On the origin of higher rotational barriers in thioamides than in amides. Remote substituent effects on the conformational stability of the thioamide group in thioacetanilides

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Cartesian coordinates and energies in Hartree for B3LYP/6-31G(d,p) fully optimized geometries of cis and trans conformers, TS1 and TS2 transition states for p-substituted thioacetanilides:

Thiocetanilide

trans

C,0,0.4417886775,0.1570280788,-0.5359882011
C,0,1.5283314566,0.3863951127,-1.3988917869
C,0,1.3190041205,0.8349903261,-2.6974926726
C,0,0.0205857605,1.0624985274,-3.1592590257
C,0,-1.0555431065,0.8348166571,-2.303085827
C,0,-0.8627188023,0.3848937316,-0.9959752114
N,0,0.7751195122,-0.2972136803,0.7621456859
C,0,0.0519537319,-0.6366035377,1.8605473022
S,0,-1.6052642329,-0.6340180583,2.0261864519
C,0,0.9325163852,-1.0140442991,3.0394391738
H,0,2.5427091072,0.2107947267,-1.0458923961
H,0,2.1714653782,1.0062483866,-3.3477687006
H,0,-0.1472491023,1.4125196349,-4.1729624809
H,0,-2.0699911929,1.0081646545,-2.6498428806
H,0,-1.7007042886,0.2099043072,-0.3372611128
H,0,1.7758063076,-0.3800409656,0.8885514525
H,0,0.4706708262,-1.829408595,3.5958335631
H,0,1.0158570985,-0.1585295486,3.7184524757
H,0,1.9443176661,-1.3147154878,2.7411245402

HF=-763.2312443 Nimag=0

cis

C,0,0.2746292307,0.3284618833,-0.5752888695
C,0,1.4178684805,0.3691045724,-1.3869049911
C,0,1.8778284801,1.5833127421,-1.8897879398
C,0,1.2106867102,2.7710535376,-1.5830109044
C,0,0.0684003665,2.729898443,-0.7831745801
C,0,-0.4108739946,1.5167118595,-0.2897450578
N,0,-0.1782666807,-0.9412418237,-0.1315656967
C,0,-0.67984274,-1.3504179977,1.0641480318
S,0,-1.1804877989,-2.9302089174,1.2576980656
C,0,-0.7469691812,-0.3501858468,2.1934976341
H,0,1.9467083928,-0.55337654,-1.6095898035
H,0,2.764893356,1.600961296,-2.5156262719
H,0,1.5730272501,3.7178830515,-1.9706040032
H,0,-0.4693995739,3.6450570368,-0.5544570162
H,0,-1.3252529478,1.4908710147,0.2902869782
H,0,-0.0793220474,-1.7010263044,-0.7961241758
H,0,-0.673759792,-0.887395565,3.138164695
H,0,-1.7131278741,0.1665276687,2.1857742224
H,0,0.0415406707,0.4048986249,2.1315662634

HF=-763.2316785 Nimag=0

TS1

6	2.598966	-0.250868	1.666535
6	1.245434	-0.573999	1.637858
6	3.210129	0.355335	0.566710
6	0.473922	-0.305075	0.494468
6	2.444443	0.624829	-0.567874
6	1.089964	0.297542	-0.614515
7	-0.880507	-0.691890	0.463734
6	-1.829025	0.041987	-0.328112
16	-2.506119	-0.619663	-1.657056
6	-2.148136	1.424609	0.177208
1	3.177405	-0.470390	2.559496
1	0.778722	-1.043431	2.500880
1	4.264611	0.610188	0.593701
1	2.903638	1.090474	-1.435339
1	0.515149	0.490525	-1.514297
1	-1.246159	-0.913627	1.384335
1	-2.846647	1.947540	-0.474993
1	-1.221514	2.003499	0.273135
1	-2.577934	1.356894	1.186172

HF=-763.1993137 Nimag=1

TS2

6	2.028206	-2.179869	-0.614016
6	1.065461	-1.761534	0.300745
6	2.130638	-1.571870	-1.866402
6	0.177444	-0.724557	-0.025560
6	1.250896	-0.538099	-2.190083
6	0.279391	-0.114501	-1.285274
7	-0.842754	-0.376852	0.886771
6	-1.372631	0.964335	0.938010
16	-0.484342	2.271185	1.359509
6	-2.830334	1.013206	0.590153
1	2.706561	-2.982871	-0.340019
1	0.996060	-2.239781	1.274979
1	2.884735	-1.896231	-2.576219
1	1.316890	-0.051558	-3.159108
1	-0.394807	0.691552	-1.556192
1	-0.641257	-0.715785	1.822308
1	-3.237880	2.021520	0.653686
1	-3.384600	0.339648	1.256743
1	-2.971375	0.609845	-0.421161

HF=-763.2005115 Nimag=1

para-methylthioacetanilide

trans

```
C,0,0.9387989701,0.3396083039,-1.5444102158
 C,0,0.1888855475,0.1791099191,-2.7020034535
 C,0,-1.156250567,-0.212056494,-2.6451226873
 C,0,-1.7083400836,-0.4399072007,-1.380551304
 C,0,-0.9735345147,-0.2852771692,-0.2049077045
 C,0,0.3678425717,0.1109251053,-0.2807104693
 N,0,1.2257817608,0.2995478762,0.8289763822
 C,0,1.0647570209,0.2071639104,2.1734037268
 S,0,-0.3255473338,-0.1835962494,3.0047844482
 C,0,2.3531212318,0.4712906678,2.9334391877
 C,0,-1.9801759658,-0.3557855796,-3.9018186111
 H,0,1.9816609098,0.642074145,-1.618942606
 H,0,0.6575244939,0.3595128721,-3.6659511187
 H,0,-2.7469888132,-0.7509641458,-1.3024822068
 H,0,-1.425047452,-0.4690843257,0.7591419859
 H,0,2.1613226483,0.559962188,0.5440301525
 H,0,2.7900971535,-0.4819229599,3.2494782093
 H,0,2.1353670671,1.0447145519,3.8345933552
 H,0,3.1007997013,1.0118428252,2.3402407131
 H,0,-2.8209224144,-1.0391038519,-3.7520814063
 H,0,-1.3795262434,-0.7359275785,-4.7340610608
 H,0,-2.396627301,0.6091723584,-4.2172626773
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HF=-802.5519725 Nimag=0

cis

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C,0,1.0024504089,-1.3794958928,0.2531704471
 C,0,2.3803368248,-1.1971619484,0.3122164811
 C,0,2.9668996365,0.0337177034,-0.0133041571
 C,0,2.1197332265,1.0697087246,-0.4239940977
 C,0,0.7390980129,0.896665387,-0.5062936583
 C,0,0.1655736846,-0.3292293707,-0.1485619519
 N,0,-1.2282639069,-0.5831223906,-0.2445574574
 C,0,-2.302871355,0.1718117856,0.1035744668
 S,0,-3.8466277824,-0.3915094121,-0.1892606675
 C,0,-2.0546537747,1.5045979674,0.7688644098
 C,0,4.4591756917,0.2376082576,0.0908178439
 H,0,0.5660453896,-2.3366278215,0.5250133858
 H,0,3.0111152745,-2.0254553506,0.6240861857
 H,0,2.5470133668,2.0281055855,-0.7070532652
 H,0,0.1160406194,1.7027317252,-0.8749017261
 H,0,-1.4877547445,-1.4978630503,-0.5974948633
 H,0,-2.9031707292,1.7362103743,1.411334217
 H,0,-1.9888373415,2.2977732757,0.0158557727
 H,0,-1.1300727599,1.5148786851,1.35266199
 H,0,4.8008018934,1.0365056704,-0.5734615451
 H,0,5.0068120701,-0.674046742,-0.1663327631
 H,0,4.7514446917,0.514459294,1.1114267922
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HF=-802.5524992 Nimag=0

TS1

```
C,0,0.666665102,-0.411307272,-1.7109993791
 C,0,-0.3762077023,-0.5224775089,-2.6249129701
 C,0,-1.7168866609,-0.4565487124,-2.221926382
 C,0,-1.9676769852,-0.2881418473,-0.8557588843
 C,0,-0.9364412592,-0.1854926429,0.0767092277
 C,0,0.4008942768,-0.2419326686,-0.3427297191
 N,0,1.469408322,-0.1947011315,0.5784269349
 C,0,1.339883934,0.5686054993,1.7893370089
 S,0,1.2675506652,-0.1678386424,3.2436973
 C,0,1.30022023,2.0631385162,1.6032727829
 C,0,-2.8421236173,-0.5417803418,-3.226005237
 H,0,1.6968215714,-0.4673561084,-2.0556434022
 H,0,-0.1397413113,-0.6597686334,-3.6774316271
 H,0,-2.9955739327,-0.2441145642,-0.5039100268
 H,0,-1.1705012813,-0.0850891163,1.1315443571
 H,0,2.3632307809,-0.029782533,0.125697674
 H,0,2.2328960266,2.3990713232,1.1293069039
 H,0,1.169132187,2.5898573264,2.5477823769
 H,0,0.4893551879,2.3261155844,0.9132167329
 H,0,-3.7697437593,-0.8836161543,-2.7573623682
 H,0,-2.6026710078,-1.2349832253,-4.0387200568
 H,0,-3.0498372659,0.4336141692,-3.6845445954
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HF=-802.5193025 Nimag=1

TS2

```
6             1.221406    1.315991    1.546349
16             0.994764    0.365347    2.858077
7             0.210481    1.546098    0.542355
6             2.486342    2.068863    1.260867
6            -0.278956    0.479972   -0.247994
6             0.536426   -0.595423   -0.627323
6             0.041357   -1.586756   -1.471544
6            -1.265763   -1.547803   -1.970987
6            -2.066482   -0.463729   -1.590304
6            -1.590191    0.531760   -0.742214
6            -1.801660   -2.645670   -2.859271
1            -0.548406    2.099638    0.928094
1             2.257178    3.138184    1.165100
1             3.243043    1.915132    2.029388
1             2.872941    1.760937    0.280531
1             1.557262   -0.661587   -0.264568
1             0.693946   -2.410961   -1.749259
1            -3.087386   -0.396528   -1.958604
1            -2.237060    1.360768   -0.464477
1            -0.999531   -3.130138   -3.424312
1            -2.304706   -3.427185   -2.275449
1            -2.531756   -2.259724   -3.577640
```

HF=-802.5205748 Nimag=1

para-methoxythioacetanilide

trans

```
C,0,0.3147464619,-1.7523136795,-0.0683948927
 C,0,0.6252388319,-1.9220900158,-1.4061988234
 C,0,0.6205939958,-0.81957631,-2.2745968283
 C,0,0.2999717323,0.4435154455,-1.7697132242
 C,0,-0.0130238302,0.6147252052,-0.4185788783
 C,0,-0.0090527152,-0.4829727781,0.4476102644
 N,0,-0.3067073069,-0.4336622502,1.8314674057
 C,0,-0.6651079045,0.5585748039,2.6818210757
 S,0,-0.8907867079,2.1720217692,2.32124
 C,0,-0.8432343095,0.0745766233,4.1104266436
 O,0,0.9390759757,-1.0872143327,-3.5737554044
 C,0,0.949755814,-0.0080960073,-4.4963820869
 H,0,0.3227646558,-2.617997028,0.5908849324
 H,0,0.8749042396,-2.8997822882,-1.8037740303
 H,0,0.2877004482,1.3139253937,-2.4144839995
 H,0,-0.2601929616,1.5947593985,-0.0364769302
 H,0,-0.2300456123,-1.3431897672,2.2682498573
 H,0,-1.7867090659,0.4520704474,4.5081673435
 H,0,-0.0425448289,0.4828781725,4.7343016237
 H,0,-0.8328425088,-1.0180156839,4.2052014041
 H,0,1.2252757725,-0.439032128,-5.4597924624
 H,0,1.6874415802,0.7551043393,-4.2178746838
 H,0,-0.0381495087,0.4622215262,-4.580431158
```

HF=-877.7561944 Nimag=0

cis

```
C,0,0.9280522755,-0.0470314228,-1.3445426946
 C,0,0.0253960626,-0.0813361231,-2.3961444848
 C,0,-1.3431974102,0.124171993,-2.1610687982
 C,0,-1.7864532889,0.3819234551,-0.8589251894
 C,0,-0.8678380222,0.4366657399,0.1916129873
 C,0,0.4906993975,0.2057362514,-0.0342037675
 N,0,1.4597497697,0.2825508984,1.0051790152
 C,0,1.474172052,-0.2819700489,2.2393000042
 S,0,2.7325169597,0.0323907453,3.2912815368
 C,0,0.3321031368,-1.197796295,2.6112722385
 O,0,-2.147995952,0.0580792658,-3.2582570593
 C,0,-3.5428305333,0.2613559875,-3.083954426
 H,0,1.983073733,-0.2260339356,-1.5305250693
 H,0,0.354031677,-0.276832507,-3.4111451495
 H,0,-2.8340780502,0.5615581994,-0.6508050368
 H,0,-1.216274348,0.6799787939,1.1889207568
 H,0,2.2956389322,0.8204833834,0.8035754309
 H,0,-0.4735986698,-0.625689124,3.0846039701
 H,0,0.6890140991,-1.9227577166,3.3416474736
 H,0,-0.0868042864,-1.7151674099,1.7436045776
 H,0,-3.9872115539,0.1582255653,-4.0745084879
 H,0,-3.7596340969,1.2637680576,-2.6938253995
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HF=-877.7565461 Nimag=0

TS1

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C,0,1.1378520137,0.1380356343,1.4219173116
 C,0,1.7200874338,-1.1186995071,1.3416694904
 C,0,1.4372059776,-1.9663864993,0.2617324811
 C,0,0.5678235648,-1.5240609162,-0.7386205412
 C,0,-0.0057108357,-0.251397296,-0.6618438364
 C,0,0.2656516737,0.5948851706,0.4184384231
 N,0,-0.2656597028,1.9080355828,0.4865051856
 C,0,-1.6041226222,2.1409830753,0.0138608231
 S,0,-1.8797253999,3.0548144045,-1.310209318
 C,0,-2.6972312091,1.5054174756,0.8338361544
 O,0,2.055332969,-3.1884813677,0.2830410853
 C,0,1.8087706005,-4.0751559073,-0.794453291
 H,0,1.3658166269,0.7796159042,2.2700094064
 H,0,2.3965046487,-1.4691080827,2.114278518
 H,0,0.3324739776,-2.1507802283,-1.5905173566
 H,0,-0.6560761156,0.0853858214,-1.462345385
 H,0,-0.1300134845,2.3185472295,1.4060974545
 H,0,-2.5146569645,0.4275566687,0.9189692526
 H,0,-3.6839434269,1.682155959,0.4074102565
 H,0,-2.6701072074,1.9076471856,1.8561280259
 H,0,2.3893976501,-4.9749595446,-0.5854141512
 H,0,2.135204431,-3.6511313313,-1.7532835741
 H,0,0.7460008478,-4.342085571,-0.8670704312
```

HF=-877.7220355 Nimag=1

TS2

```
C,0,-0.2501822607,-1.235997174,-1.2636478074
 C,0,-1.4539293202,-1.73756403,-0.7892632254
 C,0,-2.1540814461,-1.0668696038,0.222101736
 C,0,-1.6256527255,0.117310338,0.7431911622
 C,0,-0.4176120092,0.6226056194,0.2554332182
 C,0,0.2880232384,-0.0449646591,-0.7497533276
 N,0,1.4769763061,0.488091591,-1.3132188534
 C,0,2.4067647697,1.2157738856,-0.4815986049
 S,0,3.2032285282,0.5540272826,0.7851616701
 C,0,2.5768472385,2.6359286071,-0.9319563077
 O,0,-3.3274086726,-1.6482032285,0.6246346336
 C,0,-4.0638434322,-1.0117679257,1.6540299802
 H,0,0.2814091163,-1.7733633446,-2.0453535815
 H,0,-1.8677064302,-2.6590064106,-1.185312006
 H,0,-2.139431926,0.6605477896,1.5272771241
 H,0,-0.0281414915,1.5448357138,0.6747436349
 H,0,1.9744404333,-0.2212319549,-1.8435481245
 H,0,2.8962694659,2.6452520159,-1.9822341244
 H,0,3.2912004379,3.1834813776,-0.3180956442
 H,0,1.6001217911,3.1369686955,-0.9169615674
 H,0,-4.9454995255,-1.6318055258,1.823837334
 H,0,-4.3851365974,-0.0032081409,1.3614062708
 H,0,-3.4867508023,-0.9446523927,2.5858879275
```

HF=-877.7232784 Nimag=1

para-ethoxythioacetanilide

trans

C,0,0.2623634876,-1.7230159884,0.2364308928
C,0,0.5497337329,-1.7623182866,-1.1166473194
C,0,0.4961616561,-0.5871753804,-1.8826622137
C,0,0.150091178,0.6151846038,-1.2587234775
C,0,-0.1396979215,0.6547311987,0.1076914598
C,0,-0.0866721742,-0.5156913645,0.8709272342
N,0,-0.3582044995,-0.6007277901,2.2584671749
C,0,-0.7205521203,0.2997247775,3.2035427756
S,0,-0.9853713784,1.9345992833,2.9997186024
C,0,-0.8699676189,-0.3201327993,4.5821558611
O,0,0.7950865964,-0.7270829947,-3.205241243
C,0,1.1299667292,-0.0095760569,-5.4468360823
C,0,0.7593169187,0.4301060975,-4.0420438997
H,0,0.3086717796,-2.6437862991,0.814643419
H,0,0.8187668592,-2.6925411306,-1.6051414629
H,0,0.0997888171,1.5393422521,-1.8213798607
H,0,-0.4062652349,1.5887336921,0.5811530276
H,0,-0.2539383898,-1.5446736376,2.6076097386
H,0,-1.8427914515,-0.0516093061,4.9985859293
H,0,-0.1081784902,0.0917918808,5.2499486468
H,0,-0.7773816111,-1.4129923312,4.5822378598
H,0,1.1151079909,0.8489833686,-6.124914134
H,0,2.1319888229,-0.4469431018,-5.4623000078
H,0,0.4220246579,-0.7563467179,-5.8166093726
H,0,-0.2459849077,0.8737615058,-4.0222748362
H,0,1.4664087313,1.1834289716,-3.6674082503

HF=-917.078339 Nimag=0

Cis

C,0,-0.9300543814,1.2349293509,0.4088572501
C,0,0.0287239186,2.0640334955,-0.152627935
C,0,1.0953463579,1.5200123055,-0.8860853199
C,0,1.1716447086,0.1328871705,-1.0602336414
C,0,0.189761326,-0.6937086143,-0.5099141116
C,0,-0.8570633038,-0.1574479514,0.2427440582
N,0,-1.8912622076,-0.966250999,0.7929146044
C,0,-1.8197248537,-2.0995931543,1.5356320342
S,0,-3.2163285248,-2.8877840022,2.0021640221
C,0,-0.4500633704,-2.6035889935,1.9249927606
O,0,1.9886939537,2.4176421504,-1.3852751515
C,0,3.921957358,3.1403597758,-2.5656582047
C,0,3.0981062552,1.9363485781,-2.1473005945
H,0,-1.7416237475,1.6618895337,0.9909254769
H,0,-0.0193154171,3.1405243011,-0.0286857011
H,0,1.972754947,-0.3143953425,-1.6354695871
H,0,0.2350848793,-1.7622925155,-0.6874315641
H,0,-2.8425683328,-0.6507747559,0.6372178935
H,0,-0.0710664631,-3.2963170035,1.1653918816
H,0,-0.5340040273,-3.1581727121,2.858692081
H,0,0.2763247232,-1.7933602761,2.0341055047
H,0,4.7855885939,2.8174332292,-3.1546336009
H,0,3.323570375,3.8246030768,-3.1732088942
H,0,4.2834237446,3.6838431221,-1.6885428087
H,0,3.6955882612,1.2439484467,-1.5378492607
H,0,2.7349785947,1.3848429436,-3.0257745689

HF=-917.078797 Nimag=0

TS1

C,0,-0.7889897683,-1.0633638238,1.2482880522
C,0,-1.9369796936,-0.8070039105,0.5123705522
C,0,-1.8664253612,-0.0976915633,-0.6948286082
C,0,-0.6197607841,0.3394026089,-1.1514744811
C,0,0.5365730723,0.0664938536,-0.4148208488
C,0,0.4698758503,-0.6324533304,0.7950342141
N,0,1.6382089199,-0.9623006986,1.5289179888
C,0,2.7182697765,-0.0134226931,1.5766744594
S,0,4.1504705664,-0.334684162,0.8624892728
C,0,2.4288828235,1.2554577037,2.3365141243
O,0,-3.0569962543,0.1101461889,-1.3375938162
C,0,-4.4773072628,0.8890928852,-3.0758271004
C,0,-3.0445061836,0.8084526904,-2.579891478
H,0,-0.8656667462,-1.611341006,2.1846080778
H,0,-2.9077405368,-1.1439805782,0.8607731531
H,0,-0.5265500999,0.8849390681,-2.0827646797
H,0,1.4981016066,0.3893581628,-0.8001702235
H,0,1.4107777686,-1.2974222972,2.4609407604
H,0,1.5355499095,1.7370339051,1.9211730922
H,0,3.2692099071,1.9481679554,2.311084946
H,0,2.1940306165,1.0122593596,3.3820794294
H,0,-4.51588826,1.4192343252,-4.0322911918
H,0,-4.8925111258,-0.1125904326,-3.2168136937
H,0,-5.1044722231,1.4233824576,-2.3568394715
H,0,-2.6217469416,1.8143780319,-2.4418836685
H,0,-2.4099101559,0.276676495,-3.3036336006

HF=-917.0441504 Nimag=1

TS2

C,0,-0.6164697905,-1.1696659776,1.2062871195
C,0,-1.7870061662,-1.0222156918,0.4756240992
C,0,-1.7799081696,-0.344619869,-0.750920889
C,0,-0.5745473716,0.1771190565,-1.2297282845
C,0,0.6027740915,0.0181831305,-0.4940655397
C,0,0.6001315004,-0.6530879989,0.7319658142
N,0,1.7953960896,-0.8941016873,1.4593515322
C,0,2.8539071387,0.088051876,1.4555916311
S,0,2.6935091427,1.600413511,2.0591789961
C,0,4.1216429976,-0.4490914825,0.8614049165
O,0,-2.9872763019,-0.2478259121,-1.3893916156
C,0,-4.4838302116,0.4108143774,-3.1127580166
C,0,-3.0429468558,0.4418634757,-2.6347536189
H,0,-0.6434949504,-1.6943027588,2.1583987922
H,0,-2.7267193455,-1.4198388949,0.8444301472
H,0,-0.5319371117,0.7087451343,-2.1726625808
H,0,1.5260872101,0.4310417653,-0.8878885303
H,0,1.5868419674,-1.1693397554,2.4146795047
H,0,4.4248921751,-1.3487122625,1.4127721572
H,0,4.9273298585,0.2842161897,0.8692038351
H,0,3.9231531581,-0.7857307843,-0.1644664501
H,0,-4.5747991676,0.9313481532,-4.070997575
H,0,-4.8239754743,-0.6201639459,-3.2436618837
H,0,-5.1402057476,0.900106175,-2.3878778409
H,0,-2.6962022031,1.4776660721,-2.5070920424
H,0,-2.379161841,-0.044437533,-3.3645163402

HF=-917.0454036 Nimag=1

para-chlorothioacetanilide

trans

```
C,0,-1.5352721945,0.6130094376,-0.3230186674
 C,0,-1.7177122025,0.2743040299,-1.6575521739
 C,0,-0.7056515132,-0.4118038316,-2.3288523366
 C,0,0.4727859017,-0.7541080287,-1.6718014269
 C,0,0.6565002258,-0.4149157597,-0.3315854929
 C,0,-0.3517108119,0.2750281405,0.3563953127
 N,0,-0.2825061923,0.6703810631,1.7110103864
 C,0,0.6624683649,0.5516188164,2.6818834574
 S,0,2.1667824124,-0.1476713622,2.5491510629
 C,0,0.1943143892,1.1107933832,4.0136315753
 Cl,0,-0.9253367751,-0.8451562629,-4.017639555
 H,0,-2.3254922574,1.1483812121,0.19857732
 H,0,-2.634252573,0.5394367209,-2.171774201
 H,0,1.2534611404,-1.2875132222,-2.2022799699
 H,0,1.5707764805,-0.6790710234,0.1800299734
 H,0,-1.1262338059,1.1397918138,2.0145720534
 H,0,1.0414139821,1.5344494734,4.5518915763
 H,0,-0.2142008432,0.2987897258,4.6256353415
 H,0,-0.5800551566,1.8799089972,3.9051291432

HF= -1222.8250089             Nimag=0
```

Cis

```
C,0,-1.0811566746,0.0816142818,-1.1099019274
 C,0,-0.5662638383,0.9106549825,-2.1015666828
 C,0,0.763481914,1.3246428938,-2.0238931827
 C,0,1.5811213873,0.901156516,-0.9778108949
 C,0,1.0656002874,0.0553806222,0.0022879647
 C,0,-0.2758251777,-0.3471493478,-0.0444610586
 N,0,-0.8449246686,-1.2306570946,0.905681326
 C,0,-0.7218489587,-1.2978007605,2.2601652124
 S,0,-1.4917970037,-2.5132959096,3.1013658979
 C,0,0.1021541045,-0.2422326575,2.9578174051
 Cl,0,1.4174934173,2.3810786344,-3.2640310329
 H,0,-2.1211329254,-0.2282793138,-1.1539190649
 H,0,-1.193058057,1.2415873083,-2.9217264512
 H,0,2.6190084894,1.2117595083,-0.9397469076
 H,0,1.7183006553,-0.3086596321,0.7859081001
 H,0,-1.493144111,-1.917920296,0.5365370576
 H,0,1.1455021598,-0.5670231083,3.0395676909
 H,0,-0.2784085367,-0.1175545893,3.9706719714
 H,0,0.085190709,0.7174883704,2.4337904994

HF= -1222.8246718             Nimag=0
```

TS1

```
6             0.136524   -1.033289    2.482353
16            1.267614   -2.118874    2.931803
7            -0.664497   -1.243576    1.306722
6            -0.172549    0.227438    3.245849
6            -0.493674   -0.439713    0.167162
6             0.750207    0.129381   -0.152447
6             0.905502    0.884813   -1.312868
6            -0.175926    1.072178   -2.170259
6            -1.416027    0.507593   -1.874413
6            -1.572497   -0.238252   -0.710818
17            0.022346    2.026201   -3.636610
1            -1.638492   -1.419440    1.530057
1             0.480796    0.353181    4.108362
1            -0.081933    1.094292    2.579853
1            -1.217483    0.204971    3.584733
1             1.604797   -0.032673    0.495653
1             1.869412    1.320509   -1.551463
1            -2.255122    0.654772   -2.545294
1            -2.541566   -0.674916   -0.482795

HF=-1222.7932517              Nimag=1
```

TS2

```
6            -2.594960   -0.255319    0.872455
16           -2.755469    1.225167    1.545736
7            -1.878531   -0.493744   -0.358845
6            -3.190849   -1.510500    1.435331
6            -0.491708   -0.263972   -0.454373
6             0.361475   -0.407489    0.650740
6             1.737817   -0.248111    0.508518
6             2.276335    0.051439   -0.740755
6             1.445585    0.196980   -1.850217
6             0.070630    0.042075   -1.703802
17            4.016469    0.251023   -0.919875
1            -2.383395   -0.104605   -1.148739
1            -3.748152   -1.328152    2.353410
1            -3.844957   -1.969982    0.682814
1            -2.390210   -2.239731    1.615619
1            -0.044726   -0.638889    1.629605
1             2.389018   -0.357200    1.368645
1             1.868110    0.435851   -2.819776
1            -0.574391    0.158231   -2.570955

HF= -1222.7946027             Nimag=1
```

para-carboxythioacetanilide

trans

```
C,0,-3.117306834,0.139154678,-0.0713729608
 S,0,-3.295393135,-0.8918769143,1.2191028851
 N,0,-1.9525043638,0.5723882087,-0.6324629276
 C,0,-4.3341156095,0.6810299183,-0.8001919141
 C,0,-0.5886179597,0.3285167657,-0.3757182844
 C,0,-0.0991843735,-0.5266484356,0.62473074
 C,0,1.2747918904,-0.6826035267,0.7738326884
 C,0,2.1807646168,-0.0063454803,-0.0510262084
 C,0,1.6880029879,0.8468731842,-1.0492440893
 C,0,0.3211745453,1.0105152457,-1.2072845732
 C,0,3.6318719362,-0.2219881656,0.1663066891
 O,0,4.1098664896,-0.9491102045,1.0145343881
 O,0,4.4088608219,0.4874811807,-0.6940555005
 H,0,-2.085604622,1.2076518754,-1.409455289
 H,0,-4.5942852879,0.0094081626,-1.6269145557
 H,0,-5.1840272549,0.7190694757,-0.1209235625
 H,0,-4.1631077097,1.6814990714,-1.2162495354
 H,0,-0.7904961535,-1.0521669776,1.2668158106
 H,0,1.6664666707,-1.3401684273,1.5423245235
 H,0,2.3778134775,1.3769119064,-1.695284607
 H,0,-0.0526482568,1.6743381987,-1.9837196937
 H,0,5.3256041503,0.2687769705,-0.4590223848

HF= -951.8086351              Nimag=0
```

Cis

```
C,0,-1.1336838433,-0.3449208014,-0.8685781219
 C,0,-0.7963567864,0.5394800378,-1.8834866327
 C,0,0.4122548913,1.2481789504,-1.8277933165
 C,0,1.2787524308,1.0380602209,-0.7481897411
 C,0,0.9533049125,0.1445435171,0.2646986841
 C,0,-0.26996905,-0.5444188591,0.2229348884
 N,0,-0.6635089431,-1.490049593,1.1926176395
 C,0,-0.4617302662,-1.5693550252,2.5399870157
 S,0,-1.0379357271,-2.8897993122,3.3756112448
 C,0,0.2554452803,-0.4376354372,3.2344275926
 C,0,0.8233902838,2.2114720841,-2.87915923
 O,0,1.8588703811,2.8474007529,-2.8711898902
 O,0,-0.0860865925,2.3235800918,-3.8803207101
 H,0,-2.0784428007,-0.8797922179,-0.9054141655
 H,0,-1.4708288726,0.6912287002,-2.7180064928
 H,0,2.221151136,1.5744473601,-0.7282734142
 H,0,1.6593156354,-0.0381841473,1.0635593368
 H,0,-1.2509850116,-2.2419514278,0.8481247838
 H,0,1.3381139165,-0.6069535577,3.2223447691
 H,0,-0.0585282497,-0.4158018641,4.2769052339
 H,0,0.0576343547,0.5312698834,2.7672437095
 H,0,0.2833867003,2.9725985346,-4.5015491813

HF= -951.8085843              Nimag=0
```

TS1

```
6             -2.998528    0.186475   -0.036907
16            -3.916944   -1.160408   -0.055978
7             -1.915522    0.358869   -0.964322
6             -3.206742    1.341861    0.904413
6             -0.578816    0.243400   -0.592731
6             -0.188584   -0.469534    0.558183
6              1.155920   -0.588317    0.878061
6              2.147058   -0.013612    0.070276
6              1.757292    0.689581   -1.080843
6              0.416832    0.820179   -1.407195
6              3.560440   -0.175285    0.467510
8              3.948816   -0.767714    1.457215
8              4.430349    0.416470   -0.396480
1             -2.100013    1.039065   -1.692104
1             -4.023862    1.158679    1.601147
1             -2.279668    1.535195    1.458464
1             -3.417958    2.253166    0.328416
1             -0.937739   -0.941672    1.184485
1              1.463923   -1.135292    1.762778
1              2.513344    1.137552   -1.715565
1              0.125863    1.367670   -2.300218
1              5.313310    0.241567   -0.031987

HF= -951.7792065              Nimag=1
```

TS2

```
6              0.400975   -1.534658    0.469952
6              0.718841   -1.822126   -0.848764
6              0.413558   -0.909460   -1.870024
6             -0.217330    0.296422   -1.532985
6             -0.541158    0.591500   -0.217285
6             -0.235379   -0.324753    0.806385
7             -0.609428   -0.098208    2.134429
6             -0.811567    1.226449    2.669704
16             0.399778    2.306870    2.850791
6             -2.237673    1.475047    3.059298
6              0.730339   -1.164310   -3.290591
8              0.483129   -0.408296   -4.211715
8              1.344666   -2.361435   -3.495632
1              0.642298   -2.247957    1.253959
1              1.211198   -2.756067   -1.094457
1             -0.448321    0.997884   -2.327460
1             -1.025363    1.532520    0.020011
1             -0.135540   -0.705717    2.793939
1             -2.878454    1.349836    2.176570
1             -2.380872    2.465687    3.489197
1             -2.560222    0.705221    3.772392
1              1.498832   -2.410671   -4.453166

HF= -951.7803647              Nimag=1
```

para-hydroxythioacetanilide

trans

```
C,0,1.3008874623,-0.3722904732,1.9829721021
 S,0,2.6377956007,-0.8907300398,1.1307937621
 N,0,0.1082400495,0.0324017105,1.4820269268
 C,0,1.3458323869,-0.3320753528,3.500863486
 C,0,-0.4174454677,0.1592303615,0.1727794699
 C,0,0.2712602913,-0.1589499016,-1.0083294099
 C,0,-1.7319453808,0.6420110003,0.080834074
 C,0,-0.3514439926,0.0070608142,-2.2412815082
 C,0,-2.3516738691,0.806554461,-1.1524723543
 C,0,-1.6606286102,0.4883164748,-2.3264340228
 O,0,-2.2076114835,0.6255759519,-3.5704562376
 H,0,-0.5621628591,0.3073507021,2.1881372097
 H,0,2.2145024408,0.2453579732,3.8237391442
 H,0,1.4716028028,-1.347179241,3.8871792922
 H,0,0.4465987785,0.1033547451,3.9535474427
 H,0,1.2839728884,-0.5312955726,-0.9510555263
 H,0,-2.2813058997,0.8938686407,0.9855875472
 H,0,0.1758947765,-0.2370455632,-3.1572221472
 H,0,-3.3711307103,1.1822067971,-1.1990111024
 H,0,-3.1085472295,0.9644982618,-3.4877316599
```

HF= -838.4503881 Nimag=0

Cis

```
C,0,2.1937169363,0.2046103777,-0.5741064693
 S,0,3.8204299628,0.3685337286,-0.2362932984
 N,0,1.2850498754,0.1936077021,0.4342591421
 C,0,1.6795046284,0.0738064752,-1.9882929584
 C,0,-0.1282106198,0.0258418917,0.398276908
 C,0,-0.7364107529,-1.0386379162,-0.2816887706
 C,0,-0.9299527876,0.915137775,1.122636955
 C,0,-2.1182513262,-1.1897885565,-0.2665542178
 C,0,-2.3127820238,0.7551313832,1.1592431
 C,0,-2.9145272088,-0.2941409231,0.4560917511
 O,0,-4.2627939487,-0.5007803838,0.4417840533
 H,0,1.6983495949,0.3578835091,1.3457050048
 H,0,2.3785002248,0.5671446997,-2.6623070697
 H,0,1.6339997998,-0.9817356997,-2.2783378709
 H,0,0.6793129623,0.4994214621,-2.1092671356
 H,0,-0.1246014578,-1.7612999981,-0.8092998278
 H,0,-0.4676026334,1.7419665064,1.6537203463
 H,0,-2.5957362457,-2.0095562439,-0.7921313691
 H,0,-2.9233874669,1.4534876545,1.7267316651
 H,0,-4.6972327948,0.1753745651,0.9781548228
```

HF= -838.4512876 Nimag=0

TS1

```
C,0,2.143255269,0.3296687857,0.6854830327
 S,0,3.1167175379,-0.8490531692,1.2567127119
 N,0,0.8291888975,0.5342500652,1.2352169704
 C,0,2.5376021816,1.2811558693,-0.4145652403
 C,0,-0.3025921724,0.2700630387,0.4216180791
 C,0,-0.3254332798,-0.816255583,-0.4681371362
 C,0,-1.4538676697,1.0596125278,0.5398663922
 C,0,-1.4617990998,-1.0945654976,-1.2212154639
 C,0,-2.5982404334,0.7710867149,-0.2022782385
 C,0,-2.6080562605,-0.3053501981,-1.0925626291
 O,0,-3.6968631044,-0.6338864213,-1.8581763221
 H,0,0.7631571373,1.4450101063,1.6811502189
 H,0,3.528911915,1.061842894,-0.8093469733
 H,0,2.5212542398,2.3116317859,-0.0332910455
 H,0,1.7971276471,1.2371420042,-1.22234154
 H,0,0.545594263,-1.4565591105,-0.5600325736
 H,0,-1.4615082781,1.9047340078,1.2240921413
 H,0,-1.4772868003,-1.9334246,-1.9090203816
 H,0,-3.4821380633,1.3954774235,-0.0898467051
 H,0,-4.4172213232,-0.0221568354,-1.6591275234
```

HF= -838.4166276 Nimag=1

TS2

```
C,0,2.1316937563,0.2514878646,0.9298304366
 S,0,2.7589220815,1.1641848156,-0.2743597502
 N,0,0.7713782506,0.3732881227,1.4031669838
 C,0,2.9042009297,-0.7854553009,1.6888706071
 C,0,-0.3076355797,0.0955394671,0.5220199867
 C,0,-0.2438644419,-0.9540791149,-0.4077354289
 C,0,-1.4982657083,0.823381043,0.6245058054
 C,0,-1.3363471594,-1.2603235942,-1.2113200825
 C,0,-2.5995373575,0.5104367176,-0.1718757504
 C,0,-2.5243679708,-0.531898504,-1.0976462852
 O,0,-3.5672049233,-0.8851829698,-1.9146643408
 H,0,0.6472554158,1.2783234878,1.8478796022
 H,0,3.9360212779,-0.8661302187,1.348812532
 H,0,2.3961432745,-1.7540639263,1.5938634426
 H,0,2.8768172647,-0.5432109963,2.7593121332
 H,0,0.6669372009,-1.5353332316,-0.5103607381
 H,0,-1.5702345054,1.643287555,1.3348646047
 H,0,-1.2836093436,-2.0678852569,-1.9337906012
 H,0,-3.5147221852,1.090584832,-0.0746259624
 H,0,-4.3146288807,-0.2986138657,-1.7409489031
```

HF= -838.4180451 Nimag=1

para-aminothioacetanilide

trans

C,0,-1.1160941526,-0.9038833759,1.1591785596
C,0,-2.4666629721,-0.7983196099,0.8610953291
C,0,-2.895377953,-0.0647977059,-0.2589195608
C,0,-1.9163292859,0.5477520602,-1.0566897742
C,0,-0.5603528513,0.4440670281,-0.7627511526
C,0,-0.1414806708,-0.287304026,0.3575779338
N,0,1.2047938532,-0.4676397567,0.7606698033
C,0,2.3937703332,-0.0114939325,0.3013690727
S,0,2.6600784537,0.9990569533,-1.0011159812
C,0,3.5748547847,-0.5295010238,1.1039780236
N,0,-4.2466899276,0.0002216336,-0.5983283582
H,0,-0.8126450239,-1.4750964398,2.034561629
H,0,-3.1975387592,-1.2904734072,1.497116279
H,0,-2.2211428837,1.1170020092,-1.9311910407
H,0,0.1747840122,0.9282417517,-1.3895543972
H,0,1.2794822086,-1.0670295207,1.5724517521
H,0,4.2023736114,0.3095630756,1.4109215558
H,0,4.1885961837,-1.1767458362,0.4711927722
H,0,3.2815147265,-1.0946243674,1.9972602804
H,0,-4.505721968,0.7855447883,-1.1794567349
H,0,-4.8916482396,-0.1284829294,0.1691329002

HF= -818.5896059 Nimag=0

Cis

C,0,0.363345056,-1.0824569682,1.2775449553
C,0,1.3616197023,-0.7504352315,2.1851715133
C,0,1.9044293478,0.5468614573,2.2135239161
C,0,1.3970879565,1.4991323232,1.312177058
C,0,0.3830722762,1.1690776571,0.4198700998
C,0,-0.1350472228,-0.1307631901,0.3788837742
N,0,-1.1960533589,-0.4978220528,-0.4990016291
C,0,-1.3140276936,-0.3364598351,-1.8399173934
S,0,-2.7104683258,-0.8071702451,-2.6275147978
C,0,-0.1450951268,0.2711873353,-2.5791424904
N,0,2.8709857673,0.8957052123,3.1521045206
H,0,-0.0309231566,-2.0944413168,1.2558086574
H,0,1.7312717192,-1.5022507998,2.8773716197
H,0,1.7859407782,2.5138230749,1.3299282671
H,0,-0.0185144531,1.9307722928,-0.2393816229
H,0,-1.9902686754,-0.970169598,-0.0808186103
H,0,-0.241620925,1.3621886917,-2.6084620315
H,0,-0.1562903805,-0.0858091108,-3.6080960845
H,0,0.8128162367,0.0316121855,-2.108707904
H,0,3.441726651,1.6955044991,2.9174345563
H,0,3.4165227851,0.1314505991,3.5247710798

HF= -818.5904731 Nimag=0

TS1

C,0,0.8964383902,-1.5326038468,0.5711701161
C,0,2.2231959263,-1.5254372219,0.1509412649
C,0,2.7870080178,-0.3850410253,-0.4413560507
C,0,1.9730282916,0.749009799,-0.5832958979
C,0,0.6513433761,0.7501772424,-0.1456889345
C,0,0.089076804,-0.3951346805,0.4351929931
N,0,-1.2435140471,-0.3938968516,0.9337358606
C,0,-2.2597494684,0.2598520708,0.1522560586
S,0,-3.0053850667,1.6047758156,0.7006154314
C,0,-2.5820036985,-0.3932977054,-1.1675683553
N,0,4.1387205673,-0.3582593079,-0.8170137809
H,0,0.4848198797,-2.4350867108,1.0177756904
H,0,2.8290330796,-2.4188532809,0.2808076045
H,0,2.3852981869,1.6513352438,-1.0282613267
H,0,0.056599383,1.6523384674,-0.2451091922
H,0,-1.5397544443,-1.3335834033,1.1846759253
H,0,-1.6668498728,-0.4887841496,-1.7639617705
H,0,-3.332625908,0.1633700737,-1.7273664781
H,0,-2.9478281757,-1.4147105986,-0.9926232635
H,0,4.3547273148,0.313077263,-1.5422325216
H,0,4.5262701479,-1.265570632,-1.0405132952

HF= -818.5545609 Nimag=1

TS2

C,0,0.7666064503,-1.4390943874,0.7889693216
C,0,2.1281412828,-1.4799585601,0.502762248
C,0,2.7842888365,-0.3666612142,-0.0424684209
C,0,2.0254482952,0.7895359181,-0.279924672
C,0,0.6668898945,0.8348373909,0.0180486721
C,0,0.0137023106,-0.282116624,0.5551560034
N,0,-1.3577949513,-0.2350817643,0.9327658946
C,0,-2.2969528882,0.4813385126,0.100664057
S,0,-2.6338383074,0.0776632847,-1.4496476561
C,0,-2.9461825003,1.6185988081,0.8310261562
N,0,4.1676369302,-0.3867243993,-0.283342964
H,0,0.2825101373,-2.3219274404,1.2002334884
H,0,2.6876964233,-2.3911894132,0.6991160101
H,0,2.5075751175,1.669772179,-0.6980408725
H,0,0.1136773179,1.7481320262,-0.1779808952
H,0,-1.7090570005,-1.1733009156,1.1033577051
H,0,-3.4320029685,1.2330571925,1.7369272891
H,0,-3.6698116664,2.1502670095,0.2141069398
H,0,-2.1693557429,2.3084268726,1.1859658205
H,0,4.4688788018,0.2588129471,-1.0020604555
H,0,4.5407585583,-1.3108989313,-0.4586232387

HF= -818.5560641 Nimag=1

para-nitrothioacetanilide

trans

```
C,0,-0.8496158703,-1.3860453624,0.0456903499
 C,0,-1.0508365516,-1.4033083825,-1.3239393025
 C,0,-0.518508156,-0.3680125173,-2.0924793553
 C,0,0.203293836,0.6699555391,-1.5100406274
 C,0,0.405924367,0.688275787,-0.1338089985
 C,0,-0.1219263472,-0.3451192307,0.658855549
 N,0,0.0144494906,-0.4354542458,2.0552777158
 C,0,0.6314211861,0.3332996857,3.0017166688
 S,0,1.5018163268,1.7247996164,2.7581491561
 C,0,0.4045266411,-0.2060508443,4.4020572519
 N,0,-0.7264545539,-0.3778253546,-3.5433791556
 O,0,-1.3709293119,-1.3129935465,-4.0216555774
 O,0,-0.2457083031,0.5476814536,-4.1977497867
 H,0,-1.2601022457,-2.188394778,0.6537401002
 H,0,-1.6074700962,-2.1963563005,-1.8063951077
 H,0,0.6012016948,1.4565566904,-2.1387223776
 H,0,0.9649733998,1.4875015541,0.3299063318
 H,0,-0.4541427429,-1.249213184,2.4338661671
 H,0,-0.5434605048,0.1814512104,4.7941550996
 H,0,1.2024500393,0.1308626474,5.0612902977
 H,0,0.3589509594,-1.3017158037,4.4254167669
```

HF= -967.7313299 Nimag=0

Cis

```
C,0,0.6838575048,1.0375963573,0.8193882439
 C,0,-0.264225496,2.0352506608,0.6545645634
 C,0,-1.3302538505,1.8147746303,-0.2172641237
 C,0,-1.4489107839,0.6267107428,-0.9342301976
 C,0,-0.4901255244,-0.3666909404,-0.7756161731
 C,0,0.5789581971,-0.1797362827,0.1182757304
 N,0,1.6051695545,-1.1200359746,0.3166152436
 C,0,1.6417375493,-2.4869104403,0.262761218
 S,0,3.0899831264,-3.2670302617,0.5059049509
 C,0,0.3592343209,-3.2414397499,0.0146984726
 N,0,-2.3414393479,2.8616756141,-0.3921660571
 O,0,-2.1958622866,3.9072691858,0.241891112
 O,0,-3.2750079933,2.6316126963,-1.1616127358
 H,0,1.510340435,1.1880039175,1.507520877
 H,0,-0.1999480827,2.9725902013,1.1922974837
 H,0,-2.2769454781,0.5020560744,-1.6204815367
 H,0,-0.5606582132,-1.2664993509,-1.3701732534
 H,0,2.4962669082,-0.7279802598,0.6024304189
 H,0,0.46687713,-4.2492839916,0.4122216693
 H,0,0.1695791364,-3.3318976234,-1.0610224695
 H,0,-0.50602257,-2.7543671799,0.4738898784
```

HF= -967.730323 Nimag=0

TS1

6	-2.936772	0.588682	0.319617
16	-3.548971	-0.274111	-0.922898
7	-1.853837	0.106443	1.144110
6	-3.436311	1.932967	0.755504
6	-0.551931	-0.047812	0.677443
6	-0.069365	0.676096	-0.431245
6	1.253286	0.549509	-0.828018
6	2.106964	-0.298993	-0.122628
6	1.650639	-1.027903	0.977471
6	0.329498	-0.902177	1.372250
7	3.497703	-0.428542	-0.541483
8	4.224451	-1.189879	0.102289
8	3.870487	0.231330	-1.514856
1	-2.148513	-0.615668	1.791743
1	-4.266947	2.280676	0.142630
1	-3.742090	1.884856	1.808851
1	-2.610437	2.655409	0.717868
1	-0.731893	1.331815	-0.984603
1	1.638510	1.098042	-1.678313
1	2.335985	-1.682464	1.500941
1	-0.033679	-1.466025	2.227030

HF= -967.7041504 Nimag=1

TS2

6	-2.746496	-0.275547	1.205947
16	-3.034220	-1.857981	0.930470
7	-2.089497	0.576030	0.242516
6	-3.148560	0.463542	2.446446
6	-0.746915	0.445044	-0.099099
6	0.183914	-0.164471	0.765899
6	1.526731	-0.217521	0.424027
6	1.953899	0.337302	-0.782627
6	1.049575	0.944162	-1.656512
6	-0.291310	0.995562	-1.315246
7	3.366941	0.281282	-1.138324
8	3.710064	0.778265	-2.214193
8	4.140619	-0.258256	-0.343242
1	-2.691398	0.821877	-0.535274
1	-3.662904	-0.179991	3.159048
1	-2.256162	0.903676	2.910467
1	-3.791522	1.310841	2.174462
1	-0.146039	-0.601494	1.701450
1	2.253617	-0.683368	1.077413
1	1.410885	1.360663	-2.588261
1	-1.001560	1.465798	-1.989706

HF= -967.7041504 Nimag=1