triplet and BS states were fully optimized. In BS state calculations, a keyword "stable=opt" was used for ensuring the stability of BS solution, and "guess=mix" was used to generate an appropriate guess for the UB3LYP calculation, as mentioned in computational details. In our calculations, the triplet and BS calculations might have the slightly different geometries. Moreover the initial guess of BS state of our method is not consistent with Datta's results. Thus, those methodological differences can lead the different  $J$  values obtained from DFT calculations with same B3LYP functional.

It must be stressed that our calculation procedure in this study is better than that of Datta's one, even though the results studied by Datta et al. shows the quite accurate  $J$  values compared with experimental  $J$  values. Because our calculated results clearly show the same trend in magnitude of  $J$  values compare to experimental ones (Table 1). Most notably, the strong correlation between calculated and experimental  $J$  values of 9 diradicals (**i–ix**) is found on the basis of linear regression analysis, as shown in Figure 3. Further studies should be followed regarding how to generate initial guess of a BS state and the effect of self-interaction error (SIE) to the overestimation of  $J$  values.

#### 4. Calculated intramolecular magnetic coupling constants of diradicals (xiv–xvi)

**Table S2.** Calculated absolute energies in atomic unit (a.u.), the  $\langle S^2 \rangle$  value and intramolecular magnetic exchange coupling constants ( $J$  in  $\text{cm}^{-1}$ ) using UB3LYP/6-311++G(d, p) for diradicals (xiv–xvi).

Diradical	$E_T$ in au ( $\langle S^2 \rangle$ )	$E_{BS}$ in au ( $\langle S^2 \rangle$ )	$J$ ( $\text{cm}^{-1}$ )
OVER diradical with no coupler (xiv)	-900.66885706 (2.032861)	-900.67163808 (1.011537)	-597.6
Ethylene based NN diradical (xv)	-1145.3465886 (2.097798)	-1145.34993909 (1.224521)	-842.1
Hexatriene based NN diradical (xvi)	-1300.20673128 (2.132679)	-1300.20872513 (1.273903)	-509.6

## 5. Log files of triplet and BS calculations

### Triplet- (i)

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### Triplet- (ii)

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## BS state - (ii)

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cyc=800 guess=(read,mix) \\final_NN_pyridine2_NN_0_1\\0,1\C,-0.0000071
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21,-0.2605515696,-2.1343571599\H,-6.6729886001,-0.6636473327,-0.938984
0194\H,-6.2646130687,1.0281235639,-1.2740540502\C,2.4881040563,0.41021
39935,-0.0258069508\N,3.6728962812,0.9161991352,0.4000266585\N,2.68297
91251,-0.8557143596,-0.4772542775\C,4.8259947061,0.0042721342,0.047428
7912\0,3.8770495195,2.0591295219,0.9191249126\C,4.0742908582,-1.351699
5017,-0.1549883365\0,1.8153461742,-1.6256375584,-0.9977839487\C,5.8558
03007,0.0226824585,1.1744783739\C,5.4447318314,0.5775552875,-1.2391619
876\C,3.9421986876,-2.1913672904,1.1271061024\C,4.5864115001,-2.222854
7814,-1.2989454864\H,6.6729897638,-0.6636452529,0.9389818693\H,6.26461
04267,1.0281228272,1.2740607559\H,5.425835472,-0.2605587397,2.13435765
92\H,4.7305037437,0.5903378595,-2.0647916414\H,5.7649369294,1.60272535
13,-1.0461276842\H,6.3164281278,-0.0058518413,-1.5418528846\H,3.248130
1567,-3.0122384373,0.9390385547\H,4.9079666747,-2.6125048482,1.4132010
263\H,3.5575975181,-1.603363735,1.96266662975\H,4.5872578589,-1.6973293
673,-2.2529501384\H,5.6034269084,-2.5580353339,-1.0807874127\H,3.94637
12112,-3.0992434262,-1.3989942612\N,0.0000017114,3.1971334874,0.000002
1516\\Version=AM64L-G03RevD.02\\State=1-A\\HF=-1315.0648244\\S2=1.108671\\
S2-1=0.\\S2A=0.858163\\RMSD=8.917e-09\\RMSF=1.484e-05\\Thermal=0.\\Dipole=0
.0000005,-2.0338362,-0.0000014\\PG=C01 [X(C19H27N504)]\\@
```

### Triplet- (iii)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C20H28N404(3)\X543LJY\03-May
-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=2000\\Dushin_NN_mbenzene_NN_0_3\\0,3\C,-0.41154212,0.2015538
066,0.0728682166\C,-0.4671157021,1.5198952445,0.5490295488\C,-1.717897
7413,2.1200305116,0.7804771707\C,-2.8358874005,0.1119558662,0.02463110
23\H,0.5437036056,-0.2668285965,-0.0959602631\H,-1.7652047659,3.122028
2894,1.1806170537\H,-3.7468734939,-0.4202963335,-0.2059511885\C,-1.592
2551579,-0.5107045875,-0.1848080788\C,0.7682139106,2.2580664404,0.8080
177197\N,1.975175039,2.0078815259,0.2337698674\N,0.896559604,3.3108111
827,1.655930811\C,3.0784488513,2.8075011692,0.8872107224\O,2.238033918
2,1.1390327637,-0.6563299394\C,2.252571964,3.9663934307,1.5320344444\O
,-0.0064717861,3.820396794,2.3949326098\C,4.0971813505,3.234357869,-0.
1662271595\C,3.7412998281,1.8678648583,1.9090415958\C,2.0559120264,5.1
839790493,0.6123347291\C,2.7273748951,4.4248649549,2.908793615\H,4.878
0628879,3.8406497761,0.2996707152\H,4.5588430856,2.3481948376,-0.60125
05912\H,3.6436585584,3.806772136,-0.9743276302\H,3.0347871015,1.527141
0079,2.6683396056\H,4.1252625276,0.9922753224,1.3827904107\H,4.5750616
592,2.3664033649,2.4073841679\H,1.3098780995,5.8426597474,1.0600404844
\H,2.9882533658,5.7414637899,0.5029108589\H,1.7059938781,4.8925511203,
-0.3799510686\H,2.7661556306,3.6074150052,3.6276408845\H,3.7225957583,
4.8691840508,2.8274366526\H,2.0410834021,5.1783555876,3.2950841623\C,-
2.8833956342,1.4132983239,0.509757461\H,-3.844551028,1.8844505836,0.67
96601256\C,-1.5255951342,-1.8870386073,-0.6740152997\N,-2.4990677259,-
2.5251246008,-1.3732231828\N,-0.481717668,-2.7403545737,-0.4971128226\
C,-2.19322275,-3.9952887045,-1.5429563059\O,-3.6143588631,-2.044920369
8,-1.7563310043\C,-0.6473417533,-3.9990816789,-1.3166233422\O,0.585700
6241,-2.5240979838,0.1587188635\C,-2.656795827,-4.4589628343,-2.921809
7317\C,-2.9896165004,-4.7263661468,-0.4482426848\C,0.1734068393,-3.785
9189632,-2.6001436954\C,-0.1002482277,-5.1939295449,-0.5402337345\H,-2
.4058773775,-5.5135890967,-3.0607147996\H,-3.7383826128,-4.3465301948,
-2.9959363769\H,-2.2042952988,-3.8819501151,-3.7272726141\H,-2.6900551
88,-4.4105681036,0.5530193843\H,-4.0492700332,-4.4997862991,-0.5773793
967\H,-2.8549308414,-5.8069292109,-0.5274081935\H,1.2146717801,-3.6091
865492,-2.3252553275\H,0.1284029189,-4.6707145875,-3.2382337239\H,-0.1
794576958,-2.9255028062,-3.1719361223\H,-0.5770582685,-5.3107873479,0.
432060061\H,-0.2497016088,-6.1094483677,-1.1180823133\H,0.9683937649,-
5.0580341237,-0.3752896649\\Version=IBM64-G03RevC.02\\State=3-A\\HF=-129
9.0263755\\S2=2.120136\\S2-1=0.\\S2A=2.006498\\RMSD=3.508e-09\\RMSF=7.845e-
06\\Dipole=0.9998606,-0.4897972,-0.1766951\\PG=C01 [X(C20H28N404)]\\@
```

### BS state - (iii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N404\X543LJY\08-May-20
12\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=1200 GUESS=(READ,MIX) \\final_Dushin_NN_mbenzene_NN_0_1\\0,1\C,-
0.0000261419,0.4640676928,-0.0000866215\C,-1.2170933401,1.1610889237,0
.0106426149\C,-1.2097116153,2.5670978229,-0.0040548832\C,1.2096006727,
2.5671361339,0.0028556993\H,-0.0000001013,-0.6131696195,0.0001612549\H
,-2.144559935,3.1071801371,-0.0319896345\H,2.1444254159,3.1072689555,0
.0305474749\C,1.2170122661,1.1611236152,-0.0112091998\C,-2.4820074457,
0.426630815,0.0294961133\N,-2.6537404556,-0.8416658654,0.4879811505\N,
-3.6782407053,0.9028369461,-0.40066187\C,-4.0300068286,-1.3707138679,0
.1570153362\0,-1.7776879157,-1.5908798281,1.0242577341\C,-4.8112990932
,-0.0335518513,-0.049489503\0,-3.9131036864,2.040687689,-0.9217564981\
C,-4.5292747862,-2.254048078,1.2973130607\C,-3.8709133492,-2.206716750
4,-1.1244818994\C,-5.4462451975,0.5272352129,1.2347953852\C,-5.8389278
406,-0.040076314,-1.1786804959\H,-5.5380041454,-2.6103399623,1.0738334
384\H,-3.8711452291,-3.1166142708,1.3998103956\H,-4.5456468691,-1.7298
573954,2.2519430483\H,-3.4933314233,-1.6097660928,-1.9568656656\H,-3.1
59895658,-3.0119439713,-0.9319244041\H,-4.8251262941,-2.6491057115,-1.
4174136455\H,-5.7872275167,1.5453463785,1.0397434135\H,-6.3064950627,-
0.0738087496,1.5360277082\H,-4.7344782463,0.5556601736,2.062184449\H,-
5.4007361131,-0.3168041763,-2.1367388264\H,-6.64223557,-0.7427641867,-
0.9432562139\H,-6.2682463557,0.9564027585,-1.2820125688\C,-0.00066551
5,3.2511325934,-0.0007455645\H,-0.0000867988,4.3349603933,-0.000965392
9\C,2.4819272079,0.4266458792,-0.029544375\N,3.6780826109,0.9029902631
,0.4006707592\N,2.6537084874,-0.8417137319,-0.4878172142\C,4.811230255
8,-0.0335571946,0.0502626919\0,3.912852034,2.0411098914,0.9212201098\C
,4.0300220794,-1.3706763778,-0.1570066118\0,1.7778608927,-1.5907478536
,-1.024680771\C,5.8379663714,-0.0404055401,1.1802646731\C,5.4473507617
,0.5272571068,-1.2334343957\C,3.8710090664,-2.2073581803,1.1240657539\
C,4.5295249163,-2.2533880244,-1.2976809216\H,6.6406637599,-0.744171446
9,0.945985187\H,6.268332596,0.9556604984,1.2832254718\H,5.3987033404,-
0.3159405955,2.1381763509\H,4.7371069097,0.5531397151,-2.062212645\H,5
.7856376754,1.5463583434,-1.0388548524\H,6.3095479757,-0.0721520133,-1
.5323478436\H,3.1578817168,-3.0108245651,0.9319495263\H,4.8246690075,-
2.6521363464,1.4151712384\H,3.4960555952,-1.6102288486,1.9575070396\H,
4.5461408153,-1.7286673861,-2.252014892\H,5.5381883848,-2.6098394256,-
1.0741603215\H,3.8713935221,-3.1158767638,-1.4008246101\\Version=IBM64
-G03RevC.02\State=1-A\HF=-1299.0261409\S2=1.106967\S2-1=0.\S2A=0.84529
3\RMSD=4.820e-09\RMSF=2.088e-05\Dipole=-0.0002295,-1.1274503,0.0006639
\PG=C01 [X(C20H28N404)]\\@
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### Triplet- (iv)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C14H16N802(3)\X543LJY\12-Mar
-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OOPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=1200\\OVERC_mbenzene_OVERC_0_3\\0,3\C,0.2378673103,0.4118282
616,-0.000331502\C,1.6359782908,0.4024480108,0.0065543297\C,2.33093950
67,1.6187106047,0.0056060626\C,1.6286325822,2.8197104078,-0.0022670063
\C,0.2373810702,2.8279146098,-0.0091813218\C,-0.4688853131,1.618181076
2,-0.0081795304\H,-0.3023216179,-0.5234211997,0.0004203028\H,3.4127256
05,1.6129869478,0.0109732107\H,2.1708807925,3.7585233406,-0.003021652\
H,-0.3081397136,3.7620946696,-0.0152948212\C,-1.9557127721,1.614331862
1,-0.015184527\N,-2.5662507485,2.7997421083,-0.0229856308\N,-2.5624029
581,0.4273855307,-0.0131231419\N,-3.9253187409,2.7687233583,-0.0307418
173\N,-3.9211865992,0.4533213692,-0.0191475345\C,-4.5757505157,4.07492
5492,-0.0273626455\C,-4.6921411419,1.6095866503,-0.0198799277\C,-4.565
7423144,-0.8557390095,-0.0062421235\H,-4.3313406904,4.6028386754,0.896
9525381\H,-4.2141635658,4.6554253777,-0.8775224534\H,-5.6491656841,3.9
252470078,-0.0992462842\O,-5.9101573672,1.6075655146,-0.0143325516\H,-
4.2964874619,-1.3846096359,0.9103345516\H,-5.6411645065,-0.7107736806,
-0.0535126797\H,-4.2213011204,-1.4324973046,-0.8662151096\C,2.37560218
73,-0.887362629,0.0145990506\N,3.7074944047,-0.8238666142,0.0213981118
\N,1.6506205402,-2.0059869898,0.0143898694\N,4.3597444971,-2.016586921
,0.0301367636\N,2.3520615172,-3.1700033508,0.0213308552\C,5.8161938908
,-1.9273016858,0.0256406784\C,3.7388621166,-3.2600327682,0.0212068154\
C,1.5402178723,-4.3824592216,0.0104505805\H,6.1507014986,-1.4528911047
,-0.8994679301\H,6.1389355359,-1.3230206073,0.8748635919\H,6.222966981
,-2.9318058899,0.0984277855\O,4.3457382513,-4.3160998434,0.0165120701\
H,0.9469374914,-4.4146130528,-0.9056825125\H,2.2031977673,-5.241499086
8,0.0583098975\H,0.8691016085,-4.3712592304,0.8708694903\\Version=IBM6
4-G03RevC.02\State=3-A\HF=-1131.794036\S2=2.049174\S2-1=0.\S2A=2.00123
4\RMSD=8.032e-09\RMSF=1.135e-06\Di pole=0.1554205,0.2690831,-0.0002169\
PG=C01 [X(C14H16N802)]\\@
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## BS state - (iv)

```
1\1\GINC-GAIA07\F0pt\UB3LYP\6-311++G(d,p)\C14H16N802\X543LJY\19-Mar-20
12\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=800 GUESS=(READ,MIX) \\opt_OVERC_mbenzene_OVERC_0_1\\0,1\C,-0.00
00000263,0.475588,0.000000698\C,1.2153869677,1.1667320336,0.002104\C,
1.2088589289,2.5675260335,0.002159\C,-0.0000001803,3.256258,0.0000006
98\C,-1.2088590711,2.5675259665,-0.002161\C,-1.2153860323,1.1667309664
,-0.002105\H,0.0000000335,-0.604457,0.0000000698\H,2.1484949141,3.1036
260595,0.003831\H,-0.0000002403,4.340418,0.0000000698\H,-2.1484960859,
3.1036249405,-0.003833\C,-2.5009790116,0.4197589308,-0.004064\N,-3.622
5760316,1.1408898997,-0.006507\N,-2.4326729748,-0.9115000673,-0.003225
\N,-4.783952012,0.4342908676,-0.009727\N,-3.6222809566,-1.5686401003,-
0.004556\C,-6.0004590343,1.2400598339,-0.00052\C,-4.8681799736,-0.9529
841348,0.000534\C,-3.5256419163,-3.0245880976,0.006918\H,-6.0488500504
,1.8187978325,0.924416\H,-5.9813670533,1.9241758344,-0.850295\H,-6.855
4110159,0.5736238102,-0.069166\O,-5.9218609567,-1.5639351639,0.010219\
H,-3.0240039073,-3.3485250837,0.921106\H,-4.5295899049,-3.4369021254,-
0.036293\H,-2.9426389072,-3.3511520815,-0.855815\C,2.5009789884,0.4197
590692,0.004063\N,3.6225759684,1.1408901003,0.006508\N,2.4326730252,-0
.9114999327,0.003223\N,4.783951988,0.4342911324,0.009726\N,3.622281043
4,-1.5686388997,0.004556\C,6.0004589657,1.2400601661,0.000524\C,4.8681
800264,-0.9529838652,-0.000534\C,3.5256410837,-3.0245879024,-0.006919\
H,6.0488389496,1.8188181675,-0.9244\H,5.9813779467,1.9241581656,0.8503
14\H,6.8554119841,0.5736221898,0.069146\O,5.9218610433,-1.5639348361,-
0.010216\H,3.0240180927,-3.3485259163,-0.921115\H,4.5295890951,-3.4369
018746,0.036307\H,2.9426260928,-3.3511509185,0.855805\\Version=IBM64-G
03RevC.02\State=1-A\HF=-1131.7938249\S2=1.04301\S2-1=0.\S2A=0.344869\R
MSD=4.075e-09\RMSF=8.556e-05\Dipole=-0.0000011,0.3110997,-0.000001\PG=
C01 [X(C14H16N802)]\\@
```

## Triplet- (v)

1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C19H27N504(3)\X543LJY\23-Mar-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM M) SCFCYC=1200\\opt\_NN\_pyridine\_NN\_0\_3\\0,3\C,-1. 1452061572,1. 28826147 78,0. 0521858125\C,-1. 2005214968,2. 6892650005,0. 0307125297\C,1. 20055000 78,2. 6892525118,-0. 0306706456\H,-2. 1544988389,3. 1971962047,0. 024889929 \H,2. 1545328613,3. 1971733537,-0. 024840463\C,1. 1452193094,1. 2882499968, -0. 0521647084\C,-2. 3715756984,0. 4825578598,0. 1201296383\N,-2. 495939992 2,-0. 7149920229,0. 7520113239\N,-3. 5460576304,0. 8205927382,-0. 454714035 7\C,-3. 7942146433,-1. 3916492799,0. 3621943754\0,-1. 6553856784,-1. 279503 4416,1. 5093163145\C,-4. 6419522809,-0. 1558326343,-0. 0871782299\0,-3. 795 267104,1. 8693207563,-1. 1332140196\C,-4. 34789432,-2. 168839393,1. 5528123 617\C,-3. 4420330809,-2. 3569965402,-0. 7822301467\C,-5. 4366506679,0. 5049 214307,1. 0514998474\C,-5. 5477794069,-0. 3845004783,-1. 2943164608\H,-5. 3 027567507,-2. 6269879655,1. 2830602575\H,-3. 6488013458,-2. 9595233618,1. 8 24683956\H,-4. 4954670456,-1. 5388000109,2. 4291759551\H,-3. 0251106047,-1 . 8329966531,-1. 6441715947\H,-2. 6944530094,-3. 0671044445,-0. 4247356029\ H,-4. 3247296245,-2. 9137903259,-1. 1037560863\H,-5. 8310654304,1. 45845540 61,0. 6963121511\H,-6. 2749700307,-0. 1255318725,1. 3541612345\H,-4. 811466 798,0. 6947330329,1. 9263294294\H,-4. 9978493288,-0. 7459414674,-2. 1622473 225\H,-6. 3234091795,-1. 1117211713,-1. 0413769409\H,-6. 0282191977,0. 5547 205269,-1. 5686941928\C,0. 0000180565,3. 38844682,0. 0000261848\H,0. 000023 8131,4. 4722497106,0. 000034274\C,2. 3715804898,0. 482534343,-0. 1201212189 \N,3. 5460626407,0. 8205432217,0. 454736972\N,2. 4959349076,-0. 7150011842, -0. 7520313459\C,4. 641948952,-0. 155885576,0. 0871862455\0,3. 7952790585,1 . 8692531207,1. 1332624168\C,3. 7942017095,-1. 3916811237,-0. 3622281396\0, 1. 655376031,-1. 279486627,-1. 5093508185\C,5. 5477606,-0. 3845962306,1. 294 3280671\C,5. 4366677053,0. 5048894834,-1. 0514654989\C,3. 4420064268,-2. 35 70605168,0. 7821649709\C,4. 3478805683,-2. 1688396944,-1. 552867182\H,6. 32 3383481,-1. 1118205838,1. 0413779511\H,6. 0282098386,0. 554611493,1. 568734 7587\H,4. 9978167108,-0. 746052293,2. 1622439098\H,4. 8114960673,0. 6947311 199,-1. 9262972968\H,5. 8310889239,1. 4584097965,-0. 6962482683\H,6. 274983 5054,-0. 1255651723,-1. 3541338771\H,2. 6944264781,-3. 0671548641,0. 424643 2391\H,4. 3246980435,-2. 9138672688,1. 103681958\H,3. 0250788505,-1. 833084 1507,1. 6441182725\H,4. 4954619649,-1. 5387749909,-2. 429211081\H,5. 302738 2687,-2. 6270038339,-1. 2831248283\H,3. 6487826161,-2. 9595100511,-1. 82476 56172\N,0. 0000030553,0. 6047564801,0. 0000053618\\Version=IBM64-G03RevC. 02\State=3-A\HF=-1315. 0575241\S2=2. 11934\S2-1=0.\S2A=2. 006346\RMSD=6. 4 14e-09\RMSF=2. 928e-06\Dipole=-0. 0000026,-0. 7787432,-0. 0000093\PG=C01 [ X(C19H27N504)]\\@

## BS state - (v)

```
1\1\GINC-GAIA07\FOpt\UB3LYP\6-311++G(d,p)\C19H27N504\X543LJY\28-Mar-20
12\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=800 GUESS=(READ,MIX) \\opt_NN_pyridine_NN_0_1_2nd\\0,1\C,-1.1454
517155, 1.2871517725, 0.0410996646\C,-1.2006676227, 2.6878080072, 0.019190
9857\C, 1.2006673703, 2.6878081086, -0.0191907088\H,-2.1545983654, 3.19569
56181, 0.0040830634\H, 2.154598069, 3.1956958007, -0.0040827726\C, 1.145451
5748, 1.2871518693, -0.0410994653\C,-2.3732657935, 0.4817179222, 0.0973412
845\N,-2.5056956279, -0.7126896775, 0.7328974386\N,-3.5399714857, 0.81789
27181, -0.493574515\C,-3.7997614095, -1.3903737474, 0.3307669457\0,-1.673
8888569, -1.2746694023, 1.5017263556\C,-4.6410043028, -0.1561344562, -0.13
52885601\0,-3.7800510759, 1.8641262038, -1.179287589\C,-4.3685742948, -2.
1609093221, 1.5185187966\C,-3.4345286796, -2.3618351735, -0.804325605\C,-
5.4497340023, 0.5104367185, 0.9900613813\C,-5.5316085809, -0.3900264057, -
1.3527160467\H,-5.3199207641, -2.6206054135, 1.23917568\H,-3.6729978834,
-2.9500142497, 1.803708603\H, -4.5273118729, -1.5259481449, 2.3893494824\H
,-3.0065351008, -1.8426125576, -1.6637352227\H,-2.6922136709, -3.07095520
41,-0.4340989728\H, -4.31385627, -2.9193040814, -1.1338122855\H,-5.839505
2177, 1.4622218066, 0.6251905696\H, -6.2918798187, -0.118406154, 1.28534893
52\H,-4.8355567495, 0.7045667851, 1.8717188508\H, -4.9710252297, -0.756537
7103, -2.2116580364\H, -6.3112821536, -1.1150530711, -1.1060055937\H, -6.00
73439834, 0.5483435415, -1.6379894889\C, -0.0000001538, 3.3871921577, 0.000
0001629\H, -0.0000002002, 4.470986854, 0.0000001908\C, 2.3732657213, 0.4817
181252, -0.0973412001\N, 3.5399713625, 0.817892935, 0.4935746768\N, 2.50569
56555, -0.7126893626, -0.7328975314\C, 4.6410042705, -0.1561341544, 0.13528
87741\0, 3.7800508361, 1.8641263647, 1.179287878\C, 3.7997615606, -1.390373
3599, -0.3307673186\0, 1.6738889026, -1.2746690213, -1.5017265178\C, 5.5316
082003, -0.390026418, 1.352716459\C, 5.4497343478, 0.5104372007, -0.9900607
873\C, 3.4345290271, -2.3618354389, 0.8043247383\C, 4.3685746113, -2.160908
2027, -1.5185195557\H, 6.311282056, -1.1150527672, 1.1060059535\H, 6.007343
2578, 0.5483435276, 1.6379904742\H, 4.9710246682, -0.7565382596, 2.21165810
01\H, 4.8355566843, 0.7045699534, -1.871717382\H, 5.8395078566, 1.462220902
4, -0.6251888101\H, 6.2918785914, -0.1184069351, -1.2853501427\H, 2.6922136
468, -3.0709549925, 0.4340979358\H, 4.313856594, -2.9193048391, 1.133810655
4\H, 3.0065359785, -1.84261329, 1.6637348996\H, 4.5273122426, -1.5259464802
,-2.3893498375\H, 5.319921075, -2.6206044049, -1.2391766047\H, 3.672998268
7, -2.950012995, -1.8037099068\N, -0.0000000369, 0.6035537275, 0.0000000708
\\Version=IBM64-G03RevC.02\State=1-A\HF=-1315.0573722\S2=1.110697\S2-1
=0.\S2A=0.872937\RMSD=6.271e-09\RMSF=5.661e-06\Dipole=0.0000002,-0.772
8885,-0.0000001\PG=C01 [X(C19H27N504)]\\@
```

### Triplet- (vi)

1\1\GINC-GAIA20\F0pt\UB3LYP\ \C16H25N704(3)\X633KHY\02-Sep-2012\0\\# 0  
PT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT, TIGHT, NOSYMM) SCFCYC=20  
00\\NN\_triazole\_NN\_0\_3\\0,3\C,2. 4226776018,0. 1716652164,0. 0098269213\N  
,2. 9033034216,-0. 8702926212,-0. 7184503452\N,3. 4426672755,0. 9098901266,  
0. 4953831953\C,4. 4093034502,-0. 9812760799,-0. 5530731638\0,2. 2382666092  
,-1. 7389830706,-1. 3440899491\C,4. 7683355726,0. 4672547261,-0. 0727774792  
\0,3. 3337678027,1. 9619876371,1. 2162760813\C,5. 0346586525,-1. 4064597142  
,-1. 8786210078\C,4. 6357940834,-2. 0680744125,0. 5111756594\C,5. 090962201  
8,1. 4461409499,-1. 2152256581\C,5. 8432980983,0. 5529796931,1. 0084512235\  
H,6. 1206224014,-1. 4654664972,-1. 7730021249\H,4. 6598780399,-2. 392555663  
3,-2. 1528678226\H,4. 7974335,-0. 7202418789,-2. 6906566975\H,4. 1802084282  
,-1. 8051049282,1. 4678180629\H,4. 1847421663,-2. 9985639838,0. 163017269\H  
,5. 702754448,-2. 2374213365,0. 6678912935\H,5. 1359207427,2. 4574745932,-0  
. 8083391375\H,6. 0582503177,1. 209074502,-1. 6617596564\H,4. 3309656994,1.  
4249394845,-1. 9986889837\H,5. 5958350504,-0. 038608476,1. 8887963219\H,6.  
7980497611,0. 2044127402,0. 6075996132\H,5. 9581408384,1. 590773158,1. 3214  
127244\C,1. 038127442,0. 4884195142,0. 265668809\C,-1. 0487697586,0. 577147  
9817,0. 402491304\C,-2. 4621943562,0. 2353061371,0. 2356833519\N,-3. 304818  
5191,0. 8499022991,-0. 6188470548\N,-3. 0873627567,-0. 7569687806,0. 901587  
624\C,-4. 7247606822,0. 3627522039,-0. 4117484975\0,-3. 0272273253,1. 79510  
36126,-1. 4164610514\C,-4. 4683028623,-0. 9982948956,0. 3274851834\0,-2. 59  
17866057,-1. 4982437727,1. 8023796868\C,-5. 4291349471,0. 2514082015,-1. 76  
12877247\C,-5. 4116892544,1. 4297150071,0. 4566266472\C,-4. 325433171,-2. 2  
061008262,-0. 6133882131\C,-5. 4418676869,-1. 3247927405,1. 4565932475\H,-  
6. 4429117262,-0. 1310388939,-1. 6186102\H,-5. 4922318495,1. 2395284589,-2.  
217408056\H,-4. 900828305,-0. 4038339511,-2. 4525543952\H,-4. 9198826514,1  
. 5437682043,1. 4244098356\H,-5. 3648985474,2. 3869691708,-0. 0651388793\H,  
-6. 4604212558,1. 1762446883,0. 6238523943\H,-3. 9659145158,-3. 0586888065,  
-0. 0350147851\H,-5. 28876199,-2. 4674657741,-1. 0556756853\H,-3. 610659023  
6,-2. 0142037801,-1. 4156734611\H,-5. 4882398708,-0. 5366923613,2. 20713507  
54\H,-6. 4436972004,-1. 4817896489,1. 0490431291\H,-5. 121527255,-2. 241496  
8902,1. 9519516613\N,-0. 0458006671,-0. 1715354306,-0. 1192047073\N,-0. 658  
1417133,1. 650705229,1. 0841117511\H,1. 3065625998,2. 2500697364,1. 4162658  
061\N,0. 6730701087,1. 5831930506,0. 9874302425\Version=IBM64-G03RevC. 02  
\State=3-A\HF=-1309. 0300042\S2=2. 109469\S2-1=0. \S2A=2. 005259\RMSD=5. 23  
7e-09\RMSF=2. 516e-06\Dipole=1. 2361395,-0. 4099588,-0. 2482877\PG=C01 [X(  
C16H25N704)]\\@

## BS state - (vi)

```
1\1\GINC-GAIA30\F0pt\UB3LYP\ \C16H25N704\X633KHY\04-Sep-2012\0\\# OPT
UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=1200
GUESS=(READ,MIX) \\final_NN_triazole_NN_0_1\\0,1\C,2.4235019215,-0.1571
219449,-0.0385167094\N,2.9109522905,1.0076821465,0.4641087911\N,3.4388
426963,-0.9690782609,-0.4001819557\C,4.4112167414,1.0931842259,0.24141
26072\O,2.2524227314,1.9766427452,0.9286503119\C,4.7733607256,-0.41854
32606,0.0381185021\O,3.3233059011,-2.1402727834,-0.9035942642\C,5.0644
307631,1.7679735912,1.4442808778\C,4.6002660189,1.9570944702,-1.016757
2432\C,5.1338807292,-1.1586176059,1.338051973\C,5.8224281,-0.703982829
1,-1.0342278634\H,6.1467959094,1.811714326,1.3010118463\H,4.6861775669
,2.7862404245,1.5343726431\H,4.8544166817,1.2487708912,2.3785680312\H,
4.1241211946,1.5131568116,-1.893159166\H,4.1482576589,2.9345733528,-0.
8415560359\H,5.6612499228,2.0991120779,-1.2307319687\H,5.1791936703,-2
.2289246126,1.1312594568\H,6.1093515575,-0.835211559,1.7056232628\H,4.
3931434657,-0.9917284925,2.1224690921\H,5.5474067221,-0.29348267,-2.00
48339004\H,6.7830001695,-0.2797651858,-0.7324461352\H,5.9403943632,-1.
7818685802,-1.1455617112\C,1.0363649183,-0.5245096952,-0.19304948\C,-1
.0521485241,-0.6494277977,-0.2561418453\C,-2.4647567912,-0.2896091228,
-0.1222012512\N,-3.2794595193,-0.7306854594,0.8572959386\N,-3.11657606
57,0.5501576333,-0.9520597525\C,-4.709212754,-0.3013880418,0.596563515
8\O,-2.972250789,-1.5011349516,1.8158025564\C,-4.4855673583,0.89083188
7,-0.4001059304\O,-2.6509970938,1.104810647,-1.9923144052\C,-5.3812928
451,0.0667752356,1.9166294681\C,-5.4058545759,-1.5210932287,-0.0290135
587\C,-4.3327020664,2.2598012231,0.2832648174\C,-5.4898810853,0.985247
0361,-1.5454577969\H,-6.4033527548,0.4053643405,1.7292363558\H,-5.4197
362611,-0.8132150978,2.5589338218\H,-4.8448506522,0.8492165818,2.45170
41608\H,-4.9362714091,-1.8193943294,-0.9681547478\H,-5.336778884,-2.35
77042703,0.6681766861\H,-6.4608263309,-1.3107676247,-0.2156692328\H,-3
.9963183638,2.985122019,-0.4593164891\H,-5.2877463687,2.5970310752,0.6
908203435\H,-3.5967072428,2.232229912,1.0888306295\H,-5.546014633,0.06
57094724,-2.1267298038\H,-6.4831206954,1.2127957381,-1.1503535969\H,-5
.1916488323,1.7896713324,-2.2179885001\N,-0.0446650035,0.1904265721,0.
087579312\N,-0.6670756712,-1.8308751638,-0.7309993854\H,1.2950190078,-
2.471390163,-0.9943007408\N,0.6652377062,-1.7386711654,-0.6836941463\\
Version=IBM64-G03RevC.02\State=1-A\HF=-1309.0299802\S2=1.108146\S2=1=0
.\$2A=0.85304\RMSD=4.633e-09\RMSF=7.055e-06\DIPOLE=1.2372372,0.4564113
,0.1312415\PG=C01 [X(C16H25N704)]\\@
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### Triplet- (vii)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C14H16N802(3)\X543LJY\08-May
-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OOPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=1200\\opt_OVERC_pbenzene_OVERC_0_3_2nd\\0,3\C,-0.6942258119,
1.2048775876,0.0062623197\C,1.4089187777,-0.0000005968,-0.0124097973\C
,0.6942242374,-1.204874459,-0.0060802487\C,-0.6942305113,-1.204872561,
0.006236498\C,-1.4089204021,0.0000041719,0.0126142952\H,-1.2356055577,
2.1415929096,0.011081155\H,1.2356032546,-2.1415898061,-0.0109390517\H,
-1.2356128556,-2.1415860794,0.0110613711\C,-2.8939753179,0.0000096923,
0.0259618393\N,-3.5024482448,-1.1865472646,0.0325819915\N,-3.502455425
,1.1865695495,0.030724094\N,-4.8612873445,-1.157897903,0.0469966167\N,
-4.861296071,1.1579429962,0.0451805348\C,-5.5119316444,-2.4639246855,0
.0245095006\C,-5.6295195504,0.000006087,0.0290384897\C,-5.5119041645,2
.4639507257,0.0206846689\H,-5.3569087479,-2.9400048802,-0.9468509746\H
,-5.071610659,-3.0868861074,0.8034097051\H,-6.5746206176,-2.3240664408
,0.2012116751\O,-6.847259936,-0.0000331342,0.0081552306\H,-5.355565506
,2.9390972314,-0.9509130691\H,-6.5748159376,2.324231625,0.1961404988\H
,-5.072651816,3.0876853446,0.7995842477\C,2.8939741741,-0.0000011557,-
0.0257491829\N,3.5024422592,-1.186559181,-0.032477377\N,3.5024573472,1
.1865580767,-0.0306258991\N,4.8612805265,-1.1579106466,-0.04691826\N,4
.8612980853,1.1579225363,-0.0450870863\C,5.5119295334,-2.4639430814,-0
.0248807407\C,5.6295131967,-0.000012961,-0.0286342055\C,5.511914186,2
.4639346341,-0.0210570175\H,5.3570458598,-2.9402769979,0.9463776086\H,5
.0714975441,-3.0866985735,-0.8038825224\H,6.5745953229,-2.324040906,-0
.2016883577\O,6.8472665794,-0.0000590716,-0.0085300276\H,5.3555471188,
2.9394218615,0.950368239\H,6.5748311686,2.3241468316,-0.1964262516\H,5
.0726936121,3.0874009757,-0.8001910118\C,0.6942291611,1.2048756053,-0
.0060227403\H,1.2356115553,2.141589494,-0.010809258\\Version=IBM64-G03R
evC.02\State=3-A\HF=-1131.7943784\S2=2.041718\S2-1=0.\S2A=2.000882\RMS
D=3.315e-09\RMSF=1.580e-05\Dipole=-0.0000047,-0.0000217,0.0001911\PG=C
01 [X(C14H16N802)]\\@
```

## BS state - (vii)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C14H16N802\X543LJY\09-May-20
12\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=800 GUESS=(READ,MIX) \\final_OVERC_pbenzene_OVERC_0_1_2nd\\0,1\C
, 0. 6941037738, 1. 2052013743, -0. 0027830844\C, -1. 409118287, 0. 0000013383, 0
. 0049826024\C, -0. 6940980231, -1. 2051981105, 0. 0023441946\C, 0. 6941039876,
-1. 2051978371, -0. 00277386\C, 1. 4091238222, 0. 0000016215, -0. 0054483402\H,
1. 2355597294, 2. 1418639706, -0. 0048078995\H, -1. 2355532698, -2. 1418612172,
0. 004400983\H, 1. 235559581, -2. 1418610887, -0. 0048127321\C, 2. 8929283711, 0
. 0000032002, -0. 0111143919\N, 3. 5018033279, -1. 1868562298, -0. 0142639989\N
, 3. 5018052131, 1. 1868624427, -0. 0129608115\N, 4. 8606758604, -1. 1580139287,
-0. 0216240701\N, 4. 8606790925, 1. 1580338871, -0. 0203283842\C, 5. 5112214198
, -2. 4640511423, 0. 0050604872\C, 5. 6286907768, -0. 0000029848, 0. 0001388801\
C, 5. 5111860366, 2. 4640605891, 0. 0077120461\H, 5. 3509118867, -2. 9398478319,
0. 9757049214\H, 5. 0752738026, -3. 0873436252, -0. 7760404354\H, 6. 5748152085
, -2. 3241313315, -0. 1659617286\O, 6. 8462321595, -0. 0000372401, 0. 0281942183
\H, 5. 3496630541, 2. 9393682025, 0. 9783859405\H, 6. 5749781636, 2. 324199936, -
0. 1621092706\H, 5. 0762282055, 3. 0877694948, -0. 7736229565\C, -2. 8929228334
, 0. 0000028782, 0. 010630607\N, -3. 5017975752, -1. 1868570123, 0. 014026989\N,
-3. 5017996341, 1. 1868627325, 0. 0127347386\N, -4. 8606691187, -1. 1580050001,
0. 0214334653\N, -4. 8606729931, 1. 1580253219, 0. 0201309754\C, -5. 5112368326
, -2. 4640516712, -0. 0042265732\C, -5. 6286718441, -0. 0000033335, -0. 00104567
4\C, -5. 5111963945, 2. 4640657181, -0. 0068612008\H, -5. 3511248404, -2. 940482
2993, -0. 9745919454\H, -5. 0751440963, -3. 0868374708, 0. 7771981906\H, -6. 574
798797, -2. 3240124059, 0. 1668969771\O, -6. 8462520901, -0. 0000392369, -0. 027
3421962\H, -5. 3497097136, 2. 940093499, -0. 9771859817\H, -6. 5749833752, 2. 32
40678426, 0. 1628796825\H, -5. 0762241282, 3. 0872008476, 0. 7749263807\C, -0. 6
94098377, 1. 2052010638, 0. 0023110854\H, -1. 2355547539, 2. 1418635771, 0. 0043
207018\\Version=IBM64-G03RevC. 02\\State=1-A\\HF=-1131. 7947047\\S2=1. 05275
5\\S2-1=0. \\S2A=0. 423372\\RMSD=6. 410e-09\\RMSF=3. 777e-05\\Dipole=0. 000014, -
0. 0000206, -0. 00043\\PG=C01 [X(C14H16N802)]\\@
```

### Triplet- (viii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N404(3)\X543LJY\03-May
-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OOPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=2000\\Dushin_NN_pbenzene_NN_0_3\\0,3\C,0.6932012541,1.208179
8478,0.0077402092\C,1.4156329747,-0.0000040588,-0.0000033785\C,0.69319
59632,-1.2081848603,-0.0077485566\C,-1.4156308505,0.0000021411,-0.0000
042985\H,1.2242691479,2.1471977253,0.0343826453\H,1.2242595347,-2.1472
050791,-0.0343915852\C,2.8772595494,-0.0000062972,-0.0000031667\N,3.67
28628429,1.0591084641,0.3128323262\N,3.6728617057,-1.0591231823,-0.312
8350802\C,5.1255112147,0.780307179,0.0058380558\0,3.3060931316,2.21604
35756,0.6942299994\C,5.1255092631,-0.7803253576,-0.005833012\0,3.30609
08309,-2.2160599902,-0.6942263605\C,6.0093952662,1.4289545114,1.068340
8194\C,5.4019140036,1.417505476,-1.3672709458\C,5.4019034298,-1.417525
3145,1.3672770341\C,6.0093970084,-1.4289741679,-1.0683316877\H,7.05804
92145,1.1954830563,0.8677678781\H,5.88207564,2.5107125045,1.0337484548
\H,5.7619237823,1.0947331072,2.0751502991\H,4.7764210483,0.9848004231,
-2.1505124006\H,5.1864311192,2.4855367566,-1.3068503283\H,6.4492090531
,1.2906470904,-1.6480266414\H,5.1864230363,-2.4855569308,1.3068531276\
H,6.4491962371,-1.2906654915,1.6480404252\H,4.7764040556,-0.9848228095
,2.1505147471\H,5.7619308395,-1.0947520722,-2.0751422632\H,7.058050441
,-1.1955046844,-0.8677537635\H,5.8820751346,-2.5107319269,-1.033740123
9\C,-0.6931971161,-1.2081830579,0.0076599106\H,-1.2242653797,-2.147201
9846,0.0342345637\C,-0.6931918049,1.2081841914,-0.0076692803\H,-1.2242
557824,2.1472054391,-0.0342455194\C,-2.8772575833,0.0000048116,-0.0000
054348\N,-3.672865077,-1.0591525395,0.3126809681\N,-3.6728617959,1.059
1658634,-0.3126883059\C,-5.1255115042,-0.780306803,0.0057241503\0,-3.3
06102843,-2.216144307,0.6939146926\C,-5.1255078325,0.7803267619,-0.005
723275\0,-3.3060952345,2.2161595955,-0.6939118366\C,-6.0093980287,-1.4
291094838,1.0681300198\C,-5.4019118447,-1.4173125655,-1.3674762593\C,-
5.4018979241,1.4173350096,1.3674781607\C,-6.0093969867,1.4291325226,-1
.0681249656\H,-7.0580500553,-1.1955961176,0.8675961861\H,-5.8820894381
,-2.5108633707,1.0333705467\H,-5.7619197846,-1.0950468091,2.0749899935
\H,-4.7764139705,-0.9845035028,-2.1506564786\H,-5.1864362504,-2.485353
5986,-1.307203521\H,-6.4492050942,-1.2904080509,-1.6482184292\H,-5.186
4242722,2.4853762342,1.3072013596\H,-6.4491887518,1.2904298261,1.64822
906\H,-4.776393156,0.9845285705,2.1506542894\H,-5.7619245193,1.0950689
031,-2.0749860719\H,-7.0580488426,1.1956226772,-0.8675861831\H,-5.8820
845068,2.5108859695,-1.0333661761\\Version=IBM64-G03RevC.02\\State=3-A\
HF=-1299.0272692\\S2=2.103744\\S2-1=0.\\S2A=2.004653\\RMSD=7.066e-09\\RMSF=
1.314e-06\\Dipole=-0.000003,0.0000011,-0.0000015\\PG=C01 [X(C20H28N404)]
\\@
```

## BS state - (vii)

```
1\1\G INC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N404\X543LJY\15-May-20
12\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=800 GUESS=(READ,MIX) \\final_Dushin_NN_pbenzene_NN_0_1_2nd\\0,1\
C,-0.6919077149,-1.2090892157,-0.007976082\C,-1.4173658571,-0.00091387
6,-0.001602865\C,-0.6934048837,1.2081294068,0.0064024582\C,1.417335734
5,0.0008217515,0.0015531149\H,-1.2219781533,-2.1488052052,0.0056488263
\H,-1.2245861835,2.1472027597,-0.0083890498\C,-2.8757732468,-0.0017901
026,-0.0032511105\N,-3.6736380386,-1.0724639607,0.2694110581\N,-3.6743
10175,1.0678851304,-0.2777165355\C,-5.1254057167,-0.782921846,-0.03001
51902\0,-3.3084217378,-2.2425705664,0.6093403082\C,-5.1264034416,0.776
5784055,0.0183857934\0,-3.3097523068,2.2384585989,-0.6167693631\C,-6.0
116890664,-1.472323857,1.0044399044\C,-5.3988654957,-1.3669635153,-1.4
273709164\C,-5.4037787247,1.3602946737,1.415105653\C,-6.0111558814,1.4
648947866,-1.0181048496\H,-7.0596364817,-1.2288792442,0.8122042501\H,-
5.8863975542,-2.552055693,0.9265930931\H,-5.7647679278,-1.1794475388,2
.0241083043\H,-4.7718062223,-0.9048377176,-2.1923925785\H,-5.183619971
4,-2.4365672814,-1.4074628323\H,-6.4455766631,-1.2293254357,-1.7053566
057\H,-5.1897874042,2.4301585305,1.3956806252\H,-6.4509572959,1.221381
1245,1.6906840513\H,-4.7779137967,0.8989382705,2.1815683197\H,-5.76146
1526,1.1723982917,-2.0372068582\H,-7.0592311266,1.220070053,-0.8283372
915\H,-5.8874546161,2.5447836992,-0.939906024\C,0.6918752442,1.2087994
871,0.0238483728\H,1.2218729056,2.1478701685,0.0621745138\C,0.69339392
63,-1.208028282,-0.0223344565\H,1.2246610243,-2.1464375484,-0.05946307
95\C,2.8757443202,0.001747293,0.0031906303\N,3.6729061513,1.0651924099
,0.3046560249\N,3.6749883552,-1.0606521827,-0.2964011443\C,5.125441538
3,0.7833169078,0.0014920285\0,3.306808959,2.2264220392,0.6729140188\C,
5.1264398003,-0.776901764,0.0102148812\0,3.31129958,-2.2223297269,-0.6
65637205\C,6.0091003628,1.4461983554,1.0553599471\C,5.4022793144,1.402
776848,-1.3798335243\C,5.4007789505,-1.3960184647,1.3921906172\C,6.013
4574476,-1.4386316405,-1.0415516076\H,7.0575852544,1.2081465245,0.8593
272805\H,5.8835406338,2.5275279865,1.0049948678\H,5.7599898102,1.12711
06751,2.0665959201\H,4.7771354466,0.9602967523,-2.1579268568\H,5.18689
92539,2.4715194486,-1.3331997265\H,6.4496771031,1.272276693,-1.6586757
104\H,5.1868259581,-2.4650254426,1.345047742\H,6.4473571437,-1.2642290
684,1.6734936976\H,4.773260962,-0.9543097626,2.16880924\H,5.7661456118
,-1.1200644383,-2.0533931385\H,7.0611406228,-1.1989809285,-0.843194661
9\H,5.8894035266,-2.5201403208,-0.9913110058\\Version=IBM64-G03RevC.02
\State=1-A\HF=-1299.0282281\S2=1.141702\S2-1=0.\S2A=1.092346\RMSD=2.36
2e-09\RMSF=4.220e-06\Dipole=-0.0000815,0.0000298,0.00012\PG=C01 [X(C20
H28N404)]\\@\n
```

### Triplet- (ix)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C18H26N404S1(3)\X543LJY\03-M
ay-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOS
YMM) SCFCYC=2000\Dashin_NN_thiophene_NN_0_3\0,3\C,-2. 5757904201,-0. 5
280235548,-0. 334893954\N,-2. 7336075058,-1. 8004420497,0. 1031552948\N,-3
. 775160677,-0. 0514877427,-0. 7617169626\C,-4. 1062369967,-2. 3368568604,-
0. 2107699731\0,-1. 8066987613,-2. 5388837975,0. 5676807598\C,-4. 898830889
2,-1. 0009126805,-0. 4126586288\0,-4. 0087705153,1. 1045978713,-1. 23957230
92\C,-4. 5866038349,-3. 2205937245,0. 9383632039\C,-3. 9570679125,-3. 17683
40102,-1. 4913220939\C,-5. 5386891915,-0. 4509908261,0. 8737501813\C,-5. 92
69313357,-1. 0121695829,-1. 5415381857\H,-5. 5927890789,-3. 5902718813,0. 7
263408649\H,-3. 917369021,-4. 0754408674,1. 0379549065\H,-4. 6000596136,-2
. 6923941559,1. 8908399438\H,-3. 5957127749,-2. 5785355108,-2. 3299057943\H
,-3. 2358351104,-3. 973989017,-1. 3043133481\H,-4. 9108360317,-3. 629056933
2,-1. 7700233778\H,-5. 8886544608,0. 5646446201,0. 6819705991\H,-6. 3930207
796,-1. 0611735404,1. 1734416788\H,-4. 826839491,-0. 4169040755,1. 70079612
53\H,-5. 48843231,-1. 2862084694,-2. 5002722647\H,-6. 7276617434,-1. 717714
0686,-1. 3065158982\H,-6. 3604565447,-0. 0171826106,-1. 6428192372\C,-1. 33
20496489,0. 1871990212,-0. 3384268635\C,-1. 129854957,1. 486344432,-0. 7779
049267\S,0. 1509991288,-0. 5544710039,0. 2358593866\C,0. 2076551973,1. 8999
594852,-0. 6618843794\H,-1. 9315265307,2. 0933378408,-1. 1686302508\C,1. 03
08873173,0. 9186454349,-0. 1316935005\H,0. 5790188398,2. 873007747,-0. 9430
521652\C,2. 4386971768,1. 0314383228,0. 1209056193\N,3. 2107528058,2. 12409
19954,-0. 1195509539\N,3. 2109124232,0. 0476761639,0. 6421768932\C,4. 67808
86728,1. 8115162255,0. 067928154\0,2. 8268493038,3. 2355785793,-0. 60603112
14\C,4. 5962163312,0. 5376441279,0. 9758002903\0,2. 7997392121,-1. 10777230
44,0. 9829550366\C,5. 3813016656,3. 0160227066,0. 6893185683\C,5. 240990291
,1. 5438541486,-1. 338554184\C,4. 5929729833,0. 8420784777,2. 4840893058\C,
5. 6153727399,-0. 557270491,0. 6680163139\H,6. 4370682781,2. 7855539703,0. 8
518967559\H,5. 3126428673,3. 8635385038,0. 0072568979\H,4. 9369700695,3. 31
2552727,1. 6386254885\H,4. 751010174,0. 6947275651,-1. 818971472\H,5. 07349
09788,2. 4286237993,-1. 9549160549\H,6. 3144583974,1. 3492048633,-1. 296104
227\H,4. 337471733,-0. 0708602182,3. 0243384834\H,5. 5788676724,1. 17640984
56,2. 8128694297\H,3. 8599407939,1. 608735144,2. 7422822839\H,5. 5738396392
,-0. 8832541778,-0. 3704413985\H,6. 6239475235,-0. 1964421357,0. 8838901291
\H,5. 4144840931,-1. 4227081725,1. 2998532066\\Version=IBM64-G03RevC. 02\S
tate=3-A\HF=-1619. 7992627\S2=2. 101517\S2-1=0. \S2A=2. 004478\RMSD=3. 144e
-09\RMSF=5. 354e-06\Dipole=0. 139793,-0. 5132936,0. 2182674\PG=C01 [X(C18H
26N404S1)]\\@\n
```

## BS state - (ix)

```
1\1\GINC-GAIA10\F0pt\UB3LYP\6-311++G(d,p)\C18H26N404S1\X543LJY\06-May-
2012\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=20
0 SCFCYC=1200 GUESS=(READ,MIX) \\final_Dushin_NN_thiophene_NN_0_1\\0,1\
C,-2. 6324137876,-0. 2818488233,0. 0041463173\N,-3. 125175192,0. 9829074392
,0. 0024195795\N,-3. 67168309,-1. 1617000238,0. 0115086312\C,-4. 615510969,
1. 0062693111,0. 2203060022\0,-2. 422766378,2. 0444068671,-0. 0005434418\C,
-4. 9910706944,-0. 4548643165,-0. 2007997842\0,-3. 5932062939,-2. 431432501
3,0. 0159585297\C,-5. 2401800614,2. 1156386545,-0. 6230343391\C,-4. 8279002
556,1. 3011491618,1. 7155203742\C,-5. 3240160191,-0. 6101228095,-1. 6947152
478\C,-6. 0711565833,-1. 1242052487,0. 6457807618\H,-6. 32461648,2. 1178259
441,-0. 4886991122\H,-4. 8488377688,3. 0791648002,-0. 2958487489\H,-5. 0178
979813,2. 0061097588,-1. 683693972\H,-4. 376766266,0. 5348661302,2. 3488504
122\H,-4. 3613608666,2. 2586376242,1. 9525895248\H,-5. 892312259,1. 3656465
091,1. 9494943393\H,-5. 3718116836,-1. 6741247241,-1. 9322804913\H,-6. 2915
336861,-0. 1598544233,-1. 9253444165\H,-4. 5649638259,-0. 1513367122,-2. 33
13392911\H,-5. 8185958674,-1. 1394404153,1. 7052803182\H,-7. 0207101002,-0
. 5986069096,0. 5180966088\H,-6. 1989341646,-2. 1553795495,0. 3162988826\C,
-1. 242322786,-0. 6160915659,-0. 0025231984\C,-0. 7006143636,-1. 8956854435
,-0. 0019687922\S,-0. 0000006194,0. 6253648653,-0. 0000164131\C,0. 70062000
25,-1. 8956835148,0. 0019855854\H,-1. 3174597525,-2. 780777418,0. 000513177
4\C,1. 2423249266,-0. 6160881009,0. 0025231958\H,1. 3174676802,-2. 78077386
95,-0. 0004803351\C,2. 6324148935,-0. 2818407364,-0. 0041445474\N,3. 671687
8426,-1. 1616877997,-0. 011489826\N,3. 1251709032,0. 9829175448,-0. 0024337
451\C,4. 9910723366,-0. 4548426527,0. 200811044\0,3. 5932168349,-2. 4314205
598,-0. 0159193589\C,4. 6155073735,1. 0062830928,-0. 2203160239\0,2. 422757
3458,2. 0444139447,0. 0005126701\C,6. 0711627833,-1. 1241915933,-0. 6457573
176\C,5. 3240149297,-0. 6100783907,1. 6947293863\C,4. 8279004886,1. 3011437
503,-1. 7155336204\C,5. 2401688767,2. 1156668156,0. 6230112998\H,7. 0207149
58,-0. 598590267,-0. 5180755235\H,6. 1989402943,-2. 1553616944,-0. 31626217
98\H,5. 8186066083,-1. 1394399465,-1. 7052577412\H,4. 5649599016,-0. 151285
2276,2. 3313449732\H,5. 3718132073,-1. 6740766337,1. 9323105581\H,6. 291530
7814,-0. 1598038672,1. 925354264\H,4. 3613532942,2. 2586245517,-1. 95261825
6\H,5. 8923130052,1. 3656474868,-1. 9495035739\H,4. 3767764658,0. 534847699
4,-2. 3488550242\H,5. 0178849993,2. 0061511202,1. 6836719477\H,6. 324605580
1,2. 1178582031,0. 4886783902\H,4. 8488219735,3. 079186317,0. 2958116325\\Version=IBM64-G03RevC.02\\State=1-A\\HF=-1619.8009378\\S2=1.16955\\S2-1=0.\\S2A=1.276484\\RMSD=9.946e-09\\RMSF=1.848e-06\\Dipole=-0.0000018,0.5563069
,-0.0000029\\PG=C01 [X(C18H26N404S1)]\\@
```

### Triplet-(x)

```
1\1\GINC-GAIA12\F0pt\UB3LYP\ \C8H4N4S4(3)\X633KHY\24-Aug-2012\0\\# OPT
  UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=2000
  \\DTDA_mbenzene_DTDA_0_3\\0,3\C,-1.4975166651,0.1695252355,-0.00072154
  59\C,-0.1006161663,0.1742761832,-0.0001467564\C,0.6019790576,1.3816392
  451,-0.0005875001\C,-0.1021273078,2.5918709177,-0.0016233336\C,-1.4931
  274537,2.5862405433,-0.0021992406\C,-2.1935295498,1.3844343433,-0.0017
  499698\H,0.4399419999,-0.7620174505,0.0006479203\H,0.4466805605,3.5247
  007033,-0.0019682342\H,-2.0350164291,3.5248522622,-0.0030005851\H,-3.2
  75787845,1.3755858382,-0.0021912996\C,-2.2373693836,-1.1153489744,-0.0
  002332435\N,-3.5759405463,-1.0906044383,-0.0009811374\N,-1.5479518776,
  -2.2621249751,0.00072709\S,-4.3323630816,-2.5452250488,-0.0005521505\S
  ,-2.4298009842,-3.6435881351,0.0010757603\C,2.0846392615,1.3798943048,
  0.0000184294\N,2.7325253371,2.5514869961,-0.0003442478\N,2.7330380966,
  0.2094371837,0.001105889\S,4.3704730566,2.4792160686,0.000501045\S,4.3
  703468773,0.2823673959,0.0018764705\\Version=IBM64-G03RevC.02\\State=3-
  A\\HF=-2119.1878323\S2=2.038235\S2-1=0.\$2A=2.000723\\RMSD=2.993e-09\\RMS
  F=2.103e-05\\Dipole=0.0294266,-0.0509685,0.0000417\\PG=C01 [X(C8H4N4S4)]
  \\@
```

### BS state - (x)

```
1\1\GINC-GAIA16\F0pt\UB3LYP\ \C8H4N4S4\X633KHY\25-Aug-2012\0\\# OPT UB
  3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=1200 GU
  ESS=(READ,MIX) \\final_DTDA_mbenzene_DTDA_0_1\\0,1\C,-1.2121360182,0.89
  55569754,0.000067\C,-0.0000000151,0.201236,0.000004\C,1.2121379818,0.8
  955600246,-0.000034\C,1.2074619534,2.2957050245,-0.000021\C,-0.0000030
  606,2.986315,0.000037\C,-1.2074640466,2.2957059755,0.000086\H,0.000003
  0178,-0.879898,-0.000011\H,2.1491519426,2.8291670436,-0.000058\H,-0.00
  00001721,4.070121,0.000048\H,-2.1491580574,2.8291599564,0.000136\C,-2.
  4952950031,0.1527329494,0.000123\N,-3.6421680171,0.8434339261,0.000003
  \N,-2.471612976,-1.1851130501,0.000079\S,-5.0245489992,-0.0381101019,-
  0.000094\S,-3.9260389606,-1.9405880796,0.000003\C,2.4952959969,0.15273
  50506,-0.000109\N,3.6421689829,0.8434350739,-0.000065\N,2.471614024,-1
  .1851109499,-0.000021\S,5.0245490008,-0.0381098981,-0.000014\S,3.92603
  90394,-1.9405879204,0.000043\\Version=IBM64-G03RevC.02\\State=1-A\\HF=-2
  119.1876807\S2=1.033255\S2-1=0.\$2A=0.266287\\RMSD=9.069e-09\\RMSF=7.486
  e-05\\Dipole=0.0000006,-0.0589327,-0.000002\\PG=C01 [X(C8H4N4S4)]\\@
```

### Triplet- (xi)

```
1\1\GINC-GAIA12\F0pt\UB3LYP\ \C6H2N4S5(3)\X633KHY\21-Sep-2012\0\\# OPT
UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=2000
\\DTDA_fthiophene_DTDA_0_3\\0,3\C,-1.2104043867,-0.1875389224,-0.00002
54142\C,0.1585514769,-0.1611225368,-0.0008384196\C,0.6841278492,1.1637
222737,-0.0000508302\C,-0.3050804649,2.1182419893,0.0013368132\S,-1.87
86645065,1.4268566314,0.0016182371\H,0.7692899674,-1.0517971935,-0.001
9547618\H,-0.1769419558,3.189443624,0.0021320042\C,-2.0809662161,-1.36
13077098,-0.0004956853\N,-3.4068228713,-1.1793625484,0.0003430232\N,-1
.5178791811,-2.5768234915,-0.0008532164\S,-4.3221251636,-2.5417280961,
0.0003889907\S,-2.5558002941,-3.8464147493,-0.0006176298\C,2.120504516
8,1.4766654085,-0.0007117263\N,2.9962078607,0.4664831947,-0.0010213548
\N,2.5034679133,2.7612682123,0.0002122901\S,4.5835917371,0.8851479449,
-0.0008069525\S,4.1219006824,3.0304778306,0.0002779255\\Version=IBM64-
G03RevC.02\State=3-A\HF=-2439.9502492\S2=2.039691\S2-1=0.\S2A=2.000769
\RMSD=6.744e-09\RMSF=5.242e-05\Dipole=0.1421937,-0.0968257,0.0001145\P
G=C01 [X(C6H2N4S5)]\\@
```

### BS state - (xi)

```
1\1\GINC-GAIA25\F0pt\UB3LYP\ \C6H2N4S5\X633KHY\21-Sep-2012\0\\# OPT UB
3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=1200 GU
ESS=(READ,MIX) \\final_DTDA_fthiophene_DTDA_0_1\\0,1\C,1.1168030816,0.5
034052316,-0.0001135774\C,-0.0445223125,-0.2216102751,-0.0000299204\C,
-1.2081775936,0.6015135242,-0.0001035417\C,-0.9001534643,1.9410375855,
-0.0003592482\S,0.7956484768,2.2205415566,-0.0003504168\H,-0.069735054
6,-1.3012735595,0.0001221684\H,-1.5921140595,2.7687412555,-0.000487216
1\C,2.4872289903,-0.0050749093,-0.0000256443\N,3.4990263446,0.87076996
86,0.0000698303\N,2.6784822938,-1.3308862582,-0.0000002498\S,5.0094703
902,0.2283480886,0.0001262579\S,4.2409715992,-1.8284097346,0.000168257
\C,-2.5832232736,0.0804333662,0.0000278784\N,-2.7660068743,-1.24391867
02,0.0000946141\N,-3.6051374423,0.947934668,0.0000315871\S,-4.32464574
27,-1.7591123492,0.0001667165\S,-5.1083468302,0.2903203892,0.000052866
5\\Version=IBM64-G03RevC.02\State=1-A\HF=-2439.9501156\S2=1.034594\S2-
1=0.\S2A=0.276954\RMSD=5.614e-09\RMSF=1.688e-05\Dipole=-0.0660079,-0.1
588756,-0.0000051\PG=C01 [X(C6H2N4S5)]\\@
```

### Triplet- (xii)

```
1\1\GINC-GAIA17\F0pt\UB3LYP\ \C8H4N4S4(3)\X633KHY\24-Aug-2012\0\\# OPT
UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=2000
\\DTDA_pbenzene_DTDA_0_3\\0,3\C,-0.7016877138,-1.2150738666,0.00036698
42\C,0.6983887111,-1.2046515011,0.0008804884\C,1.3924530363,-0.0027848
646,0.0005482007\C,0.7016921653,1.215071317,-0.0003925228\C,-0.6983891
104,1.2046490016,-0.0009344321\C,-1.3924512395,0.0027856372,-0.0005288
277\H,1.2356515667,-2.1441126756,0.0015818225\H,2.4746826159,0.0014382
94,0.0009703082\H,-1.2356460477,2.1441135975,-0.0016427651\H,-2.474680
763,-0.0014450846,-0.0009351783\C,-1.4425536448,-2.4979794034,0.000769
6431\N,-2.7810629233,-2.4738999216,0.0000847626\N,-0.7526853391,-3.645
267259,0.0017856828\S,-3.5371486096,-3.9281103872,0.0005458712\S,-1.63
43140365,-5.0269782006,0.0021678303\C,1.4425543191,2.4979790132,-0.000
7848187\N,0.7526840178,3.6452649507,-0.0014769015\N,2.7810643439,2.473
9021378,-0.0003982675\S,1.6343110909,5.0269769112,-0.0018273955\S,3.53
71486047,3.9281138337,-0.0008543943\\Version=IBM64-G03RevC.02\State=3-
A\HF=-2119.1882159\S2=2.032037\S2-1=0.\S2A=2.000502\RMSD=6.892e-09\RMS
F=2.019e-05\Dipole=0.000002,-0.0000011,0.0000055\PG=C01 [X(C8H4N4S4)]\
\\@
```

### BS state - (xii)

```
1\1\GINC-GAIA17\F0pt\UB3LYP\ \C8H4N4S4\X633KHY\25-Aug-2012\0\\# OPT UB
3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=1200 GU
ESS=(READ,MIX) \\final_DTDA_pbenzene_DTDA_0_1\\0,1\C,1.4031519475,-0.00
00015893,0.0000005231\C,0.6938479036,-1.2074571218,-0.0000189482\C,-0.
6938481396,-1.207457158,0.000000304\C,-1.4031521439,-0.0000014577,-0.0
00013542\C,-0.6938469711,1.2074561368,-0.0000133961\C,0.6938467941,1.2
074561859,0.0000127786\H,1.2387048593,-2.1424945123,-0.0000237047\H,-1
.2387051621,-2.1424944796,-0.0000009007\H,-1.2387070165,2.1424917744,-
0.0000153469\H,1.2387068733,2.1424917322,0.000023277\C,2.8838367298,-0
.0000001189,0.0000098585\N,3.5325369251,1.1713373086,0.0001146812\N,3.
5325376917,-1.1713386279,-0.0001155719\S,5.1699742274,1.0987915622,0.0
00854651\S,5.1699743316,-1.0987907733,-0.000110135\C,-2.883836869,-0.
0000002921,-0.0000212219\N,-3.532536716,1.1713376731,-0.0001173619\N,-
3.5325375751,-1.1713384636,0.0001125596\S,-5.1699738871,1.0987924581,-
0.000071194\S,-5.1699745058,-1.0987899505,0.0001157633\\Version=IBM64-
G03RevC.02\State=1-A\HF=-2119.1884844\S2=1.041462\S2-1=0.\S2A=0.332006
\RMSD=3.123e-09\RMSF=7.383e-05\Dipole=-0.0000007,0.0000004,0.0000035\P
G=C01 [X(C8H4N4S4)]\\@
```

### Triplet- (xiii)

```
1\1\GINC-GAIA11\F0pt\UB3LYP\ \C6H2N4S5(3)\X633KHY\24-Aug-2012\0\\# OPT
UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=2000
\\DTDA_thiophene_DTDA_0_3\\0,3\C,0. 0460528961,-1. 3492804557,-0. 0009738
214\C,1. 4212984628,-1. 3199396297,-0. 0010704391\C,1. 9396655338,-0. 00536
65618,0. 0000333458\C,0. 9545707205,0. 954711002,0. 0007906919\S,-0. 636538
4794,0. 2510021699,0. 000239035\H,2. 0217845346,-2. 2186701906,-0. 00181611
09\H,2. 9919429954,0. 2416411062,0. 0002165972\C,-0. 8134230504,-2. 5314633
286,-0. 001823846\N,-2. 1412572541,-2. 3668219177,-0. 0018132913\N,-0. 2352
383782,-3. 7406162571,-0. 0017856196\S,-3. 0396056362,-3. 7396148897,-0. 00
2235027\S,-1. 257140725,-5. 0229637164,-0. 0020843604\C,1. 1332741389,2. 40
53385008,0. 0019158991\N,0. 0504342188,3. 1912821479,0. 0027804834\N,2. 381
1213907,2. 8944443803,0. 000924203\S,0. 3308219362,4. 8077515047,0. 0032315
12\S,2. 5094766806,4. 529138272,0. 0013255967\\Version=IBM64-G03RevC. 02\S
tate=3-A\HF=-2439. 9493075\S2=2. 032925\S2-1=0. \S2A=2. 00053\RMSD=5. 095e-
09\RMSF=4. 860e-05\Dipole=0. 1249388,-0. 0492656,-0. 0001045\PG=C01 [X(C6H
2N4S5)]\\@
```

### BS state - (xiii)

```
1\1\GINC-GAIA15\F0pt\UB3LYP\ \C6H2N4S5\X633KHY\25-Aug-2012\0\\# OPT UB
3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=1200 GU
ESS=(READ,MIX) \\final_DTDA_thiophene_DTDA_0_1\\0,1\C,-1. 2386034036,-0.
5364180547,0. 0001479286\C,-0. 7060201,-1. 8056405293,0. 0001643902\C,0. 70
6020053,-1. 8056405408,0. 000143496\C,1. 2386033637,-0. 5364180811,0. 00001
0703\S,0. 0000000114,0. 6857228131,0. 0002895078\H,-1. 3220615017,-2. 69380
33058,0. 0001548778\H,1. 3220614372,-2. 6938033297,0. 0000941442\C,-2. 6526
199541,-0. 1720336283,0. 0000857211\N,-2. 9875529976,1. 1240864055,-0. 0001
521307\N,-3. 5655996024,-1. 1539765205,-0. 0000258694\S,-4. 5941139597,1. 4
553893043,-0. 0004564857\S,-5. 1335756298,-0. 6740264636,-0. 0003172269\C,
2. 6526199363,-0. 1720336788,-0. 0001783009\N,2. 9875529887,1. 1240863831,0
. 0001776443\N,3. 5655996106,-1. 1539765517,-0. 0001825862\S,4. 5941139655,
1. 4553892216,0. 0003674883\S,5. 1335756562,-0. 6740263942,0. 000040963\\Ve
rsion=IBM64-G03RevC. 02\State=1-A\HF=-2439. 9496839\S2=1. 048519\S2-1=0. \
S2A=0. 386114\RMSD=2. 252e-09\RMSF=2. 225e-05\Dipole=0. , -0. 1347654,0. 0000
145\PG=C01 [X(C6H2N4S5)]\\@
```

### Triplet- (xiv)

```
1\1\GINC-GAIA16\Fopt\UB3LYP\ \C8H12N802(3)\X633KHY\25-Sep-2012\0\\# OP
T UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=200
0\\OVERC_OVERC_0_3_4th\\0,3\N,-1. 1503377689,2. 7048089934,0. 000347138\N
,-1. 1871312178,1. 3463994575,0. 000449137\C,0. 001863551,0. 7503779003,-0.
0000047574\N,1. 191586995,1. 3429800189,-0. 0004650733\N,1. 166594578,2. 70
32098795,-0. 0004539591\C,0. 0081450497,3. 4696459699,-0. 0000341097\C,-2.
4391455692,3. 3925754406,0. 0009352979\C,2. 4754229562,3. 3478167851,-0. 00
08866758\0,-0. 00804708,4. 6866297548,0. 0000686388\N,-1. 191586995,-1. 342
9800189,-0. 0004650733\N,-1. 166594578,-2. 7032098795,-0. 0004539591\C,-0.
0081450497,-3. 4696459699,-0. 0000341097\N,1. 1503377689,-2. 7048089934,0.
000347138\N,1. 1871312178,-1. 3463994575,0. 000449137\C,-0. 001863551,-0. 7
503779003,-0. 0000047574\C,-2. 4754229562,-3. 3478167851,-0. 0008866758\0,
0. 00804708,-4. 6866297548,0. 0000686388\C,2. 4391455692,-3. 3925754406,0. 0
009352979\H,-3. 2055855787,2. 622294739,0. 0006305397\H,-2. 5314584001,4. 0
236835483,-0. 8846132417\H,-2. 531227982,4. 0227064669,0. 8872150545\H,3. 0
294409611,3. 0408663821,0. 8880810463\H,2. 32849612,4. 4242426908,-0. 00094
15916\H,3. 0289155505,3. 0406942867,-0. 8901201451\H,-2. 32849612,-4. 42424
26908,-0. 0009415916\H,-3. 0294409611,-3. 0408663821,0. 8880810463\H,-3. 02
89155505,-3. 0406942867,-0. 8901201451\H,2. 5314584001,-4. 0236835483,-0. 8
846132417\H,3. 2055855787,-2. 622294739,0. 0006305397\H,2. 531227982,-4. 02
27064669,0. 8872150545\\Version=IBM64-G03RevC. 02\\State=3-\HF=-900. 66885
71\\S2=2. 032861\\S2-1=0. \\S2A=2. 000577\\RMSD=7. 338e-09\\RMSF=5. 684e-05\\Dipo
le=0. ,0. ,-0. 0000899\\PG=C02 [X(C8H12N802)]\\@
```

### BS state - (xiv)

```
1\1\GINC-GAIA17\Fopt\UB3LYP\ \C8H12N802\X633KHY\24-Sep-2012\0\\# OPT U
B3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM,CONVER=5,MAXCYCLE=1000) 0
PTCYC=200 SCFCYC=1200 GUESS=(READ,MIX) \\final_OVERC_OVERC_0_1_4th\\0,1
\N,-1. 1513789733,2. 7000194593,0. 0001611971\N,-1. 188843262,1. 3414866921
,0. 0002353913\C,0. 0013811182,0. 7462508112,-0. 0000122228\N,1. 1923822838
,1. 3378853166,-0. 0002611448\N,1. 1670974304,2. 6980688367,-0. 0002538957\
C,0. 0079333937,3. 4639820065,-0. 0000156684\C,-2. 4396048176,3. 3890175012
,0. 000512471\C,2. 4757076482,3. 3434638824,-0. 0004690768\0,-0. 0078467054
,4. 6808356796,0. 000064345\N,-1. 1923822838,-1. 3378853166,-0. 0002611448\
N,-1. 1670974304,-2. 6980688367,-0. 0002538957\C,-0. 0079333937,-3. 4639820
065,-0. 0000156684\N,1. 1513789733,-2. 7000194593,0. 0001611971\N,1. 188843
262,-1. 3414866921,0. 0002353913\C,-0. 0013811182,-0. 7462508112,-0. 000012
2228\C,-2. 4757076482,-3. 3434638824,-0. 0004690768\0,0. 0078467054,-4. 680
8356796,0. 000064345\C,2. 4396048176,-3. 3890175012,0. 000512471\H,-3. 2065
393593,2. 6192110518,0. 000096985\H,-2. 5315956527,4. 0200804765,-0. 885092
8535\H,-2. 5316635502,4. 0191486202,0. 8867850139\H,3. 0297322337,3. 036962
9124,0. 8886280151\H,2. 3283126661,4. 4198365317,-0. 0005458771\H,3. 029501
3854,3. 0367944703,-0. 8896498963\H,-2. 3283126661,-4. 4198365317,-0. 00054
58771\H,-3. 0297322337,-3. 0369629124,0. 8886280151\H,-3. 0295013854,-3. 03
67944703,-0. 8896498963\H,2. 5315956527,-4. 0200804765,-0. 8850928535\H,3.
2065393593,-2. 6192110518,0. 000096985\H,2. 5316635502,-4. 0191486202,0. 88
67850139\\Version=IBM64-G03RevC. 02\\HF=-900. 6716381\\S2=1. 011537\\S2-1=0.
\\S2A=0. 39042\\RMSD=4. 285e-06\\RMSF=7. 915e-05\\Dipole=-0. 0000048,-0. 000004
4,-0. 0000731\\PG=C02 [X(C8H12N802)]\\@
```

### Triplet- (xv)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C16H26N404(3)\JYLEE18\24-Aug
-2011\0\#\ OPT UB3LYP/6-311++G(D,P) OOPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=1200\\opt_big_cf_NN_0_3\\0,3\C,1.7221431602,0.7902984202,0.1
581974221\N,2.2863095462,2.0241959658,0.2881050444\C,3.789939903,1.959
1821253,0.1816885664\C,4.0428390577,0.4448593841,0.4990593409\N,2.6941
491838,-0.1499330196,0.160206652\0,2.530956862,-1.4073362341,0.0558370
611\0,1.6624775275,3.1279245279,0.3336784937\C,4.2744996772,0.14472382
12,1.9902231399\H,4.23967973,-0.9359438763,2.1368867935\H,5.2530265945
,0.5073287798,2.3110643715\H,3.5093364479,0.6002996701,2.6217677558\C,
5.1245572865,-0.2311696942,-0.3404440686\H,4.9397488553,-0.1372887035,
-1.4097830543\H,6.0993608813,0.2068542153,-0.1120650358\H,5.1560417288
,-1.2933404743,-0.0973062697\C,4.4175964555,2.9489314365,1.1611411693\
H,5.5071973787,2.8834777875,1.1089968994\H,4.1178401982,3.9613654399,0
.8899450404\H,4.1042549602,2.7709867376,2.1891070407\C,4.1352773784,2.
3628203618,-1.2626784506\H,3.6834226634,1.6893917779,-1.9935539692\H,3
.7549805464,3.3692617869,-1.4445930751\H,5.2164179939,2.3668685954,-1.
4136930549\C,-1.7215614709,-0.7899008974,-0.1665983782\N,-2.690561744,
0.1524450535,-0.2109621441\C,-4.0695395921,-0.4632270086,-0.1271337382
\C,-3.7633971835,-1.9409092646,-0.5520155916\N,-2.2897807289,-2.026594
1165,-0.239587472\0,-1.6710483008,-3.1338424939,-0.2140339527\0,-2.522
955857,1.4128216199,-0.1679895311\C,-3.8968327597,-2.1987379539,-2.063
3268845\H,-3.4873580561,-3.1851203606,-2.2869907514\H,-4.94545006,-2.1
805137315,-2.3662270507\H,-3.3504398763,-1.4600813476,-2.6529853672\C,
-4.5170556596,-3.0174234937,0.2264628648\H,-4.3543474847,-2.9432830554
,1.3009785743\H,-5.5885949739,-2.9394838642,0.0265526234\H,-4.17471204
13,-4.0004996739,-0.0972368648\C,-5.0256751229,0.2992887332,-1.0415791
277\H,-6.0199019359,-0.1522637469,-0.9981809483\H,-5.0990156417,1.3327
119608,-0.7024958016\H,-4.6900396956,0.3094007823,-2.0777766683\C,-4.5
127953673,-0.308837724,1.3381392627\H,-3.8419963919,-0.8294530442,2.02
43288551\H,-4.5066593642,0.7520163559,1.5933201004\H,-5.5244509131,-0.
694152547,1.479646045\C,0.3032665816,0.6038410809,0.0457592414\H,-0.27
39465307,1.5195880604,0.0466386913\C,-0.3025279142,-0.6031877833,-0.05
66514769\H,0.2749427544,-1.5187733256,-0.0620757588\\Version=IBM64-G03
RevC.02\State=3-A\HF=-1145.3465886\S2=2.097798\S2-1=0.\S2A=2.003972\RM
SD=8.716e-09\RMSF=9.718e-06\Dipole=0.0003619,0.0005427,-0.008894\PG=C0
1 [X(C16H26N404)]\\@
```

## BS state - (xv)

```
1\1\GINC-GAIA05\F0pt\UB3LYP\6-311++G(d,p)\C16H26N404\JYLEE18\26-Aug-20
11\0\\# OPT UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200
SCFCYC=800 GUESS=(READ,MIX) \\final_opt_big_cf_NN_0_1\\0,1\C,-1.8845963
561,-0.2048568536,-0.0076073351\N,-2.8256660855,-1.1959238245,0.023873
1789\C,-4.2149025002,-0.6487053922,-0.1897039063\C,-4.0003569198,0.855
8520782,0.1932632152\N,-2.5122388295,0.9994858557,-0.0299553359\0,-1.9
525262368,2.1408284019,-0.0636595615\0,-2.5917847914,-2.4417340957,0.0
614390988\C,-4.2377756208,1.164605974,1.6818720554\H,-3.8735374331,2.1
717951231,1.8906468408\H,-5.3021220997,1.1240208201,1.9215872759\H,-3.
7067937214,0.4671486453,2.3327018856\C,-4.7479849207,1.8671723941,-0.6
72688085\H,-4.519820096,1.7558183085,-1.7319458889\H,-5.8254707696,1.7
521561383,-0.5308455915\H,-4.4647171991,2.8762045071,-0.3727086244\C,-
5.2085627678,-1.4123196051,0.6832365503\H,-6.2112162155,-0.9966198192,
0.556177491\H,-5.2259557396,-2.4584686047,0.3771548431\H,-4.9453649065
,-1.3770388397,1.7396764584\C,-4.542430199,-0.8747617802,-1.6763441049
\H,-3.8390492897,-0.3578724653,-2.3321203367\H,-4.4849091199,-1.943625
5839,-1.888396955\H,-5.5520359583,-0.5287135191,-1.9058460763\C,1.8845
96841,0.2048571293,-0.0075966644\N,2.5122405259,-0.99948855,-0.0297973
834\C,4.0003536752,-0.8558288523,0.193432613\C,4.2149058828,0.64868334
6,-0.1897064029\N,2.825665498,1.195927501,0.0237847111\0,2.5917829815,
2.4417422,0.0611980371\0,1.9525294716,-2.1408352277,-0.0633877144\C,4.
5424577033,0.8745599247,-1.6763682545\H,4.4849143932,1.9433953535,-1.8
885583994\H,5.5520766937,0.5285077438,-1.9058070383\H,3.8391028511,0.3
575700975,-2.3320934023\C,5.208552841,1.4124011523,0.6831580403\H,4.94
53444533,1.3772386906,1.7395991371\H,6.2112099027,0.9966927024,0.55615
57991\H,5.2259433283,2.4585155367,0.3769580479\C,4.7479988155,-1.86724
78119,-0.6723882444\H,5.825482037,-1.7522050074,-0.5305468613\H,4.4647
362549,-2.8762466703,-0.372291424\H,4.5198455098,-1.7560222149,-1.7316
623339\C,4.2377416058,-1.1644119003,1.6820818133\H,3.7067625087,-0.466
8670247,2.332820052\H,3.8734791036,-2.1715690199,1.8909685161\H,5.3020
847054,-1.1238210755,1.9218105426\C,-0.4859382068,-0.4773900751,-0.009
7955013\H,-0.2300368928,-1.5292044214,-0.0116872181\C,0.4859386853,0.4
773887038,-0.0098382873\H,0.2300371863,1.5292029057,-0.0118468231\Ver
sion=IBM64-G03RevC.02\State=1-A\HF=-1145.3499391\S2=1.224521\S2-1=0.\S
2A=1.606663\RMSD=1.906e-09\RMSF=5.692e-06\Dipole=-0.0000019,-0.0000011
,-0.0010766\PG=C01 [X(C16H26N404)]\\@
```

## Triplet- (xvi)

```
1\1\GINC-NODE20\F0pt\UB3LYP\6-311++G(d,p)\C20H30N404(3)\ROOT\28-May-20
12\0\# opt ub3lyp/6-311++g(d,p) optcyc=200 scf=(direct,tight,nosymm)
scfcyc=1200\\\Dushin_NN_C6_NN_0_3\\0,3\N,5.3755305027,-1.2087238923,-0.
1455985135\C,4.3438497947,-0.3231297282,-0.0369426907\N,4.8444315897,0
.925128839,0.1223975296\C,6.3434916185,0.9518366197,-0.0689609835\C,6.
6997298621,-0.5580293632,0.1623307316\C,2.9752018358,-0.7305337698,-0.
0917663261\C,1.8959633534,0.0886906902,0.006669768\C,0.54683569,-0.399
3700592,-0.0505783621\C,-0.546865336,0.3993711245,0.050605784\C,-1.895
992749,-0.0886906063,-0.0066398076\C,-2.9752320252,0.7305312137,0.0918
094537\H,-2.8493029971,1.800873602,0.220172489\O,4.1705267176,1.998546
989,0.2534604219\C,6.5840564575,1.4366597088,-1.5088031319\C,6.9673130
105,1.9327777484,0.9214851466\C,7.779001109,-1.1267911307,-0.756650690
8\C,7.0216512364,-0.9082447781,1.6257101941\O,5.2612884312,-2.46417788
2,-0.3089157404\C,-4.3438795426,0.3231244548,0.0369934475\N,-4.8444598
301,-0.9251328139,-0.1223605013\C,-6.3435173561,-0.95184748,0.06901464
94\C,-6.6997621431,0.5580206546,-0.1622533099\N,-5.3755615495,1.208714
2214,0.1456736086\O,-4.1705537253,-1.9985474363,-0.2534467549\C,-6.584
0638878,-1.4366904652,1.508853215\C,-6.9673480909,-1.9327773291,-0.921
4369897\C,-7.7790269148,1.1267675976,0.7567448787\C,-7.0216965257,0.90
82556656,-1.6256252118\O,-5.2613208768,2.4641662903,0.3090062162\H,2.8
492715101,-1.8008770281,-0.2201208924\H,-7.6529861914,-1.5149806118,1.
7166735992\H,-6.134629515,-2.4241894464,1.6257425842\H,-6.1337642549,-
0.7670180644,2.2441758882\H,-8.053735505,-1.9398852793,-0.8034851147\H
,-6.7285127614,-1.6873562633,-1.9555657171\H,-6.5904158914,-2.93547294
6,-0.7192821918\H,-8.7356992764,0.6395407614,0.5530184846\H,-7.5368790
137,0.997384929,1.8108728714\H,-7.8866359921,2.1947237963,0.5657333228
\H,-7.9900162194,0.4971940395,-1.9173009385\H,-7.0614344858,1.99433119
12,-1.7237518525\H,-6.2608637099,0.5301706417,-2.3110928532\H,-2.05367
04943,-1.1530293639,-0.1387129355\H,-0.403939448,1.4702335753,0.181774
5976\H,7.6529814636,1.5149358046,-1.7166149558\H,6.1346336308,2.424162
017,-1.625708847\H,6.1337563372,0.7669830414,-2.2441216351\H,8.0537012
254,1.9398873164,0.8035407459\H,6.7284711712,1.6873662103,1.9556146199
\H,6.5903795561,2.9354703822,0.7193178011\H,8.7356706533,-0.6395567577
,-0.5529290663\H,7.5368579573,-0.99742962,-1.8107824029\H,7.8866131396
,-2.1947432477,-0.5656180464\H,7.9899637092,-0.4971706683,1.917392301\
H,7.0613983042,-1.9943188113,1.7238494972\H,6.2608070516,-0.5301589948
,2.3111648234\H,2.0536418499,1.1530302545,0.138735452\H,0.4039095405,-
1.4702325434,-0.1817466589\Version=AM64L-G03RevD.02\State=3-A\HF=-130
0.2067313\S2=2.132679\S2=1=0.\S2A=2.007683\RMSD=7.268e-09\RMSF=4.975e-
06\Thermal=0.\Dipole=0.0000035,-0.0000018,0.0000095\PG=C01 [X(C20H30N4
04)]\\@\n
```

## BS state - (xvi)

```
1\1\GINC-NODE20\F0pt\UB3LYP\6-311++G(d,p)\C20H30N404\ROOT\09-Jun-2012\
0\\# opt UB3LYP/6-311++G(d,p) scf=(direct,tight,nosymm) optcyc=200 scf
cyc=800 guess=(read,mix) \\final_NN_C6_NN_0_1\\0,1\N,-5.3710959328,1.23
00310049,-0.1446819018\C,-4.3384576657,0.3398903268,-0.0486572468\N,-4
.8474484745,-0.9120632054,0.0844152457\C,-6.3446034156,-0.9286023587,-
0.1183095517\C,-6.6968856933,0.576215594,0.14794565\C,-2.9747465851,0.
7425017721,-0.0890901037\C,-1.8918236253,-0.0829687445,-0.0030224595\C
,-0.5492516528,0.4023418036,-0.0444534283\C,0.5492510353,-0.4023406063
,0.044454525\C,1.8918230465,0.082969855,0.003023772\C,2.9747458709,-0.
7425008059,0.0890916833\H,2.8439953934,-1.8147882053,0.1948415652\O,-4
.1782157034,-1.9899529608,0.1972796924\C,-6.5775825344,-1.3756585559,-
1.5716251412\C,-6.9796056755,-1.9310326979,0.8430233014\C,-7.774500199
8,1.1685059207,-0.7579018818\C,-7.0184864069,0.8921772419,1.6191998206
\O,-5.2536796037,2.4877961795,-0.2828473401\C,4.3384570343,-0.33988958
88,0.0486594375\N,4.8474481173,0.9120638548,-0.084412518\C,6.344603013
7,0.9286028579,0.1183126239\C,6.6968852677,-0.5762152797,-0.1479417375
\N,5.3710950746,-1.2300304642,0.1446843922\O,4.1782155254,1.989953714,
-0.1972770962\C,6.5775821213,1.3756597817,1.5716279855\C,6.9796055596,
1.9310324732,-0.8430208237\C,7.7744985513,-1.168505611,0.7579072906\C,
7.0184879479,-0.8921769457,-1.6191954467\O,5.2536783942,-2.4877956485,
0.2828494337\H,-2.8439962968,1.8147891844,-0.1948401221\H,7.6453803504
,1.4446640899,1.7883401465\H,6.1309904271,2.3615680597,1.7109249536\H,
6.1201496398,0.6890832779,2.2867225373\H,8.0653076399,1.9289914269,-0.
7186965247\H,6.7454799789,1.7132990934,-1.8844008794\H,6.6072271398,2.
9304846543,-0.6176587091\H,8.7319666483,-0.6776400443,0.5670324072\H,7
.5313369721,-1.0643993179,1.8146051551\H,7.8811657625,-2.231660137,0.5
412900436\H,7.9880627676,-0.4770479923,-1.9007809628\H,7.055246937,-1.
9757061816,-1.7433885788\H,6.2589747708,-0.4955642728,-2.2956430032\H,
2.0529765623,1.1493479308,-0.1063379114\H,0.4024425569,-1.4753170168,0
.1523602517\H,-7.6453807578,-1.4446631098,-1.7883372269\H,-6.130990550
6,-2.3615666268,-1.7109227219\H,-6.1201503585,-0.6890815129,-2.2867193
693\H,-8.0653077225,-1.9289920096,0.7186987173\H,-6.7454804607,-1.7132
998259,1.8844035299\H,-6.6072268242,-2.930484626,0.6176607279\H,-8.731
9676799,0.6776393177,-0.5670266063\H,-7.5313394046,1.0644008222,-1.814
6000377\H,-7.8811682006,2.2316601723,-0.5412836036\H,-7.9880613706,0.4
770492947,1.9007863473\H,-7.0552441808,1.9757065258,1.7433930695\H,-6.
2589729099,0.4955637334,2.2956464968\H,-2.0529770062,-1.1493468292,0.1
063393125\H,-0.4024432142,1.4753182183,-0.1523591809\Version=AM64L-G0
3RevD.02\State=1-A\HF=-1300.2087251\S2=1.273903\S2-1=0.\S2A=1.996773\R
MSD=6.882e-09\RMSF=3.656e-06\Thermal=0.\Dipole=0.0000003,-0.0000001,0.
0000008\PG=C01[X(C20H30N404)]\\@
```