Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Comprehensive Insights into the Structure and Coordination Behaviour of Thiosemicarbazone Ligands: A Computational Assessment on E-Z Interconversion Mechanism during Coordination

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ELECTRONIC SUPPLEMENTARY INFORMATION

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Figure S1. Atom numbering assignment of acetaldehyde thiosemicarbazone (ATSC)

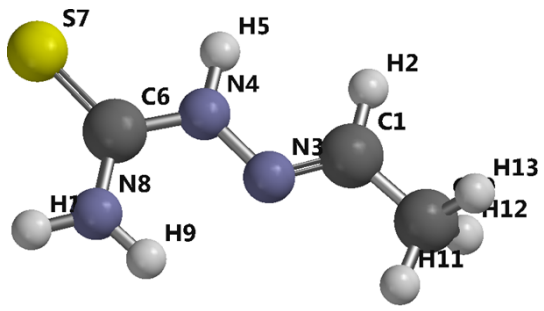


Table S1. Complete parameters for most stable thione form.

Parameters	Bond Length		Bond Angle		Torsion Angle	
	R(1,2)	1.095	A(2,1,3)	120.65	D(2,1,3,4)	-0.00
	R(1,3)	1.274	A(2,1,10)	118.02	D(10,1,3,4)	180.00
	R(1,10)	1.491	A(3,1,10)	121.32	D(2,1,10,11)	-179.99
	R(3,4)	1.361	A(1,3,4)	118.04	D(2,1,10,12)	-59.14
	R(4,5)	1.014	A(3,4,5)	121.76	D(2,1,10,13)	59.14
	R(4,6)	1.367	A(3,4,6)	121.92	D(3,1,10,11)	0.0
	R(6,7)	1.673	A(5,4,6)	116.30	D(3,1,10,12)	120.85
	R(6,8)	1.344	A(4,6,7)	120.17	D(3,1,10,13)	-120.85
	R(8,9)	1.008	A(4,6,8)	115.35	D(1,3,4,5)	-0.00
	R(8,14)	1.004	A(7,6,8)	124.47	D(1,3,4,6)	-179.99
	R(10,11)	1.089	A(6,8,9)	120.39	D(3,4,6,7)	179.99
	R(10,12)	1.094	A(6,8,14)	118.16	D(3,4,6,8)	-0.01
	R(10,13)	1.094	A(9,8,14)	121.43	D(5,4,6,7)	0.00
			A(1,10,11)	110.61	D(5,4,6,8)	179.99
			A(1,10,12)	110.69	D(4,6,8,9)	0.02
			A(1,10,13)	110.69	D(4,6,8,14)	179.98
			A(11,10,12)	108.94	D(7,6,8,9)	-179.97
			A(11,10,13)	108.94	D(7,6,8,14)	-0.02
			A(12,10,13)	106.85		

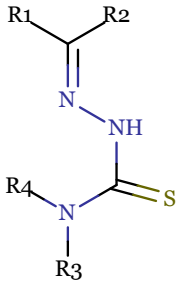
Table S1 (continued). Selected parameters compared to other TSCs.

	R(C1-N2)	R(N2-N3)	R(N3-C4)	R(C4-S6)	R(C4-N5)	A(C1-N2-N3)	A(N2-N3-C4)	A(N3-C4-N5)	A(N3-C4-S6)	A(N5-C4-S6)
Model compound	**1.275**	**1.362**	**1.367**	**1.673**	**1.344**	**118.0**	**121.9**	**115.3**	**120.1**	**124.4**
TSC1	1.286	1.398	1.342	1.690	1.334	116.6	117.6	117.8	119.3	122.8
TSC2	1.275	1.365	1.354	1.678	1.329	116.8	119.3	116.6	119.8	123.6
TSC3	1.2837	1.3783	1.3587	1.6849	1.3401	114.37	120.47	-	-	-
TSC4	1.2894	1.3846	1.3642	1.6773	1.3427	118.38	117.35	114.44	120.06	125.48
TSC5	1.299	1.352	1.367	1.675	1.330	116.8	120.2	116.4	118.4	125.1
TSC6	1.2826	1.3815	1.3417	1.6964	1.3335	116.20	118.53	117.16	120.78	122.05

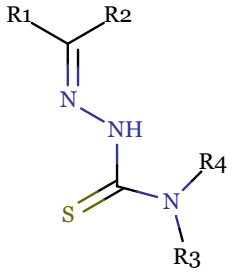
TSC1: Acetone Thiosemicarbazone (Palenic et al., 1974)
TSC2: 4-Formylpyridine Thiosemicarbazone (Restivo et al., 1970)
TSC3: Pyridine-2-carbaldehyde N4-phenethylthiosemicarbazone (Fun et al., 2005)
TSC4: N-Phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamide (Oliveira et al., 2014)
TSC5: 1-(5-Bromo-2-oxoindolin-3-ylidene) Thiosemicarbazone (Bandeira et al., 2013)
TSC6: (E)-4-(Benzyloxy)benzaldehyde Thiosemicarbazone (Tarafder et al., 2008)

** The little difference of the calculated and experimental data is owe to the hydrogen bond involve with thione S atom in solid (X-ray crystal) form.*

Table S2. Effects of alkyl & aryl N8-substituents on thiosemicarbazone rotamers (Effects of bulky substituents on stability). Calculated at B3LYP/6-31+G* level.



E(Z)-Trans configuration

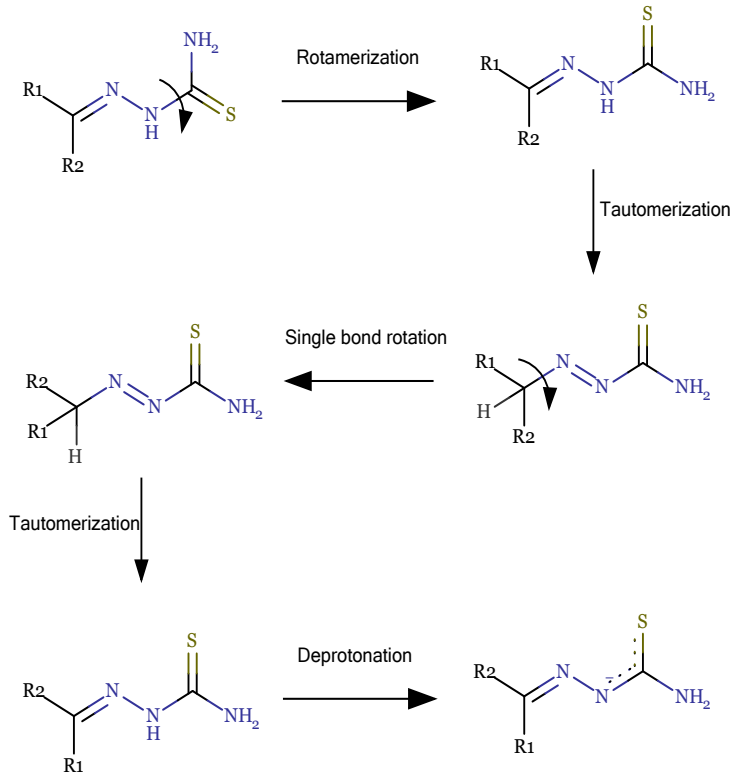


E(Z)-Cis configuration

Substituents				Energy (kcal.mol^{-1})		Substituents				Energy (kcal.mol^{-1})	
R1	**R2**	**R3**	**R4**	**E-trans**	**E-cis**	**R1**	**R2**	**R3**	**R4**	**Z-trans**	**Z-cis**
CH$_3$	*H*	*H*	*H*	*0*	*10.023*	*H*	*CH$_3$*	*H*	*H*	*0*	*10.864*
CH$_3$	*H*	*CH$_3$*	*H*	*0*	*10.534*	*H*	*CH$_3$*	*CH$_3$*	*H*	*0*	*11.429*
CH$_3$	*H*	*Ph*	*H*	*0*	*10.750*	*H*	*CH$_3$*	*Ph*	*H*	*0*	*11.797*
CH$_3$	*H*	*T-Bu*	*H*	*0*	*10.939*	*H*	*CH$_3$*	*T-Bu*	*H*	*0*	*11.992*
CH$_3$	*H*	*H*	*CH$_3$*	*0*	*4.045*	*H*	*CH$_3$*	*H*	*CH$_3$*	*0*	*4.829*
CH$_3$	*H*	*H*	*T-Bu*	*0*	*2.994*	*H*	*CH$_3$*	*H*	*T-Bu*	*0*	*5.074*
CH$_3$	*H*	*CH$_3$*	*CH$_3$*	*0*	*5.090*	*H*	*CH$_3$*	*CH$_3$*	*CH$_3$*	*0*	*5.835*
CH$_3$	*H*	*Ph*	*Ph*	*0*	*3.320*	*H*	*CH$_3$*	*Ph*	*Ph*	*0*	*4.571*
CH$_3$	*H*	*T-Bu*	*T-Bu*	*0*	*1.486*	*H*	*CH$_3$*	*T-Bu*	*T-Bu*	*0*	*2.349*

Figure S2. The route 1 (second sequence) for E-Z interconversion through tautomerization mechanism

A. 2D Sketch



B) 3D sketch of rate determining step of tautomerization (overall free energy). Calculated at B3LYP/6-311++G(2d,p) and B3LYP/6-31+G*.

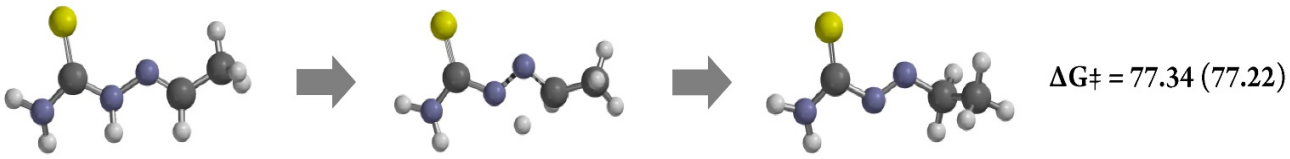
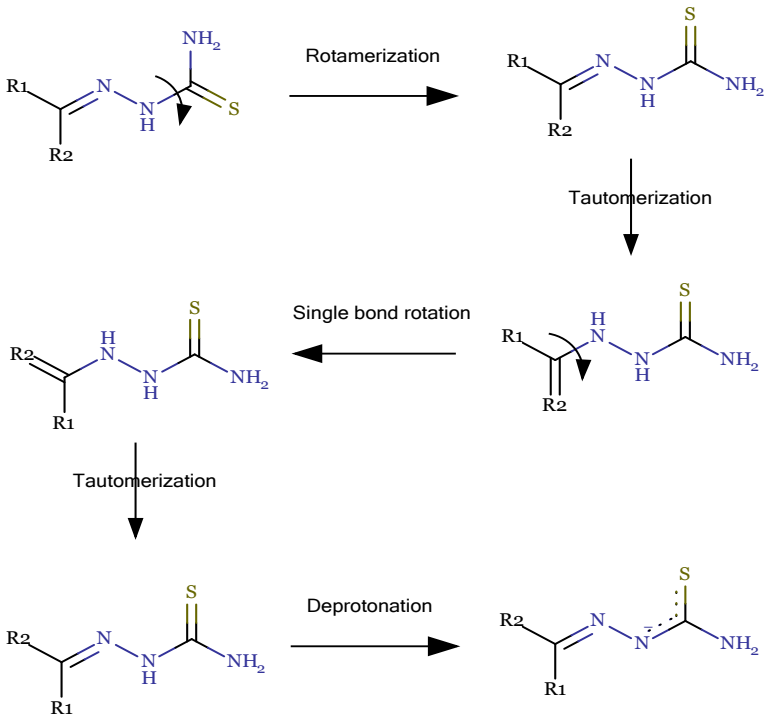
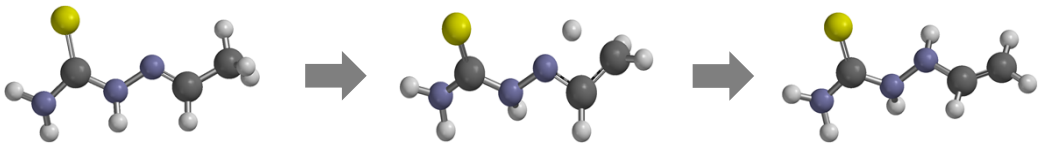


Figure S3. The route 2 for E-Z interconversion through tautomerization mechanism (This mechanism is valid on the condition that the R ≠ quaternary carbon atom).

A) 2D scheme



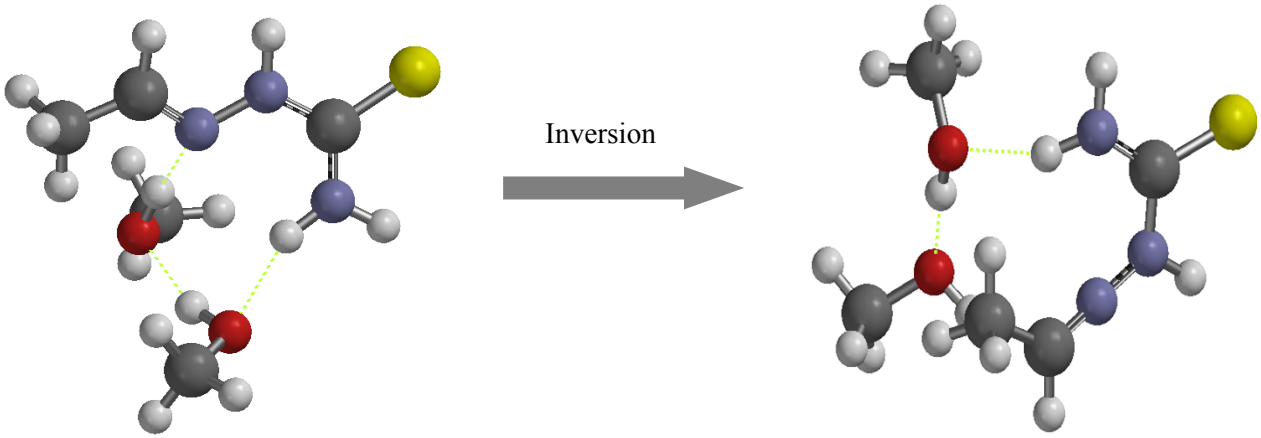
B) 3D sketch of rate determining step of tautomerization (overall free energy). Calculated at B3LYP/6-311++G(2d,p) and B3LYP/6-31+G*



ΔG‡ = 74.69 (77.40)

Figure S4. Influence of protic solvent (methanol) on inversion TS.

The minimum structure as well as transition state of ATSC inversion were treated by hybrid solvation. Two methanol molecule were utilize for microsolvation and both structures (minima and TS) were optimized by employing CPCM continuum model at B3LYP/6-311++G(2d,p) // B3LYP/6-31+G(d) level .

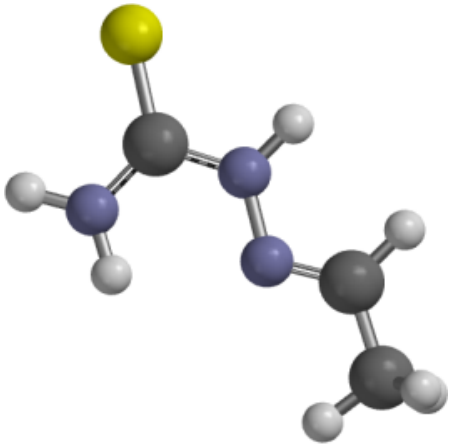


GS = <u>(0.00) kcal.mol^{-1}</u> **TS = <u>(39.89) kcal.mol^{-1}</u>**

The ground state is stabilized more efficiently due to the additional hydrogen bond of methanol (above) with nitrogen lone pair. Other methanol molecule was the same (have similar interaction) for both GS and TS.

Table S3. Optimized coordinates for all tautomers at B3LYP/6-311++G(2d,p) in *vacuo* and methanol (CPCM).

Tautomer 1 (*vacuo*)



Electronic Energy E(B3LYP): -681.08300316
Zero-point correction= 0.109444 (Hartree/Particle)
Thermal correction to Energy= 0.117883
Thermal correction to Enthalpy= 0.118828
Thermal correction to Gibbs Free Energy= 0.076108

C	-2.27236900	-0.55362800	0.00005000
H	-2.19704400	-1.64677400	0.00002200
N	-1.22309400	0.17002200	0.00000600
N	-0.01373200	-0.45592300	-0.00007200
H	0.06409300	-1.46760900	0.00000600
C	1.16159400	0.24214500	-0.00006400
S	2.62362300	-0.57234500	0.00002200
N	1.03610700	1.58031100	-0.00018700
H	0.12220700	2.00726500	0.00008700
C	-3.63358600	0.05481600	0.00013500
H	-3.56771000	1.14222700	0.00015000
H	-4.20097800	-0.26672000	-0.87882500
H	-4.20088500	-0.26675200	0.87914300
H	1.87354200	2.13501300	0.00012000

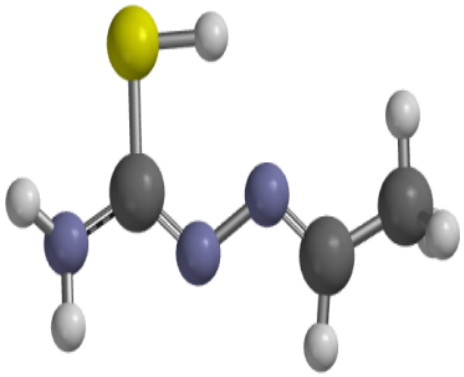
Tautomer 1 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.10001719
Zero-point correction= 0.109339 (Hartree/Particle)
Thermal correction to Energy= 0.117710
Thermal correction to Enthalpy= 0.118654
Thermal correction to Gibbs Free Energy= 0.076226

C	2.27076600	-0.54599900	-0.00032500
H	2.18258000	-1.63588200	-0.00101400
N	1.23095500	0.19235800	0.00033900
N	0.01553000	-0.44875900	0.00032600
H	-0.04017500	-1.46197100	-0.00026600
C	-1.14174700	0.24766300	0.00012200
S	-2.63185900	-0.58099000	-0.00001800
N	-1.04584500	1.57808000	0.00006500
H	-0.14009500	2.02532300	-0.00014900

C	3.63770500	0.04104500	-0.00022700
H	3.59994800	1.12959300	-0.00075400
H	4.19300400	-0.30137300	0.87799600
H	4.19358200	-0.30226300	-0.87772000
H	-1.88392500	2.13441000	-0.00032100

Tautomer 2 (*vacuo*)



Electronic Energy E(B3LYP): -681.06533092
Zero-point correction= 0.105998 (Hartree/Particle)
Thermal correction to Energy= 0.114395
Thermal correction to Enthalpy= 0.115339
Thermal correction to Gibbs Free Energy= 0.073032

C	-2.19944500	-0.50349500	0.00157400
N	-1.02761600	-0.00250800	-0.00835100
N	-0.00195500	-0.93343400	-0.01929000
C	1.18782400	-0.44226300	0.00157300
N	2.25919100	-1.29493700	0.07424600
S	1.62434400	1.28691800	0.00695200
H	-2.32422300	-1.58929900	0.00819800
H	3.13311100	-0.97502400	-0.31436000
H	2.03358900	-2.26324500	-0.10787900
H	0.32459600	1.64420300	-0.08670300
C	-3.41418900	0.36056600	0.00456500
H	-4.03916900	0.14821900	-0.86900100
H	-4.02835200	0.15629200	0.88762200
H	-3.14153300	1.41548000	-0.00160600

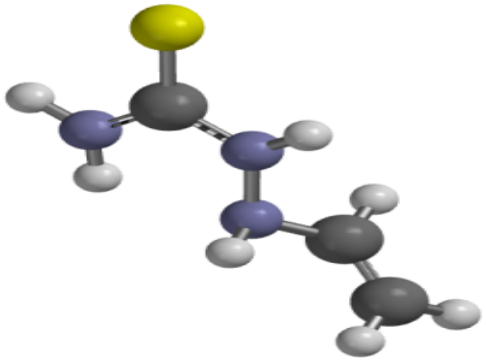
Tautomer 2 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.07590571
Zero-point correction= 0.105389 (Hartree/Particle)
Thermal correction to Energy= 0.113879
Thermal correction to Enthalpy= 0.114824
Thermal correction to Gibbs Free Energy= 0.072296

C	2.20506200	-0.50207900	0.00603500
N	1.03034300	-0.00326200	-0.00511900

N	0.00094900	-0.93791400	0.01118900
C	-1.19437800	-0.44753400	-0.00101400
N	-2.26770500	-1.28786100	-0.07164100
S	-1.62193800	1.28717700	-0.00174700
H	2.33721600	-1.58656300	0.02239700
H	-3.15070700	-0.95566300	0.28831100
H	-2.07200300	-2.26057700	0.12571700
H	-0.32504400	1.65677100	0.05049200
C	3.42018800	0.35870400	-0.00268700
H	4.03429200	0.15488400	0.88001100
H	4.04014400	0.12906400	-0.87487200
H	3.15676900	1.41596300	-0.01912000

Tautomer 3 (*vacuo*)



Electronic Energy E(B3LYP): -681.06203760
Zero-point correction= 0.110291 (Hartree/Particle)
Thermal correction to Energy= 0.118646
Thermal correction to Enthalpy= 0.119590
Thermal correction to Gibbs Free Energy= 0.076305

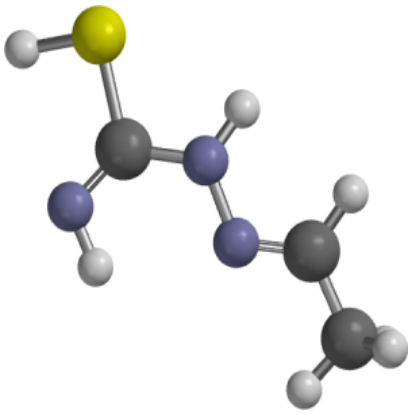
C	-2.31973200	-0.17006000	-0.42627000
N	-1.27027800	0.19846300	0.43467200
N	-0.05700500	-0.45919700	0.22673000
C	1.11289700	0.21675400	0.02242000
S	2.56364900	-0.61161800	-0.07779900
N	0.99820000	1.55291200	-0.08922800
C	-3.60047500	-0.24897700	-0.07679600
H	-1.98818200	-0.33914500	-1.44428800
H	-1.53212400	0.21911400	1.41608500
H	0.02041500	-1.45402700	0.39553200
H	1.82677400	2.08153500	-0.29784800
H	0.08999800	1.99181000	-0.06800100
H	-3.93190600	-0.09210700	0.94358700
H	-4.35591500	-0.45283700	-0.82160800

Tautomer 3 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.08082847
Zero-point correction= 0.110224 (Hartree/Particle)
Thermal correction to Energy= 0.118470
Thermal correction to Enthalpy= 0.119414
Thermal correction to Gibbs Free Energy= 0.076875

C	-2.29390700	-0.18846700	-0.42696900
N	-1.27426600	0.18701800	0.46515500
N	-0.05052000	-0.45937100	0.28940100
C	1.08440800	0.22722400	0.03400200
S	2.56798700	-0.60370600	-0.09809500
N	0.97605100	1.54762600	-0.10836900
C	-3.58866700	-0.24076700	-0.12076100
H	-1.93130500	-0.38194400	-1.43004200
H	-1.55287300	0.19874200	1.44165800
H	0.02246500	-1.45594900	0.45121200
H	1.79682600	2.09279800	-0.31114800
H	0.07612600	1.99840900	-0.01670600
H	-3.95128200	-0.05563200	0.88404500
H	-4.31760200	-0.45198200	-0.89044100

Tautomer 4 (*vacuo*)



Electronic Energy E(B3LYP): -681.05198666
Zero-point correction= 0.105552 (Hartree/Particle)
Thermal correction to Energy= 0.114256
Thermal correction to Enthalpy= 0.115200
Thermal correction to Gibbs Free Energy= 0.071774

C	2.29796800	-0.54154400	0.03058900
N	1.27256100	0.20350000	-0.08053100
N	0.04600500	-0.39055300	-0.10605000
C	-1.08889400	0.40735000	-0.01245100
N	-1.15500000	1.66833200	0.02104300
S	-2.57038400	-0.61148300	0.00828900
H	2.19636400	-1.63069900	0.11678700

H	-0.02847600	-1.37335500	0.13768100
H	-0.22021800	2.07780800	0.01396500
H	-3.37066500	0.43240900	0.27183400
C	3.67477700	0.03281000	0.04082600
H	4.27024100	-0.37608000	-0.78153400
H	3.63603100	1.11720000	-0.05530800
H	4.19480500	-0.22420200	0.96892500

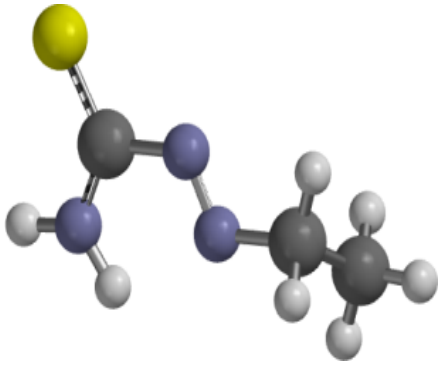
Tautomer 4 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.06582326
Zero-point correction= 0.105248 (Hartree/Particle)
Thermal correction to Energy= 0.114066
Thermal correction to Enthalpy= 0.115010
Thermal correction to Gibbs Free Energy= 0.071136

C	2.29545000	-0.53533600	0.01866900
N	1.27470900	0.22602100	-0.04108700
N	0.04367900	-0.37712000	-0.04261200
C	-1.08790600	0.39803500	-0.00244300
N	-1.15649800	1.67170600	0.01114100
S	-2.56953300	-0.61678300	-0.00095500
H	2.18266900	-1.62228100	0.07340500
H	-0.01935200	-1.38333300	0.07289300
H	-0.21520800	2.06771000	0.01556300
H	-3.39694500	0.42978400	0.13975300
C	3.67761900	0.01916200	0.01398100
H	4.24156300	-0.37927400	-0.83468900
H	3.66466400	1.10700600	-0.04398500
H	4.21092100	-0.28649400	0.91900500

Tautomer 5 (*vacuo*)

Electronic Energy E(B3LYP): -681.05425348
Zero-point correction= 0.109321 (Hartree/Particle)
Thermal correction to Energy= 0.117561
Thermal correction to Enthalpy= 0.118505



Thermal correction to Gibbs Free Energy= 0.075350

C	2.33650800	-0.42555100	-0.50575200
N	1.06651100	0.28073800	-0.32354100
N	0.08890100	-0.47242300	-0.21098400
C	-1.17152900	0.23614000	-0.02091400
N	-1.10232100	1.57042900	-0.01066500
S	-2.53423200	-0.67068100	0.15884500
H	2.16008800	-1.50233800	-0.56618700
H	2.74015100	-0.07247700	-1.46011700
H	-1.94005600	2.11186200	0.11806900
H	-0.19979800	2.01252800	-0.12706500
C	3.29893700	-0.06555100	0.62496100
H	4.26719900	-0.53739600	0.44908700
H	3.44807000	1.01379600	0.68604500
H	2.91692300	-0.41650800	1.58519900

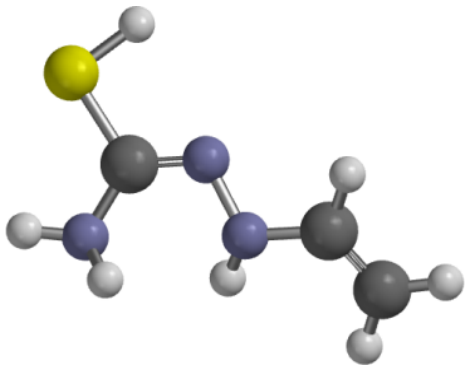
Tautomer 5 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.06741305
Zero-point correction= 0.109043 (Hartree/Particle)
Thermal correction to Energy= 0.117274
Thermal correction to Enthalpy= 0.118218
Thermal correction to Gibbs Free Energy= 0.074668

C	2.33972500	-0.43068000	-0.50158300
N	1.07106900	0.27028800	-0.31466500
N	0.08619000	-0.47264000	-0.21450500
C	-1.16944800	0.25160000	-0.02318900
N	-1.10617400	1.57001300	-0.01453500
S	-2.54093000	-0.67380900	0.16040000
H	2.17358700	-1.50888000	-0.56132700
H	2.73349000	-0.07254400	-1.45772400
H	-1.93666300	2.12690100	0.11398900
H	-0.20590900	2.02116300	-0.12995900
C	3.30776900	-0.06039000	0.62158300
H	4.27244200	-0.53418800	0.43471300
H	3.45715900	1.01916300	0.67218500

H	2.93491900	-0.40747200	1.58679100

Tautomer 6 (*vacuo*)



Electronic Energy E(B3LYP): -681.04016820
Zero-point correction= 0.106275 (Hartree/Particle)
Thermal correction to Energy= 0.114977
Thermal correction to Enthalpy= 0.115921
Thermal correction to Gibbs Free Energy= 0.072364

C	2.44826900	-0.50532800	-0.19382600
N	1.28332000	0.25747800	-0.12900300
N	0.09105200	-0.48279900	-0.08153000
C	-0.97189700	0.22109500	-0.02508800
S	-2.56370600	-0.57527200	0.07302700
N	-1.00559100	1.60958500	0.00463800
C	3.65231000	-0.11558800	0.22548000
H	2.29379000	-1.46096200	-0.67958300
H	1.31838100	1.01573900	0.54887000
H	-2.05087500	-1.79848500	0.27986600
H	-1.91672400	2.03171100	-0.10264600
H	-0.30707700	2.03684900	-0.59508400
H	3.81536700	0.83660100	0.71780500
H	4.51286400	-0.74803500	0.06420800

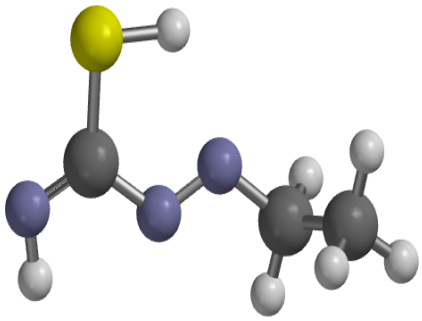
Tautomer 6 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.05290875
Zero-point correction= 0.106015 (Hartree/Particle)
Thermal correction to Energy= 0.114651
Thermal correction to Enthalpy= 0.115595
Thermal correction to Gibbs Free Energy= 0.072535

C	2.45127400	-0.51020600	-0.18107200
N	1.29011800	0.25370600	-0.14676200
N	0.09162400	-0.48222300	-0.09199900
C	-0.97389900	0.22723300	-0.02953000
S	-2.56376200	-0.57745800	0.07538600

N	-1.01864800	1.60500800	0.01220500
C	3.65869300	-0.10986000	0.22985100
H	2.30322300	-1.48229900	-0.63719100
H	1.32338300	1.04541000	0.49188100
H	-2.06287800	-1.80616100	0.27875900
H	-1.92891400	2.02962900	-0.10111000
H	-0.31039700	2.06886700	-0.54668800
H	3.82149100	0.85749200	0.69179900
H	4.51621700	-0.75204900	0.08677100

Tautomer 7 (*vacuo*)



Electronic Energy E(B3LYP): -681.03819522
Zero-point correction= 0.106153 (Hartree/Particle)
Thermal correction to Energy= 0.114371
Thermal correction to Enthalpy= 0.115316
Thermal correction to Gibbs Free Energy= 0.072629

N	2.10302000	1.47132300	0.27275000
C	1.28946500	0.52647200	0.06116200
N	-0.11734700	0.85215700	-0.12224100
N	-0.87785200	-0.09569800	-0.32567800
S	1.86421600	-1.14766600	-0.00778400
C	-2.28275300	0.28800300	-0.49562900
H	1.59766100	2.36045200	0.27884000
H	0.63768000	-1.65510200	-0.24282200
H	-2.38430000	1.37582200	-0.46108500
H	-2.56722900	-0.06841600	-1.49048900
C	-3.13868000	-0.40249500	0.56448900
H	-4.19204500	-0.17561800	0.39207500
H	-3.00889900	-1.48518600	0.52943700
H	-2.87327000	-0.05565800	1.56463500

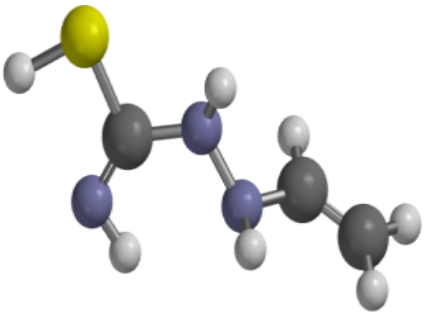
Tautomer 7 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.04714595
Zero-point correction= 0.105692 (Hartree/Particle)
Thermal correction to Energy= 0.113956
Thermal correction to Enthalpy= 0.114900

Thermal correction to Gibbs Free Energy= 0.072104

N	2.12561200	1.45682900	0.27114000
C	1.29558500	0.52266700	0.06231100
N	-0.10663900	0.86736200	-0.11263700
N	-0.87476700	-0.07399100	-0.31763700
S	1.84259500	-1.16012900	-0.01310100
C	-2.27818900	0.30723500	-0.48573700
H	1.63530700	2.35473600	0.28233100
H	0.60723700	-1.65064400	-0.24242800
H	-2.38799300	1.39265000	-0.42967100
H	-2.55293100	-0.03162500	-1.48903100
C	-3.13700700	-0.41217100	0.55286500
H	-4.18737100	-0.17800900	0.37451100
H	-3.00830200	-1.49362400	0.48820200
H	-2.87923300	-0.08920100	1.56299000

Tautomer 8 (*vacuo*)



Electronic Energy E(B3LYP): -681.03403819
Zero-point correction= 0.106872 (Hartree/Particle)
Thermal correction to Energy= 0.115244
Thermal correction to Enthalpy= 0.116189
Thermal correction to Gibbs Free Energy= 0.073365

C	-3.65824200	-0.24164500	0.01978900
C	-2.39744200	-0.21990600	-0.40751900
N	-1.30398000	0.24252400	0.33313900
N	-0.09295700	-0.41233800	0.10517600
C	1.05080700	0.37950600	-0.01286500
S	2.52668400	-0.64540800	-0.02289100
N	1.11859100	1.63414500	-0.14458700
H	-4.45446900	-0.52616700	-0.65236100
H	-3.93217000	0.04811400	1.02802100
H	-2.12511700	-0.51849300	-1.41297100
H	-1.49580400	0.40870800	1.31642600
H	0.02412900	-1.30654800	0.56980300
H	3.34887800	0.41464900	-0.02073000

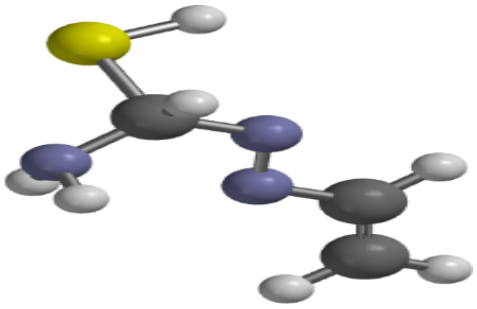
H	0.18528900	2.04820900	-0.11445600

Tautomer 8 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.04807018
Zero-point correction= 0.106599 (Hartree/Particle)
Thermal correction to Energy= 0.114991
Thermal correction to Enthalpy= 0.115935
Thermal correction to Gibbs Free Energy= 0.073183

C	-3.65321800	-0.22865800	-0.01870700
C	-2.37704500	-0.22740200	-0.40579400
N	-1.30228300	0.22177400	0.36836600
N	-0.08307600	-0.42083000	0.14297000
C	1.04112700	0.37235900	-0.00218300
S	2.53104200	-0.62800300	-0.03669900
N	1.08256100	1.63518400	-0.15112900
H	-4.42857100	-0.50803000	-0.71805800
H	-3.95355700	0.06783800	0.97992300
H	-2.08120700	-0.53217900	-1.40309700
H	-1.50572700	0.34455300	1.35573100
H	0.03780200	-1.32118400	0.59423200
H	3.35364800	0.43028600	-0.09124400
H	0.13533600	2.01607500	-0.09165300

Tautomer 9 (*vacuo*)



Electronic Energy E(B3LYP): -681.02238971
Zero-point correction= 0.106130 (Hartree/Particle)
Thermal correction to Energy= 0.114574
Thermal correction to Enthalpy= 0.115519
Thermal correction to Gibbs Free Energy= 0.072768

C	-2.35935700	-0.50591000	0.17402100
N	-1.14624800	0.20169400	0.04629500

N	-0.20359600	-0.31258100	0.66967200
C	1.08019800	0.42386100	0.52554600
S	2.23213500	-0.73057400	-0.36451500
N	1.11169700	1.67385500	-0.16124300
C	-3.44728000	-0.05568900	-0.44509300
H	-2.34353600	-1.40392300	0.78687700
H	1.45166900	0.55348200	1.54208800
H	1.71394000	-1.86076900	0.14861000
H	0.60759100	1.61434900	-1.04050100
H	0.68029900	2.40424100	0.39537600
H	-3.40709100	0.84516700	-1.04469800
H	-4.39135800	-0.57771700	-0.36542700

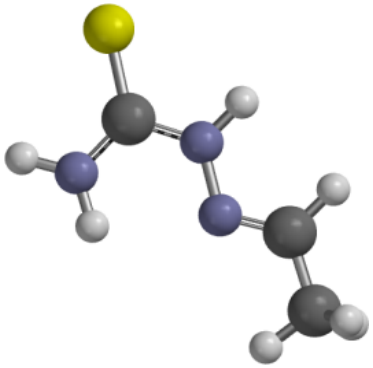
Tautomer 9 (methanol-CPCM)

Electronic Energy E(B3LYP): -681.03237468
Zero-point correction= 0.105973 (Hartree/Particle)
Thermal correction to Energy= 0.114414
Thermal correction to Enthalpy= 0.115358
Thermal correction to Gibbs Free Energy= 0.072666

C	-2.36242900	-0.49661500	0.18921100
N	-1.14441000	0.19922400	0.04442100
N	-0.20310800	-0.29597000	0.68684900
C	1.08413100	0.42869800	0.52726900
S	2.22070200	-0.74000400	-0.37380100
N	1.11733700	1.67564800	-0.16930000
C	-3.44231000	-0.06549800	-0.45933500
H	-2.36127700	-1.36955400	0.83683700
H	1.47198000	0.55826400	1.53601500
H	1.78719200	-1.86944700	0.21336600
H	0.57148700	1.62750800	-1.02480100
H	0.71989500	2.41292300	0.40497900
H	-3.39705500	0.80999600	-1.09524700
H	-4.38852900	-0.58145700	-0.36698600

Table S4. Optimized coordinates for ATSC inversion mechanism (4 sequences) at B3LYP/6-311++G(2d,p).

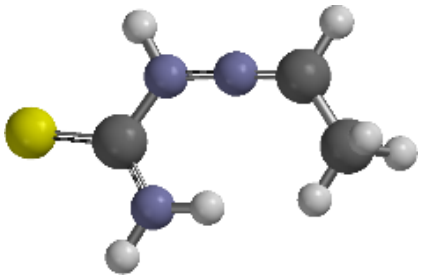
Ground structure for all sequences



Electronic Energy E(B3LYP): -681.08300316
Zero-point correction= 0.109444 (Hartree/Particle)
Thermal correction to Energy= 0.117883
Thermal correction to Enthalpy= 0.118828
Thermal correction to Gibbs Free Energy= 0.076108

C	-2.27236900	-0.55362800	0.00005000
H	-2.19704400	-1.64677400	0.00002200
N	-1.22309400	0.17002200	0.00000600
N	-0.01373200	-0.45592300	-0.00007200
H	0.06409300	-1.46760900	0.00000600
C	1.16159400	0.24214500	-0.00006400
S	2.62362300	-0.57234500	0.00002200
N	1.03610700	1.58031100	-0.00018700
H	0.12220700	2.00726500	0.00008700
C	-3.63358600	0.05481600	0.00013500
H	-3.56771000	1.14222700	0.00015000
H	-4.20097800	-0.26672000	-0.87882500
H	-4.20088500	-0.26675200	0.87914300
H	1.87354200	2.13501300	0.00012000

TS 1 (sequence 1)

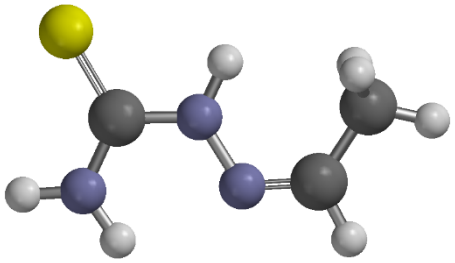


Electronic Energy E(B3LYP): -681.02462371
Zero-point correction= 0.107630 (Hartree/Particle)
Thermal correction to Energy= 0.115946
Thermal correction to Enthalpy= 0.116890
Thermal correction to Gibbs Free Energy= 0.073698

C	-2.38907800	-0.66727300	0.00017500
H	-3.03612000	-1.55901600	0.00040400
N	-1.14550500	-0.81887300	0.00012400
N	0.14567000	-0.89070200	0.00011800
H	0.60304100	-1.79957300	0.00026000
C	1.03953700	0.18048400	-0.00006600
S	2.67689800	-0.11776400	-0.00007300
N	0.46994800	1.39249300	-0.00022500

H	-0.53346000	1.48688000	-0.00004600
C	-3.16233600	0.63396800	0.00001400
H	-2.52061900	1.51683600	-0.00083500
H	-3.81324400	0.68545000	-0.87880000
H	-3.81217000	0.68632400	0.87957700
H	1.06266500	2.20381700	-0.00024400

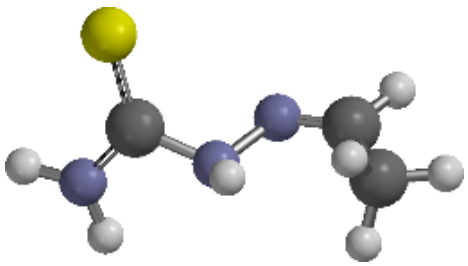
GS 1 (sequence 1)



Electronic Energy E(B3LYP): -681.08145713
Zero-point correction= 0.109920 (Hartree/Particle)
Thermal correction to Energy= 0.118230
Thermal correction to Enthalpy= 0.119174
Thermal correction to Gibbs Free Energy= 0.076599

C	2.43701400	0.44808400	0.00017500
N	1.21919900	0.83941000	0.00014700
N	0.23512000	-0.09889900	0.00004200
H	0.42333000	-1.09372500	-0.00013100
C	-1.08968300	0.25534300	-0.00002600
S	-2.27219000	-0.92711600	-0.00030900
N	-1.32915300	1.57614900	0.00021800
H	-0.56110000	2.23083700	0.00014400
C	2.91895600	-0.97288100	0.00011400
H	2.56532300	-1.51648800	0.88313600
H	2.56551900	-1.51635000	-0.88307300
H	4.00709000	-1.00893100	0.00022900
H	3.16546800	1.25188000	0.00025100
H	-2.28447000	1.88673500	-0.00004400

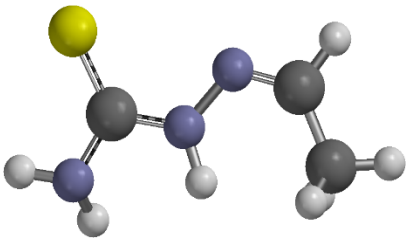
TS 2 (sequence 1)



Electronic Energy E(B3LYP): -681.05320834
Zero-point correction= 0.109421 (Hartree/Particle)
Thermal correction to Energy= 0.116870
Thermal correction to Enthalpy= 0.117814
Thermal correction to Gibbs Free Energy= 0.076953

C	2.22855300	-0.28903700	0.61379800
N	1.00255300	-0.03154100	0.84848300
N	0.27590300	0.60939200	-0.14302000
H	0.60238400	0.41865600	-1.08984600
C	-1.14422100	0.34698300	-0.06238200
S	-1.82873200	-1.15028800	-0.13340300
N	-1.82591200	1.49824900	0.03413800
H	-1.32433100	2.36303100	0.16606300
C	2.97690700	-0.02277900	-0.66142200
H	2.51736600	-0.53538700	-1.51474300
H	2.99613900	1.04738900	-0.89378100
H	4.00560400	-0.37233300	-0.58496700
H	2.75915700	-0.73985700	1.44684700
H	-2.83185000	1.47941400	0.08771700

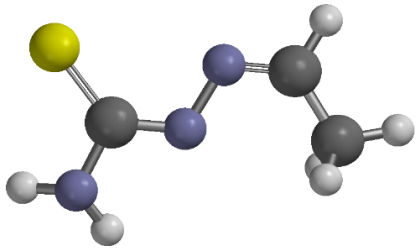
GS 2 (sequence 1)



Electronic Energy E(B3LYP): -681.06401175
Zero-point correction= 0.109408 (Hartree/Particle)
Thermal correction to Energy= 0.117791
Thermal correction to Enthalpy= 0.118735
Thermal correction to Gibbs Free Energy= 0.075661

C	-2.24791700	-0.76416800	-0.06287800
N	-0.97510000	-0.81418400	-0.14567400
N	-0.28596600	0.35433900	-0.07100300
H	-0.78279200	1.21508300	0.13268200
C	1.08830300	0.38418000	-0.01127200
S	2.08372500	-0.93415200	0.06529400
N	1.56313700	1.67605700	0.02408900
H	1.05736100	2.39091100	-0.48317000
C	-3.10187100	0.45960200	0.12661200
H	-2.85117700	0.99074300	1.05198700
H	-2.98617000	1.16560300	-0.70369300
H	-4.15435700	0.18544700	0.18129900
H	-2.73535400	-1.73027000	-0.14332100
H	2.56730200	1.73775100	-0.04714500

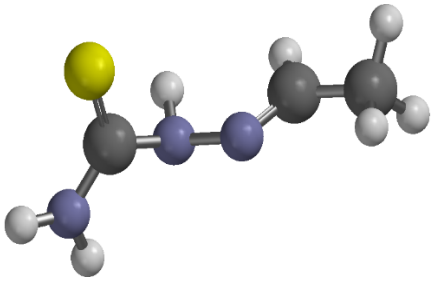
Product structure for all sequences (deprotonated)



Electronic Energy E(B3LYP): -680.51622507
Zero-point correction= 0.096256 (Hartree/Particle)
Thermal correction to Energy= 0.104213
Thermal correction to Enthalpy= 0.105157
Thermal correction to Gibbs Free Energy= 0.062789

C	2.23235500	-0.77087100	-0.00797900
N	0.94922100	-0.79762300	-0.03414400
N	0.34062700	0.42394500	-0.02228300
C	-0.98539600	0.39878200	-0.02387900
S	-2.10584000	-0.90663000	0.02284200
N	-1.53016800	1.68875100	-0.08903400
H	-0.89410300	2.40362900	0.24469400
C	3.09831300	0.46207900	0.03288800
H	2.87780000	1.12418600	-0.81038000
H	2.90696300	1.05070000	0.93668200
H	4.15844000	0.19272400	0.00726200
H	2.72065500	-1.74401500	-0.01741500
H	-2.46570200	1.73341000	0.28573600

TS 1 (sequence 2)

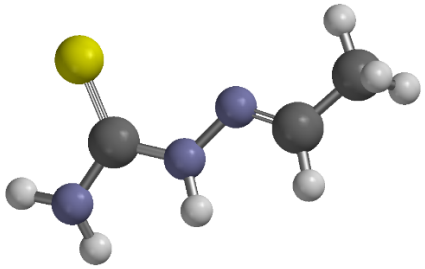


Electronic Energy E(B3LYP): -681.05539558
Zero-point correction= 0.109172 (Hartree/Particle)
Thermal correction to Energy= 0.116664
Thermal correction to Enthalpy= 0.117608
Thermal correction to Gibbs Free Energy= 0.076818

C	-2.15826900	-0.14166000	0.35633100
H	-2.23590800	-0.34032600	1.43353100
N	-1.06400000	-0.31491300	-0.26257500
N	0.00693800	-0.83508600	0.45936200
H	-0.09062700	-0.68873300	1.46621900

C	1.28194700	-0.30045800	0.02903300
S	1.67932700	1.29975200	0.02896900
N	2.10496200	-1.29522700	-0.33077200
H	1.75090000	-2.23834600	-0.37611500
C	-3.38354700	0.32899300	-0.35466900
H	-3.16543300	0.50803200	-1.40673500
H	-4.18629300	-0.41136300	-0.27802000
H	-3.75706500	1.25405500	0.09482000
H	3.03911200	-1.08401700	-0.64348000

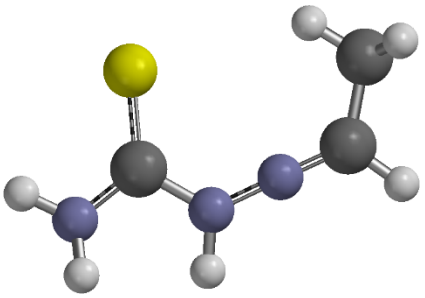
GS 1 (sequence 2)



Electronic Energy E(B3LYP): -681.06708518
Zero-point correction= 0.109134 (Hartree/Particle)
Thermal correction to Energy= 0.117499
Thermal correction to Enthalpy= 0.118443
Thermal correction to Gibbs Free Energy= 0.075815

C	-2.23953000	0.43077700	0.05746500
H	-2.36396400	1.50818000	0.23489500
N	-1.08565500	-0.08413300	-0.08587300
N	-0.01657700	0.75637100	-0.02662200
H	-0.18485600	1.73282900	0.20453800
C	1.27590900	0.29982200	-0.00117300
S	1.74317500	-1.28908100	0.01566100
N	2.18009400	1.33750900	0.05310800
H	1.95188100	2.20250000	-0.42008900
C	-3.47011800	-0.40938100	-0.01038900
H	-3.20649800	-1.45177600	-0.18338600
H	-4.04016800	-0.33396200	0.92079500
H	-4.12788200	-0.06774600	-0.81584800
H	3.13807300	1.03973300	-0.05118500

TS 2 (sequence 2)

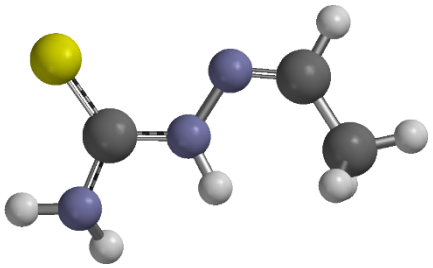


Electronic Energy E(B3LYP): -681.01559417
Zero-point correction= 0.107443 (Hartree/Particle)

Thermal correction to Energy= 0.115568
Thermal correction to Enthalpy= 0.116512
Thermal correction to Gibbs Free Energy= 0.074446

N	-2.51453600	-0.74141200	0.00360000
C	-1.27071500	-0.18355300	-0.00102500
N	-0.26537900	-1.15384100	-0.02347000
N	0.99464800	-0.90744800	-0.02449300
C	2.22372300	-0.68407200	-0.02037100
S	-0.99659700	1.44564600	-0.02440800
H	-3.28033700	-0.10307900	0.14358300
H	2.93536000	-1.52683400	-0.07332600
H	-0.57459400	-2.12428200	-0.11105700
H	-2.65123400	-1.68875800	0.32805800
C	2.86295600	0.68092100	0.05396600
H	3.51814800	0.83751300	-0.80976400
H	2.10462800	1.46149900	0.08194200
H	3.49466000	0.75272900	0.94620700

GS 2 (sequence 2)

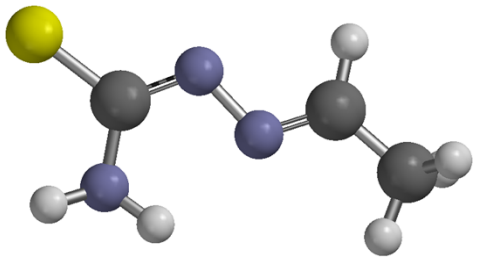


Electronic Energy E(B3LYP): -681.06401175
Zero-point correction= 0.109408 (Hartree/Particle)
Thermal correction to Energy= 0.117791
Thermal correction to Enthalpy= 0.118735
Thermal correction to Gibbs Free Energy= 0.075661

C	-2.24791700	-0.76416800	-0.06287800
N	-0.97510000	-0.81418400	-0.14567400
N	-0.28596600	0.35433900	-0.07100300
H	-0.78279200	1.21508300	0.13268200
C	1.08830300	0.38418000	-0.01127200
S	2.08372500	-0.93415200	0.06529400
N	1.56313700	1.67605700	0.02408900
H	1.05736100	2.39091100	-0.48317000
C	-3.10187100	0.45960200	0.12661200
H	-2.85117700	0.99074300	1.05198700
H	-2.98617000	1.16560300	-0.70369300

H	-4.15435700	0.18544700	0.18129900
H	-2.73535400	-1.73027000	-0.14332100
H	2.56730200	1.73775100	-0.04714500

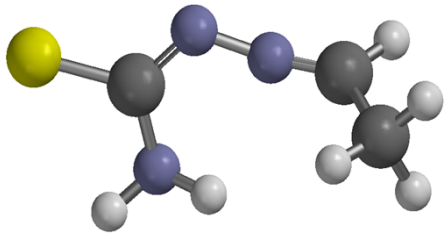
GS 1 (sequence 3)



Electronic Energy E(B3LYP): -680.52168411
Zero-point correction= 0.096135 (Hartree/Particle)
Thermal correction to Energy= 0.103998
Thermal correction to Enthalpy= 0.104942
Thermal correction to Gibbs Free Energy= 0.063551

C	-2.25992500	-0.57726300	-0.04043300
H	-2.20819700	-1.66552500	-0.15470900
N	-1.17999500	0.10535400	0.03481200
N	-0.00866400	-0.61634300	-0.01323400
C	1.07301600	0.15194600	-0.02199200
S	2.66500800	-0.50622400	0.02253300
N	0.95720700	1.53680800	-0.10370900
H	0.04890600	1.88890600	0.17391300
C	-3.60416400	0.07898400	0.03029200
H	-3.48882700	1.15878300	0.14257500
H	-4.19798800	-0.11336700	-0.87346100
H	-4.19559100	-0.29588300	0.87673300
H	1.76817400	2.02392400	0.24213000

TS 1 (sequence 3)

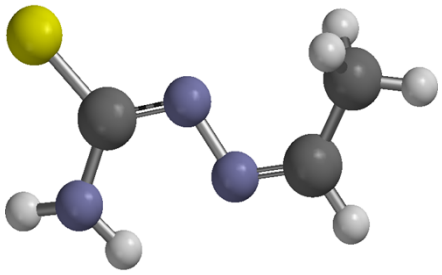


Electronic Energy E(B3LYP): -680.45898716
Zero-point correction= 0.093321 (Hartree/Particle)
Thermal correction to Energy= 0.101309
Thermal correction to Enthalpy= 0.102253
Thermal correction to Gibbs Free Energy= 0.059620

C	-2.39092300	-0.39368100	-0.40750400
H	-2.98171600	-0.77812700	-1.27872600
N	-1.16037600	-0.51231800	-0.35691700

N	0.09899200	-0.85365700	-0.12017400
C	1.02538300	0.06976900	-0.09263600
S	2.68900000	-0.25951600	0.26981000
N	0.67498200	1.39546500	-0.42994900
H	-0.27585700	1.63301500	-0.15728000
C	-3.28057300	0.27690500	0.64073800
H	-3.78601500	1.15419300	0.21477000
H	-4.06670400	-0.41415700	0.97170000
H	-2.69326300	0.58994800	1.50597600
H	1.36103900	2.04299200	-0.06770300

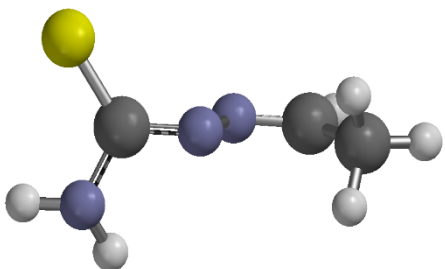
GS 2 (sequence 3)



Electronic Energy E(B3LYP): -680.52101824
Zero-point correction= 0.096379 (Hartree/Particle)
Thermal correction to Energy= 0.104250
Thermal correction to Enthalpy= 0.105194
Thermal correction to Gibbs Free Energy= 0.063287

C	-2.42380400	0.43414300	-0.05309500
N	-1.18877600	0.79156000	-0.09059100
N	-0.27316700	-0.23263500	-0.03374000
C	0.98324200	0.20350200	0.02107200
S	2.32743200	-0.87066500	-0.02291500
C	-2.91747900	-0.98068500	0.07264100
H	-2.52192400	-1.60371600	-0.73556500
H	-2.56126000	-1.44001400	1.00041100
H	-4.01062200	-1.01513000	0.05393100
H	-3.15244700	1.23983400	-0.12366800
N	1.24905300	1.55968900	0.15215800
H	2.17195500	1.82191500	-0.15316300
H	0.47385500	2.15569300	-0.11381200

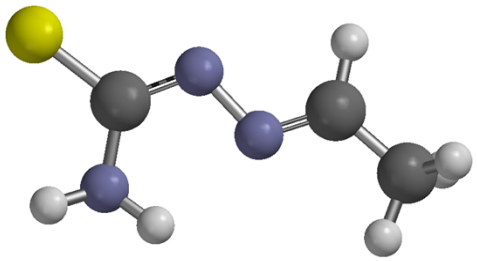
TS 2 (sequence 3)



Electronic Energy E(B3LYP): -680.48890439
Zero-point correction= 0.094583 (Hartree/Particle)
Thermal correction to Energy= 0.102158
Thermal correction to Enthalpy= 0.103103
Thermal correction to Gibbs Free Energy= 0.062117

C	2.37445700	-0.11093800	0.63776500
N	1.10193000	0.06115500	0.83641000
N	0.31034700	0.10974200	-0.23546300
C	-1.01255500	0.29079800	-0.10300700
S	-2.20553700	-0.92989500	-0.02192700
C	3.00205600	-0.26608600	-0.71551200
H	2.55091300	-1.10171000	-1.26643600
H	2.83549100	0.62215200	-1.34194100
H	4.08017200	-0.43740000	-0.63522300
H	2.98860900	-0.14823300	1.53200400
N	-1.43988100	1.59726500	-0.16443200
H	-2.40841000	1.77998300	0.04688300
H	-0.74870500	2.30374000	0.04446700

GS 1 (sequence 4)

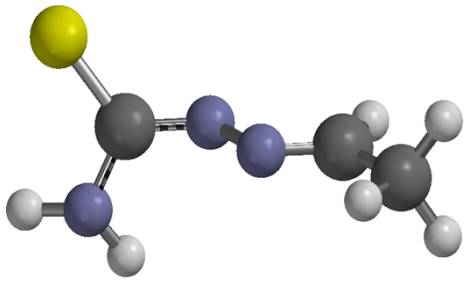


Electronic Energy E(B3LYP): -680.52168411
Zero-point correction= 0.096135 (Hartree/Particle)
Thermal correction to Energy= 0.103998
Thermal correction to Enthalpy= 0.104942
Thermal correction to Gibbs Free Energy= 0.063551

C	-2.25992500	-0.57726300	-0.04043300
H	-2.20819700	-1.66552500	-0.15470900
N	-1.17999500	0.10535400	0.03481200
N	-0.00866400	-0.61634300	-0.01323400
C	1.07301600	0.15194600	-0.02199200
S	2.66500800	-0.50622400	0.02253300
N	0.95720700	1.53680800	-0.10370900
H	0.04890600	1.88890600	0.17391300
C	-3.60416400	0.07898400	0.03029200

H	-3.48882700	1.15878300	0.14257500
H	-4.19798800	-0.11336700	-0.87346100
H	-4.19559100	-0.29588300	0.87673300
H	1.76817400	2.02392400	0.24213000

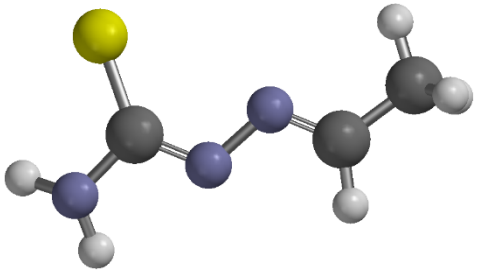
TS1 (sequence 4)



Electronic Energy E(B3LYP): -680.48715798
Zero-point correction= 0.094160 (Hartree/Particle)
Thermal correction to Energy= 0.101823
Thermal correction to Enthalpy= 0.102767
Thermal correction to Gibbs Free Energy= 0.061736

C	2.32005600	-0.05924300	0.42673300
H	2.42302400	0.01185800	1.51515700
N	1.15605000	0.01603100	-0.13223800
N	0.07677900	0.18507500	0.62453200
C	-1.14730500	0.29420900	0.08817000
S	-2.29745900	-0.95782500	-0.09418800
N	-1.53646600	1.56788900	-0.25997800
H	-0.94243900	2.31928700	0.05701300
C	3.54522900	-0.26406400	-0.41098000
H	3.25846000	-0.32665300	-1.46356500
H	4.27434600	0.55490000	-0.30792100
H	4.08421100	-1.18903500	-0.15403200
H	-2.52068100	1.74646200	-0.38939300

GS2 (sequence 4)

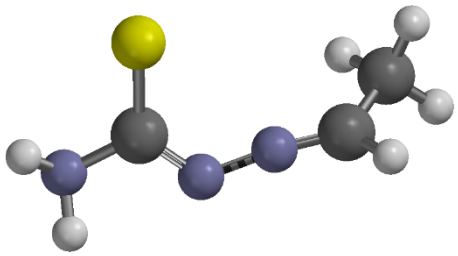


Electronic Energy E(B3LYP): -680.51841358
Zero-point correction= 0.096047 (Hartree/Particle)
Thermal correction to Energy= 0.104001
Thermal correction to Enthalpy= 0.104945
Thermal correction to Gibbs Free Energy= 0.063089

C	2.22799000	0.46250500	0.01283500

H	2.36838300	1.55119500	0.04601300
N	1.05309300	-0.03743900	-0.01956900
N	0.02868400	0.86551300	-0.00757400
C	-1.18919500	0.35113600	-0.01932700
S	-1.74634300	-1.28029200	0.00812500
N	-2.17638000	1.34747200	-0.07938200
H	-1.85286600	2.24204000	0.27077700
C	3.43965600	-0.41851700	0.00522400
H	3.13370400	-1.46518500	-0.02854800
H	4.08397400	-0.21411200	-0.86049900
H	4.05887600	-0.26376100	0.89911600
H	-3.05908200	1.03493000	0.29642400

TS2 (sequence 4)

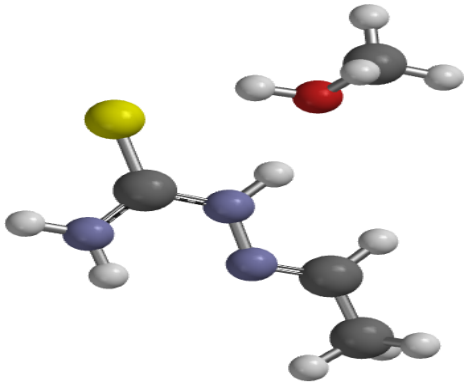


Electronic Energy E(B3LYP): -680.46187143
Zero-point correction= 0.093771 (Hartree/Particle)
Thermal correction to Energy= 0.101811
Thermal correction to Enthalpy= 0.102694
Thermal correction to Gibbs Free Energy= 0.060238

N	2.37402100	-1.08853700	0.39058700
C	1.20866300	-0.33578600	0.05257800
N	0.14456800	-1.07091300	-0.10793400
N	-1.02799900	-0.54208700	-0.34410700
C	-2.20711900	-0.22832600	-0.50927700
S	1.36579100	1.38491100	-0.07992800
H	3.19575700	-0.61695900	0.03584600
H	2.31329800	-2.03570600	0.02989400
C	-3.15306900	0.29531800	0.56902300
H	-4.06014900	-0.32226900	0.61527700
H	-2.66221900	0.29807200	1.54303200
H	-3.46860900	1.31826700	0.32921600
H	-2.69570700	-0.27645600	-1.51818100

Table S5. Optimized coordinates for ATSC tautomerization mechanism at B3LYP/6-311++G(2d,p).

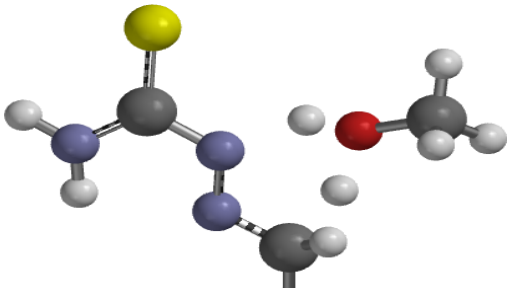
GS (methanol mediated)



Electronic Energy E(B3LYP): -796.86557160
Zero-point correction= 0.162974 (Hartree/Particle)
Thermal correction to Energy= 0.175798
Thermal correction to Enthalpy= 0.176742
Thermal correction to Gibbs Free Energy= 0.122395

C	2.36308500	0.84906000	-0.07972300
N	1.74110400	-0.25794800	0.03660900
N	0.37624700	-0.22242800	-0.04752700
C	-0.34990300	-1.36500000	0.03495600
N	0.34668800	-2.49697800	0.22581800
S	-2.03558900	-1.34768400	-0.09710800
H	-2.08096000	0.97180400	-0.49970000
H	1.81669200	1.78306800	-0.24304800
H	-0.15691800	-3.36484600	0.27239600
H	1.35364600	-2.46714400	0.27883200
H	-0.12854000	0.65979800	-0.18901300
O	-1.61719700	1.83423100	-0.51375600
C	-2.22085100	2.69597000	0.44770500
H	-2.22856600	2.24720300	1.44648300
H	-1.63290300	3.61336700	0.47715800
H	-3.24692100	2.94976800	0.16461800
C	3.85070000	0.90865400	-0.00227600
H	4.26811200	-0.08404400	0.16303400
H	4.26810700	1.32103300	-0.92626500
H	4.16881700	1.56846100	0.81101800

TS (methanol mediated)

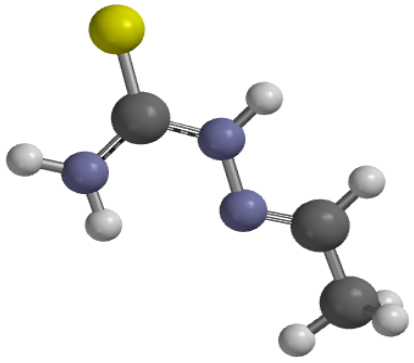


Electronic Energy E(B3LYP): -796.77578167
Zero-point correction= 0.156849 (Hartree/Particle)
Thermal correction to Energy= 0.168350
Thermal correction to Enthalpy= 0.169294
Thermal correction to Gibbs Free Energy= 0.118906

C	1.87616400	-0.77884600	0.30070500
N	0.58626800	-1.09962700	0.06047500
N	-0.28995800	-0.18996900	0.37681800
C	-1.61244300	-0.48584400	0.05191600
N	-1.90477100	-1.76002200	-0.26475600
S	-2.73504700	0.74913800	0.09127100
H	1.78429400	0.51029600	-0.42881900
H	2.05564400	-0.18742500	1.20692800
H	-2.82994800	-1.97081200	-0.59742600
H	-1.14506500	-2.41014100	-0.41067500
H	0.36180600	1.14727400	-0.15354600
O	1.20547100	1.53848900	-0.64490800
C	1.77065200	2.63366900	0.10348000
H	2.72188300	2.89272000	-0.35697900
H	1.08382000	3.47541700	0.04163600
H	1.92038600	2.35532000	1.14835000
C	2.93122900	-1.79795500	-0.04644500
H	2.67551400	-2.31838500	-0.97040400
H	3.90257000	-1.31854500	-0.18825300
H	3.05170100	-2.54864900	0.74243800

GS (*vacuo*)

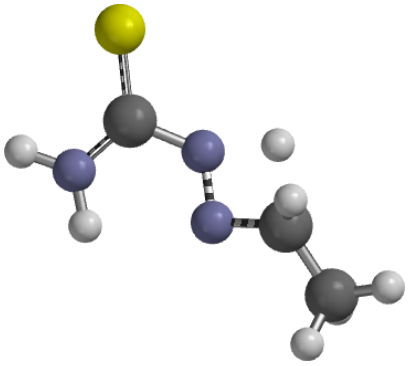
Electronic Energy E(B3LYP): -681.08300316
Zero-point correction= 0.109444 (Hartree/Particle)
Thermal correction to Energy= 0.117883
Thermal correction to Enthalpy= 0.118828



Thermal correction to Gibbs Free Energy= 0.076108

C	-2.27236900	-0.55362800	0.00005000
H	-2.19704400	-1.64677400	0.00002200
N	-1.22309400	0.17002200	0.00000600
N	-0.01373200	-0.45592300	-0.00007200
H	0.06409300	-1.46760900	0.00000600
C	1.16159400	0.24214500	-0.00006400
S	2.62362300	-0.57234500	0.00002200
N	1.03610700	1.58031100	-0.00018700
H	0.12220700	2.00726500	0.00008700
C	-3.63358600	0.05481600	0.00013500
H	-3.56771000	1.14222700	0.00015000
H	-4.20097800	-0.26672000	-0.87882500
H	-4.20088500	-0.26675200	0.87914300
H	1.87354200	2.13501300	0.00012000

TS (*vacuo*)



Electronic Energy E(B3LYP): -680.95664270
Zero-point correction= 0.102594 (Hartree/Particle)
Thermal correction to Energy= 0.110798
Thermal correction to Enthalpy= 0.111742
Thermal correction to Gibbs Free Energy= 0.069282

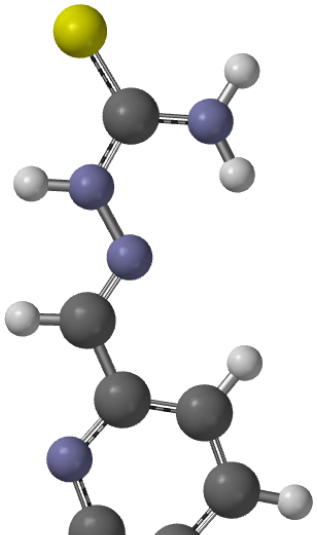
C	-2.13370200	-0.47243700	0.19551900
N	-1.14667300	0.47627500	0.01145400
N	-0.11183700	-0.24454100	-0.29677300
C	1.18256500	0.26769800	-0.05239200
N	1.25854700	1.60407400	0.05211900
S	2.45911800	-0.78270200	0.02856000
H	-0.98263500	-1.30169000	-0.27868000
H	-1.93938900	-1.03576700	1.11110100
H	2.16310700	2.03044400	0.16698500
H	0.41667900	2.16048600	0.08588600
C	-3.57330200	-0.13305800	-0.06369500
H	-4.20081600	-1.00403900	0.13090500

H	-3.92370700	0.67965200	0.58263100
H	-3.73274900	0.17027400	-1.09998100

Table S6. Optimized coordinates for FPTSC tautomerization (catalytic) and inversion mechanism at B3LYP/6-311++G(2d,p).

GS (inversion)

Electronic Energy E(B3LYP): -888.91763952
Zero-point correction= 0.151007 (Hartree/Particle)
Thermal correction to Energy= 0.162160
Thermal correction to Enthalpy= 0.163104
Thermal correction to Gibbs Free Energy= 0.112461

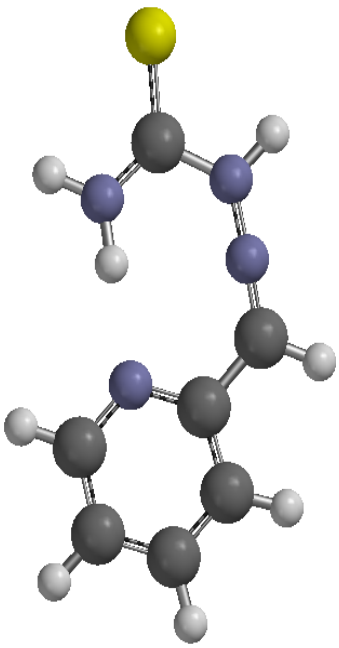


C	-0.41150000	-0.79569000	0.00000900
N	0.58294000	0.01204400	-0.00000500
N	1.82460200	-0.52092500	-0.00001200
C	2.95445300	0.25497100	-0.00002500
S	4.46178500	-0.46581600	-0.00003700
H	1.97225100	-1.52560000	-0.00000700
H	-0.28149000	-1.88049500	0.00001400
C	-1.79910700	-0.33048200	0.00001700
C	-2.14900100	1.02521500	0.00001500
C	-4.00287600	-0.96728000	0.00003600
C	-4.44408200	0.35116100	0.00003500
H	-4.71534700	-1.78642200	0.00004500
H	-5.50357500	0.57376400	0.00004200
N	2.74046000	1.58151700	-0.00002700
H	1.80103900	1.94781200	-0.00003500
H	3.53905600	2.19106100	-0.00005300
H	-1.37552100	1.78108700	0.00000700
C	-3.49065300	1.36504500	0.00002400
H	-3.79228600	2.40579900	0.00002300
N	-2.71601400	-1.31143500	0.00002800

TS (inversion)

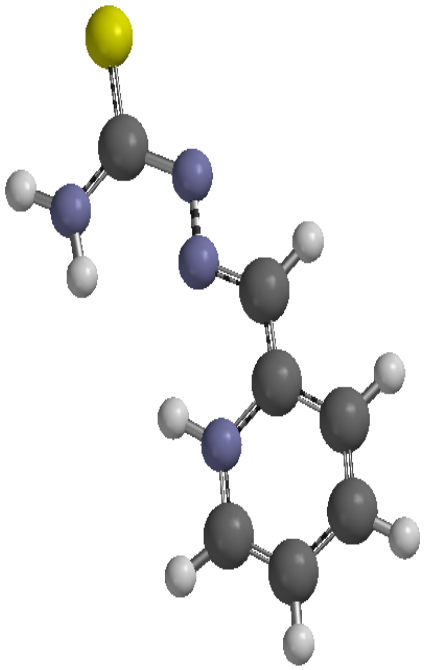
Electronic Energy E(B3LYP): -888.87125408
Zero-point correction= 0.150433 (Hartree/Particle)
Thermal correction to Energy= 0.160624
Thermal correction to Enthalpy= 0.161568
Thermal correction to Gibbs Free Energy= 0.113510

C	0.53661500	1.64150500	0.00000000
N	-0.69194500	1.37609600	0.00000000
N	-1.93318300	1.06628100	-0.00000700
C	-2.46875800	-0.23839400	0.00000200
S	-4.12809600	-0.39962200	-0.00000300
H	-2.64907300	1.79157100	-0.00001000



H	0.88219200	2.68555200	0.00000200
C	1.63360200	0.64380700	0.00000100
C	2.96124300	1.08257500	0.00000500
C	2.31548900	-1.55295000	-0.00000700
C	3.66125900	-1.20285900	-0.00000400
H	2.02132600	-2.59823600	-0.00001400
H	4.42543900	-1.96916300	-0.00000400
N	-1.57065400	-1.21768200	0.00001700
H	-0.55628400	-1.03448700	0.00000900
H	-1.92134700	-2.16036200	0.00000500
H	3.17444700	2.14489000	0.00000800
C	3.98548700	0.14862800	0.00000300
H	5.02092100	0.46820100	0.00000700
N	1.32468000	-0.66296600	-0.00000400

GS (tautomerization)

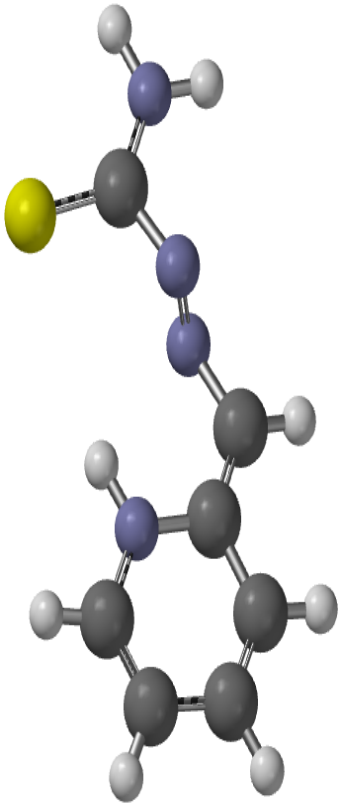


Electronic Energy E(B3LYP): -888.88245958
Zero-point correction= 0.150303 (Hartree/Particle)
Thermal correction to Energy= 0.161695
Thermal correction to Enthalpy= 0.162639
Thermal correction to Gibbs Free Energy= 0.110208

C	-0.37567500	-0.99926500	0.00053700
N	0.65593700	-0.14302300	0.00046500
N	1.82469000	-0.68962400	0.00035800
C	2.88608700	0.21825200	0.00039800
S	4.44446200	-0.37433500	-0.00119300
H	-0.19737000	-2.07001900	0.00079200
C	-1.67891800	-0.50908400	0.00016500
C	-2.84382400	-1.32977500	0.00052000
C	-3.14554300	1.41317600	-0.00094400
C	-4.26149700	0.63522600	-0.00054600

H	-3.17264300	2.49415100	-0.00154900
H	-5.24164600	1.08816600	-0.00080500
N	2.61299600	1.54110700	0.00166300
H	1.65533500	1.85184500	0.00305200
H	3.37517200	2.19558200	0.00213700
H	-2.70647100	-2.40273800	0.00110200
C	-4.09079200	-0.77666800	0.00018400
H	-4.96302400	-1.41888600	0.00049600
N	-1.91088000	0.85040400	-0.00062400
H	-1.07897300	1.42804600	-0.00105000

TS (tautomerization)

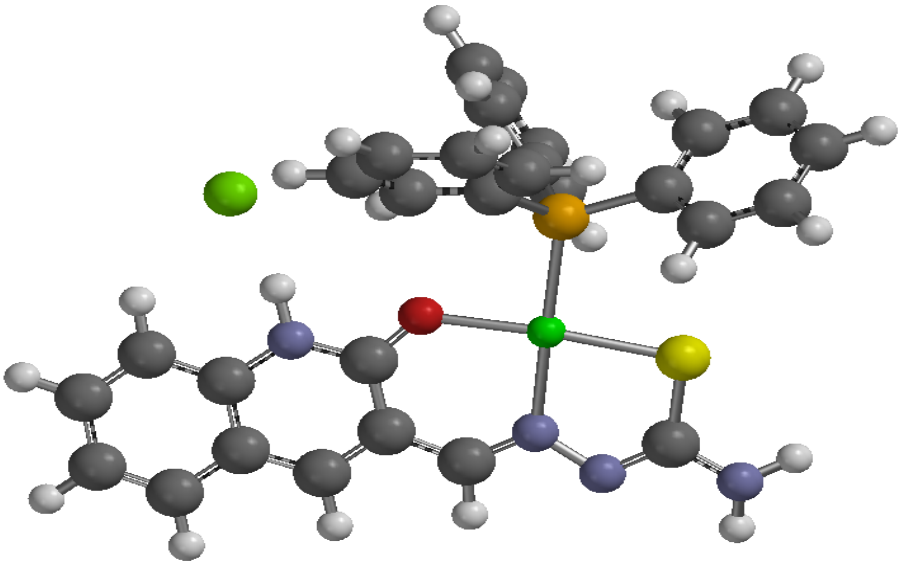


Electronic Energy E(B3LYP): -888.84465737
Zero-point correction= 0.148424 (Hartree/Particle)
Thermal correction to Energy= 0.159488
Thermal correction to Enthalpy= 0.160432
Thermal correction to Gibbs Free Energy= 0.109885

C	0.45028700	-1.55132400	0.22557800
N	-0.84304600	-1.01350300	0.55197800
N	-1.56011900	-0.77051600	-0.42955400
C	-2.79637200	-0.11612200	-0.13754800
S	-2.82303400	1.52173300	0.06128900
H	0.43550200	1.04715800	0.23497000
H	0.54687100	-2.62615900	0.26590100
C	1.51566400	-0.72633700	0.10249500
C	2.87927000	-1.18121900	-0.07212400
C	2.41183600	1.54277000	0.02687300
C	3.68252200	1.10949400	-0.13171200
H	2.14356300	2.58971800	0.07137000
H	4.49474300	1.81517700	-0.22066900

N	-3.84980800	-0.93751500	-0.17878200
H	-3.73070700	-1.92543600	-0.34507100
H	-4.77936400	-0.55316000	-0.11906500
H	3.04617700	-2.25000800	-0.10807700
C	3.90656300	-0.30951800	-0.18299800
H	4.91547700	-0.68366200	-0.31057800
N	1.36692400	0.66898800	0.13738800

Table S7. Optimized coordinates for ODCTSC metals at B3LYP/BS1.



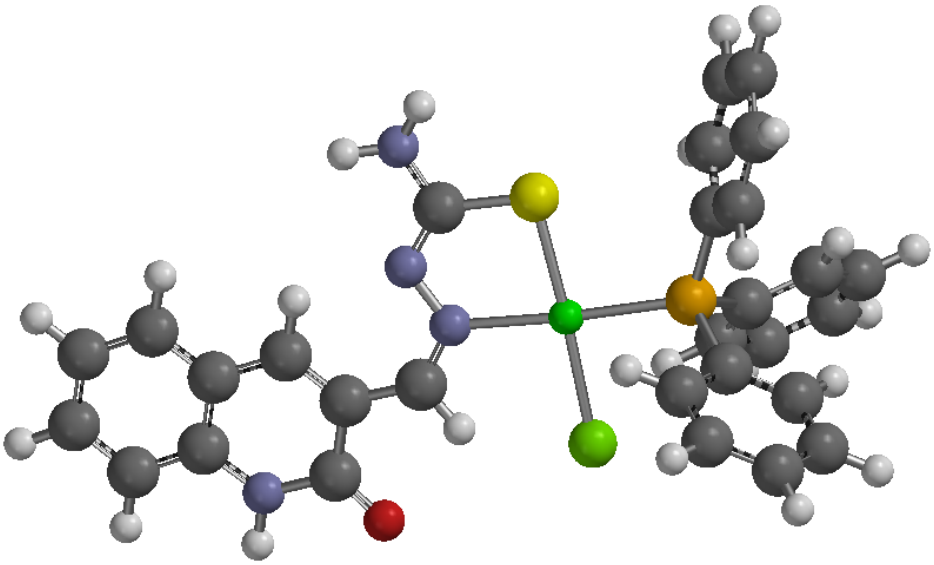
ODCTSC E Isomer (H substituted)

Electronic Energy E(B3LYP): -2740.35883527

Zero-point correction= 0.471960 (Hartree/Particle)
Thermal correction to Energy= 0.506711
Thermal correction to Enthalpy= 0.507655
Thermal correction to Gibbs Free Energy= 0.401004

C	-4.23599000	2.10796500	-0.11665700
C	-4.75236800	-0.25711300	-0.04525300
C	-2.43018800	0.46171100	-0.04728800
C	-2.87561700	1.85198000	-0.08731400
C	-5.21213700	1.08481300	-0.10177800
C	-1.99569600	2.99812300	-0.07987700
N	-0.69779500	3.00962700	-0.04924100
N	-0.12718100	4.25860400	-0.01390200
C	1.18063800	4.25167000	0.01935100
S	2.21472000	2.81186400	0.02695600
N	1.82517000	5.45169200	0.00174700
O	-1.22481200	0.06441000	-0.03336300
H	-4.57240800	3.14176700	-0.14808500
H	-2.47847000	3.97535000	-0.08975400
H	2.78943600	5.48785100	0.29937400
Pd	0.47607700	1.29383500	-0.04930800
P	1.84234600	-0.63686500	-0.03054400
C	3.65727300	-0.36324600	-0.12425200
C	4.53107000	-0.96215000	0.79595300
C	4.18724800	0.44405100	-1.14613200
C	5.90873000	-0.75938300	0.69253200
H	4.14144100	-1.58683400	1.59238400
C	5.56543100	0.63509800	-1.25057700
H	3.52586800	0.92637500	-1.85931200
C	6.42857100	0.03588500	-0.33008200
H	6.57391500	-1.22704900	1.41288100
H	5.96149000	1.25835800	-2.04713000
H	7.50095200	0.19086300	-0.40856000
C	1.54599000	-1.52890800	1.54146700
C	1.53090300	-2.93081900	1.61030200
C	1.35888600	-0.77834500	2.71496700
C	1.32944000	-3.56890700	2.83524100
H	1.66226200	-3.52486400	0.71238100

C	1.16431100	-1.42201000	3.93680200
H	1.36109400	0.30741600	2.67202000
C	1.14632800	-2.81769800	3.99774300
H	1.30791800	-4.65386800	2.87639800
H	1.01732300	-0.83324000	4.83770800
H	0.98320800	-3.31834100	4.94792600
C	1.43490900	-1.79496800	-1.39395200
C	2.33434400	-2.04953600	-2.44306900
C	0.17670100	-2.42291600	-1.39731600
C	1.97542100	-2.91222600	-3.47975700
H	3.31525700	-1.58835200	-2.45409200
C	-0.16890200	-3.29217900	-2.43196100
H	-0.53872100	-2.26376400	-0.59874000
C	0.72466900	-3.53387800	-3.47768300
H	2.68059300	-3.10265600	-4.28420400
H	-1.14027700	-3.77599100	-2.39531800
H	0.45175100	-4.20925000	-4.28408200
C	-5.66879700	-1.32714900	-0.01580600
C	-7.02344400	-1.04574100	-0.04608900
C	-7.50039000	0.28414900	-0.10475500
C	-6.60754400	1.33487600	-0.13140000
H	-5.28823400	-2.34322300	0.03139100
H	-7.73448400	-1.86650800	-0.02399600
H	-8.56900900	0.47376200	-0.12758500
H	-6.95541000	2.36330400	-0.17450500
N	-3.39601500	-0.49322000	-0.02033000
H	-3.08505200	-1.50279400	0.03432400
Cl	-2.87273400	-3.52919000	0.18000000
H	1.26626700	6.27354700	0.19244700



ODCTSC Z Isomer (H substituted)

Electronic Energy E(B3LYP): -2740.35715990
Zero-point correction= 0.472215 (Hartree/Particle)
Thermal correction to Energy= 0.507336
Thermal correction to Enthalpy= 0.508281
Thermal correction to Gibbs Free Energy= 0.399819

C	4.92035800	0.55421000	-0.03457700
C	6.92380100	-0.85119300	0.06808700
C	4.68296000	-1.90107800	0.06933000
C	4.09018400	-0.54244000	-0.00388700
C	6.34644100	0.44150700	-0.00096400
C	2.63594800	-0.55035400	-0.03157000
N	1.78334500	0.43535600	-0.07140600
N	2.27240100	1.71583800	-0.11186100
C	1.36589600	2.65720100	-0.06440400
S	-0.38229300	2.42488500	0.03357200
N	1.79613900	3.95237900	-0.04089500
O	4.04600100	-2.95219900	0.10629000
H	4.47458000	1.53878500	-0.08571300
H	2.18170900	-1.53417500	-0.01515700
H	1.14061400	4.67778500	-0.29412200

Pd	-0.34385100	0.09795700	-0.04734700
P	-2.66939100	-0.12886300	0.02159500
C	-3.61848500	1.44717400	-0.10810600
C	-4.32847400	1.78899900	-1.26813000
C	-3.60602800	2.34378400	0.97495200
C	-5.01852500	3.00165200	-1.34083800
H	-4.35041200	1.11132900	-2.11470700
C	-4.30052200	3.55053200	0.89944600
H	-3.05866500	2.09873900	1.88028100
C	-5.00829700	3.88274600	-0.25896000
H	-5.56729200	3.25165600	-2.24456100
H	-4.28622000	4.23154800	1.74568900
H	-5.54808400	4.82387200	-0.31650800
C	-3.27995600	-1.15418900	-1.37316400
C	-4.37137900	-2.02383000	-1.23908700
C	-2.64302100	-1.03434400	-2.61880700
C	-4.82244200	-2.75668700	-2.33889100
H	-4.86464300	-2.14189400	-0.27994500
C	-3.10393500	-1.76039300	-3.71684800
H	-1.77843300	-0.38500800	-2.72339000
C	-4.19350000	-2.62411400	-3.57814200
H	-5.66384700	-3.43410600	-2.22299100
H	-2.60311500	-1.66111000	-4.67562600
H	-4.54542000	-3.19742800	-4.43128600
C	-3.29468600	-0.87378400	1.58211300
C	-4.63101000	-0.68371000	1.97894200
C	-2.44238900	-1.64276200	2.38940000
C	-5.10494300	-1.26284400	3.15626400
H	-5.30018300	-0.07804500	1.37609500
C	-2.92199000	-2.21491200	3.56951800
H	-1.41442000	-1.80359500	2.08488500
C	-4.25060900	-2.02795400	3.95441100
H	-6.13944400	-1.11067400	3.45116100
H	-2.25217800	-2.80645200	4.18709700
H	-4.61960600	-2.47319700	4.87430400
C	8.31931100	-1.00623700	0.10431800
C	9.13209500	0.11895200	0.07169800

C	8.57769000	1.41070100	0.00284300
C	7.20175200	1.56491200	-0.03278200
H	8.75079300	-2.00202100	0.15748500
H	10.21098100	-0.00405100	0.09985000
H	9.22744900	2.27991500	-0.02185500
H	6.75725700	2.55516100	-0.08545100
N	6.07311100	-1.93602200	0.09845800
H	6.46267900	-2.87123000	0.14900400
Cl	-0.19885100	-2.30691200	-0.21888700
H	2.76060900	4.11591200	-0.29993500

ODCTSC E Isomer (Me substituted)

Electronic Energy E(B3LYP): -2779.6657923
Zero-point correction= 0.499770 (Hartree/Particle)
Thermal correction to Energy= 0.535575
Thermal correction to Enthalpy= 0.536519
Thermal correction to Gibbs Free Energy= 0.426909

C	-4.10536100	2.37276600	-0.11236100
C	-4.83990700	0.06563600	-0.03956000
C	-2.46142200	0.56696300	-0.04330900
C	-2.77414200	1.99284500	-0.08628500
C	-5.17257300	1.44437300	-0.09352900
C	-1.79086200	3.05139900	-0.08788800
N	-0.49540900	2.94398900	-0.05980400
N	0.19063700	4.12618000	-0.04508400
C	1.50013900	3.99839900	-0.00482200
S	2.38566400	2.46249500	0.01468900
N	2.22685800	5.13952200	0.01865800
O	-1.29769100	0.05889300	-0.02677000
H	-4.34461600	3.43316700	-0.14549200
H	-2.18058700	4.06917500	-0.10488200
H	1.68532200	5.99335900	0.00994600
Pd	0.50452200	1.12356100	-0.05059800
P	1.67703300	-0.93365500	-0.02760700
C	3.51192400	-0.84004800	-0.08131400
C	4.30417300	-1.51025300	0.86319700

C	4.13947900	-0.09647000	-1.09644500
C	5.69688800	-1.43967500	0.79051100
H	3.83923400	-2.08866200	1.65404200
C	5.53151300	-0.03794200	-1.17043800
H	3.54316600	0.43907900	-1.82874600
C	6.31290100	-0.70718600	-0.22560500
H	6.29830900	-1.96148700	1.52950400
H	6.00283600	0.53679300	-1.96253300
H	7.39667200	-0.65560200	-0.28030100
C	1.26027200	-1.81294100	1.52391300
C	1.15988700	-3.21206600	1.57950800
C	1.06695600	-1.06023600	2.69438700
C	0.86915200	-3.84492800	2.78888800
H	1.29472200	-3.80637000	0.68210700
C	0.78215900	-1.69876900	3.90129300
H	1.13313600	0.02366800	2.65890000
C	0.68025800	-3.09118900	3.94912900
H	0.78239700	-4.92696900	2.81999400
H	0.63024200	-1.10795000	4.80004000
H	0.44708300	-3.58726100	4.88701900
C	1.18581400	-2.03619300	-1.41020300
C	2.07280800	-2.37249000	-2.44671400
C	-0.12756000	-2.53805400	-1.43764300
C	1.64779100	-3.18986700	-3.49524700
H	3.09521200	-2.01217300	-2.43914700
C	-0.53989700	-3.36299200	-2.48399600
H	-0.83605500	-2.31602100	-0.64777800
C	0.34221600	-3.68536500	-3.51761600
H	2.34425500	-3.44460000	-4.28944500
H	-1.55412000	-3.75026700	-2.46630800
H	0.01742900	-4.32629600	-4.33284900
C	-5.85091900	-0.91525800	-0.01048300
C	-7.17406300	-0.51043600	-0.03700600
C	-7.52536400	0.85800600	-0.09189100
C	-6.53900600	1.82185300	-0.11945600
H	-5.56494600	-1.96203800	0.03288800
H	-7.95787700	-1.26200700	-0.01499500

H	-8.57185100	1.14619500	-0.11180800
H	-6.79086300	2.87806900	-0.16085600
N	-3.51073100	-0.29473800	-0.01656400
H	-3.29434600	-1.32832100	0.03229600
Cl	-3.27314800	-3.37439900	0.14360500
C	3.67576000	5.22849100	0.07145000
H	3.94848100	6.28529800	0.07713300
H	4.07509900	4.75872900	0.97776300
H	4.13903300	4.75229200	-0.80028700

ODCTSC Z Isomer (Me substituted)

Electronic Energy E(B3LYP): -2779.6661414
Zero-point correction= 0.500366 (Hartree/Particle)
Thermal correction to Energy= 0.537325
Thermal correction to Enthalpy= 0.538269
Thermal correction to Gibbs Free Energy= 0.425222

C	4.85076800	0.32342300	-0.03382500
C	6.81470700	-1.13735900	0.07205600
C	4.54522600	-2.12390800	0.08360400
C	3.99024000	-0.74952300	0.00494900
C	6.27380700	0.17044900	-0.00318900
C	2.53703100	-0.71685200	-0.02334500
N	1.71373700	0.29470500	-0.05090000
N	2.23865000	1.55952100	-0.06519100
C	1.35458600	2.52734400	-0.01833800
S	-0.40553800	2.33233300	0.07141800
N	1.80081200	3.80507400	-0.02909800
O	3.87933100	-3.15674400	0.12773100
H	4.43291900	1.31951900	-0.09044300
H	2.05421900	-1.68680200	-0.01911300
H	1.11058500	4.54005900	-0.00621700
Pd	-0.42120700	0.00857400	-0.03646300
P	-2.75223300	-0.16296700	0.01811400
C	-3.66592300	1.43678600	-0.07697100
C	-4.36588600	1.82264600	-1.22914900

C	-3.63724500	2.30547900	1.02829400
C	-5.03068500	3.05076800	-1.27229200
H	-4.39988400	1.16752300	-2.09284200
C	-4.30661100	3.52776700	0.98234600
H	-3.09706300	2.02619800	1.92798500
C	-5.00496600	3.90375400	-0.16840900
H	-5.57199700	3.33486600	-2.17042700
H	-4.28036500	4.18662000	1.84571400
H	-5.52535700	4.85687000	-0.20290600
C	-3.37519300	-1.13851500	-1.40674300
C	-4.47518800	-2.00093200	-1.30009500
C	-2.73575700	-0.98719800	-2.64780200
C	-4.93191800	-2.69598500	-2.42192900
H	-4.97072900	-2.14289400	-0.34541400
C	-3.20217100	-1.67548000	-3.76762300
H	-1.86522500	-0.34274100	-2.73234300
C	-4.30013900	-2.53251300	-3.65599000
H	-5.78000800	-3.36836300	-2.32728000
H	-2.69936600	-1.55201900	-4.72255700
H	-4.65646100	-3.07653400	-4.52632200
C	-3.40874200	-0.92966600	1.55538300
C	-4.74809700	-0.72875800	1.93652900
C	-2.57807900	-1.72271400	2.36177600
C	-5.24659400	-1.32176200	3.09665300
H	-5.40038600	-0.10358800	1.33497100
C	-3.08199300	-2.30833700	3.52513500
H	-1.54795900	-1.89176400	2.06940600
C	-4.41368700	-2.11121800	3.89379900
H	-6.28330100	-1.16133900	3.37919800
H	-2.42871400	-2.91867500	4.14215100
H	-4.80175000	-2.56740800	4.80040100
C	8.20528000	-1.33191500	0.10626400
C	9.05001900	-0.23076000	0.06519800
C	8.53214000	1.07555100	-0.01029300
C	7.16086500	1.26851600	-0.04372400
H	8.60803200	-2.33939600	0.16428700
H	10.12502900	-0.38428400	0.09172100

H	9.20611200	1.92595400	-0.04183600
H	6.74471500	2.27077300	-0.10158700
N	5.93376500	-2.19773400	0.11019800
H	6.29714800	-3.14321300	0.16428800
Cl	-0.33857600	-2.39873200	-0.23631600
C	3.20725800	4.16340400	-0.08743000
H	3.75046900	3.76289500	0.77623000
H	3.67523300	3.77474100	-0.99929100
H	3.28576900	5.25226400	-0.08342800

Table S8. Optimized coordinates for influence of terminal nitrogen substitution (N5-substituents effect study for ODCTSC and MSTSC) at B3LYP/6-311++G(2d,p).

ODCTSC GS (N5=H)

Electronic Energy E(B3LYP): -1117.87312578
Zero-point correction= 0.202525 (Hartree/Particle)
Thermal correction to Energy= 0.217430
Thermal correction to Enthalpy= 0.218374
Thermal correction to Gibbs Free Energy= 0.158683

C	1.03658200	0.95159400	-0.00062100
N	1.89716100	-0.00142100	-0.00008600
N	3.20494500	0.34214500	-0.00078500
C	4.20545500	-0.59249600	0.00020600
S	5.80520300	-0.10742500	-0.00058300
H	3.49941600	1.31409800	-0.00162300
H	1.33581200	2.00081100	-0.00132400
C	-0.39600200	0.69947100	-0.00006100
C	-1.25180500	1.89829500	0.00098800

C	-0.96216400	-0.54001800	-0.00036400
C	-2.37512500	-0.74078000	-0.00006500
H	-0.31715600	-1.41171700	-0.00097700
C	-3.21076600	0.39831100	0.00029600
O	-0.83813700	3.05014800	-0.00020900
N	-2.61447200	1.64076400	0.00060900
H	-3.19408100	2.47026700	0.00062800
N	3.79581300	-1.87287600	0.00161700
H	2.81204300	-2.09357000	0.00212900
C	-4.60219800	0.25375500	0.00032700
C	-5.15861100	-1.01235000	0.00007900
H	-6.23650600	-1.11928100	0.00013400
C	-4.34525300	-2.15344600	-0.00026900
H	-4.79436200	-3.13835700	-0.00050400
C	-2.97247300	-2.01475900	-0.00037200
H	-2.33262000	-2.88980300	-0.00071300
H	-5.23523100	1.13394400	0.00059800
H	4.49456100	-2.59453600	0.00231500

ODCTSC TS (N5=H)

Electronic Energy E(B3LYP): -1117.81233834
Zero-point correction= 0.201430 (Hartree/Particle)
Thermal correction to Energy= 0.215755
Thermal correction to Enthalpy= 0.216699
Thermal correction to Gibbs Free Energy= 0.158820

C	-1.02730300	1.84680700	-0.58989300
N	-2.15801200	1.29523100	-0.50856400
N	-3.27885500	0.67218600	-0.38808900
C	-3.48181000	-0.56596900	0.22787900
S	-4.99943800	-1.24411200	0.22504900
H	-4.14322000	1.11708700	-0.69208900
H	-0.94689400	2.89282200	-0.90173500
C	0.27793100	1.20283800	-0.31053100
C	1.35215100	2.08719200	0.17265700
C	0.54300000	-0.10815000	-0.55897600
C	1.82570100	-0.70001800	-0.32072600

H	-0.23661900	-0.73617800	-0.97827400
C	2.85625600	0.12775500	0.17458200
O	1.22651400	3.28450800	0.38656800
N	2.57237200	1.45906200	0.39104800
H	3.30043000	2.07309700	0.73335000
N	-2.38701900	-1.10015900	0.79352400
H	-1.55282100	-0.54408900	0.91238000
C	4.12691800	-0.40192200	0.42621100
C	4.37092000	-1.74126400	0.18265300
H	5.35638700	-2.14618000	0.37816100
C	3.36147800	-2.57498600	-0.31507800
H	3.56667600	-3.62080200	-0.50460700
C	2.10648000	-2.05575900	-0.56350400
H	1.31729300	-2.69058800	-0.95026800
H	4.91240900	0.24071000	0.80758600
H	-2.50448700	-1.93952100	1.33508000

ODCTSC GS (N5=Me)

Electronic Energy E(B3LYP): -1157.19087259
Zero-point correction= 0.230816 (Hartree/Particle)
Thermal correction to Energy= 0.247152
Thermal correction to Enthalpy= 0.248097
Thermal correction to Gibbs Free Energy= 0.184742

C	-0.66296400	-1.19577900	-0.00034600
N	-1.59606500	-0.31280300	-0.00015100
N	-2.87262500	-0.75060100	-0.00041300
C	-3.94746100	0.11044700	-0.00003700
S	-5.49975900	-0.51571500	-0.00034700
H	-3.09576700	-1.74111900	-0.00071000
H	-0.87962100	-2.26484400	-0.00061100
C	0.74519700	-0.83194500	-0.00018700
C	1.69288800	-1.95965500	0.00022300
C	1.21321300	0.44785900	-0.00046200
C	2.60630900	0.75845300	-0.00027800
H	0.50253100	1.26686800	-0.00084300
C	3.52887000	-0.31125600	0.00017300

O	1.37116300	-3.14064500	0.00045900
N	3.03130400	-1.59645000	0.00039600
H	3.67382100	-2.37816000	0.00069800
N	-3.63353700	1.41334900	0.00048800
H	-2.64928200	1.63910300	0.00067900
C	4.90474100	-0.05777400	0.00037000
C	5.36015400	1.24807000	0.00011300
H	6.42632600	1.43920100	0.00026500
C	4.45960800	2.32145900	-0.00034100
H	4.82977700	3.33867600	-0.00054200
C	3.10187600	2.07510700	-0.00053500
H	2.39526600	2.89716400	-0.00088600
H	5.60504800	-0.88547300	0.00071800
C	-4.61718400	2.48028300	0.00093100
H	-5.25577100	2.42441800	-0.88221600
H	-5.25568600	2.42377900	0.88410100
H	-4.08483400	3.43091400	0.00124800

ODCTSC TS (N5=Me)

Electronic Energy E(B3LYP): -1157.13088483
Zero-point correction= 0.229415 (Hartree/Particle)
Thermal correction to Energy= 0.245372
Thermal correction to Enthalpy= 0.246316
Thermal correction to Gibbs Free Energy= 0.184385

C	-0.76095200	2.09523800	-0.54231900
N	-1.92080200	1.59938800	-0.52994700
N	-3.07246700	1.02876200	-0.48026300
C	-3.35436000	-0.25101200	0.03219100
S	-4.90965800	-0.83650100	-0.07689400
H	-3.90813500	1.54037200	-0.75791400
H	-0.61875500	3.15695200	-0.76608200
C	0.50015100	1.35907000	-0.29009800
C	1.60428400	2.13281000	0.30355300
C	0.70316700	0.06366500	-0.65222800
C	1.94251100	-0.62073600	-0.43136800

H	-0.09359200	-0.47634400	-1.15426500
C	2.99816200	0.09731700	0.17071300
O	1.53786800	3.31146400	0.62158400
N	2.77969100	1.41766400	0.50072200
H	3.52744300	1.95517900	0.92045200
N	-2.31157100	-0.86876000	0.59321000
H	-1.45386900	-0.34026300	0.67271700
C	4.22806200	-0.52572300	0.41110300
C	4.40756300	-1.84886300	0.05069600
H	5.36171600	-2.32613300	0.23810300
C	3.37307000	-2.57342600	-0.55450200
H	3.52797500	-3.60718500	-0.83579900
C	2.15791500	-1.96186500	-0.79186800
H	1.35049300	-2.51167500	-1.26229000
H	5.03313500	0.03291400	0.87508600
C	-2.39403100	-2.17400300	1.22474400
H	-3.07581000	-2.15432800	2.07745800
H	-2.75934700	-2.91885500	0.51710200
H	-1.39688300	-2.45251900	1.56329900

ODCTSC GS (N5=Ph)

Electronic Energy E(B3LYP): -1348.97783704
Zero-point correction= 0.283503 (Hartree/Particle)
Thermal correction to Energy= 0.302634
Thermal correction to Enthalpy= 0.303578
Thermal correction to Gibbs Free Energy= 0.232479

C	-0.87269500	-1.82030700	0.01115200
N	0.27492600	-1.24254500	-0.00506000
N	1.37206900	-2.02795100	-0.01098200
C	2.65808400	-1.52412600	-0.00892000
S	3.91874300	-2.62116800	0.00718900
H	1.30177900	-3.04111000	0.00432500
H	-0.97069900	-2.90646200	0.02951800
C	-2.11790600	-1.06997900	0.00668300
C	-3.34597200	-1.88043600	0.07835600

C	-2.20324400	0.28833800	-0.06417400
C	-3.45054800	0.98178900	-0.06771400
H	-1.29017300	0.87025800	-0.12323900
C	-4.63802000	0.21979900	0.00330300
O	-3.37159300	-3.10251900	0.14027700
N	-4.52577400	-1.15206000	0.07174600
H	-5.36353600	-1.71739700	0.12194100
N	2.69354500	-0.17257700	-0.00964400
H	1.77076900	0.24469100	0.04162900
C	-5.88520400	0.85346000	0.00223400
C	-5.95152300	2.23290900	-0.06956400
H	-6.91938100	2.71921400	-0.07019400
C	-4.78414800	3.00465700	-0.14143100
H	-4.85118000	4.08357700	-0.19746900
C	-3.55228700	2.38315500	-0.14056200
H	-2.64208900	2.96915200	-0.19666000
H	-6.79100500	0.26025900	0.05723700
C	3.76190200	0.74836200	0.00931300
C	3.43927800	2.06085300	0.37598300
C	5.07682200	0.44227800	-0.34588300
C	4.41141300	3.04910500	0.39241600
H	2.41935600	2.30222200	0.65708900
C	6.04306300	1.44254400	-0.32061500
H	5.33572300	-0.56520300	-0.62965300
C	5.72440800	2.74467500	0.04599700
H	4.14173000	4.05769600	0.68203700
H	7.06041800	1.19216400	-0.59712300
H	6.48723700	3.51324400	0.06146300

ODCTSC TS (N5=Ph)

Electronic Energy E(B3LYP): -1348.91778746
Zero-point correction= 0.282020 (Hartree/Particle)
Thermal correction to Energy= 0.300799
Thermal correction to Enthalpy= 0.301743
Thermal correction to Gibbs Free Energy= 0.232143

C	-0.58249100	-2.90125200	-0.05554800
N	0.67197200	-2.84592900	-0.19254100
N	1.93990000	-2.69443000	-0.34809700
C	2.68022400	-1.49551300	-0.26302000
S	4.29934900	-1.57014900	-0.63153700
H	2.53501500	-3.50844400	-0.49325900
H	-1.07625600	-3.87265300	0.03892400
C	-1.51589100	-1.75266300	-0.02223500
C	-2.77056300	-1.95639300	0.72318300
C	-1.31907200	-0.59254200	-0.70581700
C	-2.26269900	0.48457600	-0.69766600
H	-0.42427400	-0.47635300	-1.30890900
C	-3.45899800	0.31292200	0.03174700
O	-3.05822400	-2.97241000	1.34009700
N	-3.65067600	-0.88198100	0.69203700
H	-4.50541900	-1.03017400	1.21325400
N	1.93726900	-0.45636400	0.16269600
H	1.00430300	-0.71679800	0.46181700
C	-4.41581100	1.33330400	0.06860400
C	-4.18505400	2.51232800	-0.61678400
H	-4.92876400	3.29931100	-0.58603700
C	-3.00478200	2.69763000	-1.34776300
H	-2.83669100	3.62543000	-1.87940000
C	-2.05845300	1.69307000	-1.38577700
H	-1.13988000	1.82612100	-1.94554100
H	-5.33161100	1.19296100	0.63168900
C	2.27464400	0.89843400	0.38850100
C	1.49330800	1.59580200	1.31507400
C	3.29400000	1.56349900	-0.29347300
C	1.73308400	2.93917300	1.56466900
H	0.70043500	1.07901800	1.84496600
C	3.52615700	2.90911300	-0.03127000
H	3.90111300	1.03141700	-1.00889700
C	2.75530100	3.60363400	0.89419600
H	1.12185200	3.46414500	2.28869800
H	4.32186900	3.41688900	-0.56317900
H	2.94783800	4.65099500	1.09129200

MSTSC GS (N5=H)

Electronic Energy E(B3LYP): -1062.65802381
Zero-point correction= 0.199660 (Hartree/Particle)
Thermal correction to Energy= 0.214243
Thermal correction to Enthalpy= 0.215187
Thermal correction to Gibbs Free Energy= 0.156504

C	-2.78097800	-0.29198700	-0.02081900
C	-1.43431700	2.19211500	0.24182600
C	-3.44100200	0.84617000	0.35049100
C	-1.34403100	-0.26674900	-0.29537300
C	-0.69129500	1.03200000	-0.14999100
C	-2.76567000	2.09877400	0.48398500
C	0.66822100	1.13406400	-0.39887500
N	1.42406200	0.10238500	-0.76491600
N	2.77871800	0.26277600	-0.99029800
C	3.70188500	-0.20096500	-0.06073500
S	3.31798900	-0.70749100	1.46480800
N	4.97240400	-0.19202600	-0.55787000
H	5.21253100	0.43537700	-1.31314600
O	-0.72267700	-1.29773100	-0.63750500
O	-3.33910700	-1.51734500	-0.17290500
C	-4.72685900	-1.65136900	0.07999800
H	-0.91415200	3.13826400	0.34384700
H	-4.50356900	0.81553300	0.55314100
H	-3.33547500	2.96926700	0.78309100
H	1.18099700	2.08555500	-0.30473000
H	5.69939800	-0.37468300	0.11547300
H	-5.31835500	-1.02744200	-0.59847500
H	-4.96258000	-2.69904400	-0.09418900
H	-4.97038800	-1.39065200	1.11529400
H	0.94681700	-0.81787300	-0.78023500
H	3.02921600	0.14190100	-1.96516300

MSTSC TS (N5=H)

Electronic Energy E(B3LYP): -1062.62239159
Zero-point correction= 0.198796 (Hartree/Particle)
Thermal correction to Energy= 0.213077
Thermal correction to Enthalpy= 0.214021
Thermal correction to Gibbs Free Energy= 0.156478

C	-2.98003900	-0.20853100	0.05991300
C	-1.31609600	2.05155900	-0.49181600
C	-3.50076200	1.02951700	-0.12298400
C	-1.52018000	-0.45573200	-0.12776500
C	-0.66227100	0.78138400	-0.22426800
C	-2.65617900	2.15996000	-0.43556900
C	0.67635300	0.76515900	-0.04843500
N	1.41339700	-0.36300300	0.41208100
N	2.44750200	-0.68093700	-0.49512800
C	3.75048800	-0.39459900	-0.22262700
S	4.22944200	0.56568600	1.06166700
N	4.64195700	-0.99225200	-1.06439000
H	4.34415000	-1.28429400	-1.98470000
O	-1.09321100	-1.58517400	-0.26878000
O	-3.66642800	-1.33445700	0.33641900
C	-5.07575300	-1.23544100	0.47980800
H	-0.69331200	2.91803500	-0.68092800
H	-4.56791700	1.19490300	-0.05666700
H	-3.13223400	3.11867600	-0.60203600
H	1.24107000	1.68121800	-0.22946500
H	5.59656400	-0.68273500	-0.97923100
H	-5.54238800	-0.89287800	-0.44903300
H	-5.42287600	-2.23906800	0.71360500
H	-5.34328500	-0.55520900	1.29448100
H	1.87525700	-0.13678700	1.29840400
H	2.23766500	-1.52210400	-1.01772300

MSTSC GS (N5=Me)

Electronic Energy E(B3LYP): -1101.97475346
Zero-point correction= 0.227702 (Hartree/Particle)

Thermal correction to Energy= 0.243917
Thermal correction to Enthalpy= 0.244861
Thermal correction to Gibbs Free Energy= 0.181965

C	-3.12060000	-0.28765700	-0.08467600
C	-1.74690000	2.18830200	0.09104500
C	-3.77860900	0.88007000	0.18500500
C	-1.67352000	-0.29806200	-0.29736700
C	-1.00635000	0.99678600	-0.19539400
C	-3.08992100	2.12892800	0.27366400
C	0.36753100	1.06240800	-0.37065200
N	1.11762200	-0.00061500	-0.64508800
N	2.49158200	0.11084200	-0.75701300
C	3.31585100	-0.21615300	0.31057900
S	2.77099900	-0.41863400	1.86951100
N	4.62358000	-0.31661500	-0.02491200
O	-1.05517100	-1.35661900	-0.55307300
O	-3.69125300	-1.51307500	-0.18521100
C	-5.08896200	-1.61378900	0.02336700
H	-1.21568700	3.13106400	0.16313300
H	-4.84967400	0.87603500	0.33945700
H	-3.65826500	3.02394000	0.49237800
H	0.89478800	2.00703100	-0.29095100
H	5.22908900	-0.50237800	0.75803100
H	-5.64662100	-1.02956700	-0.71646000
H	-5.33303000	-2.66792900	-0.09002500
H	-5.36682900	-1.28187800	1.02930400
H	0.61906300	-0.91031700	-0.62327100
H	2.82469200	-0.09194100	-1.69006200
C	5.21257100	-0.07516600	-1.33137200
H	4.88324700	-0.81128200	-2.07297200
H	4.98552500	0.92962900	-1.69954300
H	6.29307000	-0.16597300	-1.24102200

MSTSC TS (N5=Me)

Electronic Energy E(B3LYP): -1101.93976234

Zero-point correction= 0.226809 (Hartree/Particle)
Thermal correction to Energy= 0.242722
Thermal correction to Enthalpy= 0.243666
Thermal correction to Gibbs Free Energy= 0.181928

C	3.25256200	-0.25017400	-0.08044100
C	1.68102300	1.89644100	0.96833800
C	3.82625500	0.86182300	0.44100100
C	1.77329700	-0.43973200	-0.02833700
C	0.97810600	0.78420100	0.35103300
C	3.02598300	1.92726600	1.00027400
C	-0.34765700	0.90262100	0.12195300
N	-1.11632900	-0.01333800	-0.65038900
N	-2.21790200	-0.48059100	0.10336000
C	-3.48729800	-0.06120900	-0.16237800
S	-3.82111100	1.22441100	-1.19685800
N	-4.46909900	-0.75240200	0.46093500
H	-5.39913700	-0.42122500	0.26509300
O	1.27993600	-1.53675100	-0.20673700
O	3.89462800	-1.31013500	-0.61016900
C	5.31309800	-1.27053500	-0.65982700
H	1.09440900	2.72406700	1.34959900
H	4.90274800	0.96733100	0.46648700
H	3.54123300	2.77726800	1.43092100
H	-0.87315900	1.77448800	0.51536800
H	5.74053300	-1.20909100	0.34589900
H	5.62111100	-2.20119500	-1.13048300
H	5.66451800	-0.42317600	-1.25700500
H	-1.52031000	0.47359000	-1.45784400
H	-2.06829900	-1.42731200	0.42482200
C	-4.28106200	-1.81982500	1.42772200
H	-3.65241100	-1.49828200	2.26310000
H	-5.25514300	-2.10083400	1.82287700
H	-3.83736000	-2.71206400	0.97278000

MSTSC GS (N5=Ph)

Electronic Energy E(B3LYP): -1293.76570936
Zero-point correction= 0.280337 (Hartree/Particle)
Thermal correction to Energy= 0.299423
Thermal correction to Enthalpy= 0.300367
Thermal correction to Gibbs Free Energy= 0.229311

C	-4.37683100	-0.29283200	0.48458400
C	-3.12453600	-0.78549300	-2.01298500
C	-5.10131500	-0.60582200	-0.63189900
C	-2.91791600	-0.20348400	0.42790600
C	-2.31539900	-0.46309100	-0.87655000
C	-4.47393700	-0.85424000	-1.89147100
C	-0.93763300	-0.38503500	-1.00988800
N	-0.12260500	-0.09455200	-0.00020200
N	1.24079300	0.01932100	-0.19855000
C	1.82474600	1.26202800	-0.35107400
S	0.97221700	2.65334100	-0.66679700
N	3.18657900	1.26796900	-0.24383900
O	-2.23712000	0.07612900	1.44088300
O	-4.88740600	-0.04264300	1.71505900
C	-6.29421000	-0.09684600	1.87363200
H	-2.64066600	-0.96711700	-2.96645700
H	-6.18023800	-0.66978600	-0.57806300
H	-5.09459300	-1.09463400	-2.74523100
H	-0.46055300	-0.56368200	-1.96761200
H	3.56712100	2.20298300	-0.26157300
H	-6.68322800	-1.09491900	1.64546100
H	-6.48655600	0.13623600	2.91875600
H	-6.79621500	0.64020800	1.23796200
H	-0.59203100	0.16379400	0.88799000
H	1.78035100	-0.69533300	0.27542600
C	4.08228600	0.20431800	0.04852600
C	4.06450500	-0.99231000	-0.67303500
C	5.04438900	0.39295200	1.04385800
C	4.98045900	-1.99546500	-0.37506700
H	3.35595900	-1.12490900	-1.48047200
C	5.96964200	-0.60541100	1.31843800

H	5.05760500	1.32125200	1.60305600
C	5.93547700	-1.80749500	0.61803300
H	4.95797900	-2.92006600	-0.93917300
H	6.71215300	-0.44674000	2.09106400
H	6.65193500	-2.58844300	0.84016900

MSTSC TS (N5=Ph)

Electronic Energy E(B3LYP): -1293.73019358
Zero-point correction= 0.279595 (Hartree/Particle)
Thermal correction to Energy= 0.298301
Thermal correction to Enthalpy= 0.299245
Thermal correction to Gibbs Free Energy= 0.230038

C	4.16794600	-0.66568200	-0.21564100
C	3.05549300	1.14356800	1.70033000
C	4.91648400	-0.14301300	0.78630400
C	2.70177500	-0.39646300	-0.29031500
C	2.20002900	0.70445000	0.61035700
C	4.33835600	0.74340500	1.77070500
C	1.01044900	1.31769400	0.43191200
N	0.16977100	1.13242400	-0.70330100
N	-1.12216200	0.73163900	-0.29683400
C	-2.17170700	1.59056200	-0.32275500
S	-1.99167400	3.24061900	-0.59470300
N	-3.41371400	1.04994000	-0.14049100
H	-4.15248600	1.71366100	-0.31992100
O	1.97627200	-1.08601200	-0.98002900
O	4.59052700	-1.51314600	-1.17412100
C	5.95803200	-1.89563000	-1.16726300
H	2.64947800	1.84599300	2.41880900
H	5.96435500	-0.39466100	0.88168800
H	4.97836200	1.10504500	2.56637800
H	0.67460300	2.04000700	1.17793000
H	6.21362200	-2.42481200	-0.24396400
H	6.08530300	-2.56231300	-2.01684000
H	6.61263500	-1.02590200	-1.28193300

H	0.04565900	2.02822100	-1.18562200
H	-1.28719400	-0.25405500	-0.45923400
C	-3.79850800	-0.29502600	0.08680700
C	-4.91810300	-0.78719700	-0.58991100
C	-3.13698100	-1.11530400	1.00477100
C	-5.36308400	-2.08137700	-0.35814700
H	-5.43147500	-0.15223900	-1.30290900
C	-3.57757800	-2.41771800	1.21316200
H	-2.29999100	-0.73024400	1.57185500
C	-4.68922300	-2.90701400	0.53682100
H	-6.23285000	-2.44904100	-0.88908800
H	-3.05447900	-3.04578800	1.92412100
H	-5.03069500	-3.92008400	0.70875100

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