

Supporting Information
for

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

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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 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 (cm^{-1})
2,4-thiophene based NN diradical (i)	-1619.79833644 (2.127578)	-1619.7980298 (1.110525)	66.2
3,5-pyridine based NN diradical (ii)	-1315.0650742 (2.122624)	-1315.06482439 (1.108671)	54.1
1,3-phenylene based NN diradical (iii)	1299.02637548 (2.120136)	-1299.02614091 (1.106967)	50.8
1,3-phenylene based OVER diradical (iv)	-1131.79403604 (2.049175)	-1131.79382485 (1.04301)	46.1
2,6-pyridine based NN diradical (v)	-1315.0575241 (2.11934)	-1315.05737224 (1.110697)	33.0
1,2,4-triazole based NN diradical (vi)	-1309.03000419 (2.109469)	-1309.02998017 (1.108146)	5.3
1,4-phenylene based OVER diradical (vii)	-1131.79437842 (2.041718)	-1131.79470467 (1.052755)	-72.4
1,4-phenylene based NN diradical (viii)	-1299.02726918 (2.103744)	-1299.02822813 (1.141702)	-218.8
2,5-thiophene based NN diradical (ix)	-1619.79926274 (2.101517)	-1619.80093782 (1.16955)	-394.5
1,3-phenylene based DTDA diradical (x)	-2119.18783234 (2.038235)	-2119.18768073 (1.033255)	33.1
2,4-thiophene based DTDA diradical (xi)	-2439.95024916 (2.039691)	-2439.95011558 (1.034594)	29.2
1,4-phenylene based DTDA diradical (xii)	-2119.18821589 (2.032037)	-2119.18848437 (1.041462)	-59.5
2,5-thiophene based DTDA 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..

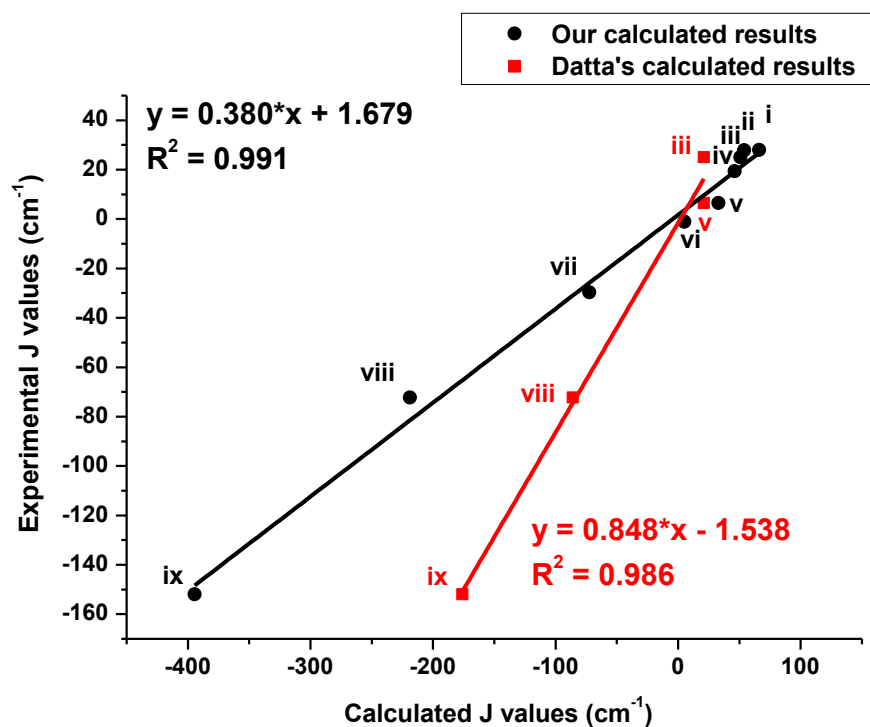


Figure S1. Comparison of our calculated results and Datta's calculated results.

Diradical	Datta's calculated J value ^a (cm ⁻¹)	Experimental J value (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

^aThe 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 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 (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)

```
1\1\GINC-GAIA23\F0pt\UB3LYP\ C18H26N4O4S1(3)\X633KHY\01-Sep-2012\0\#\n
OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=\n
2000\NN_fthiophene_NN_0_3\0,3\C,-1.3324570693,-0.0493910884,0.000280\n
3647\C,0.04596205,-0.0313746735,-0.0017261041\C,0.5781329346,1.2959813\n
741,0.0039591117\C,-0.4217308992,2.2559367156,0.0089312489\S,-1.996043\n
4142,1.5815327393,0.0126991218\H,0.6468571386,-0.924965697,-0.00699309\n
29\H,-0.2811525626,3.3239750332,0.0147224017\C,-2.1832934364,-1.202969\n
9695,-0.0027306317\N,-3.536355006,-1.1588400801,0.0073339756\N,-1.7771\n
53462,-2.5001765941,-0.0167982192\C,-4.1412679909,-2.5244573734,0.2069\n
231065\0,-4.2380190429,-0.0943140803,0.0258453839\C,-2.9451229324,-3.4\n
365656153,-0.2322315957\0,-0.577289372,-2.9189721422,-0.0278315354\C,-\n
5.4098425875,-2.6502993048,-0.6343320581\C,-4.49150633,-2.6255190407,1\n
.7016064724\C,-2.9441111635,-3.7858971057,-1.7301500985\C,-2.743966128\n
6,-4.7016261058,0.5986079048\H,-5.8395025622,-3.6475186077,-0.51173563\n
86\H,-6.1396983918,-1.9148383861,-0.2952383266\H,-5.2247735448,-2.4754\n
021955,-1.6933808008\H,-3.6076584346,-2.5231588619,2.3341324502\H,-5.1\n
86846467,-1.8229345944,1.9528110252\H,-4.9702672219,-3.5813555954,1.92\n
28510813\H,-1.9893832612,-4.2513909296,-1.9802720695\H,-3.7456288387,-\n
4.4895093995,-1.9633164856\H,-3.0660468427,-2.8986375475,-2.3545109478\n
\H,-2.6303649776,-4.4875285242,1.6606196085\H,-3.5950518898,-5.3737295\n
966,0.4637897217\H,-1.8421326475,-5.2125542019,0.2610734347\C,1.990393\n
3211,1.6161218049,0.0043751757\N,3.0116495217,0.7178747465,0.015590563\n
2\N,2.5067676908,2.8700468325,-0.0059912331\C,4.3445447912,1.396934979\n
5,0.2285182835\0,2.9138777385,-0.5497369783,0.016679061\C,4.0020641315\n
,2.8573972913,-0.2123722054\0,1.8516585969,3.9637207125,-0.0139121347\C,\n
5.4161652099,0.6930891534,-0.6007139035\C,4.662925871,1.2545378316,1\n
.7268888377\C,4.2298829018,3.1302077079,-1.7092161084\C,4.644252076,3.\n
964232173,0.6211358415\H,6.3769359762,1.197067302,-0.4693789393\H,5.51\n
5404809,-0.3372961752,-0.2593565191\H,5.1729915891,0.6722672415,-1.662\n
3584968\H,3.9050804514,1.7327323977,2.3505618274\H,4.6937192958,0.1932\n
100245,1.9787149507\H,5.6344694561,1.6951789027,1.9588321751\H,3.78123\n
81385,4.0924862239,-1.9611054579\H,5.2967872009,3.1745853744,-1.936359\n
0155\H,3.7712660542,2.363485485,-2.3366548725\H,4.4108673438,3.8740238\n
185,1.6812844963\H,5.7296661893,3.9396522073,0.4962964208\H,4.27758555\n
53,4.9316855189,0.2780714643\Version=IBM64-G03RevC.02\State=3-A\HF=-1\n
619.7983364\S2=2.127578\S2-1=0.\S2A=2.007287\RMSD=3.796e-09\RMSF=1.923\n
e-06\Dipole=0.4636521,-0.7798377,0.0003574\PG=C01 [X(C18H26N4O4S1)]\@\n
```

BS state - (i)

```
1\1\GINC-GAIA30\F0pt\UB3LYP\ \C18H26N4O4S1\X633KHY\03-Sep-2012\0\#\# OP
T UB3LYP/6-311++G(D,P) SCF=(DIRECT,TIGHT,NOSYMM) OPTCYC=200 SCFCYC=120
0 GUESS=(READ,MIX)\final_NN_fthiophene_NN_0_1\0,1\C,-1.1410299977,-0
.6879514204,0.003115078\C,0.020744647,0.0531895346,0.0014636838\C,1.19
41009247,-0.7648190628,-0.0027809035\C,0.884667461,-2.115167709,-0.003
0163498\S,-0.8008415478,-2.4152499005,-0.0041515788\H,0.032835655,1.12
99713759,0.0031915512\H,1.5882970778,-2.9309803182,-0.0066917963\C,-2.
4864697137,-0.191099918,0.0060556898\N,-3.5925742313,-0.9710336629,-0.
0003897402\N,-2.8589192788,1.115850261,0.0164569928\C,-4.8484321397,-0
.162515998,-0.200478842\O,-3.5947838078,-2.2460579902,-0.0145681625\C,
-4.3489382913,1.2581221424,0.232923033\O,-2.0858224724,2.1246865906,0.
023524561\C,-5.9762140338,-0.7511796962,0.6447564418\C,-5.1991945768,-
0.2756471244,-1.6941788622\C,-4.5383010602,1.5562418096,1.7299455858\C
,-4.8761765501,2.4228924761,-0.6016477679\H,-6.8831187642,-0.154134596
1,0.5217162207\H,-6.182858841,-1.7677638487,0.3094620044\H,-5.72366651
69,-0.7921059614,1.7035152885\H,-4.4057658066,0.122680292,-2.329433048
7\H,-5.3392203814,-1.3291675897,-1.941613538\H,-6.1250079005,0.2588239
836,-1.9155241522\H,-3.9947371297,2.4698117655,1.9762604113\H,-5.59415
99495,1.7061863272,1.9635107222\H,-4.1533294482,0.749602787,2.35688228
51\H,-4.664836953,2.3023988321,-1.6634520539\H,-5.956362601,2.51800244
77,-0.4660069153\H,-4.4024346326,3.346220852,-0.2680126683\C,2.5517549
76,-0.2588133475,-0.0063875466\N,2.9133703481,1.0518823564,-0.02262046
18\N,3.6703364528,-1.0247727507,0.0055401499\C,4.4001846532,1.21383692
12,-0.2373764211\O,2.1367283101,2.0586383157,-0.0264659543\C,4.9145975
372,-0.1941194303,0.2072174046\O,3.721900313,-2.2986269002,0.017715280
8\C,4.9114903232,2.3923699795,0.5878906514\C,4.587048503,1.5030719318,
-1.736778095\C,5.2570017528,-0.2927943292,1.7038499022\C,6.0569432711,
-0.7708825209,-0.6262311212\H,5.9911994025,2.4970653363,0.4552618785\H
,4.4293898461,3.307544786,0.2442350387\H,4.6976444823,2.2796701725,1.6
500703938\H,4.2155899508,0.68547809,-2.3576817391\H,4.0299914681,2.406
33426,-1.9909032598\H,5.6408399897,1.6673500455,-1.9700187352\H,5.4089
197284,-1.3428309403,1.9588940564\H,6.1744055055,0.2550185751,1.927723
7561\H,4.4544170426,0.0996882788,2.3312872645\H,5.8106170185,-0.826750
0443,-1.6858181952\H,6.9516274555,-0.1551660502,-0.5048138326\H,6.2808
511707,-1.7799594356,-0.2802194261\Version=IBM64-G03RevC.02\State=1-A
\HF=-1619.7980298\S2=1.110525\S2-1=0.\S2A=0.871219\RMSD=4.963e-09\RMSF
=4.792e-06\Dipole=-0.0412558,0.8939019,-0.0032492\PG=C01 [X(C18H26N4O4
S1)]\@
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Triplet- (ii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C19H27N5O4(3)\X543LJY\26-May
-2012\0\#\# OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYM
M) SCFCYC=1200\Dushin_NN_pyridine2_NN_0_3\0,3\C,0.0000022583,0.40041
03093,0.0000187118\C,-1.2068739238,1.1103735662,0.005128627\C,-1.14636
80114,2.5168491952,-0.013537145\C,1.1463964121,2.5168352471,0.01369291
73\H,-0.0000039818,-0.677300162,-0.0000112905\H,-2.056146645,3.1004726
372,-0.0509422401\H,2.0561819225,3.1004462363,0.0511346317\C,1.2068846
406,1.1103611091,-0.005051741\C,-2.4877798862,0.4099017467,0.023582513
4\N,-2.6832791581,-0.8575062092,0.4719214887\N,-3.6733714617,0.9172366
104,-0.399779182\C,-4.0750358527,-1.3519931593,0.1494335017\0,-1.81614
23779,-1.6290246023,0.9907699688\C,-4.8263795278,0.0047765031,-0.04835
42338\0,-3.8778878059,2.0611597544,-0.9164124913\C,-4.586691798,-2.226
0653153,1.2913319149\C,-3.9444180434,-2.1880272993,-1.1351628775\C,-5.
4433480699,0.5746429418,1.2406061122\C,-5.8575489433,0.0266236676,-1.1
740813225\H,-5.6040305121,-2.5601690845,1.0730246597\H,-3.9470056104,-
3.1030322231,1.3885645566\H,-4.5865983333,-1.7030955236,2.2467379007\H
,-3.5602661411,-1.5977978158,-1.9693649887\H,-3.25052247,-3.0097099703
,-0.9499915109\H,-4.9105804217,-2.6079870307,-1.4216675394\H,-5.763263
6401,1.6005305726,1.0509021931\H,-6.3150003263,-0.0091670594,1.5426357
561\H,-4.7281727339,0.5846989784,2.065465993\H,-5.4288527363,-0.254033
7626,-2.1352892592\H,-6.6746165694,-0.6601585445,-0.9394973359\H,-6.26
6215678,1.0324437698,-1.2703484329\C,2.4877833735,0.4098772483,-0.0235
47449\N,3.6733754291,0.9171692817,0.3998624745\N,2.6832739271,-0.85749
54509,-0.4719884725\C,4.8263773559,0.0047321707,0.0483631175\0,3.87789
49136,2.0610498288,0.9165896121\C,4.0750244586,-1.3520179631,-0.149533
2499\0,1.8161335816,-1.6289627917,-0.9909070558\C,5.8575487368,0.02647
99671,1.1740894302\C,5.443346648,0.5746979462,-1.2405532825\C,3.944395
386,-2.1881490182,1.134999068\C,4.5866802719,-2.2260052806,-1.29149612
09\H,6.6746010901,-0.6603038725,0.9394566354\H,6.2662389746,1.03228386
75,1.2704269263\H,5.4288474977,-0.2542346722,2.1352784502\H,4.72817118
55,0.5848183287,-2.0654121804\H,5.7632640425,1.6005704146,-1.050770123
8\H,6.3149982144,-0.009089752,-1.5426279848\H,3.2504903377,-3.00980944
69,0.9497642284\H,4.9105525837,-2.608142299,1.4214720048\H,3.560250284
3,-1.5979786545,1.9692460739\H,4.5865802701,-1.7029663809,-2.246864367
4\H,5.6040217009,-2.5601189943,-1.0732166381\H,3.9469997344,-3.1029695
095,-1.3887908684\N,0.0000182003,3.1966244744,0.0000970523\Version=IB
M64-G03RevC.02\State=3-A\HF=-1315.0650742\S2=2.122624\S2-1=0.\S2A=2.00
6746\RMSD=4.471e-09\RMSF=6.659e-06\Dipole=-0.0000096,-2.0340558,-0.000
0715\PG=C01 [X(C19H27N5O4)]\@\
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BS state - (ii)

```
1\1\GINC-NODE20\F0pt\UB3LYP\6-311++G(d,p)\C19H27N5O4\ROOT\29-May-2012\
0\#\# opt UB3LYP/6-311++G(d,p) scf=(direct,tight,nosymm) optcyc=200 scf
cyc=800 guess=(read,mix)\final_NN_pyridine2_NN_0_1\0,1\C,-0.00000071
59,0.4013217669,0.0000022001\C,-1.2065963361,1.1112827809,0.0064195207
\C,-1.1463438025,2.5171688271,-0.0121569821\C,1.1463459343,2.517166723
3,0.0121605785\H,-0.0000020128,-0.6764365919,0.0000026043\H,-2.0562525
964,3.1007459227,-0.0487412492\H,2.0562558962,3.100742157,0.0487460287
\C,1.2065958041,1.1112808246,-0.0064159273\C,-2.488105034,0.4102167063
,0.0258104797\N,-2.6829780254,-0.8557141721,0.4772518768\N,-3.67289881
63,0.9162017082,-0.4000198326\C,-4.0742892354,-1.3517003568,0.15498428
74\0,-1.8153427933,-1.6256389176,0.9977756699\C,-4.8259955227,0.0042703
674,-0.047426557\0,-3.8770552295,2.0591326651,-0.919115454\C,-4.586408
3045,-2.2228611927,1.2989379092\C,-3.9421966056,-2.1913623305,-1.12711
39734\C,-5.4447344417,0.5775457326,1.2391667485\C,-5.8558032761,0.0226
836801,-1.1744766098\H,-5.6034229412,-2.5580432013,1.080778217\H,-3.94
63660735,-3.0992487069,1.3989836297\H,-4.587256464,-1.6973392511,2.252
9446792\H,-3.5575979818,-1.6033542936,-1.9626720632\H,-3.2481257919,-3
.0122324772,-0.9390507482\H,-4.9079639887,-2.6125011194,-1.4132095443\
H,-5.7649395412,1.6027165964,1.0461380768\H,-6.3164307924,-0.005863649
3,1.5418532302\H,-4.7305072413,0.5903235575,2.0647972617\H,-5.42583469
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,-1.603363735,1.9626662975\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(C19H27N5O4)]\@\
```

Triplet- (iii)

1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C20H28N4O4(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(C20H28N4O4)]\@

BS state - (iii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N4O4\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
598956658,-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,-0.000066551
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(C20H28N4O4)]\@
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Triplet- (iv)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C14H16N8O2(3)\X543LJY\12-Mar
-2012\0\#\# OPT UB3LYP/6-311++G(D,P) OPTCYC=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,4.35974444971,-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\Dipole=0.1554205,0.2690831,-0.0002169\
PG=C01 [X(C14H16N8O2)]\@\
```

BS state - (iv)

```
1\1\GINC-GAIA07\F0pt\UB3LYP\6-311++G(d,p)\C14H16N8O2\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,-0.0000001803,3.256258,0.00000006
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(C14H16N8O2)]\@
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Triplet- (v)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C19H27N5O4(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\O,-1.6553856784,-1.279503
4416,1.5093163145\C,-4.6419522809,-0.1558326343,-0.0871782299\O,-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\O,3.7952790585,1
.8692531207,1.1332624168\C,3.7942017095,-1.3916811237,-0.3622281396\O,
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(C19H27N5O4)]\@
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BS state - (v)

```
1\1\GINC-GAIA07\F0pt\UB3LYP\6-311++G(d,p)\C19H27N5O4\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\O,-1.673
888569,-1.2746694023,1.5017263556\C,-4.6410043028,-0.1561344562,-0.13
52885601\O,-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\O,3.7800508361,1.8641263647,1.179287878\C,3.7997615606,-1.390373
3599,-0.3307673186\O,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(C19H27N5O4)]\@
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Triplet- (vi)

```
1\1\GINC-GAIA20\F0pt\UB3LYP\ C16H25N7O4(3)\X633KHY\02-Sep-2012\0\#\# 0
PT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOSYMM) SCFCYC=20
00\N\N_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(
C16H25N7O4)]\@
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BS state - (vi)

```
1\1\GINC-GAIA30\F0pt\UB3LYP\ \C16H25N7O4\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\0,2.2524227314,1.9766427452,0.9286503119\C,4.7733607256,-0.41854
32606,0.0381185021\0,3.3233059011,-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\0,-2.972250789,-1.5011349516,1.8158025564\C,-4.4855673583,0.89083188
7,-0.4001059304\0,-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
.\S2A=0.85304\RMSD=4.633e-09\RMSF=7.055e-06\Dipole=1.2372372,0.4564113
,0.1312415\PG=C01 [X(C16H25N7O4)]\@
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Triplet- (vii)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C14H16N8O2(3)\X543LJY\08-May
-2012\0\#\# OPT UB3LYP/6-311++G(D,P) OPTCYC=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,-0.000005968,-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\0,-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\0,6.8472665794,-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(C14H16N8O2)]\@\@
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BS state - (vii)

```
1\1\GINC-GAIA06\F0pt\UB3LYP\6-311++G(d,p)\C14H16N8O2\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(C14H16N8O2)]\@\@
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Triplet- (viii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N4O4(3)\X543LJY\03-May
-2012\0\#\# OPT UB3LYP/6-311++G(D,P) OPTCYC=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\O,3.3060931316,2.21604
35756,0.6942299994\C,5.1255092631,-0.7803253576,-0.005833012\O,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\O,-3.3
06102843,-2.216144307,0.6939146926\C,-5.1255078325,0.7803267619,-0.005
723275\O,-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(C20H28N4O4)]
\@
```

BS state - (vii)

```
1\1\GINC-GAIA09\F0pt\UB3LYP\6-311++G(d,p)\C20H28N4O4\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
H28N4O4)]\@
```

Triplet- (ix)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C18H26N4O4S1(3)\X543LJY\03-M
ay-2012\0\#\ OPT UB3LYP/6-311++G(D,P) OPTCYC=200 SCF=(DIRECT,TIGHT,NOS
YMM) SCFCYC=2000\Dushin_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
26N4O4S1)]\@\
```

BS state - (ix)

```
1\1\GINC-GAIA10\F0pt\UB3LYP\6-311++G(d,p)\C18H26N4O4S1\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(C18H26N4O4S1)]\@\
```

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.\S2A=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,-0.000030
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.\S2A=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\PG
=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
000854651\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\F0pt\UB3LYP\ \C8H12N8O2(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(C8H12N8O2)]\ \@
```

BS state - (xiv)

```
1\1\GINC-GAIA17\F0pt\UB3LYP\ \C8H12N8O2\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(C8H12N8O2)]\ \@
```

Triplet- (xv)

```
1\1\GINC-GAIA08\F0pt\UB3LYP\6-311++G(d,p)\C16H26N4O4(3)\JYLEE18\24-Aug
-2011\0\#\# OPT UB3LYP/6-311++G(D,P) OPTCYC=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=CO
1 [X(C16H26N4O4)]\@\
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BS state - (xv)

```
I\1\GINC-GAIA05\FOpt\UB3LYP\6-311++G(d,p)\C16H26N4O4\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(C16H26N4O4)]\@\
```

Triplet- (xvi)

```
I\1\GINC-NODE20\F0pt\UB3LYP\6-311++G(d,p)\C20H30N4O4(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
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BS state - (xvi)

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