

# Conformational Preferences and Internal Rotation in Alkyl- and Phenyl-Substituted Thiourea Derivatives

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**Supporting Information Available.** Cartesian coordinates and energies (Hartrees) for the MP2/aug-cc-pVDZ optimized equilibrium and transition state geometries, and a Table comparing calculated geometric data for **6** to that observed in X-ray crystal structures.

**1** anti conformer MP2/aug-cc-pVDZ T.E.= -547.320362486 a.u.

S	0.00000	0.00000	1.48838
N	0.01245	-1.15089	-0.92883
C	0.00000	0.00000	-0.17690
H	-0.37630	-1.12189	-1.86520
H	-0.14815	-2.00331	-0.40706
N	-0.01245	1.15089	-0.92883
H	0.37630	1.12189	-1.86520
H	0.14815	2.00331	-0.40706

**1** syn conformer MP2/aug-cc-pVDZ T.E.= -547.319557638 a.u. (-232.4 cm<sup>-1</sup>)

S	0.00286	-1.35876	0.00000
N	0.01933	1.04791	-1.15082
C	0.00033	0.31253	0.00000
H	-0.09614	2.05246	-1.15357
H	-0.06297	0.54436	-2.02196
N	0.01933	1.04791	1.15082
H	-0.09614	2.05246	1.15357
H	-0.06297	0.54436	2.02196

**1** planar conformer MP2/aug-cc-pVDZ T.E.= -547.319544158 a.u. (-275.9; -1065 cm<sup>-1</sup>)

S	0.00000	0.00000	1.47985
N	0.00000	1.15002	-0.92648
C	0.00000	0.00000	-0.19225
H	0.00000	1.15614	-1.93714
H	0.00000	2.02580	-0.42518
N	0.00000	-1.15002	-0.92648
H	0.00000	-1.15614	-1.93714
H	0.00000	-2.02580	-0.42518

**1** TS1 conformer MP2/aug-cc-pVDZ T.E.= -547.306608625 a.u. (-334.4 cm<sup>-1</sup>)

S	-0.09362	-1.47565	0.00000
N	-1.06679	1.11306	0.00000
C	0.03951	0.17651	0.00000
H	-1.65216	0.87353	-0.80439
H	-1.65216	0.87353	0.80439
N	1.21240	0.84542	0.00000
H	1.19994	1.85726	0.00000
H	2.08441	0.33264	0.00000

**1 TS2 conformer MP2/aug-cc-pVDZ T.E.= -547.295848636 a.u. (-403.5 cm-1)**

S	-0.06291	1.37053	0.00027
N	-1.17827	-1.09480	0.00068
C	0.00958	-0.27717	-0.00037
H	-1.18776	-1.70030	-0.82297
H	-1.18395	-1.70193	0.82319
N	1.18688	-0.96691	0.00309
H	1.20183	-1.97770	-0.01949
H	2.05919	-0.45346	-0.00915

**2 cis conformer MP2/aug-cc-pVDZ T.E.= -586.502773780 a.u.**

S	1.45529	-0.68237	-0.08186
N	-1.11094	-1.46855	-0.05886
N	-0.76482	0.80612	0.03747
C	-0.19341	-0.42945	-0.02055
H	-1.98275	-1.33366	0.44484
H	-0.68882	-2.38050	0.07306
H	-1.74934	0.86924	-0.19681
C	0.02905	2.02440	-0.04546
H	0.76749	2.03797	0.76633
H	0.56890	2.08594	-1.00273
H	-0.64943	2.88075	0.05979

**2 trans conformer MP2/aug-cc-pVDZ T.E.= -586.501661824 a.u.**

S	0.54536	1.85487	-0.05113
N	0.68468	-0.80869	-0.05421
N	-1.44662	0.06698	0.02640
C	-0.09443	0.30616	-0.03945
C	0.19416	-2.16953	0.09027
H	1.67933	-0.62348	-0.04605
H	-1.82486	-0.82041	-0.28363
H	-2.02668	0.88308	-0.11962
H	-0.40085	-2.48271	-0.78423
H	1.05629	-2.84239	0.16625
H	-0.41648	-2.27729	1.00107

**2 TS1 conformer MP2/aug-cc-pVDZ T.E.= -586.486518199 a.u. (-140.8 cm-1)**

S	0.78140	-1.35022	-0.03496
N	-1.72252	-0.45405	-0.17237
N	-0.23339	1.17122	0.46575
C	-0.41839	-0.21164	0.08391
H	-2.38414	0.30739	-0.08447
H	-2.01941	-1.38126	-0.44887
H	0.10357	1.15407	1.43129
C	0.80048	1.83531	-0.35675
H	0.44963	1.86937	-1.39744
H	0.91492	2.86567	0.00626
H	1.77164	1.31547	-0.32468

**2 TS2 conformer MP2/aug-cc-pVDZ T.E.= -586.474498354 a.u. (-166.0 cm-1)**

S	0.45164	1.67960	-0.09126
N	-1.54245	-0.06580	-0.04066
N	0.57484	-0.94801	0.53568
C	-0.21406	0.18720	0.13857
H	-1.92301	-0.99467	0.08429

H	-2.15015	0.68189	-0.35032
H	0.29676	-1.24144	1.47368
C	0.51909	-2.07391	-0.41012
H	-0.47768	-2.53919	-0.53732
H	0.85951	-1.71209	-1.39040
H	1.21856	-2.84830	-0.06788

**3a** cis conformer MP2/aug-cc-pVDZ T.E.= -625.697091653 a.u.

S	-1.31273	-1.07793	-0.10762
N	1.22335	-1.80523	0.34909
N	0.93589	0.38013	-0.31224
C	0.33613	-0.81165	-0.03450
H	2.15529	-1.77715	-0.05438
H	0.80454	-2.72785	0.37622
H	1.89872	0.48672	-0.00762
C	0.18278	1.60483	-0.57266
C	-0.30471	2.27644	0.71128
H	0.84188	2.27380	-1.14621
H	-0.66732	1.32646	-1.20974
H	0.54387	2.56262	1.35145
H	-0.87728	3.18527	0.47069
H	-0.95596	1.58653	1.26524

**3a** trans conformer MP2/aug-cc-pVDZ T.E.= -625.694666369 a.u.

S	-0.36815	-2.18892	-0.29582
N	1.48898	-0.31739	0.15864
N	-0.71191	0.39349	0.26374
C	0.15363	-0.63137	0.03847
H	1.80251	0.63160	-0.00624
H	2.11461	-1.05278	-0.14510
H	-1.68746	0.13372	0.18085
C	-0.35420	1.76533	0.60293
C	-0.05021	2.63366	-0.62312
H	-1.20005	2.19021	1.16259
H	0.50054	1.74295	1.29796
H	-0.93086	2.68977	-1.27869
H	0.22168	3.65405	-0.31230
H	0.77978	2.21977	-1.21553

**3a** TS1 conformer MP2/aug-cc-pVDZ T.E.= -625.677167590 a.u (-130.6 cm-1)

S	-1.30481	1.11687	0.20467
N	1.25397	1.82643	0.15404
N	0.94839	-0.35436	-0.47254
C	0.31915	0.86959	-0.04325
H	2.22651	1.59509	-0.00632
H	0.97375	2.75187	0.45349
H	0.60967	-0.55139	-1.41720
C	0.62976	-1.52097	0.39500
C	-0.59294	-2.32579	-0.04442
H	1.52195	-2.16698	0.40232
H	0.49338	-1.13741	1.41756
H	-0.45536	-2.69551	-1.07394
H	-0.72704	-3.20085	0.61050
H	-1.49919	-1.70782	-0.00914

**3a** TS2 conformer MP2/aug-cc-pVDZ T.E.= -625.665549401 a.u (-195.4 cm-1)

S	0.29990	2.17879	0.17259
N	-1.49448	0.25063	-0.09588
N	0.74402	-0.38502	-0.54358
C	-0.18571	0.63801	-0.17668
H	-1.78964	-0.63565	-0.48275
H	-2.19177	0.95446	0.11556
H	0.68460	-0.61017	-1.53605
C	0.82479	-1.57373	0.32076
C	-0.25090	-2.65843	0.16001
H	1.81102	-2.02454	0.12723
H	0.84513	-1.20391	1.35786
H	-0.35688	-2.94992	-0.89755
H	0.04085	-3.55790	0.72472
H	-1.23024	-2.33975	0.54533

**3b** cis conformer MP2/aug-cc-pVDZ T.E.= -625.696530740 a.u.

S	-1.35273	-1.01809	0.27566
N	1.10957	-1.92958	-0.25207
N	0.97209	0.31732	0.23173
C	0.29857	-0.85174	0.06489
H	1.95255	-1.74478	-0.78727
H	0.59368	-2.75127	-0.54400
H	1.98529	0.28719	0.21269
C	0.32365	1.57283	0.60358
C	-0.26742	2.29892	-0.60433
H	-0.46426	1.33670	1.33329
H	1.08553	2.19163	1.10066
H	-1.01078	1.65575	-1.09467
H	-0.76374	3.22726	-0.28232
H	0.51922	2.55714	-1.32888

**3b** trans conformer MP2/aug-cc-pVDZ T.E.= -625.695082892 a.u.

S	-0.43036	-2.15920	0.06013
N	1.51575	-0.32598	0.04729
N	-0.57017	0.40758	-0.65071
C	0.19610	-0.62870	-0.19991
H	1.94494	0.46033	-0.42728
H	2.10535	-1.13678	0.18809
H	-1.55413	0.16784	-0.70947
C	-0.21587	1.82183	-0.54873
C	-0.23614	2.34516	0.89026
H	0.77007	1.98568	-1.01350
H	-0.93558	2.37170	-1.17233
H	0.46734	1.77964	1.51722
H	0.04470	3.40926	0.91525
H	-1.24337	2.23998	1.31867

**3b** TS1 conformer MP2/aug-cc-pVDZ T.E.= -625.681986392 a.u (-89.9 cm<sup>-1</sup>)

S	0.82001	1.56925	-0.31953
N	-1.72572	0.81160	-0.14459
N	-0.30094	-0.59975	0.97500
C	-0.43040	0.59599	0.17009
H	-2.42154	0.15681	0.19109
H	-1.98481	1.62231	-0.69254
H	0.05124	-0.28868	1.88402
C	0.69373	-1.54367	0.40723

C	0.18506	-2.10651	-0.91470
H	1.67103	-1.05062	0.26219
H	0.81333	-2.34948	1.14704
H	0.06163	-1.30279	-1.65664
H	0.90460	-2.83200	-1.32228
H	-0.78233	-2.61105	-0.77412

**3b** TS2 conformer MP2/aug-cc-pVDZ T.E.= -625.669900567 a.u (-94.3 cm-1)

S	0.69860	1.80141	0.01785
N	-1.55456	0.51868	0.56470
N	-0.14734	-0.56128	-0.99831
C	-0.38187	0.56342	-0.13037
H	-2.19070	-0.26262	0.47130
H	-1.77451	1.26484	1.21225
H	-0.86255	-0.56997	-1.72894
C	-0.11466	-1.86174	-0.29388
C	1.02843	-1.88386	0.71554
H	-1.06703	-2.11183	0.21845
H	0.04633	-2.62767	-1.06725
H	0.87936	-1.12582	1.49884
H	1.08683	-2.87047	1.19880
H	1.98137	-1.67106	0.21141

**3c** cis conformer MP2/aug-cc-pVDZ T.E.= -625.696163571 a.u.

S	-1.10615	1.55533	-0.14996
N	1.57463	1.54899	-0.03381
N	0.57120	-0.52367	0.02242
C	0.39133	0.82557	-0.03858
H	2.35158	1.16012	0.49261
H	1.43529	2.54410	0.09933
H	1.50191	-0.87499	-0.18332
C	-0.53602	-1.46647	-0.11012
C	-0.01778	-2.89091	0.05506
H	-1.28087	-1.22140	0.66003
H	-1.02706	-1.32828	-1.08766
H	0.44191	-3.03041	1.04485
H	-0.84762	-3.60456	-0.04337
H	0.72742	-3.13625	-0.71840

**3c** trans conformer MP2/aug-cc-pVDZ T.E.= -625.695552754 a.u.

S	0.68365	-2.15132	0.11177
N	-1.58619	-0.74555	-0.08926
N	0.34472	0.49511	0.12569
C	-0.21986	-0.74036	0.06123
H	-2.13409	0.05954	0.19045
H	-2.02040	-1.65293	0.01956
H	1.35671	0.49206	0.18290
C	-0.36097	1.75988	-0.03869
C	0.64361	2.90682	-0.06827
H	-0.94400	1.73683	-0.97540
H	-1.06749	1.90912	0.79793
H	1.34120	2.78741	-0.91033
H	0.12164	3.86637	-0.18619
H	1.22033	2.94120	0.86795

**3c** TS1 conformer MP2/aug-cc-pVDZ T.E.= -625.680470683 a.u (-136.8 cm-1)

S	1.02632	1.66028	-0.03499
N	-1.61483	1.34818	-0.15420
N	-0.51955	-0.58587	0.41751
C	-0.39546	0.81326	0.07598
H	-2.42943	0.75190	-0.07409
H	-1.69961	2.32688	-0.39784
H	-0.19689	-0.67289	1.38584
C	0.35167	-1.44757	-0.41523
C	0.20964	-2.89682	0.03449
H	0.01621	-1.33164	-1.45753
H	1.40379	-1.11876	-0.36494
H	-0.83549	-3.22950	-0.03964
H	0.83521	-3.55173	-0.58981
H	0.53822	-3.01452	1.07948

**3c** TS2 conformer MP2/aug-cc-pVDZ T.E.= -625.668853107 a.u (-157.8 cm-1)

S	0.75899	2.02200	0.10702
N	-1.61511	0.84572	0.03666
N	0.21056	-0.55165	-0.51577
C	-0.26465	0.74899	-0.12900
H	-2.21737	0.04167	-0.08202
H	-2.01359	1.72494	0.34091
H	-0.12434	-0.77065	-1.45727
C	-0.14177	-1.63052	0.42571
C	0.55985	-2.91838	0.00853
H	0.20858	-1.30695	1.41824
H	-1.23310	-1.81375	0.50724
H	1.64719	-2.76430	-0.01797
H	0.32760	-3.72960	0.71444
H	0.22935	-3.23571	-0.99323

**4a** cis conformer MP2/aug-cc-pVDZ T.E.= -664.893584147 a.u.

S	1.08153	-1.67640	0.39728
N	-1.47647	-1.91683	-0.35473
N	-0.75815	0.24176	-0.00611
C	-0.43244	-1.08050	0.01019
H	-2.41814	-1.61184	-0.12575
H	-1.29247	-2.89482	-0.16185
H	-1.62540	0.49430	-0.47355
C	0.22004	1.31674	0.17649
C	1.00377	1.56564	-1.11418
C	-0.51663	2.56540	0.65721
H	0.90888	0.96012	0.95623
H	0.32791	1.91878	-1.91015
H	1.77724	2.33198	-0.95101
H	1.49294	0.63783	-1.44101
H	-1.24925	2.90149	-0.09606
H	-1.04554	2.37338	1.60199
H	0.19782	3.38619	0.81553

**4a** trans conformer MP2/aug-cc-pVDZ T.E.= -664.891450424 a.u.

S	-0.44448	-2.47760	-0.38023
N	1.44957	-0.88575	0.63586
N	-0.46536	0.17413	-0.12020
C	0.21127	-0.99358	0.04479
H	1.97185	-0.02064	0.56910

H	1.99122	-1.74058	0.62399
H	-1.38285	0.06289	-0.53896
C	-0.01040	1.51226	0.25310
C	0.89630	2.12097	-0.82502
C	-1.24045	2.38505	0.50106
H	0.54426	1.41784	1.20259
H	0.32321	2.26649	-1.75349
H	1.28745	3.09641	-0.49638
H	1.74890	1.46624	-1.05999
H	-1.84557	2.45744	-0.41741
H	-1.86377	1.96497	1.30305
H	-0.93548	3.40208	0.78646

**4a** TS1 conformer MP2/aug-cc-pVDZ T.E.= -664.873861159 a.u (-123.7 cm-1)

S	-0.85642	1.89979	0.37454
N	1.76519	1.56474	0.11300
N	0.58472	-0.27528	-0.56882
C	0.51842	1.06213	-0.03525
H	2.55469	0.99110	-0.15690
H	1.89166	2.50448	0.46755
H	0.13131	-0.25509	-1.48598
C	-0.11307	-1.29263	0.27482
C	-1.56191	-1.51830	-0.16196
C	0.69535	-2.58934	0.22437
H	-0.10290	-0.89737	1.30367
H	-1.58364	-1.88848	-1.20176
H	-2.04537	-2.27534	0.47484
H	-2.13502	-0.58382	-0.10428
H	0.73767	-2.97133	-0.80814
H	1.72450	-2.41942	0.57079
H	0.22899	-3.35989	0.85831

**4a** TS2 conformer MP2/aug-cc-pVDZ T.E.= -664.862081611 a.u (-170.0 cm-1)

S	-0.71689	-2.33759	-0.01059
N	1.57276	-1.01813	0.14127
N	-0.25923	0.23878	-0.67660
C	0.24894	-1.00918	-0.19418
H	2.16677	-0.22803	-0.06979
H	1.98458	-1.87523	0.48911
H	0.11081	0.45260	-1.60394
C	-0.15094	1.39078	0.25213
C	1.05366	2.29847	-0.02829
C	-1.45478	2.18885	0.17605
H	-0.05886	0.96064	1.26336
H	1.00492	2.67870	-1.06233
H	1.05365	3.16623	0.64937
H	2.01662	1.78145	0.10356
H	-1.58972	2.59436	-0.83956
H	-2.30769	1.53450	0.39997
H	-1.44499	3.02961	0.88773

**4b** cis conformer MP2/aug-cc-pVDZ T.E.= -664.893121939 a.u.

S	1.02655	1.66402	0.58602
N	-1.49121	1.93912	-0.28471
N	-0.75013	-0.23118	-0.08383
C	-0.44622	1.08756	0.03921

H	-2.14475	1.63074	-0.99830
H	-1.21110	2.91012	-0.35901
H	-1.71521	-0.47849	-0.28103
C	0.17563	-1.31800	0.24580
C	-0.64344	-2.55537	0.60697
C	1.13504	-1.57951	-0.91638
H	0.75239	-0.97834	1.12023
H	-1.26213	-2.87696	-0.24779
H	0.02774	-3.38696	0.86473
H	-1.29990	-2.36060	1.46823
H	0.57838	-1.93504	-1.79812
H	1.67105	-0.65639	-1.17535
H	1.87371	-2.34613	-0.63510

**4b** trans conformer MP2/aug-cc-pVDZ T.E.= -664.891931849 a.u.

S	-0.65005	-2.43060	0.11880
N	1.45028	-0.93315	-0.58328
N	-0.53535	0.21064	-0.23159
C	0.11546	-0.98839	-0.25365
H	1.80077	-0.14666	-1.11828
H	1.86420	-1.83426	-0.78685
H	-1.48564	0.13517	0.11985
C	0.09691	1.53194	-0.18606
C	-0.98624	2.58003	-0.43776
C	0.81748	1.76536	1.14663
H	0.82273	1.59207	-1.01611
H	-1.74990	2.53248	0.35557
H	-0.54963	3.58886	-0.42685
H	-1.47566	2.41575	-1.40834
H	0.08484	1.76323	1.96843
H	1.55606	0.97463	1.33848
H	1.33432	2.73764	1.14018

**4b** TS1 conformer MP2/aug-cc-pVDZ T.E.= -664.879138901 a.u (-92.1 cm-1)

S	-0.96671	1.84685	0.30586
N	1.60199	1.49122	-0.29272
N	0.31330	-0.34397	-0.78801
C	0.34269	1.00386	-0.26517
H	2.34329	0.89869	-0.64645
H	1.78620	2.43470	0.02451
H	-0.23857	-0.30007	-1.65003
C	-0.36754	-1.29768	0.12669
C	-0.51322	-2.62582	-0.60987
C	0.46939	-1.44115	1.39436
H	-1.36747	-0.90981	0.39557
H	0.47613	-3.01966	-0.88877
H	-1.01920	-3.36202	0.03251
H	-1.11362	-2.50819	-1.52616
H	1.46717	-1.83608	1.14594
H	0.58630	-0.47243	1.90323
H	-0.02027	-2.13303	2.09618

**4b** TS2 conformer MP2/aug-cc-pVDZ T.E.= -664.867445376 a.u (-90.5 cm-1)

S	0.73327	-2.17092	0.12986
N	-1.59609	-1.04602	-0.44449
N	-0.10346	0.32212	0.77384



C	-0.37020	-0.94432	0.14456
H	-2.24217	-0.26726	-0.44618
H	-1.84521	-1.90181	-0.92425
H	-0.76183	0.45172	1.54712
C	-0.16390	1.48753	-0.14011
C	0.12807	2.73589	0.68839
C	0.86336	1.29664	-1.25314
H	-1.16722	1.60548	-0.60504
H	1.13076	2.65903	1.13408
H	0.08340	3.63473	0.05519
H	-0.60626	2.85547	1.50114
H	1.86487	1.17422	-0.81437
H	0.64360	0.40449	-1.85782
H	0.86237	2.17318	-1.91857

**4c cis conformer** MP2/aug-cc-pVDZ T.E.= -664.888075283 a.u.

S	-1.35669	1.20569	-0.15230
N	1.09301	2.24298	0.03731
N	1.03316	-0.04747	0.10353
C	0.30441	1.09808	0.01453
H	1.93444	2.21500	0.60622
H	0.55025	3.09328	0.13892
H	2.03575	0.06645	-0.00546
C	0.54175	-1.43612	0.02550
C	-0.39311	-1.78669	1.18653
C	-0.06759	-1.76350	-1.34195
H	1.45987	-2.03535	0.14387
H	-1.34669	-1.25333	1.09367
H	-0.58674	-2.87037	1.17658
H	0.07003	-1.52382	2.14885
H	-0.99048	-1.19069	-1.49637
H	0.63940	-1.52357	-2.15009
H	-0.29967	-2.83871	-1.39031

**4c trans conformer** MP2/aug-cc-pVDZ T.E.= -664.886684373 a.u.

S	0.25222	2.48069	-0.20351
N	-1.31229	0.50581	0.68960
N	0.38855	-0.12159	-0.77278
C	-0.24594	0.88743	-0.09600
H	-1.84988	-0.30152	0.39732
H	-1.85563	1.28861	1.03419
H	1.20286	0.23933	-1.26099
C	0.49319	-1.53659	-0.35509
C	1.05970	-1.67382	1.06290
C	-0.80644	-2.33309	-0.53682
H	1.22305	-1.95371	-1.06722
H	0.37561	-1.22216	1.79550
H	1.19213	-2.73721	1.31599
H	2.03436	-1.17097	1.14099
H	-1.50422	-2.18887	0.30237
H	-1.30496	-2.06644	-1.47994
H	-0.57163	-3.40781	-0.56233

**4c TS1 conformer** MP2/aug-cc-pVDZ T.E.= -664.873179382 a.u (-123.9 cm<sup>-1</sup>)

S	1.13933	-1.45610	0.39039
N	-1.44157	-1.80204	-0.09227

N	-0.70212	0.21308	-0.87232
C	-0.35027	-1.00694	-0.19327
H	-2.32799	-1.45819	-0.44041
H	-1.35697	-2.72209	0.32158
H	-0.30996	0.16288	-1.81539
C	-0.28873	1.49652	-0.24008
C	-0.75009	1.51923	1.21651
C	1.19521	1.85753	-0.37875
H	-0.87339	2.25197	-0.79291
H	-0.18762	0.78776	1.81529
H	-0.57716	2.51768	1.64483
H	-1.82407	1.29176	1.28992
H	1.82436	1.20138	0.23512
H	1.52364	1.76925	-1.42681
H	1.34625	2.90252	-0.06334

**4c** TS2 conformer MP2/aug-cc-pVDZ T.E.= -664.863075121 a.u (-164.5 cm-1)

S	-0.42576	2.29199	-0.04247
N	1.50164	0.54491	-0.52527
N	-0.16966	-0.18742	0.99233
C	0.34781	0.84355	0.14467
H	2.05190	-0.26105	-0.26031
H	1.92849	1.27040	-1.08919
H	0.37287	-0.26022	1.85294
C	-0.47681	-1.50659	0.39485
C	-1.37020	-1.29886	-0.82809
C	0.72049	-2.41454	0.06109
H	-1.06900	-2.01697	1.17328
H	-0.82361	-0.76910	-1.62412
H	-1.69340	-2.27244	-1.22635
H	-2.25645	-0.70619	-0.56317
H	1.24015	-2.08607	-0.85228
H	1.43875	-2.45297	0.89655
H	0.36690	-3.44193	-0.11973

**5** cis conformer MP2/aug-cc-pVDZ T.E.= -704.086858530 a.u.

S	1.04960	-1.89373	-0.08277
N	-1.60516	-2.10258	0.01316
N	-0.83895	0.05528	0.05002
C	-0.49684	-1.26154	0.00939
H	-2.41602	-1.79770	0.54443
H	-1.35947	-3.07640	0.15218
H	-1.82658	0.24610	-0.09724
C	0.03986	1.24374	-0.02817
C	0.79188	1.27892	-1.36537
C	-0.91007	2.44423	0.06063
C	1.00919	1.27563	1.15954
H	0.07882	1.26999	-2.20435
H	1.45812	0.41223	-1.45671
H	1.39186	2.20051	-1.42537
H	-1.62952	2.43977	-0.77519
H	-0.33402	3.37884	0.00605
H	-1.46579	2.43468	1.01189
H	0.45089	1.22973	2.10700
H	1.58108	2.21633	1.13365
H	1.70858	0.43229	1.11818

**5** trans conformer MP2/aug-cc-pVDZ T.E.= -704.085400023 a.u.

S	-0.58596	-2.64660	-0.11995
N	1.55726	-1.06382	0.07732
N	-0.44795	-0.00978	-0.48597
C	0.20878	-1.17568	-0.18275
H	2.06910	-0.32943	-0.39677
H	2.02887	-1.95940	0.12772
H	-1.44271	-0.19565	-0.59112
C	-0.14121	1.35508	0.01504
C	1.12292	1.93904	-0.63729
C	-1.34367	2.20569	-0.41319
C	-0.01652	1.35049	1.54500
H	1.12998	1.73572	-1.71852
H	2.04812	1.55437	-0.18350
H	1.13685	3.02979	-0.48954
H	-1.43546	2.22208	-1.51028
H	-1.22119	3.23801	-0.05494
H	-2.27626	1.80398	0.01437
H	-0.95272	0.99628	2.00222
H	0.19062	2.36876	1.91036
H	0.80031	0.69002	1.86856

**5** TS1 conformer MP2/aug-cc-pVDZ T.E.= -704.071927963 a.u (-126.3 cm-1)

S	-0.89149	-2.03858	-0.16426
N	1.72999	-1.76533	0.07242
N	0.63572	0.14440	0.67190
C	0.50223	-1.20601	0.19142
H	2.54447	-1.19687	0.26958
H	1.81614	-2.73288	-0.21304
H	0.36005	0.15008	1.65772
C	-0.09358	1.23694	-0.03885
C	-1.60381	1.26022	0.24120
C	0.53845	2.53141	0.48856
C	0.18010	1.10416	-1.53881
H	-1.79101	1.31514	1.32653
H	-2.09519	0.36078	-0.14815
H	-2.05459	2.15002	-0.22707
H	0.40797	2.60953	1.58056
H	0.05653	3.40675	0.02606
H	1.61523	2.55300	0.26574
H	1.26413	1.06981	-1.72936
H	-0.23753	1.97467	-2.06703
H	-0.28431	0.19652	-1.94996

**5** TS2 conformer MP2/aug-cc-pVDZ T.E.= -704.061889655 a.u (-197.4 cm-1)

S	0.63401	2.48895	0.07717
N	-1.62795	1.12258	-0.03984
N	0.30744	-0.05746	-0.74614
C	-0.27778	1.14967	-0.25252
H	-2.18940	0.37789	-0.43087
H	-2.08129	1.98018	0.25287
H	0.13131	-0.17564	-1.74453
C	0.15597	-1.32119	0.01708
C	-1.24687	-1.96009	-0.03920
C	1.16394	-2.28893	-0.61571

C	0.54473	-1.03629	1.47055
H	-1.60340	-2.02807	-1.08069
H	-1.97825	-1.39967	0.56175
H	-1.21192	-2.98264	0.36886
H	0.90661	-2.48183	-1.67085
H	1.15948	-3.25294	-0.08409
H	2.17380	-1.85707	-0.57767
H	1.55674	-0.60922	1.51736
H	0.52003	-1.97136	2.05115
H	-0.15401	-0.32501	1.93726

**6** trans conformer MP2/aug-cc-pVDZ T.E.= -777.703065323 a.u.

S	0.29693	-3.39679	-0.15525
N	-1.25429	-1.45623	0.83773
N	0.53041	-0.76544	-0.47576
C	-0.16242	-1.80813	0.09313
H	-1.35013	-0.50617	1.18147
H	-1.66472	-2.20503	1.37982
H	1.40445	-1.05070	-0.90541
C	0.29168	0.61829	-0.26117
C	-0.96056	1.18506	-0.57823
C	-1.17891	2.55588	-0.36110
C	-0.14580	3.37110	0.13528
C	1.11009	2.80737	0.42378
C	1.32751	1.43206	0.24002
H	-1.74256	0.55313	-1.00642
H	-2.15071	2.99198	-0.60586
H	-0.31624	4.43913	0.29026
H	1.91834	3.43558	0.80664
H	2.29331	0.98147	0.48502

**6** cis1 conformer MP2/aug-cc-pVDZ T.E.= -777.698838713 a.u.

S	-0.95066	-1.99849	1.06080
N	1.22145	-3.00765	-0.12978
N	0.97332	-0.74433	-0.37224
C	0.43624	-1.90165	0.14890
H	1.72924	-3.01331	-1.00941
H	0.78636	-3.88839	0.11903
H	1.96553	-0.78365	-0.58953
C	0.44410	0.56026	-0.18919
C	-0.89150	0.84924	-0.52490
C	-1.37122	2.15899	-0.37066
C	-0.52579	3.18298	0.09495
C	0.81155	2.89023	0.41272
C	1.29509	1.57774	0.28068
H	-1.53856	0.05380	-0.89580
H	-2.41030	2.38222	-0.62568
H	-0.90626	4.20113	0.20721
H	1.47680	3.67769	0.77584
H	2.32885	1.33900	0.54880

**6** cis2 conformer MP2/aug-cc-pVDZ T.E.= -777.697961677 a.u.

S	-1.22409	2.05916	0.54862
N	1.09138	3.04733	-0.32795
N	0.95505	0.75624	-0.38020
C	0.32320	1.93104	-0.05817

H	2.10300	2.96531	-0.33705
H	0.72275	3.90713	0.06007
H	1.93084	0.81360	-0.65536
C	0.44293	-0.55629	-0.19900
C	1.26620	-1.51543	0.42057
C	0.81683	-2.83882	0.56094
C	-0.46210	-3.19961	0.10254
C	-1.27970	-2.23393	-0.51232
C	-0.83146	-0.91368	-0.67700
H	2.25041	-1.22067	0.79696
H	1.46001	-3.58096	1.04060
H	-0.81818	-4.22587	0.22119
H	-2.27176	-2.51124	-0.87772
H	-1.45486	-0.16397	-1.16385

**6 TS1 conformer MP2/aug-cc-pVDZ T.E.= -777.687394440 a.u (-93.5 cm-1)**

S	-0.83580	2.17784	-1.02985
N	0.54762	2.66381	1.19924
N	1.18808	0.72679	0.14031
C	0.30390	1.87462	0.12728
H	1.25980	2.38531	1.86320
H	0.03384	3.52850	1.31383
H	1.84895	0.82278	-0.63242
C	0.54269	-0.54166	0.07441
C	-0.61124	-0.78694	0.84461
C	-1.19863	-2.06107	0.83746
C	-0.64089	-3.10242	0.07307
C	0.51058	-2.85428	-0.69376
C	1.09717	-1.57784	-0.69953
H	-1.04838	0.01845	1.44112
H	-2.09680	-2.24070	1.43410
H	-1.10103	-4.09328	0.07182
H	0.95036	-3.65096	-1.29942
H	1.98876	-1.38513	-1.30463

**6 TS2 conformer MP2/aug-cc-pVDZ T.E.= -777.681739577 a.u (-83.8 cm-1)**

S	-0.57006	2.93893	0.56855
N	0.69439	1.76333	-1.45922
N	0.91779	0.67588	0.60182
C	0.36132	1.77817	-0.13712
H	1.08138	0.91887	-1.86592
H	0.27804	2.45465	-2.07209
H	1.93744	0.68915	0.58378
C	0.38724	-0.60660	0.31146
C	-0.96437	-0.75499	-0.06674
C	-1.48892	-2.03708	-0.29658
C	-0.68468	-3.18123	-0.14953
C	0.66087	-3.03032	0.23065
C	1.19730	-1.75272	0.45586
H	-1.59975	0.12965	-0.16113
H	-2.53815	-2.13904	-0.58623
H	-1.09990	-4.17582	-0.32728
H	1.30060	-3.90884	0.34949
H	2.24405	-1.64134	0.75694