Theoretical study of the mechanism for the sequential N−O and N−N bond cleavage within N2O adducts of N−heterocyclic carbenes by a vanadium(III) complex

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Supporting Information

Contents:

Full citation for the Gaussian09 program

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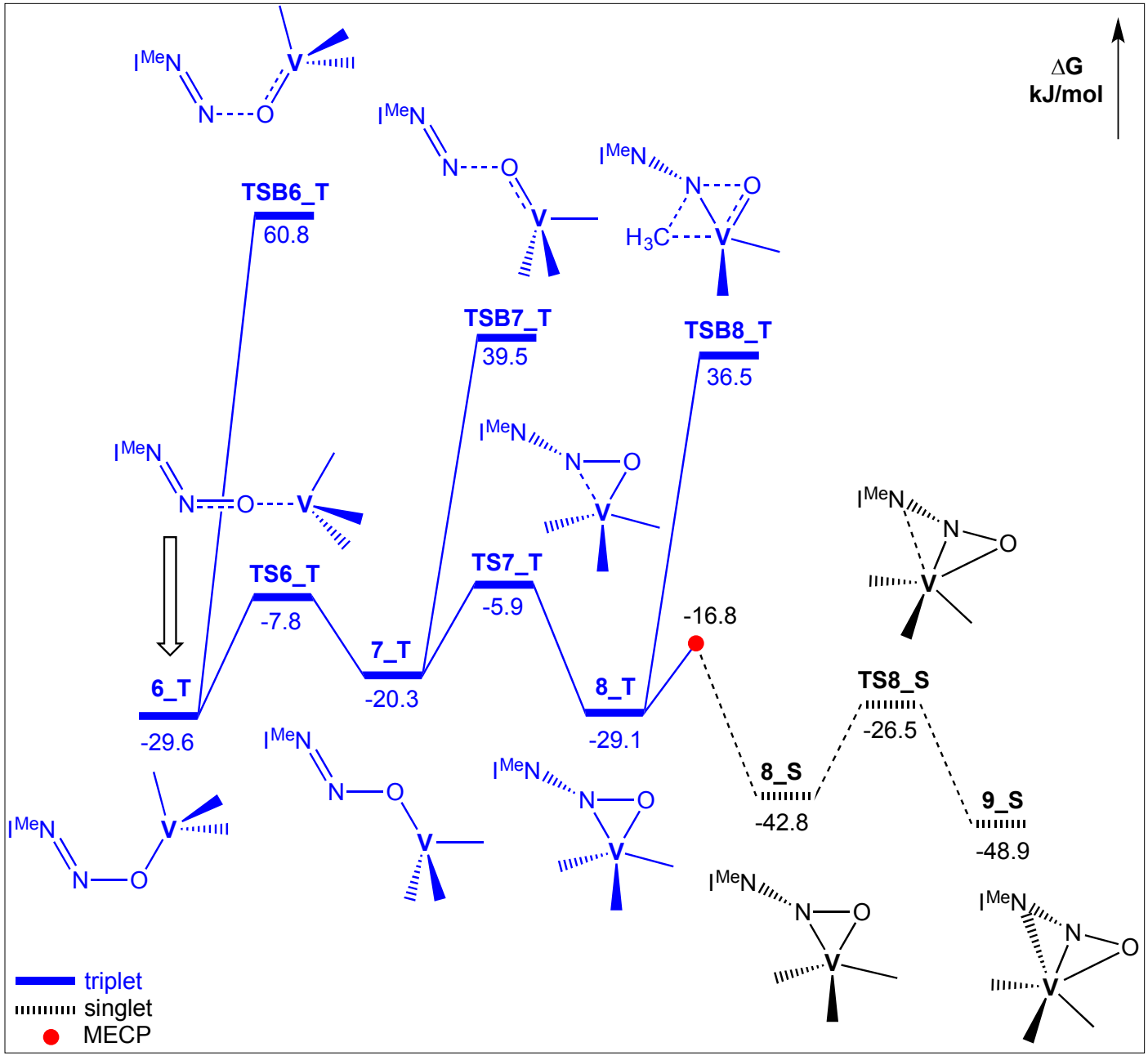

Fig. S1. Calculated reaction profile for N−O bond cleavage from **6_T**-**8_T**. All energies are relative to **1_T−thf** and *normal* $\mathbf{I^{Me}–N_2O}$ in THF.

Table S1. Calculated energies (kJ/mol) and selected bond lengths (Å) for all stable I^{Me}-N_2O-$V(CH_3)_3$ complexes[a,b]

Triplet-state							*Singlet-state*						
Normal	**η**	**ΔG**	**N2-O**	**N1-N2**	**V-O**	**V-N**	*Normal*	**η**	**ΔG**	**N2-O**	**N1-N2**	**V-O**	**V-N**
4_T	N1	-20.9	1.227	1.348	-	2.057	**4_S**	N1	99.4	1.219	1.367	-	1.962
5_T	N1,O	-22.3	1.337	1.343	1.890	2.253							
6_T	O_{syn}	-29.6	1.324	1.327	1.830	-	**6_S**	O_{syn}	51.8	1.298	1.347	1.768	-
7_T	O_{anti}	-20.3	1.340	1.315	1.815	-	**7_S**	O_{anti}	50.6	1.298	1.346	1.724	-
8_T	N2,O	-29.1	1.343	1.321	1.899	2.025	**8_S**	N2,O	-42.8	1.395	1.375	1.775	1.909
9_T	N1,N2,O	-11.5	1.357	1.337	1.858	2.026 1.888	**9_S**	N1,N2,O	-48.9	1.377	1.423	1.858	2.026 1.888
11_T	N2	-11.3	1.226	1.345	-	2.056							
Inverted							*Inverted*						
4i_T	N1	-11.2	1.227	1.345	-	2.055							
7i_T	O_{anti}	-1.7	1.342	1.309	1.833	-	**7i_S**	O_{anti}	87.5	1.321	1.337	1.751	-
8i_T	N2,O	-17.5	1.357	1.319	1.911	2.001	**8i_S**	N2,O	-29.4	1.442	1.382	1.761	1.894
							9i_S	N1,N2,O	-43.8	1.409	1.418	1.837	1.985 1.895
10i_T	N1,N2	9.6	1.248	1.407	-	1.989 2.032							
11i_T	N2	-15.7	1.257	1.323	-	1.950							

[a]All ΔG energies are relative to **1_T−thf** and *normal* $\mathbf{I^{Me}–N_2O}$ in THF.
[b]Attempts to locate **9i_T** led to formation of **8i_T**. Complex **10_T** led to **9_T**. Both **5_S** and **11_S** led to **8_S**. Complex **11i_S** to **8i_S**. Complexes **10_S**, **4i_S** and **10i_S** to the unobserved N−N insertion product, $(I^{Me}–N)V(CH_3)_3(NO)$.

As discussed in the computational details section, the calculated energy values throughout the article were obtained at the M06/BS2//M06/BS1 level of theory in THF solvation. As such, the methodology of the calculated Gibbs energies for the formation of $O{=}V(Me)_2(I^{Me}N_2Me)$ **(2_S)** were carried out on the corresponding stationary points (**1_T-thf**, **I^{Me}–N_2O**, **2_S** and thf) at different levels of theory and the results are shown below in Table S1.

Table S2. Effect of DFT functional method on the calculated Gibbs energy values

Level of theory		**ΔG** (kJ/mol)
G_{corr}[a]	**SPE**[b]	**1_T-thf+I^{Me}–N_2O → 2_S+thf**
M06	B3LYP	-213.9
M06	M06	-308.1
B3LYP	B3LYP	-219.9
B3LYP	M06	-320.7

[a]All energies calculated with BS1 (SDD for Mo; 6-31G(d) for all other elements).
[b]All energies calculated with BS2 (def2-QZVP for Mo; 6-311+G(2d,p) for all other elements).

Similarly, calculations were carried out on the corresponding stationary points with Ph substituents/ligands (**1_T_P-thf**, **I^{Ph}–N_2O**, **2_S_P**) at different levels of theory and the results are shown below in Table S2.

Table S3. Effect of DFT functional method on the calculated Gibbs energy values

Level of theory		**ΔG** (kJ/mol)
G_{corr}[a]	**SPE**[b]	**1_T_P-thf+ I^{Ph}–N_2O → 2_S_P+thf**
M06	M06	-357.5
B3LYP	B3LYP	-231.4
B3LYP-D3BJ	M06	-363.4
B3LYP-D3BJ	B3LYP-D3BJ	-294.5

[a]All energies calculated with BS1 (SDD for Mo; 6-31G(d) for all other elements).
[b]All energies calculated with BS2 (def2-QZVP for Mo; 6-311+G(2d,p) for all other elements).

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for $I^{Me}–N_2O$ (*normal/inverted*), $TSI^{Me}–N_2O$ and $I^{Ph}–N_2O$ (singlet) in Solvent = THF

I^{Me}-N_2O (*normal*)

E_{elec} (M06/BS1) = -489.47945068 au
H_{corr} (M06/BS1) = 0.152303 au
G_{corr} (M06/BS1) = 0.405391 au
SPE (M06/BS2//M06/BS1) = -489.31808050 au

0 1

O	4.11474600	6.35269700	1.42644000
N	7.05135500	4.35916700	3.35175800
N	6.02499500	2.53217700	2.75157400
N	4.92211400	4.47156500	2.06366300
N	5.06637200	5.80100400	1.97831700
C	5.95780800	3.88672800	2.68828800
C	7.79311400	3.28109400	3.81949200
H	8.70835000	3.43353000	4.37430200
C	7.15710900	2.15053400	3.44860700
H	7.39665400	1.10964800	3.61344400
C	7.41867900	5.74665800	3.59173500
H	7.64229700	6.25822800	2.65267200
H	8.30334900	5.74804000	4.23477600
H	6.60293200	6.27671400	4.08979900
C	5.03831900	1.65037800	2.15752500
H	4.04885100	1.85317800	2.57780800
H	5.32463100	0.61892400	2.37578200
H	4.99852700	1.79943800	1.07431800

TSI^{Me}-N_2O

E_{elec} (M06/BS1) = -486.15652588 au
H_{corr} (M06/BS1) = 0.150396 au
G_{corr} (M06/BS1) = 0.105228 au
SPE (M06/BS2//M06/BS1) = -489.29184585 au

0 1

C	2.18750900	0.60903500	-0.14738000
C	1.34064900	1.65293200	-0.10412700
C	0.10549500	-0.22317400	0.10438200
N	1.42982300	-0.55140200	-0.01969800
H	3.26220500	0.56801500	-0.25537500
H	1.51773100	2.71737800	-0.16790300
N	0.04613600	1.14838900	0.05429300
C	1.90053000	-1.91538300	-0.00708100
H	1.70312500	-2.38621700	0.96352400
H	1.39493900	-2.49768600	-0.78627700
H	2.97683700	-1.91712000	-0.19627200
C	-1.15966700	1.94728000	0.12689100
H	-1.72227600	1.72463600	1.03972700
H	-0.86974200	3.00091600	0.14707200
H	-1.80457600	1.77065800	-0.74155100
N	-0.82387300	-1.12075600	0.24723800
N	-2.14148300	-0.81481000	0.42734800
O	-2.78608500	-0.75905400	-0.60243800

I^{Me}-N_2O (inverted)

E_{elec} (M06/BS1) = -489.17786517 au
H_{corr} (M06/BS1) = 0.151561 au
G_{corr} (M06/BS1) = 0.105799 au
SPE (M06/BS2//M06/BS1) = -489.31367020 au

0 1

O	6.10796100	5.89174500	1.14658200
N	7.10018000	4.35429700	3.39251800
N	6.04009700	2.56413900	2.76655500
N	4.85697800	4.59376800	2.40683700
N	4.98198700	5.65098700	1.62112400
C	5.97470000	3.91545300	2.78012700
C	7.87604000	3.26586300	3.75462500
H	8.82487000	3.39210200	4.25705200
C	7.21719300	2.15135500	3.36266700
H	7.47278800	1.10471100	3.44975800
C	7.39353700	5.74262100	3.69150000
H	7.67866900	6.26851800	2.77534600
H	8.19482000	5.77727500	4.43322000
H	6.49722800	6.21835200	4.10275500
C	5.02141700	1.71577200	2.17462000
H	4.03545300	2.05803300	2.49924600
H	5.18590400	0.68907600	2.50892700
H	5.07322000	1.75849800	1.08224200

I^{Ph}-N_2O (*normal*)

E_{elec} (M06/BS1) = -872.35858883 au
H_{corr} (M06/BS1) = 0.262389 au
G_{corr} (M06/BS1) = 0.201261 au
SPE (M06/BS2//M06/BS1) = -872.58514436 au

0 1

O	0.88256300	3.18678600	0.04373200
N	0.97753600	-0.79597900	-0.22294000
N	-1.20505200	-0.77909300	-0.15043700
N	-0.18727400	1.32984800	0.20446400
N	0.86777700	2.00664100	-0.28987800
C	-0.10464000	0.02371500	-0.06011300
C	0.53750100	-2.10446200	-0.42304800
H	1.24324100	-2.91014000	-0.56846900
C	-0.80701100	-2.09494800	-0.37046700
H	-1.53158900	-2.88674300	-0.49589500
C	2.36014700	-0.46621800	-0.05225100
C	3.24740000	-0.74126700	-1.08540800
C	4.60371500	-0.49276800	-0.89928500
H	5.30439700	-0.70405700	-1.70426000
C	5.05902100	0.03061400	0.30617700
C	4.15825000	0.29931400	1.33478500
H	4.51370600	0.70301100	2.28047800
C	2.80443600	0.04239400	1.16478100
C	-2.56195800	-0.35550600	-0.03436400
C	-3.42500500	-1.10344000	0.76183900
C	-4.76101700	-0.73117100	0.85683500
H	-5.43676500	-1.31424400	1.47886200
C	-5.22500400	0.38673600	0.17091600
C	-4.35072700	1.13075700	-0.61701000
H	-4.71002600	2.00403000	-1.15723800
C	-3.01611200	0.76106500	-0.73069100
H	-3.04653000	-1.96186200	1.31433200
H	-2.32891400	1.33137300	-1.34943800
H	-6.26969600	0.67999400	0.25034200
H	2.87183800	-1.13710600	-2.02764900
H	2.08935200	0.23999100	1.96111200
H	6.11947700	0.22901700	0.44726200

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 1-thf, 1, 1-thf$_P$ & 1$_P$ (triplet) in Solvent = THF

1-thf_T

E_{elec} (M06/BS1) = -423.54065376 au
H_{corr} (M06/BS1) = 0.236754 au
G_{corr} (M06/BS1) = 0.176691 au
SPE (M06/BS2//M06/BS1) = -423.10393712 au

0 3

V	-0.41331500	-0.45515600	0.22919800
C	0.02736400	0.72004000	-1.40704600
H	-0.28428100	1.76431200	-1.22702800
H	1.11694900	0.72352800	-1.58536600
H	-0.46784300	0.37315100	-2.32864200
C	0.29695600	-2.38991200	0.14209800
H	1.38719500	-2.37392800	-0.03098400
H	0.12012600	-2.90772300	1.10141200
H	-0.16713000	-2.98983700	-0.65733600
C	-2.32628400	-0.23433400	0.96003300
H	-2.43015800	-0.72872700	1.94175200
H	-2.54308800	0.83910800	1.10298300
H	-3.09531100	-0.64841900	0.28754800
O	0.85695600	0.35230500	1.61348200
C	0.99998100	1.79162200	1.73434200
C	1.03631000	-0.28274200	2.90844900
C	1.66828800	1.99037000	3.07736200
H	1.57694800	2.13556800	0.87039000
H	-0.00401600	2.24136400	1.70404600
C	1.05522300	0.86227400	3.90030700
H	0.21530000	-0.99398500	3.05810800
H	1.98567900	-0.83264200	2.87458500
H	1.47610500	2.98522800	3.49135900
H	2.75468500	1.85673700	2.98778400
H	0.03071100	1.12295900	4.20024800
H	1.62557000	0.61757300	4.80193400

1_T

E_{elec} (M06/BS1) = -191.21552336 au
H_{corr} (M06/BS1) = 0.111711 au
G_{corr} (M06/BS1) = 0.066878 au
SPE (M06/BS2//M06/BS1) = -190.70294840 au

0 3

V	0.21208100	0.08900800	0.63252500
C	2.16881800	0.14764800	0.06387800
H	2.60358300	-0.81333100	0.38909400
H	2.28656000	0.22855800	-1.02568300
H	2.72547400	0.96538700	0.54805200
C	-0.67025600	1.70368400	-0.24453600
H	-1.75596400	1.54202200	-0.12663900
H	-0.40293900	2.65782200	0.23567300
H	-0.44724400	1.76638500	-1.31895700
C	-0.72744200	-1.68601800	0.25601900
H	-1.16685300	-2.07085900	1.19372800
H	-1.53703700	-1.55230800	-0.47618400
H	-0.01747000	-2.43466800	-0.12605500

1-thf_T_P

E_{elec} (M06/BS1) = -998.30395409 au
H_{corr} (M06/BS1) = 0.411241 au
G_{corr} (M06/BS1) = 0.328097 au
SPE (M06/BS2//M06/BS1) = -998.02115452 au

0 3

V	0.00345800	-0.01357900	-0.12817100
C	-0.94609500	-1.71979000	-0.73719600
C	-0.27386800	-2.73305900	-1.44372200
C	-0.79117400	1.70721400	-0.89185100
C	-0.92791100	-3.89182700	-1.86446200
C	-2.18101000	1.90468200	-0.99314300
C	-2.28089300	-4.06754900	-1.58715700
C	-2.72079000	3.11217300	-1.43113600
C	-2.97490900	-3.08220400	-0.88561300
C	-1.87688900	4.16440600	-1.78372000
C	-2.31183700	-1.93071400	-0.46817800
C	-0.49686700	3.99935800	-1.69678500
C	0.03435800	2.78607600	-1.25714200
C	2.04166000	-0.11066400	-0.26961000
C	2.68123700	-0.16885100	-1.52212600
O	-0.59213100	0.09216600	1.80182800
C	4.06752500	-0.23956900	-1.63398100
C	-0.53785800	1.33292300	2.56469900
C	4.85734700	-0.25050300	-0.48416700
C	-0.26768100	0.89435800	3.98966900
C	4.25623800	-0.18780400	0.76976500
C	-0.93930600	-0.47461900	4.04553100
C	2.86561200	-0.11883200	0.86760800
C	-0.58747800	-1.05718200	2.69440200
H	-0.38018100	-4.66109000	-2.40923200
H	-3.80193700	3.23515200	-1.50001300
H	-4.03375600	-3.21638700	-0.66297600
H	0.16746400	4.81828300	-1.97370700
H	4.53688800	-0.28725900	-2.61667000
H	0.24340700	1.96573500	2.12731700
H	-1.50958600	1.82795900	2.44464400
H	0.81254800	0.79762500	4.16447200
H	-0.66881700	1.60534000	4.71879200
H	4.87075300	-0.19348700	1.67008100
H	-0.58048500	-1.09989400	4.86901600
H	-2.02782000	-0.36687300	4.14256400
H	0.42048100	-1.49834600	2.67733800
H	-1.30560300	-1.77944700	2.29434600

H	-2.87831600	-1.17466200	0.08704500
H	-2.79491300	-4.97078200	-1.91386400
H	0.79006100	-2.62211300	-1.66995100
H	2.07956100	-0.15933000	-2.43784800
H	5.94195300	-0.30693600	-0.56847300
H	1.12145800	2.68139700	-1.19806900
H	-2.86501700	1.09352500	-0.72385400
H	-2.29491500	5.10956500	-2.12847200
H	2.41816200	-0.07073500	1.86617600

1_T_P

E_{elec} (M06/BS1) = -765.97197072 au
H_{corr} (M06/BS1) = 0.286546 au
G_{corr} (M06/BS1) = 0.219363 au
SPE (M06/BS2//M06/BS1) = -765.61753425 au

0 3

V	0.20550600	0.26019800	0.58620800
C	-0.87002900	1.67213700	-0.38586100
C	-0.48303400	3.00101800	-0.13758900
C	-1.98044400	1.46074500	-1.22201000
C	-1.17070900	4.07701400	-0.69787000
H	0.37971100	3.21091600	0.50345100
C	-2.66601000	2.52932700	-1.79252200
H	-2.31302100	0.44337100	-1.43849100
C	-2.26263600	3.83814500	-1.52785400
H	-0.85479300	5.09901400	-0.49072600
H	-3.51950600	2.34513100	-2.44441300
H	-2.80155400	4.67370700	-1.97259200
C	-0.24772800	-1.62174900	0.00605500
C	-1.58445700	-1.93318600	0.31666000
C	0.51086400	-2.60168400	-0.65291600
C	-2.14664800	-3.16208100	-0.02823000
H	-2.22049800	-1.20332900	0.83250200
C	-0.04267400	-3.83349100	-0.99434000
H	1.55312400	-2.39840200	-0.90623500
C	-1.37257900	-4.11505900	-0.68526100
H	-3.18584900	-3.37765300	0.21960100
H	0.56394500	-4.57857500	-1.50905200
H	-1.80468500	-5.07758000	-0.95571000
C	2.20505400	0.37671400	0.27883300
C	3.01911700	-0.45165000	1.07295400
C	2.84465800	1.27265200	-0.59526100
C	4.41015600	-0.38710000	1.00551300
H	2.55909800	-1.17806800	1.75122200
C	4.23345000	1.34725600	-0.66402300
H	2.24627000	1.92752200	-1.23269300
C	5.01678200	0.51625600	0.13643800
H	5.02158600	-1.03951000	1.62858300
H	4.70939800	2.05053600	-1.34709700
H	6.10309700	0.57177400	0.07883800

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 1-thf, free THF & N2O (singlet) in Solvent = THF

1-thf_S

E_{elec} (M06/BS1) = -423.49811973 au
H_{corr} (M06/BS1) = 0.236408 au
G_{corr} (M06/BS1) = 0.178777 au
SPE (M06/BS2//M06/BS1) = -423.05748730 au

0 1

V	-0.43395600	-0.42215800	0.20047100
C	0.04700000	0.58012900	-1.50670300
H	-0.52098700	1.50840500	-1.28703300
H	1.09947000	0.86060900	-1.67712000
H	-0.35833700	0.15331000	-2.43996200
C	0.40402500	-2.28636000	0.14512200
H	1.50025900	-2.32499400	0.27329900
H	-0.05925000	-2.70481700	1.06228000
H	0.12698900	-2.94565500	-0.69319900
C	-2.31908700	-0.13819600	0.94720600
H	-2.50653900	-0.63866200	1.91137900
H	-2.55615000	0.93433800	1.05918900
H	-3.00509000	-0.56579800	0.19562100
O	0.64068100	0.38576900	1.67164400
C	0.89141500	1.81378300	1.80812700
C	0.97880800	-0.30236200	2.90984000
C	1.70389700	1.93985400	3.07941300
H	1.39992900	2.14338200	0.89691100
H	-0.08419300	2.31441300	1.88534000
C	1.14270200	0.80359900	3.92914400
H	0.16925900	-1.00742100	3.12627900
H	1.90945900	-0.85773400	2.73515500
H	1.59278200	2.92492700	3.54371600
H	2.76955000	1.77400700	2.87226800
H	0.16687000	1.08500600	4.34792900
H	1.79941200	0.51135900	4.75470500

THF (free)

E_{elec} (M06/BS1) = -232.28834496 au
H_{corr} (M06/BS1) = 0.122816 au
G_{corr} (M06/BS1) = 0.088775 au
SPE (M06/BS2//M06/BS1) = -232.35651638 au

0 1

C	-1.48234400	1.50140800	0.77638400
O	-0.71486000	0.73946800	-0.13454400
C	0.37049500	1.57589100	-0.49426600
C	-0.17709500	3.01366700	-0.52938600
C	-1.54982600	2.88966300	0.15428800
H	-2.45393100	1.01096300	0.90232700
H	-0.98018100	1.53991500	1.76210600
H	1.17513100	1.48755300	0.25766800
H	0.76328300	1.22290000	-1.45445000
H	0.48802900	3.69896700	0.00874100
H	-0.27189600	3.39006100	-1.55398400
H	-1.73727300	3.67675800	0.89301200
H	-2.35671300	2.92619700	-0.58790700

N_2O (free)

E_{elec} (M06/BS1) = -184.57266064 au
H_{corr} (M06/BS1) = 0.015198 au
G_{corr} (M06/BS1) = -0.009690 au
SPE (M06/BS2//M06/BS1) = -184.62841534 au

0 1

O	0.00000000	0.00000000	1.11193100
N	0.00000000	0.00000000	-1.20143700
N	0.00000000	0.00000000	-0.06934100

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 4-9, 11, 6-thf, 4i, 7i, 8i, 10i, 11i, 6-thf$_P$ & 8$_P$ (triplet) in Solvent = THF

4_T ($\eta^{\square}$-N1)

E_{elec} (M06/BS1) = -680.44150014 au
H_{corr} (M06/BS1) = 0.265933 au
G_{corr} (M06/BS1) = 0.195336 au
SPE (M06/BS2//M06/BS1) = -680.07567208 au

0 3

C	-4.46952200	0.30929000	-0.17242500
C	-3.62150700	1.28621200	-0.57906700
C	-2.39986800	-0.38814500	0.21099700
N	-3.69763500	-0.72121200	0.32510100
H	-5.54890100	0.25485000	-0.18098900
H	-3.81028900	2.25815000	-1.01278800
N	-2.33690800	0.83891100	-0.33794900
C	-4.19487900	-1.97977800	0.86034400
H	-4.49763800	-2.64156400	0.04228500
H	-3.39624900	-2.45430100	1.43522800
H	-5.04849500	-1.77693100	1.51180100
C	-1.10239100	1.53175700	-0.67984400
H	-0.37452500	0.80053600	-1.04710500
H	-1.31978200	2.25560700	-1.46811500
H	-0.69398900	2.04551200	0.19450800
N	-1.34553100	-1.21355600	0.49140500
N	-0.52335300	-0.74861200	1.45280000
O	0.44849900	-1.47897400	1.61815900
V	-0.67697000	-2.70709100	-0.75434900
C	-2.14274000	-2.46934500	-2.20222800
C	-0.74869200	-4.57969400	0.08895800
C	1.09978800	-2.22893100	-1.67330300
H	-1.92574300	-3.08381600	-3.09192600
H	-3.15427600	-2.74046900	-1.85175100
H	-2.18043100	-1.41251100	-2.53041600
H	-0.52296300	-5.35521700	-0.66292700
H	-0.02754300	-4.67465600	0.91718900
H	-1.75843800	-4.78078400	0.48751100
H	1.29581800	-2.97289600	-2.46595100
H	1.03416700	-1.23955000	-2.15877600
H	1.95662500	-2.21953000	-0.98172800

5_T (η^2-N1,O)

E_{elec} (M06/BS1) = -680.44452861 au
H_{corr} (M06/BS1) = 0.266182 au
G_{corr} (M06/BS1) = 0.198137 au
SPE (M06/BS2//M06/BS1) = -680.07262792 au

0 3

O	6.67819300	3.32407600	4.95286400
N	4.96921400	2.83195000	1.29921300
N	4.12518600	4.81856000	1.61024000
N	5.34038400	3.91145600	3.44852800
N	6.54040700	3.28218800	3.67249100
C	4.85536100	3.84254800	2.19210100
C	4.29630600	3.18618900	0.14095900
H	4.26280300	2.52406200	-0.71264500
C	3.76495500	4.41398400	0.33713200
H	3.16824200	5.04414400	-0.30687600
C	5.59300800	1.53573000	1.53239200
H	5.18366400	0.83119800	0.80401500
H	6.67788900	1.59954500	1.42215800
H	5.35470600	1.19375800	2.54312700
C	3.82053700	6.10562700	2.21231700
H	2.90821000	6.04517400	2.81363700
H	4.65551900	6.40477400	2.85357500
H	3.69231300	6.83989700	1.41320400
V	4.82522400	4.18553400	5.39450500
C	4.36487100	2.59409400	6.58899200
H	4.12362100	3.08721600	7.54786900
H	3.45757800	2.07713600	6.24188000
H	5.17864400	1.87473600	6.74265300
C	5.60603300	5.80012700	6.36171500
H	5.33335400	6.71282200	5.80693100
H	5.09526400	5.83194300	7.33927300
H	6.69213200	5.77223100	6.51502100
C	2.83629500	4.78353100	5.29471900
H	2.28558400	4.20750100	4.52936500
H	2.31036600	4.66172700	6.25515900
H	2.78253200	5.85036600	5.01620800

6_T ($\eta^{\square}$-O_{syn})

E_{elec} (M06/BS1) = -680.45080082 au
H_{corr} (M06/BS1) = 0.265707 au
G_{corr} (M06/BS1) = 0.196647 au
SPE (M06/BS2//M06/BS1) = -680.08028061 au

0 3

C	-4.07604100	0.65917000	-1.12759300
C	-3.68169700	1.57491300	-0.21753500
C	-2.11328300	-0.02139600	-0.28421900
N	-3.10543600	-0.32530100	-1.16696800
H	-4.95552400	0.61250900	-1.75424900
H	-4.14659400	2.49318900	0.11334900
N	-2.46557400	1.15852400	0.30946700
C	-3.10795300	-1.51155200	-1.99784500
H	-2.20232200	-1.54337800	-2.61413500
H	-3.14470600	-2.41241200	-1.37566800
H	-3.98820400	-1.47817600	-2.64419100
C	-1.73463800	1.89967300	1.32611200
H	-0.76612300	2.23163800	0.94331000
H	-2.33796600	2.77066800	1.59652100
H	-1.56980600	1.28224400	2.21237500
N	-1.05516700	-0.82491000	-0.14775400
N	-0.14121100	-0.39544300	0.71280400
O	0.84474200	-1.27784500	0.75486500
V	0.91931000	-2.91180700	-0.06573100
C	1.84727200	-2.46426000	-1.81704500
H	2.03247300	-3.42774900	-2.32041600
H	1.19562700	-1.84706200	-2.45580600
H	2.80666100	-1.94813400	-1.66842500
C	-0.57327100	-4.16755000	-0.62861000
H	-0.14058600	-5.16229900	-0.82368600
H	-1.37001500	-4.25419700	0.12547600
H	-0.99932400	-3.77965100	-1.56647200
C	2.22213500	-4.04944000	0.98076300
H	2.56060400	-4.90634700	0.37898800
H	3.09030600	-3.41152900	1.21148300
H	1.78466300	-4.41200100	1.92397600

7_T ($\eta^{\square}$-O_{anti})

E_{elec} (M06/BS1) = -680.44728977 au
H_{corr} (M06/BS1) = 0.265636 au
G_{corr} (M06/BS1) = 0.196601 au
SPE (M06/BS2//M06/BS1) = -680.07669441 au

0 3

C	-4.39759900	0.11541700	-0.34294600
C	-3.84294200	1.29116100	0.02320000
C	-2.23527400	-0.26678300	0.11404800
N	-3.40464200	-0.84397500	-0.28677200
H	-5.40743800	-0.13190400	-0.63890700
H	-4.27161200	2.27964300	0.11382900
N	-2.50243700	1.06279200	0.30677900
C	-3.53912500	-2.25166300	-0.59900900
H	-2.88195200	-2.52110500	-1.43237200
H	-3.27236900	-2.86079800	0.27072900
H	-4.57835900	-2.44557200	-0.87497200
C	-1.58258900	2.10113900	0.74471700
H	-0.75361700	2.20864000	0.03989100
H	-2.14241000	3.03921300	0.79485500
H	-1.17527600	1.86784300	1.73230600
N	-1.13357400	-1.00613100	0.24655800
N	-0.06913200	-0.33152600	0.62183400
O	0.96339600	-1.17742200	0.73709200
V	2.55415300	-0.45154100	1.22189100
C	2.73597800	1.54651500	1.48923800
H	3.74362300	1.84873400	1.81174800
H	2.48759900	2.05195400	0.54203500
H	2.00153000	1.84854600	2.25405000
C	3.95570300	-0.97391200	-0.14429700
H	4.93115600	-0.62975200	0.23623000
H	3.98504500	-2.06925100	-0.24951600
H	3.77213300	-0.52053500	-1.13027600
C	3.09677000	-1.28919700	2.98596800
H	4.10360400	-0.91181200	3.22810800
H	2.40729000	-1.02715700	3.80283200
H	3.14427800	-2.38454400	2.88947900

8_T (η^2-N2,O)

E_{elec} (M06/BS1) = -680.45516855 au
H_{corr} (M06/BS1) = 0.266289 au
G_{corr} (M06/BS1) = 0.199501 au
SPE (M06/BS2//M06/BS1) = -680.08294883 au

0 3

C	-4.33765100	-0.73794800	0.15147800
C	-4.19268200	0.57201800	0.45175600
C	-2.17799100	-0.21410000	-0.11826300
N	-3.09334800	-1.21775200	-0.20451900
H	-5.21054000	-1.37532300	0.15569200
H	-4.91502700	1.31149200	0.76810400
N	-2.85506900	0.90196900	0.28450600
C	-2.76259500	-2.57580600	-0.59187900
H	-2.29633200	-2.58033200	-1.58182900
H	-2.06717400	-3.01699700	0.12931800
H	-3.68492800	-3.16044600	-0.61719000
C	-2.32934600	2.24737000	0.46307500
H	-1.71012400	2.52982500	-0.39175600
H	-3.17988100	2.93007400	0.53880900
H	-1.72937600	2.31459400	1.37673300
N	-0.90127500	-0.44911600	-0.43279000
N	-0.07861100	0.55806200	-0.20284000
O	1.19051900	0.26228700	-0.52662100
V	1.29407000	1.00432600	1.21815300
C	1.72465400	2.96204400	1.47564100
H	2.16519000	3.11213200	2.47401300
H	2.44820900	3.28593600	0.71272200
H	0.81089000	3.57062200	1.38787100
C	3.05384500	0.05503200	1.61420400
H	3.42113900	0.43336000	2.58312100
H	2.88198300	-1.02817400	1.70229800
H	3.81199800	0.23992900	0.83865400
C	0.17133700	0.27771600	2.75893600
H	0.70441600	0.48367400	3.70154800
H	-0.85020700	0.68399700	2.82213700
H	0.10699300	-0.81559000	2.63174100

9_T (η^3-N1,N2,O)

E_{elec} (M06/BS1) = -680.44765714 au
H_{corr} (M06/BS1) = 0.266323 au
G_{corr} (M06/BS1) = 0.199577 au
SPE (M06/BS2//M06/BS1) = -680.07631802 au

0 3

C	-4.42217400	1.23251300	-0.46785000
C	-3.43787500	2.01839900	0.02539700
C	-2.67179000	-0.07589900	-0.00468800
N	-3.94288500	-0.06047000	-0.48635300
H	-5.42004400	1.47039300	-0.80870000
H	-3.40152000	3.08460800	0.19983600
N	-2.35192400	1.20927500	0.31413900
C	-4.68387800	-1.22526200	-0.94006000
H	-4.01437800	-2.08768700	-0.93421300
H	-5.52840900	-1.41479900	-0.26968200
H	-5.05327000	-1.05036700	-1.95505900
C	-1.09225700	1.70895300	0.85469600
H	-0.26480900	1.46468400	0.18475300
H	-1.18318200	2.79426900	0.94633000
H	-0.89870700	1.26859800	1.83646200
N	-1.97816700	-1.22579200	0.06734100
N	-0.76892000	-1.11872200	0.62786300
O	-0.24246800	-2.36545200	0.72263500
V	-1.56854100	-2.55880200	2.04146300
C	-0.57156400	-3.80823700	3.30917200
H	-1.19507500	-4.00155500	4.19583600
H	-0.32644700	-4.76510200	2.82199200
H	0.35969900	-3.32189000	3.63715000
C	-3.32717000	-3.56429800	1.82961800
H	-3.54405600	-4.13994200	2.74209600
H	-4.15005000	-2.85565900	1.64945600
H	-3.25565800	-4.25414700	0.97456700
C	-1.83692400	-1.08660100	3.43604100
H	-2.37135000	-1.53232800	4.29079400
H	-0.86382100	-0.71583900	3.79462500
H	-2.42650200	-0.24057400	3.04574500

11_T (η^{2}-N2)

E_{elec} (M06/BS1) = -680.44176620 au
H_{corr} (M06/BS1) = 0.266436 au
G_{corr} (M06/BS1) = 0.199022 au
SPE (M06/BS2//M06/BS1) = -680.07569946 au

0 3

C	-4.41706200	-0.62175700	-0.03052800
C	-4.29691900	0.71003000	-0.24041600
C	-2.24591300	-0.16459600	-0.24610400
N	-3.14063100	-1.15391100	-0.03438300
H	-5.28780700	-1.24307700	0.12488300
H	-5.04222500	1.49001100	-0.31192400
N	-2.94852700	0.98567400	-0.38165500
C	-2.79605200	-2.54453400	0.21064300
H	-1.71879300	-2.65894300	0.07012900
H	-3.06258700	-2.81797200	1.23653400
H	-3.33098200	-3.18652500	-0.49484400
C	-2.38082700	2.28392600	-0.70310500
H	-1.45437300	2.13743200	-1.26524200
H	-3.09570700	2.83528200	-1.31933000
H	-2.16657600	2.85351500	0.20915800
N	-0.91605600	-0.35721000	-0.43658200
N	-0.17034100	0.33041000	0.40781800
O	1.05933700	0.36781100	0.19231300
V	-0.42695500	1.07360000	2.20664100
C	-0.00619500	-0.73549900	3.06644600
C	-2.28723400	1.51862300	2.93317100
C	0.80484500	2.62489700	2.68957000
H	-0.01057100	-0.63552400	4.16410900
H	-0.79163300	-1.45780000	2.77988600
H	0.96740100	-1.13346200	2.74106900
H	-2.16786500	1.73480000	4.00917600
H	-2.80403200	2.37116500	2.46470700
H	-2.93167500	0.62660800	2.84691400
H	0.72731400	2.83326200	3.76929000
H	1.85388700	2.41383100	2.43684700
H	0.48088400	3.52208000	2.13408800

6-thf_T

E_{elec} (M06/BS1) = -912.75225537 au
H_{corr} (M06/BS1) = 0.391670 au
G_{corr} (M06/BS1) = 0.310498 au
SPE (M06/BS2//M06/BS1) = -912.45129512 au

0 3

O	0.72097000	-0.99616700	0.70357000
N	-3.75982700	-0.60491500	0.69240600
N	-2.85512600	-0.23045000	-1.26964000
N	-1.42896400	-0.79084800	0.68165800
N	-0.33978100	-0.73690900	-0.06796800
C	-2.56408600	-0.55272000	0.03189100
C	-4.78744100	-0.31287700	-0.18600200
H	-5.81959500	-0.30021900	0.13501100
C	-4.23204400	-0.08183200	-1.39435400
H	-4.68148400	0.17345100	-2.34404900
C	-1.92289900	-0.04793700	-2.36953100
H	-2.50484300	0.20640700	-3.26007700
H	-1.22235800	0.76476900	-2.15410100
H	-1.35267000	-0.96175800	-2.55700200
C	-3.88241200	-0.92146600	2.09913900
H	-3.43842300	-1.90071900	2.30652600
H	-3.37005800	-0.16834000	2.70752100
H	-4.94378900	-0.93894100	2.35826100
V	2.38251300	-0.80049300	-0.00357900
C	3.91317500	-0.63859500	1.33470400
H	4.71483200	-1.35623600	1.10945600
H	4.32449600	0.38041600	1.38756200
H	3.47834400	-0.89877200	2.31471900
C	2.68229400	-2.80612700	-0.36128700
H	2.58281700	-3.37488500	0.57731800
H	1.93340400	-3.17769800	-1.08101400
H	3.68697600	-2.98221200	-0.77416300
C	2.88891300	-0.31610100	-1.92710300
H	3.12881800	0.74700300	-2.07322600
H	3.72165100	-0.93695500	-2.28700900
H	1.99117800	-0.56816500	-2.51948900
O	1.99308500	1.46223800	0.30562900
C	1.65025600	1.86806600	1.64617700
C	1.15548100	2.15818900	-0.63802300
C	0.77082500	3.09302000	1.48671200
H	1.10369200	1.04227100	2.12757500
H	2.58040600	2.04949200	2.19628000
C	0.04292600	2.77394300	0.18622300

H	1.76279700	2.92376600	-1.14414000
H	0.80537100	1.43378200	-1.38369400
H	1.38238200	3.99851100	1.37027500
H	0.10159900	3.23793800	2.34142700
H	-0.40533300	3.64882500	-0.29706400
H	-0.74586600	2.02720000	0.36464500

4i_T ($\eta^{\square}$-N1)

E_{elec} (M06/BS1) = -680.43785883 au
H_{corr} (M06/BS1) = 0.266056 au
G_{corr} (M06/BS1) = 0.197272 au
SPE (M06/BS2//M06/BS1) = -680.07389436 au

0 3

C	-4.48039200	0.17496300	-0.10147700
C	-3.70110300	1.15345800	-0.62523900
C	-2.36359900	-0.41586300	0.18630400
N	-3.63413400	-0.78979700	0.40927600
H	-5.55485900	0.07717000	-0.03814400
H	-3.95776100	2.08565200	-1.10860700
N	-2.38762300	0.77269800	-0.43907000
C	-4.04439100	-2.04243300	1.02511400
H	-4.39063400	-2.74123000	0.25596700
H	-3.18741000	-2.47270200	1.54870900
H	-4.84917700	-1.84470300	1.73757200
C	-1.20193500	1.51267900	-0.83927400
H	-0.46222700	0.81005700	-1.23784200
H	-1.48165200	2.22737100	-1.61570800
H	-0.77933100	2.03442200	0.02463900
N	-1.24426700	-1.18986300	0.43218000
N	-0.38236500	-0.75236800	1.36703800
O	-0.70258200	0.26782300	1.96844900
V	-0.76215600	-2.69998300	-0.87568300
C	-2.14009300	-2.23762300	-2.36059500
C	-0.98225600	-4.55659100	-0.02261900
C	1.17466900	-2.27431300	-1.42073600
H	-2.03915000	-2.91223900	-3.22722500
H	-3.18822400	-2.29862500	-2.01457500
H	-1.97671600	-1.20633300	-2.72478900
H	-0.70717100	-5.35823500	-0.72889100
H	-0.32920500	-4.63937600	0.86328400
H	-2.02104000	-4.73183100	0.30522300
H	1.55491300	-2.94654500	-2.20768200
H	1.25453400	-1.23668200	-1.78883000
H	1.82852100	-2.36486400	-0.53599500

7i_T ($\eta^{\square}$-O_{anti})

E_{elec} (M06/BS1) = -680.43800125 au
H_{corr} (M06/BS1) = 0.265018 au
G_{corr} (M06/BS1) = 0.195247 au
SPE (M06/BS2//M06/BS1) = -680.06825318 au

0 3

C	-4.60900600	0.09140600	-0.02382400
C	-4.12898800	1.28610800	-0.43448500
C	-2.37456700	-0.06225400	-0.09505800
N	-3.52289400	-0.73962900	0.17751900
H	-5.62074600	-0.24913000	0.14687800
H	-4.63750900	2.19997200	-0.70927000
N	-2.74716900	1.19094500	-0.48112400
C	-3.57938800	-2.10201700	0.67201600
H	-2.60714000	-2.56926800	0.50076600
H	-3.80483400	-2.11178500	1.74386800
H	-4.35396800	-2.65291700	0.13067000
C	-1.87384900	2.21187300	-1.03124400
H	-1.02166300	1.73425200	-1.52351800
H	-2.43872000	2.78702900	-1.77002400
H	-1.50061300	2.87324500	-0.24342300
N	-1.18018200	-0.68185200	-0.12228900
N	-0.07254400	-0.11332100	0.28091800
O	-0.25804100	1.02004400	0.97589800
V	1.20597000	1.95869800	1.55435400
C	3.08637500	1.26882400	1.24337900
H	3.84618900	1.97864900	1.60584800
H	3.21859900	0.30247100	1.75559600
H	3.22461100	1.11648700	0.16074600
C	1.04999200	2.37657800	3.53522100
H	1.87598000	3.05533300	3.80364600
H	0.09661800	2.89152100	3.73267500
H	1.10767200	1.47507400	4.16454000
C	1.11729400	3.74029300	0.57480200
H	1.98229300	4.33950000	0.90365000
H	1.16840200	3.61542100	-0.51880800
H	0.19733200	4.28930200	0.83265500

8i_T (η^2-N2,O)

E_{elec} (M06/BS1) = -680.44661873 au
H_{corr} (M06/BS1) = 0.265767 au
G_{corr} (M06/BS1) = 0.195889 au
SPE (M06/BS2//M06/BS1) = -680.07491620 au

0 3

C	-4.33388700	-0.22960900	0.56195600
C	-4.22810600	1.10540800	0.37427500
C	-2.26394200	0.19159700	-0.17550600
N	-3.11894000	-0.78959800	0.21743200
H	-5.15721900	-0.83508900	0.91387800
H	-4.94611200	1.90077700	0.51809200
N	-2.94630000	1.36771700	-0.08307600
C	-2.75906900	-2.19345000	0.28025100
H	-2.62668900	-2.60118600	-0.72726000
H	-1.82422000	-2.31189900	0.83692500
H	-3.56091500	-2.73223800	0.79036900
C	-2.49218800	2.66290200	-0.56149400
H	-1.95456800	2.53386400	-1.50627100
H	-3.37096700	3.28916300	-0.73270900
H	-1.82103700	3.12919900	0.16426300
N	-1.05767600	-0.11122100	-0.67688100
N	-0.05460900	0.73602100	-0.54780900
O	-0.09255200	1.60992600	0.48963000
V	1.62692700	0.77683200	0.53581100
C	1.85138500	-1.24417600	0.52338800
H	2.80613000	-1.49108000	1.01596600
H	1.03096400	-1.68711900	1.11132800
H	1.82838400	-1.67227900	-0.48963700
C	1.84099500	1.11557600	2.53794500
H	2.87508900	0.84277200	2.80849200
H	1.65813600	2.16563900	2.81154400
H	1.15263100	0.47078800	3.10484600
C	3.22747700	1.65459200	-0.32324500
H	4.14971000	1.29916200	0.16265100
H	3.25142900	1.38359000	-1.39019000
H	3.16682100	2.74867500	-0.22711400

10i_T ($\eta^{\square}$-N1,N2)

E_{elec} (M06/BS1) = -680.43431574 au
H_{corr} (M06/BS1) = 0.266051 au
G_{corr} (M06/BS1) = 0.198785 au
SPE (M06/BS2//M06/BS1) = -680.06748685 au

0 3

V	5.86085400	0.55811000	5.80257700
N	4.75457100	2.08890000	5.05211400
N	5.61289300	1.53167900	4.08648300
N	4.13562300	4.20743000	5.98297400
N	3.85294300	3.96898900	3.83110200
C	4.31928600	3.34860300	4.94838300
C	3.54853600	5.36918200	5.51230000
H	3.31478300	6.19128600	6.17402300
C	3.38111000	5.22437200	4.17960600
H	2.97112900	5.89545900	3.43790600
C	4.47186800	3.91997700	7.36353600
C	3.68317600	3.35232300	2.52665200
C	4.86743600	-1.19365700	5.92034600
H	3.91849000	-1.03501500	6.45599900
H	4.66171300	-1.60336300	4.92113500
H	5.48456700	-1.90764300	6.48827600
C	7.79395500	0.19899800	5.27207500
H	8.36612500	1.13687600	5.35664700
H	8.19748700	-0.52276200	6.00096900
H	7.90238500	-0.19520000	4.25199800
C	6.29241000	1.03997600	7.75409900
H	6.77173900	0.14333000	8.18370300
H	7.02675800	1.86007300	7.80626100
H	5.41992100	1.29990400	8.37308000
O	6.21484500	2.28679400	3.29623300
H	5.48621900	3.51613400	7.42254300
H	4.41397400	4.85019600	7.93328100
H	3.77242300	3.18917900	7.78475300
H	4.61718500	3.37832000	1.96035500
H	3.38120800	2.30897400	2.66257700
H	2.89238400	3.88850600	1.99614700

11i_T ($\eta^{\square}$-N2)

E_{elec} (M06/BS1) = -680.44110162 au
H_{corr} (M06/BS1) = 0.265817 au
G_{corr} (M06/BS1) = 0.195355au
SPE (M06/BS2//M06/BS1) = -680.07371014 au

0 3

C	-4.36197700	-0.37828400	0.65687000
C	-4.19137500	0.96329500	0.70112100
C	-2.33084400	0.07659900	-0.15138200
N	-3.20654400	-0.91822100	0.12749000
H	-5.19422500	-0.99945300	0.95670300
H	-4.84654300	1.75201800	1.04389000
N	-2.93275500	1.24201800	0.19563100
C	-2.93562600	-2.32552400	-0.11021600
H	-2.91645500	-2.53227800	-1.18486400
H	-1.96822000	-2.59456800	0.32318700
H	-3.72558600	-2.91288000	0.36287400
C	-2.41221800	2.57704800	-0.04497400
H	-1.96511600	2.61870900	-1.04337200
H	-3.24578700	3.28166100	0.00389600
H	-1.64785800	2.82563800	0.69542400
N	-1.17667600	-0.17127500	-0.81485900
N	-0.07930800	0.45375400	-0.42155100
O	-0.05774900	1.15304700	0.62309900
V	1.62357500	0.14878900	-1.32080100
C	2.91427400	1.71397100	-1.15461300
C	1.46315600	-0.40907500	-3.26963600
C	2.14125900	-1.43726200	-0.14288700
H	3.88952900	1.44544800	-1.59297600
H	2.53290700	2.61606400	-1.65904000
H	3.05838200	1.94296100	-0.08673700
H	2.43972500	-0.71078800	-3.68154400
H	0.77862300	-1.27202400	-3.31651100
H	1.04657000	0.40020400	-3.89041300
H	3.12982900	-1.82294700	-0.44121400
H	2.18361200	-1.13028200	0.91524000
H	1.40018400	-2.24814900	-0.24140300

6-thf_T_P

E_{elec} (M06/BS1) = -1870.69169431 au
H_{corr} (M06/BS1) = 0.675869 au
G_{corr} (M06/BS1) = 0.559550 au
SPE (M06/BS2//M06/BS1) = -1870.64924756 au

0 3

O	0.31514300	-1.53621400	0.66505600
N	-4.08122800	-0.84173100	0.07185200
N	-2.75641600	0.16864700	-1.34300700
N	-1.76691900	-1.03173800	0.56668800
N	-0.65615100	-1.21978300	-0.11886900
C	-2.77337800	-0.58073200	-0.20292300
C	-4.88093900	-0.27982700	-0.91464900
H	-5.95760600	-0.36623400	-0.87645300
C	-4.06505600	0.34523900	-1.78712300
H	-4.27838300	0.93646700	-2.66660800
V	0.42052800	-1.73825700	2.52348700
O	-0.43834200	-3.80091100	2.24385800
C	0.26678400	-4.70166200	1.36217900
C	-1.86274300	-3.99719700	2.10569400
C	-0.78292900	-5.67115400	0.85336000
H	0.70091800	-4.10975500	0.54218600
H	1.08237800	-5.16585900	1.92857700
C	-2.02653100	-4.79006300	0.82772100
H	-2.22691400	-4.55091700	2.98523800
H	-2.33906800	-3.01202100	2.08328300
H	-0.92063300	-6.49936400	1.56243600
H	-0.51806000	-6.09412100	-0.12159600
H	-2.96812800	-5.35016200	0.79937800
H	-2.00080600	-4.11064100	-0.03864500
C	-1.63733800	0.83967000	-1.93392900
C	-0.86791000	1.70898000	-1.16647500
C	-1.38654900	0.65490800	-3.28820800
C	0.18428300	2.38632200	-1.77023000
H	-1.08633700	1.84754200	-0.10811400
C	-0.33885100	1.35015900	-3.88443200
H	-2.00189700	-0.03463900	-3.86393700
C	0.44903700	2.21103400	-3.12689700
H	0.79461200	3.06428700	-1.17662800
H	-0.13570300	1.20979500	-4.94398700
H	1.27140300	2.74848600	-3.59446700
C	-4.55185300	-1.67204200	1.13538500
C	-5.27480400	-2.82042800	0.82470400
C	-4.27922100	-1.32254600	2.45295700

C	-5.72433200	-3.63506200	1.85904300
H	-5.46612300	-3.07634200	-0.21655700
C	-4.72024500	-2.15140500	3.47817500
H	-3.70375500	-0.42569300	2.67344200
C	-5.44235600	-3.30514400	3.18282800
H	-6.28865600	-4.53584900	1.62621600
H	-4.47666300	-1.89236100	4.50827200
H	-5.78638300	-3.95195400	3.98756900
C	-0.90152800	-1.50990800	4.09580500
C	-1.11665500	-2.54832400	5.01727100
C	-1.58864000	-0.30658200	4.33182500
C	-1.94819500	-2.39271900	6.12777300
H	-0.62893100	-3.51583600	4.86761400
C	-2.44026900	-0.14415000	5.42315900
H	-1.44720900	0.53283100	3.64580900
C	-2.61426100	-1.18726100	6.33323000
H	-2.08038300	-3.21521000	6.83133100
H	-2.95835800	0.80354500	5.57500700
H	-3.26505300	-1.05894700	7.19778900
C	1.22672800	0.16401200	2.78661200
C	1.69148400	0.58638100	4.04801500
C	1.35185500	1.09830000	1.74282600
C	2.22697100	1.85443100	4.26049300
H	1.62971900	-0.10010100	4.89822400
C	1.88133100	2.37583600	1.94224700
H	1.03707100	0.82402200	0.73197400
C	2.31960100	2.76160500	3.20487200
H	2.57600000	2.13920400	5.25417200
H	1.96000000	3.07176000	1.10466000
H	2.73671700	3.75557000	3.36585900
C	2.18199800	-2.63724600	2.99918400
C	2.39784500	-3.35182500	4.18741800
C	3.22757000	-2.61250100	2.06146200
C	3.59830800	-4.02240100	4.42503200
H	1.61568900	-3.39367700	4.95015000
C	4.42357300	-3.29171500	2.28608400
H	3.10781500	-2.05294800	1.12911100
C	4.61293700	-3.99993600	3.47175200
H	3.74027500	-4.56677200	5.35924000
H	5.21543900	-3.26086400	1.53710000
H	5.54929500	-4.52643100	3.65332500

8_T_P

E_{elec} (M06/BS1) = -1638.38669728 au
H_{corr} (M06/BS1) = 0.551350 au
G_{corr} (M06/BS1) = 0.450334 au
SPE (M06/BS2//M06/BS1) = -1638.27149235 au

0 3

O	0.30208900	0.82407700	-2.05015000
N	-1.63323400	-2.08251700	0.17094400
N	-3.41978600	-0.83073300	-0.06137000
N	-1.57259500	-0.12079500	-1.33586700
N	-0.25950800	-0.17174100	-1.35991300
C	-2.12976900	-0.99151000	-0.48877200
C	-2.60774000	-2.56026000	1.04347300
H	-2.43051300	-3.44203100	1.64296100
C	-3.70315200	-1.78856800	0.90250700
H	-4.67854600	-1.84935700	1.36390400
V	1.27845300	0.66896100	-0.41403500
C	-0.40944000	-2.78635100	-0.06714500
C	0.38647600	-3.12346100	1.02147000
C	-0.07062700	-3.18497800	-1.35800800
C	1.55477100	-3.85098500	0.81138600
C	1.09820400	-3.90811500	-1.55590100
C	1.91291300	-4.24040200	-0.47453100
H	2.18710900	-4.10712500	1.65934400
H	1.37529700	-4.21411000	-2.56309700
C	-4.29077000	0.24400700	-0.40706800
C	-4.95593600	0.91703000	0.61527900
C	-4.49703300	0.58405100	-1.74163100
C	-5.83999800	1.94153800	0.29596300
C	-5.37391300	1.61776600	-2.04709000
C	-6.04810100	2.29508500	-1.03372100
H	-6.35950900	2.46947100	1.09286600
H	-5.53741800	1.88886500	-3.08801100
C	2.99035000	-0.38606900	-0.49193800
C	3.92955400	-0.40777600	0.55324200
C	3.24228100	-1.18147700	-1.62135400
C	5.05929100	-1.21898400	0.48780800
C	4.37831400	-1.98518100	-1.69771000
C	5.28283600	-2.00928000	-0.63955600
H	5.77280500	-1.23030900	1.31124200
H	4.55260400	-2.60232700	-2.57915800
C	0.29277200	0.56926500	1.36934300
C	-0.97027700	1.16086500	1.54203600
C	0.83619200	-0.11719700	2.46704700

C	-1.66419900	1.06248300	2.74617300
C	0.14922400	-0.21502900	3.67891400
C	-1.10606100	0.36914100	3.81990400
H	-2.64291000	1.53316500	2.85059900
H	0.59679000	-0.75575000	4.51341800
C	1.86166000	2.61786200	-0.41018800
C	2.10631900	3.30630800	-1.61106200
C	2.20423000	3.26705000	0.78926100
C	2.67166300	4.57920000	-1.61859800
C	2.77557500	4.53964100	0.78968000
C	3.00807600	5.19788300	-0.41545200
H	2.85186100	5.09175600	-2.56375100
H	3.03332700	5.02223000	1.73261000
H	6.16807400	-2.64181600	-0.69228500
H	3.77825200	0.21824600	1.43690400
H	2.53304100	-1.18850500	-2.45250700
H	-0.71601200	-2.92535400	-2.19532700
H	0.10140900	-2.79158100	2.01856000
H	2.83359900	-4.79698800	-0.63886500
H	-4.77013500	0.64320300	1.65265400
H	-3.97533100	0.04364000	-2.52698300
H	-6.73539900	3.10123500	-1.28182500
H	-1.64639800	0.28863100	4.76233400
H	-1.43538900	1.70256200	0.71160800
H	1.80962900	-0.60769900	2.38126700
H	2.02029500	2.77175100	1.74627100
H	1.84933900	2.83829400	-2.56424700
H	3.44809200	6.19454000	-0.41786900

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TS4-9 (triplet) in Solvent = THF

TS4_T

E_{elec} (M06/BS1) = -680.44128457 au
H_{corr} (M06/BS1) = 0.265015 au
G_{corr} (M06/BS1) = 0.197618 au
SPE (M06/BS2//M06/BS1) = -680.07545209 au

0 3

C	-4.46659000	0.44145800	-0.20189700
C	-3.57933600	1.42026700	-0.50434100
C	-2.43133600	-0.34559100	0.19183300
N	-3.74061700	-0.64939400	0.23505600
H	-5.54605500	0.41895700	-0.24990700
H	-3.72648000	2.42637700	-0.87112800
N	-2.31545800	0.91670900	-0.26185800
C	-4.30059300	-1.91748100	0.67834600
H	-4.77933900	-2.42537500	-0.16436500
H	-3.49127900	-2.54073300	1.06654600
H	-5.03435800	-1.73258100	1.46761200
C	-1.05237200	1.59298200	-0.52648100
H	-0.34140600	0.86823800	-0.93718100
H	-1.23173100	2.38148400	-1.26054000
H	-0.64491400	2.02188400	0.39257700
N	-1.41071400	-1.21126700	0.46022400
N	-0.52210700	-0.76216600	1.36593600
O	0.43147800	-1.53761700	1.46055700
V	-0.66149600	-2.75252800	-0.68351600
C	-2.14696100	-2.76301200	-2.12283500
C	-0.57268900	-4.61746300	0.17626700
C	0.99874400	-2.16205400	-1.74781200
H	-1.90641300	-3.44279600	-2.95710900
H	-3.12651400	-3.06843700	-1.71433300
H	-2.26594400	-1.74692200	-2.54561100
H	-0.30698600	-5.35785900	-0.59862800
H	0.16156700	-4.68648600	0.99403600
H	-1.56481600	-4.89435500	0.57436800
H	1.22521300	-2.93687300	-2.50157800
H	0.76885000	-1.23094900	-2.29582900
H	1.89628900	-1.99315300	-1.13376000

TS5_T

E_{elec} (M06/BS1) = -680.45058139 au
H_{corr} (M06/BS1) = 0.264835 au
G_{corr} (M06/BS1) = 0.198458 au
SPE (M06/BS2//M06/BS1) = -680.07936615 au

0 3

O	-0.50278500	-1.29966200	0.17768900
N	-0.05610600	0.40960400	3.91145600
N	2.03098400	-0.21727400	3.71699900
N	0.69007500	-0.71898200	1.84931300
N	-0.56797700	-0.86469300	1.43278200
C	0.83085900	-0.20408500	3.07372600
C	0.61117100	0.78116100	5.07190900
H	0.09392000	1.28435000	5.87699700
C	1.89928100	0.39747600	4.94969000
H	2.73860900	0.49329300	5.62392700
C	-1.45587600	0.71078200	3.65006400
H	-1.81413300	1.34934100	4.46193700
H	-1.55919300	1.23960500	2.69899900
H	-2.05224500	-0.20405700	3.61011700
C	3.25339900	-0.77753100	3.17668200
H	3.00922600	-1.64239600	2.55380500
H	3.78867400	-0.03715000	2.57141500
H	3.89011900	-1.09280400	4.00769800
V	1.15842700	-1.29818900	-0.63946600
C	0.78999300	-1.38260300	-2.62567000
H	1.68123500	-1.67726200	-3.19930000
H	0.01630400	-2.15962700	-2.74552000
H	0.39691400	-0.43018200	-3.01315700
C	2.62207500	0.11779600	-0.57382600
H	3.32648500	-0.07899800	-1.39798400
H	2.19040000	1.12254400	-0.70416900
H	3.16253400	0.07897200	0.38113800
C	1.92908300	-3.14634300	-0.28975800
H	2.03138400	-3.38633100	0.77780900
H	1.32426500	-3.92363000	-0.78064700
H	2.92946200	-3.13276800	-0.75530100

TS6_T

E_{elec} (M06/BS1) = -680.43944178 au
H_{corr} (M06/BS1) = 0.244841 au
G_{corr} (M06/BS1) = 0.194116 au
SPE (M06/BS2//M06/BS1) = -680.06943954 au

0 3

C	4.42396400	0.56382400	0.04846300
C	4.30259600	-0.78155500	0.04543300
C	2.23685100	0.07831000	-0.03058000
N	3.14804500	1.09186100	0.00114400
H	5.29838900	1.19845800	0.07818600
H	5.05089800	-1.56136400	0.07448900
N	2.94972300	-1.08879400	-0.00345900
C	2.79150000	2.49618800	-0.00767900
H	2.21464500	2.73579700	-0.90666000
H	2.18984200	2.74174000	0.87350500
H	3.71202500	3.08454100	0.00310700
C	2.43151600	-2.44806400	-0.02083500
H	1.84681400	-2.62797800	-0.92652900
H	3.28788400	-3.12744900	0.00126100
H	1.79745800	-2.63269500	0.85008100
N	0.93149700	0.35321600	-0.07642500
N	0.15119000	-0.71047100	-0.10129900
O	-1.10187900	-0.32978800	-0.15103300
V	-2.84465600	0.04210800	-0.15573600
C	-4.12562900	-1.40417700	-0.78381400
H	-5.14634500	-1.13545300	-0.46627400
H	-4.10663800	-1.51584900	-1.87952800
H	-3.86179400	-2.36779500	-0.32257500
C	-3.47964500	1.88323600	-0.74101300
H	-4.52454900	2.01645100	-0.41643200
H	-2.86470900	2.65972900	-0.26162500
H	-3.42274600	2.00765100	-1.83395200
C	-3.19875100	0.08112200	1.84601300
H	-4.27928700	0.27267900	1.95319000
H	-2.95892400	-0.88005500	2.32412900
H	-2.64147000	0.88847700	2.34350000

TS7_T

E_{elec} (M06/BS1) = -680.44630794 au
H_{corr} (M06/BS1) = 0.265013au
G_{corr} (M06/BS1) = 0.198443 au
SPE (M06/BS2//M06/BS1) = -680.07307168 au

0 3

C	-4.08705800	-0.39438200	0.31071900
C	-4.01854500	0.93782900	0.53205100
C	-2.05076100	0.29566400	-0.31841200
N	-2.87127400	-0.78768300	-0.21057000
H	-4.88673900	-1.10232000	0.47654500
H	-4.74751300	1.62843100	0.93283800
N	-2.75929400	1.37105400	0.14571000
C	-2.49326700	-2.12931400	-0.60909700
H	-2.27594300	-2.16087800	-1.68168200
H	-1.60430000	-2.45024700	-0.05739800
H	-3.32543900	-2.80067200	-0.38487700
C	-2.31399600	2.75343500	0.25338000
H	-2.10264000	3.17329300	-0.73486200
H	-3.11877600	3.32287000	0.72622200
H	-1.41049800	2.81976000	0.86421600
N	-0.81865700	0.16086200	-0.81081900
N	-0.12185100	1.28392500	-0.85419800
O	1.08754200	1.03669900	-1.46304400
V	0.50922500	2.09941100	-2.82611000
C	-1.25080000	1.81588500	-3.78780600
H	-1.28681000	2.38854800	-4.72715400
H	-1.36799600	0.74216900	-4.00387000
H	-2.07997100	2.13422800	-3.13664100
C	2.01640000	2.12989200	-4.19942500
H	1.83317000	2.94742100	-4.91496000
H	2.96456000	2.33734400	-3.67985100
H	2.10538400	1.17652000	-4.74311600
C	0.69508600	4.03692200	-2.25847100
H	0.14340700	4.59286800	-3.03649000
H	0.23797200	4.23180800	-1.27791700
H	1.74019400	4.37633000	-2.26417200

TS8_T

E_{elec} (M06/BS1) = -680.44782567 au
H_{corr} (M06/BS1) = 0.265203 au
G_{corr} (M06/BS1) = 0.199707 au
SPE (M06/BS2//M06/BS1) = -680.07659021 au

0 3

C	-4.21003900	-0.08748500	0.50686200
C	-4.02161800	1.20560200	0.15176800
C	-2.07055000	0.15285000	-0.08482900
N	-3.00131500	-0.73213500	0.35845000
H	-5.09254400	-0.60826300	0.85081900
H	-4.70773200	2.04061200	0.12472500
N	-2.69467900	1.35718500	-0.21419100
C	-2.73071700	-2.13890300	0.60101400
H	-2.43637500	-2.63086000	-0.33123600
H	-1.92241800	-2.24698500	1.33083400
H	-3.64165400	-2.59929700	0.98956000
C	-2.12846000	2.60614800	-0.70975900
H	-1.68233200	2.45463000	-1.69535600
H	-2.94350200	3.33072000	-0.78204300
H	-1.36136200	2.97808100	-0.02600200
N	-0.81255800	-0.25717300	-0.31679100
N	0.03737500	0.71905300	-0.63981400
O	1.28387300	0.18711400	-0.74196400
V	1.19148300	0.33187200	1.12933900
C	0.47782800	2.02230600	2.03065600
H	0.89235000	2.06772200	3.05081100
H	0.81157000	2.91700100	1.48188500
H	-0.62348200	2.02353600	2.08943500
C	3.15614700	0.73323300	1.47853400
H	3.30334100	0.85388200	2.56302500
H	3.80540200	-0.07483400	1.10743000
H	3.42868600	1.67552000	0.98019900
C	0.83156700	-1.21748000	2.39576900
H	1.46025800	-1.12718600	3.29457500
H	-0.22737200	-1.19473900	2.69989100
H	1.04191200	-2.17685500	1.89922400

TS9_T

E_{elec} (M06/BS1) = -680.42839143 au
H_{corr} (M06/BS1) = 0.265411 au
G_{corr} (M06/BS1) = 0.200626 au
SPE (M06/BS2//M06/BS1) = -680.05975005 au

0 3

C	-4.74855200	0.51350200	-1.01857100
C	-4.25899700	1.42422900	-0.15043800
C	-3.01216800	-0.42363000	0.04047900
N	-3.97140400	-0.62524800	-0.90001500
H	-5.57107800	0.56657600	-1.71774300
H	-4.56503500	2.43845200	0.06486600
N	-3.17598600	0.84749900	0.50396600
C	-4.14745900	-1.87730700	-1.61009900
H	-4.34309000	-2.68999800	-0.90135100
H	-4.99704900	-1.77172000	-2.28844600
H	-3.24720000	-2.11859100	-2.18375800
C	-2.36116500	1.54969600	1.48489100
H	-1.30136400	1.36100300	1.29925400
H	-2.56122000	2.61955400	1.37963600
H	-2.60729100	1.23177900	2.50391200
N	-2.13425200	-1.39763700	0.33500300
N	-1.46532800	-1.19027600	1.52557200
O	-0.52085500	-2.03063700	1.71478700
V	-2.78247000	-2.21894300	2.54707900
C	-2.85424800	-4.20784500	2.19933000
H	-3.55098000	-4.72723800	2.87279000
H	-3.13237300	-4.39425500	1.15105500
H	-1.82849800	-4.57113300	2.36788300
C	-4.76743700	-1.81320000	2.42565700
H	-5.33375400	-2.29890900	3.23355700
H	-4.83897600	-0.71648600	2.55328600
H	-5.21611700	-2.07790700	1.45627800
C	-2.39136800	-1.89416800	4.50196800
H	-3.07379300	-2.56814200	5.04521300
H	-1.35366300	-2.12453700	4.77944200
H	-2.63235000	-0.85355400	4.77198400

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TSB6-8 (triplet) in Solvent = THF

TSB6_T

E_{elec} (M06/BS1) = -680.42100767 au
H_{corr} (M06/BS1) = 0.264482 au
G_{corr} (M06/BS1) = 0.196041 au
SPE (M06/BS2//M06/BS1) = -680.04584812 au

0 3

C	-3.16854700	1.34528100	-0.04026400
C	-3.61664100	0.13090800	-0.42989300
C	-1.50933400	-0.11686300	0.25270100
N	-1.86110400	1.18719200	0.38499400
H	-3.65574500	2.30982400	-0.01890100
H	-4.57459000	-0.18050700	-0.82243600
N	-2.58686000	-0.78009500	-0.24512200
C	-1.00470000	2.21066900	0.95619900
H	-0.51533000	1.81481300	1.85191700
H	-0.23734500	2.52272700	0.23870100
H	-1.62374000	3.06968500	1.22535700
C	-2.64457600	-2.19009700	-0.60275000
H	-1.82434700	-2.44320000	-1.28035700
H	-2.57832700	-2.81816800	0.28984800
H	-3.59810100	-2.36720600	-1.10638100
N	-0.29331600	-0.56625200	0.59551300
N	-0.09811400	-1.84206400	0.72175700
O	1.65340100	-1.84265900	0.29586800
V	1.97701500	-0.19240500	0.12107200
C	2.28707700	0.74985300	1.89750400
H	2.29975300	1.82428900	1.64297900
H	1.49740700	0.56518900	2.63813800
H	3.26158700	0.47482800	2.32698800
C	1.30536000	0.88377200	-1.51595000
H	1.69088400	0.45045200	-2.44941000
H	0.21169500	0.96389000	-1.59116600
H	1.73545800	1.89496900	-1.41335100
C	3.83862300	-0.13388800	-0.68042300
H	4.19873900	0.89751900	-0.80685400
H	4.45266800	-0.64124700	0.08442800
H	3.93046100	-0.68000900	-1.62839600

TSB7_T

E_{elec} (M06/BS1) = -680.42853236 au
H_{corr} (M06/BS1) = 0.264006 au
G_{corr} (M06/BS1) = 0.196397 au
SPE (M06/BS2//M06/BS1) = -680.05372917 au

0 3

C	-3.75345000	0.78777700	-0.45225000
C	-3.44489300	1.49887300	0.65702900
C	-2.01542100	-0.21355300	0.53263500
N	-2.86939100	-0.27059000	-0.52720900
H	-4.52429900	0.93390000	-1.19585600
H	-3.89148300	2.39129900	1.07326200
N	-2.37195000	0.87616100	1.27588700
C	-2.80090000	-1.28596700	-1.55874500
H	-1.82978800	-1.24489700	-2.06372400
H	-2.93156600	-2.28027600	-1.11968900
H	-3.59722700	-1.09843900	-2.28260700
C	-1.70536400	1.35502400	2.47505200
H	-0.71655000	1.76215200	2.23555800
H	-2.32389800	2.14246400	2.91349200
H	-1.58875600	0.54031000	3.19448300
N	-1.08263900	-1.14412200	0.73014400
N	-0.30497300	-1.08672700	1.72795700
O	1.12119700	-2.03744800	1.21348500
V	2.30348100	-0.86993100	0.99819600
C	1.69290100	0.44350200	-0.42698800
H	2.53886100	1.12149100	-0.62573000
H	1.40313800	-0.05985600	-1.36124600
H	0.84076000	1.03549900	-0.05828800
C	4.09668000	-1.56904400	0.37449800
H	4.82865300	-0.75365700	0.26995100
H	4.47369700	-2.31064900	1.09478500
H	3.96041200	-2.06349900	-0.59981000
C	2.65690500	0.07263100	2.75906200
H	1.72637800	0.51740700	3.14109300
H	3.06698700	-0.61155900	3.51683300
H	3.38760500	0.87285900	2.55837800

TSB8_T

E_{elec} (M06/BS1) = -680.42820879 au
H_{corr} (M06/BS1) = 0.263961 au
G_{corr} (M06/BS1) = 0.195267 au
SPE (M06/BS2//M06/BS1) = -680.05373333 au

0 3

C	-4.42233500	-0.71909900	0.10999400
C	-4.33193600	0.59328700	0.42563200
C	-2.30045300	-0.09221100	-0.19970700
N	-3.16510400	-1.13992400	-0.27839300
H	-5.26646400	-1.39392000	0.12060700
H	-5.07974900	1.29177900	0.77498700
N	-3.01860100	0.98915600	0.22419700
C	-2.77641300	-2.47318300	-0.69477700
H	-2.32753100	-2.43799500	-1.69241000
H	-2.04884600	-2.89272600	0.00799100
H	-3.66910100	-3.10241200	-0.71618700
C	-2.50187800	2.32194700	0.49056500
H	-1.96293400	2.70310300	-0.38067800
H	-3.35220800	2.97392500	0.70619000
H	-1.82578300	2.31322000	1.35330700
N	-1.01654700	-0.21944700	-0.54355100
N	-0.24971500	0.79024700	-0.53560700
O	1.36754900	0.10589100	-0.21877500
V	1.67697400	0.71052400	1.31713900
C	1.77338800	2.73557900	1.23409900
H	2.65486500	3.07321700	0.66825200
H	0.86686600	3.14737300	0.76815500
H	1.84761400	3.09955200	2.27174700
C	3.42373400	0.13331700	2.16006400
H	3.54965300	0.58138300	3.15762800
H	3.43251600	-0.96394400	2.24861400
H	4.25956900	0.43957600	1.51280000
C	0.24460000	0.06115400	2.60806800
H	0.54968200	0.39063800	3.61462100
H	-0.73644300	0.50167900	2.37278600
H	0.15576800	-1.03550200	2.59932100

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 4, 6-9, 7i-9i, 8_P, 9_P, $8i_P$ & $9i_P$ (singlet) in Solvent = THF

4_S ($\eta^{\square}$-N1)

E_{elec} (M06/BS1) = -680.40104237 au
H_{corr} (M06/BS1) = 0.265296 au
G_{corr} (M06/BS1) = 0.198231 au
SPE (M06/BS2//M06/BS1) = -680.03272459 au

0 1

C	-4.40601600	0.12806500	-0.16926300
C	-3.59141400	1.06954700	-0.70416500
C	-2.30236900	-0.49571900	0.21996400
N	-3.60149100	-0.82483000	0.42885200
H	-5.48422200	0.05531300	-0.14237300
H	-3.81768400	1.98432000	-1.23419900
N	-2.28914000	0.69188800	-0.43668000
C	-4.05370700	-2.04514500	1.07074300
H	-4.16506900	-2.84940700	0.33326800
H	-3.32275600	-2.34822200	1.82455400
H	-5.01539500	-1.85537800	1.55412200
C	-1.07874900	1.37879800	-0.84040300
H	-0.51334700	0.76132500	-1.55012900
H	-1.35646600	2.31987700	-1.31963600
H	-0.45170400	1.58515900	0.03249000
N	-1.21230800	-1.24347700	0.57085600
N	-0.62399700	-0.91399500	1.75968400
O	0.38930300	-1.55134200	1.99017600
V	-0.77809600	-2.50542100	-0.86685900
C	-2.20431200	-2.39360800	-2.31738200
C	-0.97961500	-4.34610900	-0.06378200
C	1.03677800	-2.02079400	-1.62431200
H	-2.11588700	-3.20549600	-3.06071900
H	-3.26553300	-2.28331900	-2.04268200
H	-1.88499500	-1.45471000	-2.81378900
H	-0.81475400	-5.15456100	-0.79402900
H	-0.11586700	-4.31087200	0.62816400
H	-1.88840000	-4.56439000	0.51974100
H	1.22238800	-2.78682300	-2.39813500
H	1.08486400	-1.02583000	-2.09982200
H	1.82799900	-2.09196300	-0.86120900

6_S ($\eta^{\square}$-O_{syn})

E_{elec} (M06/BS1) = -680.42287957 au
H_{corr} (M06/BS1) = 0.265870 au
G_{corr} (M06/BS1) = 0.199613 au
SPE (M06/BS2//M06/BS1) = -680.05224005 au

0 1

C	-4.41931000	0.64721600	-0.68181700
C	-3.80076900	1.62342800	0.01321600
C	-2.31877000	-0.04624100	-0.25861700
N	-3.50799400	-0.38231500	-0.84992600
H	-5.42385600	0.58130700	-1.07587100
H	-4.15609600	2.58659700	0.35284500
N	-2.49988700	1.20449900	0.28040500
C	-3.72511300	-1.63429900	-1.53607300
H	-3.02245100	-1.73889400	-2.37129800
H	-3.57613600	-2.47712800	-0.85073500
H	-4.74967500	-1.64976500	-1.91634700
C	-1.53380200	1.99591000	1.02208200
H	-0.66686400	2.24138700	0.40211700
H	-2.03022300	2.92070300	1.33044800
H	-1.18807300	1.45806200	1.90885900
N	-1.29569900	-0.88396000	-0.29399100
N	-0.17732400	-0.44245300	0.31293500
O	0.74745300	-1.34674400	0.20721900
V	1.17296000	-2.94803800	-0.41030800
C	2.80736600	-2.69864500	-1.54111600
H	3.24000200	-3.66899700	-1.83004300
H	2.38168000	-2.21502700	-2.43878100
H	3.58384300	-2.04737400	-1.11825500
C	-0.24790900	-3.92216400	-1.42139200
H	0.21876700	-4.87123800	-1.73719800
H	-1.12959700	-4.13158200	-0.79505200
H	-0.56264200	-3.34923900	-2.30862400
C	1.82946100	-4.00536900	1.15836900
H	2.27170000	-4.95914900	0.83124400
H	2.51932900	-3.47796200	1.83066600
H	0.88798100	-4.21243800	1.69818000

7_S ($\eta^{\square}$-O_{anti})

E_{elec} (M06/BS1) = -680.42045295 au
H_{corr} (M06/BS1) = 0.265656 au
G_{corr} (M06/BS1) = 0.196400 au
SPE (M06/BS2//M06/BS1) = -680.04949413 au

0 1

C	-4.36420900	-0.31108300	-0.39455000
C	-4.16619000	1.00548800	-0.18039200
C	-2.19841900	-0.03295500	0.16381900
N	-3.15514600	-0.95280700	-0.18205400
H	-5.25199600	-0.86003700	-0.67639200
H	-4.84637800	1.84402200	-0.23908400
N	-2.82969300	1.18961000	0.16551000
C	-2.89103800	-2.36797100	-0.29900800
H	-2.13668100	-2.55572200	-1.07166200
H	-2.52178200	-2.76897100	0.65177500
H	-3.82144500	-2.87370700	-0.56985300
C	-2.24322300	2.48618000	0.45455000
H	-1.42516800	2.70739700	-0.23682700
H	-3.02809900	3.23944600	0.33865900
H	-1.85415600	2.52225700	1.47603700
N	-0.95965100	-0.41447000	0.41292200
N	-0.12793900	0.58375300	0.76442900
O	1.05530900	0.08988700	0.96940900
V	2.70623400	-0.25462000	1.32823600
C	3.61433100	1.45066800	1.86534300
H	4.64783500	1.11772700	2.07056300
H	3.63142500	2.20702800	1.06729200
H	3.19000500	1.88850600	2.78074900
C	3.53207500	-1.06808800	-0.30862000
H	4.55548500	-1.40826100	-0.08054900
H	2.96127500	-1.88073900	-0.77708900
H	3.58853500	-0.21713200	-1.00913900
C	2.74772700	-1.63689500	2.78148000
H	3.79056600	-1.94108300	2.96933100
H	2.36877700	-1.09685800	3.66577100
H	2.12354300	-2.52355400	2.60769700

8_S (η^2-N2,O)

E_{elec} (M06/BS1) = -680.46445013 au
H_{corr} (M06/BS1) = 0.266855 au
G_{corr} (M06/BS1) = 0.201574 au
SPE (M06/BS2//M06/BS1) = -680.09025100 au

0 1

O	1.31767700	3.01636500	4.96872700
N	-1.50947800	1.53099700	7.67807700
N	-0.45310600	2.73892600	9.17190400
N	0.45294100	2.88912000	7.02542200
N	0.18750100	2.64560200	5.69806300
C	-0.45439200	2.39513700	7.84603500
C	-2.13840000	1.34373900	8.90904100
H	-2.99136200	0.68583300	9.00225300
C	-1.49097300	2.08994000	9.82497200
H	-1.66527000	2.22840700	10.88297800
C	-1.86437900	0.79922500	6.47519500
H	-2.17903400	1.47898500	5.67707700
H	-1.01794400	0.20655200	6.11529000
H	-2.69155400	0.12875300	6.72612300
C	0.45314000	3.71490600	9.73116700
H	1.49137200	3.37770400	9.63906800
H	0.35023300	4.67265000	9.20491300
H	0.20862300	3.85175900	10.78770600
V	0.09623200	4.27769100	4.71170500
C	-1.67797100	4.61963100	5.63995600
H	-2.36966500	3.79821900	5.40118400
H	-1.55874900	4.69185800	6.73021300
H	-2.07433800	5.56714000	5.24232400
C	0.91608200	6.03883300	5.21507200
H	0.29872300	6.85407800	4.80942200
H	1.04592700	6.15680100	6.29819800
H	1.90157500	6.04247400	4.72111000
C	-0.39875000	4.24708900	2.77379700
H	-1.00301400	5.15239400	2.60461400
H	0.50361300	4.28417600	2.14719500
H	-0.98945600	3.35412800	2.52577000

9_S (η^3-N1,N2,O)

E_{elec} (M06/BS1) = -680.47185721 au
H_{corr} (M06/BS1) = 0.267709 au
G_{corr} (M06/BS1) = 0.205724 au
SPE (M06/BS2//M06/BS1) = -680.09673253 au

0 1

C	-4.45270500	0.89417600	-0.60405700
C	-3.60617800	1.79456600	-0.06315800
C	-2.64091000	-0.21475500	0.10100600
N	-3.84928500	-0.34758200	-0.50453800
H	-5.42763000	1.01184200	-1.05559500
H	-3.68578300	2.86626400	0.05301900
N	-2.48193800	1.10800800	0.38094200
C	-4.37797400	-1.58706700	-1.04679800
H	-3.54681000	-2.27753400	-1.20939100
H	-5.09314000	-2.04196500	-0.35433100
H	-4.87269500	-1.37256300	-1.99848000
C	-1.33346800	1.76768600	0.99337600
H	-0.45447900	1.69211500	0.34902700
H	-1.59670800	2.81959500	1.13095800
H	-1.10313800	1.31845400	1.96221000
N	-1.83124500	-1.27383800	0.28017300
N	-0.59276900	-0.98678100	0.91836700
O	-0.01761400	-2.23484300	1.00565400
V	-1.52579600	-2.14028600	2.08644800
C	-0.93506400	-4.00043700	2.69579600
H	-1.54457100	-4.30030900	3.56165700
H	-1.12692900	-4.69429900	1.86509900
H	0.13297800	-4.02092100	2.94730600
C	-3.47516300	-2.78273600	2.06481800
H	-3.67968500	-3.18819500	3.06875300
H	-4.20091800	-1.98615900	1.84016400
H	-3.59219000	-3.59385900	1.33168500
C	-1.37964400	-1.01962100	3.74848100
H	-1.69819300	-1.61447400	4.61778000
H	-0.36335600	-0.63391600	3.89964100
H	-2.08111800	-0.17830000	3.61539100

7i_S ($\eta^{\square}$-O_{anti})

E_{elec} (M06/BS1) = -680.40804987 au
H_{corr} (M06/BS1) = 0.265512 au
G_{corr} (M06/BS1) = 0.198639 au
SPE (M06/BS2//M06/BS1) = -680.03767883 au

0 1

C	-4.40803300	-0.12909200	0.48758400
C	-4.28167700	1.04303700	-0.16241100
C	-2.20850900	0.20820400	0.11812700
N	-3.13030100	-0.64317200	0.66637100
H	-5.28151900	-0.65060900	0.85343400
H	-5.02299900	1.75812400	-0.49160100
N	-2.92139200	1.26727700	-0.38645000
C	-2.77076600	-1.86962100	1.33815800
H	-2.35625500	-2.59745600	0.63052400
H	-2.01775000	-1.66832600	2.10909000
H	-3.66716300	-2.28830500	1.80368400
C	-2.41464300	2.35166200	-1.20923800
H	-2.02674300	1.97506600	-2.16213900
H	-3.24699000	3.03282000	-1.40993600
H	-1.62097100	2.89644300	-0.69209100
N	-0.92268000	-0.07926000	0.14590600
N	-0.07502200	0.90572100	-0.32431000
O	0.09707200	1.90593200	0.70018700
V	1.52830200	0.87981400	0.68444200
C	1.96158500	-0.83222400	-0.30742100
H	2.93171400	-1.18920500	0.07237300
H	1.18144600	-1.58851300	-0.16407400
H	2.03890800	-0.58292500	-1.37517500
C	1.81233000	0.12964100	2.52419700
H	2.85285800	-0.21877500	2.60231200
H	1.64600900	0.96591300	3.22155000
H	1.11631100	-0.68711400	2.75110500
C	3.05361400	2.04756400	0.13744100
H	3.96939900	1.45484600	0.28423900
H	2.96670800	2.35249600	-0.91379900
H	3.07423900	2.93529500	0.78577100

8i_S (η^2-N2,O)

E_{elec} (M06/BS1) = -680.45832992 au
H_{corr} (M06/BS1) = 0.266493 au
G_{corr} (M06/BS1) = 0.200000 au
SPE (M06/BS2//M06/BS1) = -680.03767883 au

0 1

C	-4.46817300	0.35521300	0.27454000
C	-3.91891700	1.46716600	-0.25727300
C	-2.27578200	-0.05404800	-0.03358500
N	-3.45725100	-0.58082500	0.41441700
H	-5.48323600	0.14045600	0.57873000
H	-4.35898900	2.41785600	-0.52577300
N	-2.56206100	1.22410800	-0.44714100
C	-3.57701400	-1.91616600	0.95612700
H	-2.80985400	-2.07688600	1.72085400
H	-4.56862900	-2.02431600	1.40320200
H	-3.44915300	-2.66904400	0.16991800
C	-1.69690900	2.05511200	-1.26352700
H	-1.03662800	1.41697000	-1.85907400
H	-2.32152200	2.64706600	-1.93877100
H	-1.08490000	2.72243600	-0.64873500
N	-1.18154700	-0.79773700	-0.11000200
N	0.06169400	-0.31020500	-0.04114900
O	0.15062200	0.84992600	0.58466700
V	1.20150700	1.98108700	1.41002300
C	3.08116800	1.37332700	1.06845500
H	3.68964900	2.08131900	1.65928900
H	3.26353100	0.35170400	1.43389000
H	3.37248100	1.44604300	0.01004900
C	0.71705000	2.01563600	3.35752700
H	1.36522700	2.73129400	3.88854900
H	-0.33783100	2.24027900	3.56840000
H	0.94554800	0.99552900	3.70941500
C	0.90872200	3.85424400	0.73630500
H	1.53027100	4.56842200	1.30001300
H	1.28011100	3.80817500	-0.30283300
H	-0.13368100	4.20671200	0.72607300

9i_S (η^3-N1,N2,O)

E_{elec} (M06/BS1) = -680.47054937 au
H_{corr} (M06/BS1) = 0.268014 au
G_{corr} (M06/BS1) = 0.205866 au
SPE (M06/BS2//M06/BS1) = -680.09489757 au

0 1

C	-2.28225500	-2.01899300	2.37457900
C	-3.05102100	-0.98518300	1.97787500
C	-1.09307600	-0.80569200	0.91450600
N	-1.07221100	-1.90911400	1.70772500
H	-2.47280600	-2.82736500	3.06630300
H	-4.05774200	-0.70073400	2.25018500
N	-2.31730400	-0.23273000	1.06824400
C	-0.01374400	-2.90145500	1.73097000
H	0.49716600	-2.89141900	0.76399700
H	0.71081800	-2.69332100	2.52395900
H	-0.46369900	-3.88481400	1.89413700
C	-2.86729000	0.91739700	0.35854200
H	-2.85262300	0.73949900	-0.71967900
H	-3.90088900	1.04102600	0.69035300
H	-2.28856500	1.81555100	0.58229400
N	-0.07434500	-0.48768000	0.10321900
N	-0.16122600	0.66407300	-0.71850700
O	-0.05414800	1.75809400	0.16294500
V	1.47647500	0.74488200	0.23070000
C	2.71959500	0.75135200	-1.34345300
H	3.75169700	0.81991000	-0.96684000
H	2.57556900	-0.20061200	-1.87618500
H	2.50361800	1.59036100	-2.01717400
C	2.29478900	-0.46876000	1.67226800
H	3.29609900	-0.07864400	1.90656800
H	1.69157700	-0.45627300	2.59218500
H	2.37778700	-1.50211900	1.30865600
C	2.18475600	2.32737700	1.32902800
H	3.27169300	2.20741200	1.45062300
H	1.95752400	3.28284500	0.83942200
H	1.71240800	2.30322900	2.32102600

8_S_P (η^2-N2,O)

E_{elec} (M06/BS1) = -1638.39215979 au
H_{corr} (M06/BS1) = 0.550848 au
G_{corr} (M06/BS1) = 0.449997 au
SPE (M06/BS2//M06/BS1) = -1638.27508739 au

0 1

O	1.38116300	0.28657700	-1.34814600
N	-1.87522100	-1.62684200	0.56317100
N	-3.08214300	-0.22224300	-0.62662200
N	-0.76606800	0.08610400	-0.84032200
N	0.44577600	-0.56001100	-0.75023900
C	-1.78066200	-0.55466200	-0.30091300
C	-3.22410100	-1.97728100	0.70757900
H	-3.52056700	-2.77401100	1.37493600
C	-3.95649800	-1.12318800	-0.02515300
H	-5.02631800	-1.03180100	-0.15099000
V	0.95205600	-0.94839000	-2.55149000
C	-0.86084400	-2.18481800	1.39160000
C	0.06093500	-1.36610100	2.03992700
C	-0.84911000	-3.56267700	1.59428700
C	1.01434900	-1.93953100	2.87252800
C	0.10098300	-4.12614900	2.43890500
C	1.03893100	-3.31778500	3.07449200
H	1.73770500	-1.30044600	3.37512000
H	0.11100600	-5.20359900	2.59204900
C	-3.46129300	0.73224200	-1.60675000
C	-3.01845100	2.05017500	-1.51196400
C	-4.29608500	0.33746000	-2.65069500
C	-3.40911400	2.97131600	-2.47685000
C	-4.69162100	1.26924100	-3.60459100
C	-4.24680700	2.58588400	-3.52172000
H	-3.06307400	4.00074500	-2.40550200
H	-5.34264200	0.96064400	-4.42009900
C	0.29400900	0.02480800	-4.16729800
C	0.72812300	-0.39097900	-5.43827300
C	-0.63504400	1.07389800	-4.08740500
C	0.23813000	0.21738200	-6.59240500
C	-1.12712100	1.68000200	-5.23892900
C	-0.69075000	1.25029400	-6.49203900
H	0.58239800	-0.11548700	-7.57087200
H	-1.85719900	2.48563800	-5.15514400
C	-0.44424200	-2.44218700	-2.46738100
C	-0.10246600	-3.59040400	-1.73882600
C	-1.70467600	-2.40570600	-3.08424500

C	-0.97230800	-4.67654900	-1.65074300
C	-2.59023800	-3.47704900	-2.97030800
C	-2.22393500	-4.61699200	-2.25878300
H	-0.67823300	-5.56283600	-1.08749800
H	-3.56871600	-3.42424600	-3.44861700
C	2.71518300	-1.82865200	-2.90774300
C	2.79448800	-2.91616300	-3.79693300
C	3.90397500	-1.36136400	-2.32279400
C	4.01834400	-3.50970100	-4.09263000
C	5.12916800	-1.95372100	-2.62093200
C	5.18709000	-3.02708800	-3.50587200
H	4.06098400	-4.35257100	-4.78144100
H	6.04184200	-1.57544400	-2.16184400
H	6.14450500	-3.49138500	-3.73779400
H	3.87198700	-0.52194200	-1.62791100
H	-1.07521200	1.72378900	-7.39452800
H	-2.37209600	2.34260800	-0.68802000
H	-0.98251000	1.40613200	-3.10678500
H	-4.55496400	3.31370800	-4.27022200
H	1.45475100	-1.19926600	-5.53795400
H	-2.01267700	-1.52429600	-3.65178800
H	0.85368900	-3.64001800	-1.21066100
H	-2.91279000	-5.45698800	-2.17830300
H	-4.62362100	-0.69966900	-2.71385900
H	0.02806000	-0.28949900	1.89065700
H	-1.57004800	-4.18717100	1.06942900
H	1.78570300	-3.75954600	3.73135200
H	1.88985500	-3.31553900	-4.26190600

9_S_P (η^3-N1,N2,O)

E_{elec} (M06/BS1) = -1638.39743833 au
H_{corr} (M06/BS1) = 0.551298 au
G_{corr} (M06/BS1) = 0.453241 au
SPE (M06/BS2//M06/BS1) = -1638.27929159 au

0 1

C	-4.02549300	0.55377000	-1.13517700
C	-3.35098900	1.54782000	-0.52633400
C	-2.25609800	-0.36436600	-0.10209300
N	-3.33798900	-0.62888100	-0.89203500
H	-4.90602000	0.57229600	-1.76133100
H	-3.51271100	2.61637700	-0.50595700
N	-2.24485000	0.98323500	0.10875400
N	-1.45957900	-1.35111300	0.32599000
N	-0.33957800	-1.01007900	1.12343700
O	0.19844600	-2.24774500	1.37535600
V	-1.46241500	-2.08547100	2.20410800
C	-1.32842800	1.76788000	0.88423600
C	-1.82096200	2.45180700	1.99047400
C	-0.00029200	1.88789500	0.48946800
C	-0.96090800	3.26314100	2.72381200
C	0.85249800	2.69312100	1.23427100
C	0.37390800	3.38053500	2.34857900
H	-1.33549400	3.79564400	3.59555600
H	1.89473500	2.78973100	0.93784900
C	-3.76813700	-1.91728800	-1.33809900
C	-2.85316900	-2.83313800	-1.85410400
C	-5.12337100	-2.22216900	-1.26792600
C	-3.30880700	-4.07477600	-2.28054800
C	-5.56794100	-3.46366200	-1.70844000
C	-4.66326800	-4.39396600	-2.20917700
H	-2.59722300	-4.79492600	-2.67974500
H	-6.62659500	-3.70678000	-1.64047700
C	-3.46867800	-2.52888300	2.01140100
C	-4.08008700	-3.78497200	1.87564700
C	-4.32138700	-1.41551000	2.13939300
C	-5.46580200	-3.92677000	1.88119800
C	-5.70943700	-1.54940200	2.17086000
C	-6.28492200	-2.81050900	2.03784600
H	-5.91056900	-4.91595100	1.77008400
H	-6.34018900	-0.66838100	2.29160200
C	-1.06869700	-4.00088500	2.77419600
C	-1.22012300	-4.46214700	4.08938300
C	-0.80368200	-4.94413600	1.77213100

C	-1.12188600	-5.82200200	4.38701600
C	-0.72352200	-6.30467800	2.06388400
C	-0.88180000	-6.74760800	3.37536800
H	-1.23674400	-6.15845800	5.41766300
H	-0.53263300	-7.02214600	1.26556000
C	-1.31776300	-0.94667500	3.86108200
C	-0.29425400	0.00042800	4.02291100
C	-2.20526300	-1.15027400	4.93505500
C	-0.15032100	0.70813800	5.21264900
C	-2.06395800	-0.44356100	6.12721600
C	-1.03417300	0.48517000	6.26644800
H	0.64696700	1.44444700	5.31444100
H	-2.76100100	-0.61425700	6.94695200
H	-0.68325700	-4.61215300	0.73780300
H	-1.41863800	-3.75936300	4.90078200
H	-0.81390700	-7.80950600	3.60835600
H	-3.90411500	-0.40681700	2.23824600
H	-3.45927900	-4.67701300	1.77040200
H	-7.36854600	-2.92280400	2.05285500
H	-0.92466600	1.03968100	7.19765600
H	-3.02125700	-1.87074300	4.84321800
H	0.38751000	0.19889600	3.19423400
H	-2.86684700	2.33803200	2.27413200
H	0.35324100	1.34955500	-0.38717500
H	1.04588600	4.01265800	2.92594100
H	-5.82069300	-1.50720800	-0.83456700
H	-5.01213700	-5.36831700	-2.54553300
H	-1.79835800	-2.57938900	-1.90679000

8i_S$_P$ (η^2-N2,O)

E_{elec} (M06/BS1) = -1638.37888734 au
H_{corr} (M06/BS1) = 0.551229 au
G_{corr} (M06/BS1) = 0.448111 au
SPE (M06/BS2//M06/BS1) = -1638.260706520 au

0 1

C	-0.47908100	2.96971000	2.93649300
C	0.74854500	2.45059500	3.08829000
C	-0.54527900	0.84248000	2.14848300
N	-1.29399400	1.98524900	2.37447400
H	-0.87956800	3.93409900	3.21530900
H	1.64603200	2.86200600	3.52889200
N	0.72153400	1.12975400	2.62019600
N	-1.05351000	-0.20533800	1.54994500
N	-0.21527200	-1.24216600	1.27433700
O	0.79854200	-0.88300700	0.33765500
V	-0.20281600	-2.16192700	-0.36323400
C	1.82820700	0.24539900	2.76610300
C	1.67703200	-0.98278100	3.40458000
C	3.07107600	0.64791600	2.28383800
C	2.77522600	-1.82808000	3.52248500
C	4.16783900	-0.19458400	2.42544900
C	4.01993800	-1.43830900	3.03444200
H	2.65516400	-2.79764400	4.00339100
H	5.13804000	0.11763400	2.04392200
C	-2.64756000	2.18322200	2.00295900
C	-3.59925000	1.18539000	2.21800000
C	-3.02658200	3.41043700	1.45870700
C	-4.92670800	1.42350700	1.88121600
C	-4.36013600	3.64189700	1.13963200
C	-5.31397300	2.64974900	1.34660600
H	-5.66779900	0.64496300	2.05393200
H	-4.65023100	4.60172700	0.71645900
C	-0.59737500	-1.49055100	-2.21373700
C	-0.76700800	-2.37462800	-3.29223600
C	-0.65114400	-0.11122700	-2.46570400
C	-0.95895700	-1.89425000	-4.58493200
C	-0.85452300	0.37212600	-3.75564800
C	-1.00379500	-0.52040400	-4.81543000
H	-1.08245300	-2.59147800	-5.41270500
H	-0.89023600	1.44551600	-3.93776300
C	0.95468800	-3.78305900	-0.22228100
C	1.59888600	-4.35404300	-1.32878800
C	1.10923500	-4.38172900	1.03737300

C	2.36392200	-5.50972200	-1.18194100
C	1.87576100	-5.53424400	1.18437800
C	2.50068900	-6.09840600	0.07305700
H	2.85667900	-5.95051200	-2.04764600
H	1.98879900	-5.99321500	2.16598300
C	-2.13458100	-2.72206000	-0.05750100
C	-3.22628700	-1.86529800	0.15006700
C	-2.39866800	-4.08893300	-0.25452000
C	-4.52932900	-2.35060000	0.15536400
C	-3.70605300	-4.58017200	-0.23531700
C	-4.77278500	-3.71163600	-0.03262000
H	-5.36323400	-1.66427700	0.30487900
H	-3.88646400	-5.64499100	-0.38111600
H	3.09983300	-7.00062200	0.18646000
H	0.62031900	-3.94267300	1.90982600
H	1.50908000	-3.89738500	-2.31633300
H	4.87608200	-2.10295300	3.13218200
H	3.16724900	1.60917000	1.78066100
H	0.70450000	-1.27350300	3.79542900
H	-1.58280400	-4.79507400	-0.42459200
H	-5.79337100	-4.09208300	-0.02080800
H	-3.04754500	-0.80133400	0.30826700
H	-3.29449900	0.23225700	2.64177900
H	-6.35607600	2.83143000	1.09123000
H	-2.27446600	4.17606200	1.27452800
H	-0.75753300	-3.45553700	-3.12891900
H	-1.15801700	-0.14343000	-5.82543400
H	-0.52267800	0.59407500	-1.64156900

9i_S$_P$ (η^3-N1,N2,O)

E_{elec} (M06/BS1) = -1638.39414691 au
H_{corr} (M06/BS1) = 0.550522 au
G_{corr} (M06/BS1) = 0.450454 au
SPE (M06/BS2//M06/BS1) = -1638.27713140 au

0 1

C	-4.33721000	0.65749300	-0.68111900
C	-3.43680900	1.62538900	-0.42639200
C	-2.55749000	-0.31247300	0.28727100
N	-3.80465000	-0.54042900	-0.21754500
H	-5.33031500	0.70302200	-1.10479400
H	-3.46831400	2.69467400	-0.58113400
N	-2.33709000	1.02860300	0.18950400
N	-1.79442900	-1.30718200	0.74495400
N	-0.56475400	-1.12923600	1.40883400
O	0.36607900	-0.68362900	0.45543300
V	-0.29157700	-2.31051900	-0.04395600
C	-1.17709600	1.76637000	0.58701800
C	-0.83007700	1.84387700	1.92987300
C	-0.43990000	2.41812500	-0.39551000
C	0.30278100	2.56505500	2.28955100
C	0.68504900	3.14525600	-0.02375300
C	1.05939900	3.21266800	1.31614100
H	0.59221100	2.62445500	3.33650400
H	1.27367000	3.65415400	-0.78419300
C	-4.47647900	-1.79923300	-0.28791600
C	-4.49640700	-2.65099200	0.81518200
C	-5.14683100	-2.12949800	-1.46013700
C	-5.17533800	-3.85996800	0.72170600
C	-5.83165100	-3.33700500	-1.53762500
C	-5.84251500	-4.20651800	-0.45192300
H	-5.19082600	-4.53033400	1.57919700
H	-6.34573800	-3.60199200	-2.45955400
C	1.20461900	-2.25009600	-1.45699200
C	1.90593000	-1.10717900	-1.86044000
C	1.57998600	-3.47780000	-2.02965200
C	2.94598500	-1.18120200	-2.78443800
C	2.63645600	-3.56258100	-2.93561400
C	3.31997200	-2.41207500	-3.31979900
H	3.47406800	-0.27524600	-3.08284600
H	2.91745000	-4.53036600	-3.35137400
C	0.09695400	-3.98445200	0.99559100
C	1.34409200	-4.54789600	1.29818200
C	-1.06222200	-4.61966200	1.46982000

C	1.43011500	-5.72177000	2.04160100
C	-0.97800200	-5.79750600	2.21081100
C	0.26941700	-6.34716100	2.49578500
H	2.40443700	-6.15431800	2.26634400
H	-1.88505700	-6.28237100	2.57056400
C	-1.48476300	-2.55748100	-1.69519300
C	-1.95906600	-3.83170200	-2.03139300
C	-1.78523800	-1.49742900	-2.56218900
C	-2.70115900	-4.03916800	-3.19619400
C	-2.52548400	-1.69890200	-3.72394000
C	-2.98623400	-2.97565900	-4.04595100
H	-3.06076000	-5.04040900	-3.43491500
H	-2.73865600	-0.85855600	-4.38536200
H	0.33807900	-7.26608600	3.07632300
H	-2.04959700	-4.19219000	1.26647400
H	2.25783500	-4.07045400	0.94087500
H	1.94415100	3.77740500	1.60352000
H	-1.43326700	1.33060400	2.67588900
H	-0.73990500	2.33510800	-1.43980200
H	-3.98183100	-2.36916400	1.73035200
H	-5.09973800	-1.46230400	-2.31894400
H	-3.56416500	-3.13835800	-4.95492700
H	-1.74590900	-4.68982700	-1.38836900
H	-6.37299000	-5.15445500	-0.51696400
H	4.13689100	-2.47389200	-4.03783900
H	1.63462600	-0.13588600	-1.44148900
H	1.04729400	-4.39447700	-1.76546800
H	-1.41545500	-0.49017200	-2.33835000

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TS8, *a*TSB8 & *a*TSB9 (singlet) in Solvent = THF

TS8_S

E_{elec} (M06/BS1) = -680.46301127 au
H_{corr} (M06/BS1) = 0.266287 au
G_{corr} (M06/BS1) = 0.1204836 au
SPE (M06/BS2//M06/BS1) = -680.08728352 au

0 1

C	3.38820700	0.87410700	0.42957300
C	3.53674600	-0.46526000	0.47031000
C	1.47041700	-0.04346200	-0.28671400
N	2.10585900	1.13176200	-0.03289200
H	4.06457300	1.67612400	0.68927200
H	4.37561300	-1.07879300	0.76798800
N	2.34680200	-1.03922500	0.03345200
C	1.48306800	2.42942700	-0.17727600
H	1.19946900	2.60648700	-1.22106100
H	0.58478200	2.48593700	0.44864600
H	2.19689200	3.19368300	0.13914900
C	2.16777800	-2.46413000	-0.19855700
H	1.78094800	-2.63385300	-1.20766800
H	3.14674900	-2.94189800	-0.10315900
H	1.47180200	-2.89750400	0.52375100
N	0.24962100	-0.10399000	-0.82370900
N	-0.43584800	-1.27149500	-0.47606400
O	-1.57369400	-1.30074300	-1.29051900
V	-1.80843000	-0.03752400	-0.01408100
C	-1.38004600	-0.26645100	1.94616500
H	-1.98001400	0.43860500	2.54094400
H	-1.57243600	-1.29796900	2.26842800
H	-0.30751400	-0.04230100	2.06518400
C	-3.80152600	-0.33345400	0.20402100
H	-4.23538300	0.44802300	0.84559800
H	-4.25583000	-0.27074600	-0.79692800
H	-4.00516300	-1.32765600	0.62629800
C	-1.99012700	1.92284600	-0.52080900
H	-1.99808800	2.43634800	0.45766300
H	-1.20459500	2.34697700	-1.15285400
H	-2.97484600	2.06009000	-0.99077700

***a*TS8_S**

E_{elec} (M06/BS1) = -680.37197868 au
H_{corr} (M06/BS1) = 0.266935 au
G_{corr} (M06/BS1) = 0.205579 au
SPE (M06/BS2//M06/BS1) = -679.99922651 au

0 1

O	1.22489100	4.01325200	6.18472000
N	-1.23305400	0.72330900	6.48905000
N	-1.33868200	0.74197300	4.30594000
N	0.06430600	2.39112800	5.26322200
N	0.11088500	3.24992700	6.39815600
C	-0.79876000	1.38042400	5.37573000
C	-2.04549000	-0.33453000	6.09373700
H	-2.50168200	-0.98951300	6.82270200
C	-2.10615700	-0.32605300	4.74678100
H	-2.62776900	-0.96865400	4.05176800
C	-0.77976300	0.93318100	7.85605200
H	0.31293000	0.96932100	7.88828300
H	-1.17740800	1.86370300	8.27050400
H	-1.12853700	0.08692000	8.45380200
C	-1.11134500	1.12859800	2.92956500
H	-1.28425600	2.20510800	2.81737400
H	-0.08058400	0.90783800	2.63044500
H	-1.80389300	0.57088000	2.29459400
V	0.24595900	4.34523300	4.62224700
C	-1.45455400	4.25628800	6.40423800
H	-2.03831900	3.40028500	6.75504200
H	-1.16265000	4.90719300	7.23206300
H	-2.05146900	4.81465200	5.67370500
C	-0.39394600	6.27117700	4.56382000
H	-1.23100200	6.22670800	3.84089000
H	-0.71757400	6.83515700	5.44751600
H	0.45276100	6.79548100	4.08310000
C	0.75014300	4.05095800	2.68230700
H	-0.15353400	4.22242800	2.07067300
H	1.45447700	4.88551200	2.50787800
H	1.22638000	3.11234700	2.37409500

***a*TS9_S**

E_{elec} (M06/BS1) = -680.36864091 au
H_{corr} (M06/BS1) = 0.266346 au
G_{corr} (M06/BS1) = 0.204244 au
SPE (M06/BS2//M06/BS1) = -679.99589656

0 1

C	-4.22139800	0.91991400	-0.80683900
C	-3.46512700	1.89458500	-0.26382700
C	-2.52539200	-0.06127800	0.27683200
N	-3.64017900	-0.29399000	-0.46452300
H	-5.12282400	0.96194100	-1.40182000
H	-3.56949900	2.97031100	-0.28197300
N	-2.40728800	1.28934700	0.41022600
C	-4.09458100	-1.61216000	-0.85171700
H	-4.14421000	-2.25974500	0.03391500
H	-5.08779900	-1.51947700	-1.29783000
H	-3.40791000	-2.06269700	-1.57692300
C	-1.30542800	2.01417100	1.02480300
H	-0.35127600	1.68103100	0.60638600
H	-1.44534300	3.07554200	0.80359300
H	-1.28828200	1.86588200	2.10834300
N	-1.71654900	-1.03403700	0.69251200
N	-0.86321400	-0.74252100	1.80309900
O	-0.00099400	-1.78874200	1.85227000
V	-1.75561900	-2.61336700	1.86394700
C	-0.95952400	-4.46136900	1.68909800
H	-0.82095700	-4.79174100	2.73481300
H	-1.75650400	-5.06839100	1.22410400
H	-0.01898300	-4.59441400	1.14274500
C	-3.53091800	-3.02196400	2.80325900
H	-3.23778100	-3.53865900	3.73610200
H	-4.25027600	-2.23120300	3.05984500
H	-4.02512200	-3.76272700	2.14624500
C	-1.77309300	-0.72533400	3.42947100
H	-2.19713800	-1.46681800	4.11623600
H	-0.90887900	-0.25088500	3.90003600
H	-2.54203700	0.01106000	3.16897800

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TSB8, TSB9i, $TSB8_P$, $TSB9_P$ & $TSB9i_P$ (singlet) in Solvent = THF

TSB8_S

E_{elec} (M06/BS1) = -680.45596783 au
H_{corr} (M06/BS1) = 0.265512 au
G_{corr} (M06/BS1) = 0.200415 au
SPE (M06/BS2//M06/BS1) = -680.07950200 au

0 1

O	-2.28712900	2.41108500	5.44289800
N	-0.30311500	1.07889800	8.20680400
N	-0.93588400	2.50111100	9.73783500
N	-2.35997600	2.41919600	7.88064300
N	-2.73906600	1.69140100	6.84523500
C	-1.26881700	1.98471500	8.52589800
C	0.62765500	1.03447900	9.24044600
H	1.48431200	0.37662700	9.19160900
C	0.23735700	1.91549400	10.18463200
H	0.68023200	2.18886500	11.13205300
C	-0.20759700	0.26835300	7.00113600
H	-0.86419400	-0.60526400	7.06233900
H	-0.48446700	0.86106000	6.12716900
H	0.83030800	-0.06427300	6.90580700
C	-1.72247500	3.50594000	10.42478900
H	-1.76230200	4.42734400	9.83461300
H	-2.74320300	3.14373800	10.58416900
H	-1.25273600	3.70963900	11.39011700
V	-3.99256400	2.46613400	5.67627300
C	-5.30112800	2.27238600	7.24561800
H	-5.32774200	1.21442300	7.54684600
H	-4.99794500	2.87828500	8.10888400
H	-6.29565500	2.58723600	6.89251000
C	-4.49213600	4.40689100	5.44529800
H	-5.57947200	4.49336900	5.31048700
H	-4.17094900	5.00454300	6.30817800
H	-3.97152100	4.75611200	4.54016300
C	-4.82551400	1.29405500	4.27917300
H	-5.88666100	1.58855500	4.25505100
H	-4.36807800	1.46462200	3.29584000
H	-4.74084200	0.23355500	4.55217100

TSB9i_S

E_{elec} (M06/BS1) = -680.45611944 au
H_{corr} (M06/BS1) = 0.266061 au
G_{corr} (M06/BS1) = 0.202372 au
SPE (M06/BS2//M06/BS1) = -680.07872577 au

0 1

C	-4.16386200	0.86555200	-1.24318500
C	-2.98981800	1.53248600	-1.27754200
C	-2.97002900	0.23657700	0.53414300
N	-4.14290000	0.05823900	-0.11902600
H	-5.01200300	0.87843500	-1.91306700
H	-2.59916200	2.24944600	-1.98621800
N	-2.24386000	1.13562600	-0.17481100
C	-5.22228600	-0.78865500	0.35873900
H	-4.88520300	-1.82671700	0.43735200
H	-5.56427300	-0.44538200	1.34037400
H	-6.04534700	-0.72684300	-0.35648600
C	-0.95088600	1.71032100	0.18165400
H	-0.27637200	0.92381500	0.52390000
H	-0.54390800	2.18812300	-0.71322200
H	-1.07142700	2.45939200	0.97093300
N	-2.70673900	-0.41920800	1.67877500
N	-1.56418500	-0.25336400	2.31738700
O	-0.40816900	-1.16165500	1.46613600
V	-1.53127800	-2.17312200	2.28811200
C	-0.32737200	-3.65304700	3.00264300
H	-0.92004200	-4.50734000	3.35805000
H	0.29040800	-3.97139900	2.14667000
H	0.32982100	-3.29540700	3.80671300
C	-2.60089800	-3.32408300	0.99596800
H	-2.02925100	-4.23846600	0.78151100
H	-3.51811500	-3.58925900	1.54844800
H	-2.87126200	-2.82506900	0.05779900
C	-2.36256200	-2.08080400	4.16893100
H	-2.70219800	-3.08180600	4.47442700
H	-1.61949400	-1.71108800	4.88847200
H	-3.21144700	-1.38302700	4.13782200

TSB8_S_P

E_{elec} (M06/BS1) = -1638.37787842 au
H_{corr} (M06/BS1) = 0.549409 au
G_{corr} (M06/BS1) = 0.446844 au
SPE (M06/BS2//M06/BS1) = -1638.25856315 au

0 1

O	-0.15935000	0.68721400	-1.98419500
N	1.65962700	-2.72078200	-0.13803300
N	3.43501100	-1.44573800	-0.27022700
N	1.37392700	-0.29680200	-0.40478700
N	0.13042500	-0.42143400	-0.78180000
C	2.06964600	-1.42811400	-0.31125000
C	2.78103500	-3.53778300	0.00435500
H	2.67396100	-4.60359100	0.15096700
C	3.87265100	-2.75231100	-0.06700500
H	4.92589500	-2.99153900	-0.02544200
V	-1.14668300	0.92086900	-0.60073400
C	0.31791300	-3.19622500	0.02314700
C	-0.18421300	-4.10632200	-0.90148200
C	-0.43662600	-2.78880200	1.11974600
C	-1.47110500	-4.60852100	-0.73111600
C	-1.72569700	-3.28641000	1.27206100
C	-2.24294400	-4.19612600	0.35206100
H	-1.87159900	-5.32039500	-1.45011400
H	-2.32616000	-2.95348300	2.11707100
C	4.28478100	-0.31249100	-0.43050700
C	4.06402300	0.59386200	-1.46615900
C	5.35116200	-0.14785600	0.44985000
C	4.91921000	1.68021400	-1.60678600
C	6.20837100	0.93559000	0.28926800
C	5.99172100	1.85245700	-0.73479100
H	4.75085500	2.39111100	-2.41319300
H	7.04209200	1.06628400	0.97599700
C	-0.92215500	2.89672300	-0.24145300
C	-1.93075400	3.63585100	0.39720900
C	0.23542900	3.57327100	-0.65419600
C	-1.80043600	5.00845600	0.59227300
C	0.37540500	4.94421500	-0.44756500
C	-0.64470100	5.66356200	0.17069700
H	-2.59601500	5.56642900	1.08514700
H	1.28018300	5.45489800	-0.77629800
C	-0.99506600	0.59409500	1.43965600
C	-2.16352900	0.17262800	2.09593800
C	0.15707600	0.76514500	2.22293700

C	-2.17348900	-0.08807600	3.46930000
C	0.15418600	0.50989600	3.59069700
C	-1.01362200	0.07330600	4.21859000
H	-3.09292200	-0.42350500	3.95017000
H	1.06438900	0.65264100	4.17350600
C	-2.95942900	0.27996900	-1.16380400
C	-4.07758800	1.12251000	-1.24256600
C	-3.13725200	-1.09790700	-1.36471200
C	-5.34434300	0.59818000	-1.49568700
C	-4.40256500	-1.62206600	-1.61381900
C	-5.50650300	-0.77314300	-1.67858400
H	-6.20619900	1.26200900	-1.55400300
H	-4.52679100	-2.69507700	-1.76015500
H	-6.49675700	-1.18152700	-1.87573800
H	-2.28047400	-1.77402900	-1.30868700
H	-0.53771600	6.73595800	0.32852900
H	3.23410800	0.44503600	-2.15249200
H	1.03691700	3.02099500	-1.14980000
H	6.65968400	2.70297600	-0.85467300
H	-2.83014500	3.13495300	0.76574600
H	1.07996700	1.10119700	1.74683500
H	-3.09019100	0.02199800	1.53694600
H	-1.01726900	-0.13280000	5.28830300
H	5.49588900	-0.85558100	1.26473300
H	0.42929300	-4.40526900	-1.75003500
H	-0.02913900	-2.06739000	1.82844400
H	-3.25191400	-4.58380900	0.48088200
H	-3.96791200	2.20042100	-1.10610700

TSB9_S_P

E_{elec} (M06/BS1) = -1638.37649410 au
H_{corr} (M06/BS1) = 0.549593 au
G_{corr} (M06/BS1) = 0.448423 au
SPE (M06/BS2//M06/BS1) = -1638.25697973 au

0 1

C	-0.70990200	-4.58211200	-0.26166100
C	-1.82076500	-4.19431500	-0.91728900
C	-0.67189800	-2.33671200	-0.38598400
N	0.00542400	-3.43102200	0.05790000
H	-0.33194400	-5.56243200	-0.00751500
H	-2.64183900	-4.75921200	-1.33620000
N	-1.80282700	-2.80098300	-0.99254400
N	-0.25556100	-1.09191600	-0.15813900
N	-0.68193800	-0.12220000	-0.94876400
O	0.66010600	0.35063300	-1.79486500
V	0.58527800	1.12984700	-0.26658800
C	-2.90050000	-2.02995500	-1.49226600
C	-3.66776900	-1.27439300	-0.61150800
C	-3.21872500	-2.11136000	-2.84327600
C	-4.76033400	-0.56994000	-1.10316000
C	-4.32055400	-1.41041700	-3.32314300
C	-5.08758900	-0.63733300	-2.45585400
H	-5.36426300	0.02964400	-0.42421800
H	-4.57585800	-1.46514000	-4.37927100
C	1.31702800	-3.41557400	0.62382100
C	2.36076100	-2.81221900	-0.07323800
C	1.53178600	-4.04639200	1.84452500
C	3.63944000	-2.84618300	0.46750700
C	2.81857400	-4.07769200	2.37406800
C	3.86972300	-3.47691900	1.68821900
H	4.45944600	-2.36579400	-0.06275200
H	2.99488600	-4.56833900	3.32922100
C	2.23995700	0.66743100	0.79207600
C	3.46996500	1.07417400	0.25635300
C	2.23086700	0.04660300	2.04849300
C	4.65642100	0.88904000	0.96675900
C	3.40983100	-0.12292200	2.76835500
C	4.62446600	0.29642900	2.22651100
H	5.60480300	1.21044100	0.53701600
H	3.38586800	-0.60361700	3.74630800
C	0.72181400	3.05446800	-0.85564000
C	1.47353400	4.01094700	-0.15442300
C	-0.00323700	3.47864000	-1.98026000

C	1.50831200	5.34000700	-0.56982300
C	0.01940000	4.80878300	-2.39156200
C	0.77890100	5.74112200	-1.68724400
H	2.10307400	6.06692100	-0.01735500
H	-0.55065300	5.11850400	-3.26707700
C	-0.90473000	1.65698000	1.06261100
C	-2.27435900	1.61274000	0.77034000
C	-0.52848200	2.16098800	2.31991300
C	-3.23239900	2.03624100	1.68824700
C	-1.48068800	2.57408600	3.25151700
C	-2.83590700	2.51329200	2.93647200
H	-4.29154800	1.99578100	1.43156100
H	-1.16226200	2.94948200	4.22412400
H	-0.59344800	2.75351100	-2.54504900
H	2.04536100	3.72129400	0.72967900
H	0.80311600	6.78109700	-2.00997000
H	1.28986000	-0.31761900	2.46592700
H	3.51165800	1.54588000	-0.72862200
H	5.54912000	0.15246800	2.78423900
H	-3.58101400	2.84063400	3.66069900
H	0.52755600	2.23021900	2.59246500
H	-2.59759500	1.23688800	-0.20350300
H	-3.39860200	-1.23167500	0.44297300
H	-2.59992400	-2.71400900	-3.50618100
H	-5.94670600	-0.08695900	-2.83408700
H	0.69545300	-4.50376700	2.37141400
H	4.87368800	-3.49340800	2.10871000
H	2.16350200	-2.32097200	-1.02461000

TSB9i_S_P

E_{elec} (M06/BS1) = -1638.38030299 au
H_{corr} (M06/BS1) = 0.549515 au
G_{corr} (M06/BS1) = 0.448649 au
SPE (M06/BS2//M06/BS1) = -1638.26169704 au

0 1

C	0.37422100	-4.03697100	0.13904500
C	1.69991500	-3.81326100	0.03873800
C	0.65256800	-2.00657000	-0.75491900
N	-0.27490500	-2.92092300	-0.37167600
H	-0.17962600	-4.89895400	0.48275200
H	2.55221100	-4.43446900	0.27562400
N	1.87420300	-2.55276300	-0.53033500
N	0.29341200	-0.77737800	-1.17505800
N	1.12102600	0.15162200	-1.59849400
O	1.87884000	0.82805600	-0.20077700
V	0.18951600	1.06190400	-0.20007100
C	3.16374500	-1.98960500	-0.80280000
C	3.50715400	-1.63367600	-2.10133100
C	4.05837900	-1.85060100	0.25221000
C	4.76979300	-1.10308300	-2.33899500
C	5.32242400	-1.32938500	0.00041900
C	5.67566000	-0.95144600	-1.29219800
H	5.04807900	-0.81377700	-3.35002700
H	6.02915000	-1.21048900	0.81874200
C	-1.69266300	-2.74194700	-0.40008700
C	-2.31228200	-2.23960500	-1.54192100
C	-2.42818300	-3.09023000	0.72725200
C	-3.69117300	-2.06588400	-1.53665200
C	-3.80836100	-2.92558800	0.71371400
C	-4.44059500	-2.40807700	-0.41265800
H	-4.18265400	-1.67016100	-2.42329400
H	-4.38637500	-3.18288700	1.59923700
C	0.35604200	2.69422900	1.11265500
C	1.57645500	2.94131600	1.76296700
C	-0.71233600	3.54721900	1.44277600
C	1.72705600	3.97452900	2.68835700
C	-0.57505800	4.57945500	2.36718100
C	0.64920900	4.79841900	2.99647900
H	2.69285200	4.13529700	3.16894000
H	-1.42735500	5.22051100	2.59517700
C	-0.85713100	2.26944500	-1.40043900
C	-0.66815800	3.47069800	-2.09066300
C	-2.06615200	1.58111800	-1.54838900

C	-1.66668100	3.96532100	-2.91986400
C	-3.07491700	2.07725500	-2.38136900
C	-2.87141800	3.26927700	-3.06443500
H	-1.51610900	4.90238300	-3.45506200
H	-4.01478000	1.53612900	-2.48778500
C	-0.69977600	0.08522100	1.39219400
C	-2.02201200	0.29554300	1.81014700
C	0.07326800	-0.81587800	2.14267900
C	-2.55041400	-0.36503200	2.91771500
C	-0.44721500	-1.47887800	3.25410900
C	-1.76513600	-1.25606800	3.64571600
H	-3.58375200	-0.18156700	3.21344800
H	0.18281900	-2.16683300	3.81896900
H	-3.65263200	3.66591200	-3.71119700
H	-2.24438000	0.63302900	-1.02391800
H	0.26330700	4.02544900	-1.96914800
H	6.66316500	-0.53706400	-1.48486400
H	2.78961200	-1.76607600	-2.90811700
H	3.75596300	-2.13120000	1.26031300
H	-1.72060900	-1.98106100	-2.41711500
H	-1.91697900	-3.42933700	1.62707400
H	-2.17629400	-1.76890600	4.51448900
H	-2.66390400	0.99649000	1.27059600
H	-5.52006200	-2.27139400	-0.41711600
H	0.76112200	5.60665100	3.71858500
H	2.43555700	2.30509600	1.53875700
H	-1.68428900	3.41122800	0.96195500
H	1.11650100	-1.00013300	1.86913500

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for Int, TSInt, 2, Int_P, $TSInt_P$ & 2_P (singlet) in Solvent = THF

Int_S

E_{elec} (M06/BS1) = -680.56780250 au
H_{corr} (M06/BS1) = 0.270615 au
G_{corr} (M06/BS1) = 0.206883 au
SPE (M06/BS2//M06/BS1) = -680.19277464 au

0 1

O	-1.74242900	3.27893200	5.56819900
N	-0.98509700	1.19257300	8.07901200
N	-0.97288700	2.65329800	9.71262500
N	-3.00644500	2.51865000	8.56651900
N	-3.58950500	2.30143800	7.33940400
C	-1.75502900	2.13698400	8.71311500
C	0.26091200	1.12943800	8.70357800
H	1.02458400	0.44882800	8.35295100
C	0.26430700	2.02326800	9.71077700
H	1.03297600	2.29040200	10.42250400
C	-1.45301200	0.22156700	7.11344100
H	-2.45063000	-0.14029500	7.38990700
H	-1.49798200	0.64536700	6.10318800
H	-0.76001800	-0.62526100	7.11852900
C	-1.41463000	3.69669700	10.60825700
H	-1.90671100	4.48874200	10.03411400
H	-2.12551800	3.31022700	11.34882900
H	-0.54311800	4.10734500	11.12533400
V	-3.23871600	2.77608700	5.63310300
C	-4.96142500	1.82377300	7.47816400
H	-4.96345100	0.79993400	7.88224600
H	-5.52207400	2.48138700	8.15671500
H	-5.46665900	1.80704300	6.50211100
C	-4.48074300	4.33492500	5.22911500
H	-5.53135700	4.05739900	5.39745000
H	-4.23710400	5.21974800	5.83039100
H	-4.33736100	4.58424200	4.16502700
C	-3.58052800	1.19734500	4.38838600
H	-3.93302800	0.30253400	4.92158600
H	-4.39821700	1.55634000	3.73669000
H	-2.72284700	0.93350900	3.75789300

TSInt_S

E_{elec} (M06/BS1) = -680.55281170 au
H_{corr} (M06/BS1) = 0.269015 au
G_{corr} (M06/BS1) = 0.204053 au
SPE (M06/BS2//M06/BS1) = -680.17525567 au

0 1

V	-2.01495000	1.17724500	0.80792100
O	-1.16059000	0.61187400	2.02907100
N	-0.54328300	0.25842000	-0.90919000
N	-1.00988300	1.56387500	-0.64877800
N	1.24550800	-1.22441700	-0.77431700
N	1.66777300	0.70571800	0.16286500
C	0.70389100	0.00152600	-0.51053300
C	2.53742500	-1.28701900	-0.27813500
H	3.14219600	-2.17655500	-0.38580000
C	2.79970000	-0.09871900	0.29896800
H	3.68291300	0.26669200	0.80448700
C	-3.42801700	-0.19192000	0.34005800
H	-3.89818000	0.11803000	-0.60423800
H	-3.00156400	-1.19542800	0.22874000
H	-4.17115000	-0.19325500	1.15297100
C	-2.88206400	2.92651500	1.32050900
H	-2.13838600	3.66484200	1.65139700
H	-3.42805600	3.31358400	0.44708300
H	-3.58730300	2.74475600	2.14597700
C	-0.70792200	2.58791400	-1.61031700
H	-1.12631100	3.53934300	-1.25898200
H	0.37926100	2.71075600	-1.75709900
H	-1.14844000	2.34379600	-2.58993200
C	0.52850700	-2.27709400	-1.45988000
H	1.18391700	-3.14858500	-1.53464600
H	-0.37539500	-2.54666500	-0.90217700
H	0.23533700	-1.95189000	-2.46380200
C	1.58511700	2.03746600	0.74529200
H	1.48353300	2.80992500	-0.02393300
H	0.75239800	2.10083000	1.44867800
H	2.51939700	2.21492900	1.28564800

2_S

E_{elec} (M06/BS1) = -680.57712304 au
H_{corr} (M06/BS1) = 0.271120 au
G_{corr} (M06/BS1) = 0.208814 au
SPE (M06/BS2//M06/BS1) = -680.19852548 au

0 1

V	6.06947600	1.05237000	5.77419400
O	4.65115500	0.37989300	6.01694600
N	5.76876400	2.86690500	5.13911500
N	6.18378200	2.01009800	4.08458300
N	3.85027200	3.87876700	6.09246200
N	3.77081500	3.60126000	3.92976700
C	4.53212300	3.38718900	5.03037000
C	2.64215800	4.39940700	5.65822700
H	1.93624000	4.83720200	6.34974100
C	2.59322200	4.22852000	4.32045800
H	1.83503300	4.49067600	3.59611400
C	7.17103300	1.24883000	7.48441900
H	8.13448400	1.71618500	7.22963700
H	6.66248400	1.86747700	8.23792400
H	7.35539800	0.25466600	7.91792600
C	7.21463400	-0.40300000	4.89312900
H	6.87322200	-0.70604600	3.89654700
H	8.24887500	-0.03376600	4.82884700
H	7.18159500	-1.26944400	5.57175200
C	7.50923400	2.39841600	3.62829200
H	7.89484300	1.60515100	2.97748800
H	7.45746500	3.32966100	3.04039100
H	8.23517800	2.56734900	4.44635600
C	4.33214800	3.85105900	7.46042200
H	3.70054100	4.51032400	8.06061200
H	4.28566400	2.83501400	7.86768900
H	5.36596900	4.20845000	7.49543900
C	4.11709600	3.32738700	2.54033100
H	5.11385200	3.71649800	2.31705200
H	4.09669400	2.25565000	2.33630000
H	3.38251500	3.84193500	1.91448700

Int_S_P

E_{elec} (M06/BS1) = -1638.50031575 au
H_{corr} (M06/BS1) = 0.5529520 au
G_{corr} (M06/BS1) = 0.451906 au
SPE (M06/BS2//M06/BS1) = -1638.38108082 au

0 1

O	-2.02673400	3.03035500	5.56397500
N	-0.91958300	1.22373400	8.07237500
N	-0.97339100	2.82726500	9.58808800
N	-3.02878400	2.41820300	8.54051000
N	-3.69825700	1.91907800	7.43523900
C	-1.76625700	2.13109600	8.68464900
C	0.37947200	1.39567200	8.57636900
H	1.18669400	0.75296600	8.25428000
C	0.34262400	2.37027400	9.49582600
H	1.11729600	2.76449000	10.13823500
V	-3.49598200	2.49052300	5.68729700
C	-1.27480400	0.10985600	7.26526600
C	-0.49104500	-0.18512900	6.15139500
C	-2.34839000	-0.70968800	7.60905300
C	-0.78796700	-1.30081000	5.37631100
H	0.33476000	0.47361600	5.88498600
C	-2.64954400	-1.81167900	6.81671100
H	-2.94420300	-0.47939300	8.49093000
C	-1.87230600	-2.11124400	5.69991600
H	-0.17964500	-1.52459100	4.50160500
H	-3.49462700	-2.44476000	7.08325000
H	-2.11116900	-2.97634600	5.08432700
C	-1.38201900	3.93487800	10.37125400
C	-2.59754700	3.91443000	11.05726200
C	-0.53418000	5.03790400	10.47887300
C	-2.95781700	5.00285000	11.84270900
H	-3.24836700	3.04873900	10.97122600
C	-0.89951300	6.11504000	11.27853200
H	0.40061800	5.05703300	9.92081900
C	-2.11273900	6.10356400	11.96028700
H	-3.90639100	4.98415700	12.37638000
H	-0.23443800	6.97308200	11.35597200
H	-2.40029400	6.95128500	12.57916600
C	-3.75119500	1.18377500	4.14873400
C	-2.65681200	0.81000700	3.34589000
C	-5.02575600	0.74111200	3.74293400
C	-2.82171100	0.02022800	2.21090800
H	-1.65269700	1.13308100	3.62149000

C	-5.19883800	-0.03514700	2.60035700
H	-5.91153700	1.00518700	4.32576200
C	-4.09410400	-0.40314400	1.83546200
H	-1.95448300	-0.26224700	1.61433100
H	-6.19772500	-0.35789400	2.30849000
H	-4.22601000	-1.01804500	0.94622600
C	-4.68944100	4.10893500	5.52607500
C	-4.18619500	5.38547600	5.21591500
C	-6.08611700	3.95929200	5.61812100
C	-5.04002100	6.46288200	4.99655400
H	-3.10870000	5.53737200	5.14738700
C	-6.94298400	5.03300200	5.39255700
H	-6.52422100	2.98906000	5.86834900
C	-6.41942200	6.28635100	5.08251400
H	-4.62950300	7.44355600	4.75866300
H	-8.02117400	4.89400700	5.46323900
H	-7.08888600	7.12784800	4.90967100
C	-5.02868500	1.52369300	7.73533400
C	-5.79363000	2.22573300	8.68001400
C	-5.59495900	0.45112200	7.04260000
C	-7.11840200	1.87543600	8.88552700
H	-5.33125000	3.04690700	9.22357200
C	-6.93599500	0.12301200	7.24212600
H	-4.97200800	-0.13254100	6.36590300
C	-7.70078600	0.83254500	8.15979600
H	-7.71156800	2.42766200	9.61276200
H	-7.37127500	-0.70940400	6.69137500
H	-8.74375000	0.56910700	8.32523300

TSInt_S$_P$

E_{elec} (M06/BS1) = -1638.49596031 au
H_{corr} (M06/BS1) = 0.551614 au
G_{corr} (M06/BS1) = 0.451299 au
SPE (M06/BS2//M06/BS1) = -1638.37619730 au

0 1

V	-2.10818100	1.10507100	0.80057300
O	-1.37917900	0.33202900	1.97616100
N	-0.49200100	0.24438000	-0.91884300
N	-0.97121900	1.52514600	-0.59519700
N	1.29040000	-1.26769600	-0.68712400
N	1.70675100	0.73457000	0.11053900
C	0.73886400	-0.01470200	-0.51757500
C	2.58571100	-1.28195800	-0.17090900
H	3.20124500	-2.16854800	-0.22665300
C	2.84560600	-0.05483000	0.30772200
H	3.72814600	0.36165300	0.77315000
C	0.63332600	-2.40583500	-1.22874100
C	-0.10650500	-2.31154900	-2.40727100
C	0.77909500	-3.63194200	-0.58162500
C	-0.70553600	-3.45230000	-2.92791100
H	-0.21400600	-1.34903400	-2.89982100
C	0.18696200	-4.76926700	-1.11995800
H	1.34228700	-3.68765100	0.34871700
C	-0.55880000	-4.68246000	-2.29137800
H	-1.28545900	-3.37918400	-3.84599700
H	0.30240500	-5.72518400	-0.61272400
H	-1.02708800	-5.57222600	-2.70778200
C	1.70553900	2.13150700	0.43449900
C	2.37553400	3.01055100	-0.41103400
C	1.11331400	2.58011500	1.61092300
C	2.42976800	4.36303400	-0.08858800
H	2.83075100	2.62963200	-1.32445800
C	1.16727600	3.93427000	1.92336900
H	0.60130700	1.86669800	2.25514700
C	1.82347300	4.82482600	1.07552500
H	2.93956500	5.05608400	-0.75502900
H	0.70218500	4.29553800	2.83897100
H	1.86305200	5.88327800	1.32647700
C	-0.70503800	2.58513900	-1.46277300
C	-1.03337300	3.89553400	-1.08068000
C	-0.10343800	2.36771800	-2.71115400
C	-0.76741300	4.95592500	-1.93345700
H	-1.47326400	4.06934100	-0.09860000

C	0.16034800	3.44254100	-3.55296600
H	0.14879100	1.35134500	-3.00742700
C	-0.16610600	4.74148400	-3.17420400
H	-1.01867200	5.96766800	-1.61742900
H	0.62634900	3.25799500	-4.52034500
H	0.04626800	5.57923800	-3.83574600
C	-3.04844700	2.66997000	1.61950900
C	-3.99619700	3.34730500	0.82777900
C	-2.75667500	3.18979000	2.89331400
C	-4.62053500	4.50349600	1.28639100
H	-4.24958200	2.96944400	-0.16687400
C	-3.37454700	4.34835100	3.35307000
H	-2.03094300	2.67851800	3.52784000
C	-4.30615300	5.00396900	2.54866100
H	-5.35200000	5.01556200	0.66281800
H	-3.13602300	4.74213500	4.34027300
H	-4.79193700	5.90956400	2.90926400
C	-3.50536100	-0.11917800	0.03902700
C	-4.28134100	-0.93843700	0.87299000
C	-3.84326600	-0.03488400	-1.32212000
C	-5.37862200	-1.63323300	0.36928400
H	-4.02938600	-1.03231600	1.93092400
C	-4.93967700	-0.72916800	-1.82708900
H	-3.23734900	0.57491800	-1.99699900
C	-5.70793200	-1.52671200	-0.98041600
H	-5.97588700	-2.26298600	1.02782100
H	-5.19395400	-0.65395300	-2.88390800
H	-6.56290300	-2.07326500	-1.37618100

2_S_P

E_{elec} (M06/BS1) = -1638.51676575 au
H_{corr} (M06/BS1) = 0.552449 au
G_{corr} (M06/BS1) = 0.451755 au
SPE (M06/BS2//M06/BS1) = -1638.39710834 au

0 1

V	0.65111300	0.67831200	-0.80207100
O	0.97277300	0.12592500	-2.24527300
N	-0.03233600	-0.80581600	0.27086400
N	-1.09646200	0.02700400	-0.15523000
N	0.97324900	-2.87379800	-0.38452600
N	-1.20597400	-2.77911000	-0.52064000
C	-0.10004700	-2.06373600	-0.18674500
C	0.53217300	-4.10035400	-0.87690500
H	1.23201700	-4.89407600	-1.09729700
C	-0.81117500	-4.04311700	-0.95862500
H	-1.54453900	-4.77570700	-1.26499800
C	2.34259900	-2.52409000	-0.17337400
C	3.24279100	-2.68598200	-1.22257300
C	4.58576700	-2.39138600	-1.01407600
H	5.29675900	-2.51612800	-1.82814300
C	5.01460800	-1.92968000	0.22727500
C	4.10192100	-1.76416800	1.26547100
H	4.43516100	-1.39236100	2.23228000
C	2.75938400	-2.06607200	1.07254800
C	-2.57543700	-2.40643000	-0.30578900
C	-3.05148800	-2.30506500	0.99622300
C	-4.38644400	-1.97552900	1.20520100
H	-4.76428400	-1.88087600	2.22130600
C	-5.23208600	-1.76894600	0.11934400
C	-4.74474000	-1.89038500	-1.18100200
H	-5.40572000	-1.72795200	-2.02978400
C	-3.40984600	-2.21152300	-1.40050300
C	-1.79014400	0.65348600	0.89347400
C	-1.53448800	0.42738900	2.25157400
C	-2.31744600	1.04477100	3.22484400
H	-2.10980400	0.85143900	4.27717400
C	-3.35807600	1.89451400	2.86542500
C	-3.61148000	2.12390400	1.51099700
H	-4.42640100	2.78314600	1.21393400
C	-2.84219100	1.51079600	0.53489200
C	-0.25203400	2.47397600	-1.16655000
C	-0.83144900	2.78400400	-2.40648500
C	-1.45281200	4.01169700	-2.62718800

H	-1.90273200	4.22673700	-3.59659100
C	-1.50000800	4.96371000	-1.61093600
C	-0.92045000	4.68274200	-0.37587100
H	-0.94948200	5.42404100	0.42267100
C	-0.31320500	3.44790500	-0.15696200
C	2.36244000	1.18933600	0.15166100
C	3.59435700	1.29542000	-0.51737100
C	4.74978700	1.68850600	0.15428400
H	5.69597100	1.76219000	-0.38162700
C	4.69630100	1.98259700	1.51462400
C	3.48771900	1.87920000	2.20479600
H	3.44727100	2.10613400	3.26986800
C	2.33907700	1.48302400	1.52765900
H	0.11873000	3.24663900	0.82741500
H	-1.98492500	5.92425800	-1.78177500
H	-0.80836500	2.04680200	-3.21065600
H	-3.96914000	2.37227900	3.62931800
H	-3.04114700	1.67987800	-0.52382600
H	-0.72761400	-0.24817600	2.53436600
H	-2.37671700	-2.47247800	1.83412400
H	-6.27666200	-1.51302300	0.28558700
H	-3.00446600	-2.29601600	-2.40744400
H	1.40172600	1.39651500	2.08690500
H	5.59868000	2.28934900	2.04240200
H	3.65239000	1.05500900	-1.58037100
H	2.88502000	-3.02823600	-2.19265900
H	6.06476300	-1.69099400	0.38552000
H	2.03597700	-1.94242300	1.87636400

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 2, TSB2, 3, 2_P, $TSB2_P$ & 3_P (singlet) in Solvent = toluene

2_S

E_{elec} (M06/BS1) = -680.57058441 au
H_{corr} (M06/BS1) = 0.271027 au
G_{corr} (M06/BS1) = 0.208182 au
SPE (M06/BS2//M06/BS1) = -680.19250772 au

0 1

V	6.07521600	1.05603900	5.76444300
O	4.64776600	0.41688400	6.01077700
N	5.78558100	2.88596800	5.13443000
N	6.18944100	2.02342600	4.07731600
N	3.86378200	3.88216600	6.09503500
N	3.77991000	3.60427000	3.93220400
C	4.54850300	3.39478800	5.03084000
C	2.64940300	4.39102100	5.66453000
H	1.94097600	4.82062000	6.35878000
C	2.59829200	4.22134300	4.32709100
H	1.83517700	4.47701400	3.60550300
C	7.15406700	1.29353000	7.48356600
H	8.10590600	1.78875300	7.23817600
H	6.62917000	1.88610300	8.24573100
H	7.36337800	0.29846900	7.90484600
C	7.19862700	-0.40998800	4.88442700
H	6.84196100	-0.71155800	3.89303100
H	8.23987700	-0.06221200	4.81247800
H	7.14986600	-1.27219700	5.56763300
C	7.51899300	2.39925700	3.62508300
H	7.89777600	1.60171100	2.97538900
H	7.47794200	3.33150100	3.03671700
H	8.24520300	2.56251900	4.44430200
C	4.33541400	3.82259600	7.46436500
H	3.73758300	4.51295100	8.06527300
H	4.23527400	2.80709900	7.86450800
H	5.38751700	4.12110300	7.50407900
C	4.12264400	3.32174600	2.54457200
H	5.11150900	3.72567600	2.31063900
H	4.12455200	2.24735100	2.35410900
H	3.37465600	3.81613200	1.91714500

TSB2_S

E_{elec} (M06/BS1) = -680.51194402 au
H_{corr} (M06/BS1) = 0.268651 au
G_{corr} (M06/BS1) = 0.205637 au
SPE (M06/BS2//M06/BS1) = -680.13494843 au

0 1

C	3.62531800	-0.25205200	0.00996200
C	3.30730700	1.05887600	0.10583400
C	1.38123000	-0.07437200	-0.20065600
N	2.44266000	-0.95255100	-0.14942200
H	4.58278200	-0.75365700	0.03947100
H	3.93226700	1.92792600	0.25994000
N	1.93648600	1.17422800	-0.04179300
C	2.29549100	-2.38045700	-0.30667700
H	1.33964200	-2.68305500	0.13431600
H	2.29813600	-2.67049800	-1.36436700
H	3.11783000	-2.88447900	0.21004700
C	1.17069000	2.40148300	0.02544900
H	0.72150300	2.52561100	1.01831800
H	1.83841900	3.24068800	-0.18919800
H	0.36267700	2.36951200	-0.71190400
N	0.14428400	-0.43231500	-0.38342600
N	-0.97044100	0.25188000	1.25706000
O	-1.81830300	1.53433100	-1.15208600
V	-1.64187000	0.13730400	-0.41656300
C	-2.68666000	-1.35497100	-1.36189200
H	-2.61357700	-2.28077400	-0.77179700
H	-3.74371000	-1.10654000	-1.52037500
H	-2.20724200	-1.51611800	-2.34044500
C	-3.29064000	0.17977500	1.02125100
H	-3.52413100	-0.85922900	1.27984000
H	-3.21595000	0.80402800	1.91612200
H	-4.03655200	0.60135000	0.33658100
C	-0.81865900	-0.86406000	2.13423700
H	-1.13531400	-1.83937300	1.72459300
H	0.23061200	-0.92707700	2.46387500
H	-1.40230100	-0.64413900	3.04284200

3_S

E_{elec} (M06/BS1) = -680.64966776 au
H_{corr} (M06/BS1) = 0.274214 au
G_{corr} (M06/BS1) = 0.209239 au
SPE (M06/BS2//M06/BS1) = -680.27044765 au

0 1

V	4.95831000	2.51023900	5.33324800
O	5.37995100	2.30272200	6.84789600
N	6.08502900	3.50828600	4.39204100
N	3.21769200	3.07749500	5.22671900
N	7.36659500	5.26540400	5.41386200
N	8.42769400	3.88365300	4.09940200
C	7.19406000	4.15419800	4.63031600
C	8.69638800	5.66044300	5.38079100
H	9.04410900	6.52107500	5.93556500
C	9.35393700	4.80358400	4.56944200
H	10.39299600	4.76372300	4.27284700
C	2.24261800	3.19238900	6.28592900
H	2.65954400	2.82773900	7.22986900
H	1.92528400	4.24167800	6.42105400
H	1.33914900	2.60398000	6.05099700
C	2.72970600	3.56955400	3.95560800
H	1.83459200	3.00848900	3.63730900
H	2.45490600	4.63767200	4.01853100
H	3.49496400	3.46123900	3.17646100
C	4.96710000	0.66471200	4.44932300
H	4.61082100	0.77886600	3.41479200
H	5.98535500	0.25282200	4.43435500
H	4.30541600	-0.02518400	4.98862400
C	8.68060400	2.73405200	3.26126600
H	8.68601700	1.81142200	3.85500900
H	7.89470100	2.65456400	2.50318900
H	9.65076200	2.85741800	2.77182600
C	6.29774500	5.86479500	6.18083000
H	5.38825800	5.89653800	5.57008400
H	6.08855600	5.28315500	7.08654200
H	6.58678500	6.88302600	6.45662100

2_S_P

E_{elec} (M06/BS1) = -1638.50822457 au
H_{corr} (M06/BS1) = 0.552404 au
G_{corr} (M06/BS1) = 0.453434 au
SPE (M06/BS2//M06/BS1) = -1638.38957440 au

0 1

V	0.62998900	0.68083200	-0.81154500
O	0.91316600	0.08274200	-2.24119100
N	-0.01252500	-0.80296700	0.31549300
N	-1.08431100	0.02890200	-0.09854400
N	0.98677300	-2.86111700	-0.37271100
N	-1.19144800	-2.75175800	-0.53015300
C	-0.08507500	-2.04809300	-0.16742400
C	0.54440300	-4.07257800	-0.89955400
H	1.24252500	-4.86524700	-1.12905600
C	-0.79743300	-4.00650400	-0.99416300
H	-1.53138200	-4.72794200	-1.32486500
C	2.35547700	-2.51919000	-0.15194300
C	3.26300100	-2.68895900	-1.19330200
C	4.60638300	-2.40503400	-0.97488500
H	5.32225300	-2.53361800	-1.78418800
C	5.02916700	-1.94547600	0.26885500
C	4.10900100	-1.76793600	1.29815600
H	4.43773000	-1.39624900	2.26643000
C	2.76550600	-2.05663700	1.09441700
C	-2.56124400	-2.37284800	-0.33284500
C	-3.05612400	-2.27323100	0.96205500
C	-4.38949900	-1.92886600	1.15320100
H	-4.77838400	-1.82607900	2.16434000
C	-5.21759200	-1.71155100	0.05639800
C	-4.71330400	-1.83526300	-1.23668500
H	-5.35956500	-1.66104700	-2.09455800
C	-3.37860100	-2.16720700	-1.43826600
C	-1.76741200	0.65275200	0.95692100
C	-1.51003900	0.40798400	2.31143100
C	-2.28950300	1.01416300	3.29445000
H	-2.08010500	0.80648100	4.34386200
C	-3.32615300	1.87336600	2.94872100
C	-3.57897600	2.12363000	1.59806200
H	-4.38937800	2.79278200	1.31098500
C	-2.81606500	1.52008300	0.61171900
C	-0.28767200	2.45843500	-1.18704600
C	-0.88942000	2.74036600	-2.42309200
C	-1.52064100	3.95999100	-2.65546200

H	-1.98689600	4.15589100	-3.62128300
C	-1.55605500	4.92950300	-1.65550900
C	-0.95607200	4.67497800	-0.42499900
H	-0.97797000	5.43021700	0.36050300
C	-0.33823800	3.44839300	-0.19303700
C	2.35804800	1.15318300	0.12840300
C	3.58988500	1.26321700	-0.53776400
C	4.73950200	1.66829300	0.13658500
H	5.68712400	1.74741000	-0.39631800
C	4.67885000	1.97077500	1.49472700
C	3.46908300	1.86248900	2.18137400
H	3.42264400	2.09718700	3.24471900
C	2.32644000	1.45213100	1.50237100
H	0.10757200	3.26671500	0.78868000
H	-2.04923500	5.88424400	-1.83585800
H	-0.87284800	1.98727800	-3.21214800
H	-3.93310800	2.34458000	3.72001800
H	-3.01511800	1.70432400	-0.44432300
H	-0.70322100	-0.27285400	2.58225300
H	-2.39459200	-2.44525200	1.80952100
H	-6.26092600	-1.44204900	0.20856000
H	-2.95738600	-2.24401700	-2.43936400
H	1.38661100	1.35809100	2.05655600
H	5.57697200	2.28899600	2.02339600
H	3.65200300	1.01818500	-1.59939100
H	2.90886100	-3.02212600	-2.16780600
H	6.07978000	-1.71447400	0.43550100
H	2.03347300	-1.91342200	1.88713300

TSB2_S_P

E_{elec} (M06/BS1) = -1638.45039939 au
H_{corr} (M06/BS1) = 0.549981 au
G_{corr} (M06/BS1) = 0.449370 au
SPE (M06/BS2//M06/BS1) = -1638.32907965 au

0 1

V	5.83815900	0.59093000	5.34541500
O	4.81992800	-0.52169200	4.87173400
N	5.01225400	2.27357300	5.42688100
N	6.40398500	1.71397000	3.97608600
N	4.37304600	4.54641300	5.68853200
N	3.76557800	3.58538700	3.80367300
C	4.42994500	3.33983700	4.99837300
C	3.68126900	5.48688500	4.93728800
H	3.45847700	6.46910200	5.33033200
C	3.33043400	4.90358500	3.77376600
H	2.75909200	5.28394900	2.93840100
C	5.00524700	4.80191000	6.93178300
C	4.96738100	3.85892900	7.95651700
C	5.60904000	4.13779500	9.15936100
H	5.58826400	3.39225500	9.95227300
C	6.26807600	5.34842500	9.34637200
C	6.29714900	6.28689900	8.31705900
H	6.81903100	7.23254100	8.45140800
C	5.67380500	6.01516600	7.10602200
C	3.63281200	2.67071100	2.72306700
C	3.92926800	3.10717700	1.43298900
C	3.80201300	2.22517000	0.36671300
H	4.03335800	2.56257500	-0.64190600
C	3.39995200	0.91093200	0.59240700
C	3.11015900	0.48589600	1.88559000
H	2.80497700	-0.54175100	2.07192200
C	3.21143700	1.36545500	2.95624200
C	7.19636700	2.79070400	3.75521300
C	7.77002200	3.58677800	4.78202100
C	8.58174800	4.65803500	4.46497800
H	9.00181100	5.27526100	5.25729900
C	8.88051800	4.93917800	3.12695300
C	8.33745200	4.16670100	2.10205800
H	8.57037300	4.39646800	1.06407100
C	7.47390800	3.12614000	2.40842500
C	7.68747100	-0.30656000	4.84177200
C	7.67922600	-1.56840700	4.23314500
C	8.87148900	-2.24487800	3.97337600

H	8.84143600	-3.23098100	3.50897800
C	10.09365000	-1.66629300	4.30068800
C	10.11803500	-0.40364300	4.89000100
H	11.06986100	0.06080600	5.14888500
C	8.92605500	0.26885800	5.14476900
C	6.31131800	0.16846800	7.29444800
C	5.94008200	-1.05047300	7.88791900
C	6.22681100	-1.32562000	9.22311500
H	5.92535000	-2.27806000	9.65921800
C	6.90171600	-0.38717200	10.00009300
C	7.28724400	0.82616000	9.43424100
H	7.81649600	1.56713400	10.03499800
C	6.99359800	1.09406200	8.09944800
H	8.97349700	1.25880300	5.60740400
H	6.73103200	-2.03562600	3.96678100
H	3.31628700	0.21622400	-0.24109500
H	2.99792300	1.02886500	3.96723200
H	4.28349400	4.12570600	1.27586200
H	7.52022100	3.36298900	5.81934800
H	9.53484700	5.77509100	2.88516400
H	7.00447400	2.52257100	1.63309400
H	11.02459900	-2.19299900	4.09347500
H	5.72736400	6.72457200	6.28114600
H	4.45073600	2.91328000	7.81067800
H	6.76297000	5.56048100	10.29214900
H	7.30065700	2.05929800	7.68581100
H	7.12930200	-0.60149000	11.04388800
H	5.42020300	-1.80028500	7.28939400

3_S_P

E_{elec} (M06/BS1) = -1638.59203532 au
H_{corr} (M06/BS1) = 0.553772 au
G_{corr} (M06/BS1) = 0.453844 au
SPE (M06/BS2//M06/BS1) = -1638.47170318 au

0 1

V	4.89675900	2.22463200	5.35061300
O	5.45942400	1.77072400	6.75656900
N	6.00682000	3.33884400	4.56041900
N	3.14693700	2.89310800	5.51323100
N	7.17037600	5.24612300	5.42965100
N	8.34152600	3.80824800	4.25878200
C	7.07818100	4.04072500	4.76148600
C	8.45780300	5.75993600	5.29618200
H	8.74080800	6.68791400	5.77367500
C	9.17797600	4.87587500	4.57927800
H	10.22396000	4.86941200	4.30594600
C	6.06104800	5.92979600	6.00235200
C	5.29298300	5.31625100	6.98986100
C	5.75065400	7.20987500	5.54804600
C	4.18794900	5.98585100	7.50564100
H	5.55574600	4.31956000	7.34325900
C	4.65394000	7.87773900	6.08307200
H	6.35807400	7.66524500	4.76679300
C	3.86614500	7.26274800	7.05270300
H	3.57272200	5.50006600	8.26168100
H	4.40737700	8.87700200	5.72916800
H	2.99875700	7.77979200	7.45892100
C	8.69681300	2.69715200	3.44558200
C	8.32289700	1.40893300	3.82064500
C	9.42493600	2.91686500	2.27845300
C	8.66152400	0.33785200	3.00292900
H	7.76747300	1.24961800	4.74208700
C	9.78227400	1.83472200	1.48192400
H	9.69092400	3.93309400	1.99037700
C	9.39400600	0.54603600	1.83721700
H	8.34369700	-0.66497600	3.28363900
H	10.35191800	2.00442300	0.57020000
H	9.66153300	-0.29766000	1.20393200
C	2.35011900	3.16732500	6.63810400
C	1.29758100	4.09535200	6.58443700
C	2.61390400	2.53016100	7.86240300
C	0.55342800	4.38749500	7.72220200
H	1.06959100	4.60038600	5.64781100

C	1.86626200	2.83240500	8.99128800
H	3.42082800	1.80151100	7.91338600
C	0.83176300	3.76589700	8.93505500
H	-0.25404300	5.11567100	7.65350200
H	2.09214200	2.32432500	9.92806100
H	0.24638800	3.99756200	9.82299900
C	2.69059900	3.37376900	4.24577000
C	1.84675100	2.56882600	3.47660500
C	3.08974600	4.62239500	3.76144500
C	1.41496800	3.00262600	2.22821200
H	1.55271800	1.59571100	3.86927800
C	2.65685600	5.05044900	2.51124200
H	3.74743700	5.23994400	4.37473400
C	1.82310400	4.24210700	1.74178600
H	0.76422400	2.36701200	1.62988400
H	2.97426700	6.02168300	2.13473800
H	1.49000700	4.58006400	0.76181900
C	4.88532600	0.54914200	4.20150000
C	5.07665700	-0.74068300	4.71855400
C	4.72579800	0.68407400	2.81216400
C	5.09874800	-1.85638800	3.88237000
H	5.21543200	-0.87480800	5.79235900
C	4.74645600	-0.42660900	1.97367400
H	4.59284300	1.67664400	2.37291600
C	4.93315300	-1.70010500	2.50862500
H	5.24665100	-2.85020900	4.30512600
H	4.62386000	-0.29951800	0.89815900
H	4.95285700	-2.57044300	1.85348800

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TS7c, TS8c & TS11c (triplet) in Solvent = THF

TS7c_T

E_{elec} (M06/BS1) = -680.42917888 au
H_{corr} (M06/BS1) = 0.263908 au
G_{corr} (M06/BS1) = 0.195048 au
SPE (M06/BS2//M06/BS1) = -680.05831562 au

0 3

C	-0.00963700	0.01549900	-0.04100700
C	-0.04244100	-0.05702200	1.30252700
C	2.12370800	-0.01667000	0.68513300
N	1.32628400	0.04218000	-0.42412200
H	-0.80507600	0.05487300	-0.77211000
H	-0.87285000	-0.09349000	1.99378500
N	1.27687600	-0.07481400	1.76349200
C	1.85315900	0.11712300	-1.76647100
H	2.47184700	1.01407800	-1.88545800
H	2.46894800	-0.76251400	-1.98764900
H	1.01603000	0.15887200	-2.46793200
C	1.65607600	-0.14568900	3.16116800
H	2.28438400	0.70557600	3.44155800
H	0.74068400	-0.12161500	3.75967800
H	2.19398700	-1.07721100	3.37963400
N	3.43307600	0.00427200	0.59086000
N	4.18110500	-0.00092000	1.70661000
O	4.48693000	-1.31043500	2.03510600
V	5.40390800	-1.58828900	3.54932900
C	5.28959300	-0.20848900	5.00602800
H	5.99679600	-0.39863500	5.82635300
H	5.54751800	0.74080100	4.50833600
H	4.26482300	-0.13948600	5.40110800
C	7.33073200	-1.63924800	2.97145700
H	7.89935800	-1.82558800	3.89729800
H	7.52291600	-2.44966400	2.25465000
H	7.64201900	-0.67662900	2.53943100
C	4.91987700	-3.34658000	4.39125100
H	5.60707500	-3.56469700	5.22229000
H	3.88024800	-3.35779400	4.75094600
H	5.04307700	-4.11238600	3.60925500

TS8c_T

E_{elec} (M06/BS1) = -680.43611321 au
H_{corr} (M06/BS1) = 0.264681 au
G_{corr} (M06/BS1) = 0.196649 au
SPE (M06/BS2//M06/BS1) = -680.06439847 au

0 3

C	0.27706200	0.95088300	-0.14755100
C	0.33337200	1.22482400	1.16914700
C	2.14908900	0.00299100	0.65917800
N	1.40095700	0.19580300	-0.46395600
H	-0.44870000	1.22002300	-0.90196800
H	-0.33443900	1.78365200	1.80984400
N	1.49692100	0.64210100	1.67775200
C	1.76852700	-0.32727100	-1.76059800
H	2.75180700	0.05209100	-2.06059200
H	1.80733500	-1.42222700	-1.73648900
H	1.01941600	-0.00672100	-2.48885600
C	1.88500300	0.66722400	3.07643800
H	2.87545800	1.11661200	3.20316900
H	1.15144500	1.27276800	3.61572000
H	1.89084000	-0.34196500	3.50318000
N	3.26016800	-0.70792700	0.62713800
N	3.96009500	-0.82433200	1.77225600
O	4.97774800	0.00933300	1.95326900
V	5.45083900	-1.76420500	2.61815900
C	5.29309200	-2.10764700	4.59173500
H	5.89115400	-2.98849300	4.87225600
H	5.64234700	-1.23123700	5.15756700
H	4.23348000	-2.29536700	4.82540100
C	7.41204900	-1.51882500	2.15388400
H	7.96157600	-2.37900900	2.57135000
H	7.52369200	-1.52704500	1.05944200
H	7.82502700	-0.58139000	2.55398200
C	5.01561200	-3.47950100	1.63179300
H	5.71280800	-4.24102400	2.02019000
H	3.97738200	-3.81082200	1.77565700
H	5.20415300	-3.34357000	0.55597700

TS11c_T

E_{elec} (M06/BS1) = -680.43088695 au
H_{corr} (M06/BS1) = 0.265221 au
G_{corr} (M06/BS1) = 0.199701 au
SPE (M06/BS2//M06/BS1) = -680.06361863 au

0 3

C	-4.59856900	-0.45112900	-0.62250000
C	-4.25930300	0.82023400	-0.90787700
C	-2.42789600	-0.19326600	-0.08687600
N	-3.46781100	-1.07648000	-0.11457500
H	-5.53385100	-0.98161800	-0.73404400
H	-4.83469100	1.63630500	-1.32197400
N	-2.91149200	0.98652700	-0.58350600
C	-3.36655000	-2.43034200	0.38337600
H	-2.61684200	-2.99349500	-0.18281400
H	-3.07615000	-2.42415000	1.44078800
H	-4.34125000	-2.91266300	0.27575400
C	-2.19061100	2.23660700	-0.75147000
H	-1.22877800	2.05923200	-1.24096600
H	-2.80067600	2.89488600	-1.37590500
H	-2.01564900	2.72826800	0.21374400
N	-1.24925000	-0.55955300	0.38906300
N	-0.28646700	0.41611800	0.56852300
O	0.45702800	0.74461900	-0.37895100
V	-0.30349600	0.91520300	2.39662200
C	0.83076700	-0.55226700	3.19255600
C	-2.16269500	0.96363600	3.20100400
C	0.55957100	2.69439200	2.78763700
H	0.81556300	-0.36925400	4.28066600
H	0.41030800	-1.54740600	2.98583800
H	1.87001900	-0.50729800	2.83433300
H	-2.09883600	1.23054200	4.26750600
H	-2.82163200	1.68142900	2.68703900
H	-2.59215100	-0.04637400	3.10641200
H	0.63680900	2.89705900	3.86641500
H	1.57452100	2.62229600	2.36150300
H	0.02618900	3.52008500	2.29196000

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for TS8c & TS9c (singlet) in Solvent = THF

TS8c_S

E_{elec} (M06/BS1) = -680.44583483 au
H_{corr} (M06/BS1) = 0.265524 au
G_{corr} (M06/BS1) = 0.200851 au
SPE (M06/BS2//M06/BS1) = -680.07263101 au

0 1

C	0.03858600	0.08101500	0.10588200
C	0.23502900	0.16098100	1.43550300
C	2.24842100	-0.10778800	0.47547000
N	1.28358700	-0.08465900	-0.48784800
H	-0.86474500	0.12890300	-0.48595300
H	-0.46262600	0.29116200	2.25103300
N	1.60684600	0.05025500	1.67290100
C	1.56762900	-0.22016500	-1.89913400
H	2.24503900	0.57431100	-2.23097900
H	2.03641800	-1.18926100	-2.10422300
H	0.62669500	-0.14914100	-2.45050900
C	2.20486400	0.02547700	2.99701900
H	3.02982600	0.74142900	3.06338900
H	1.43038300	0.30458000	3.71720500
H	2.57833000	-0.97516800	3.24324300
N	3.52245700	-0.27294100	0.15095500
N	4.38925500	-0.25157800	1.19185700
O	5.00720400	0.92582200	1.54268300
V	6.02375700	-0.67973600	1.70245700
C	7.48265100	0.56878900	2.37611300
H	8.36194100	-0.09092200	2.47760000
H	7.70003400	1.39142200	1.68499900
H	7.21563600	0.96771300	3.36354200
C	6.76134700	-1.53450300	0.05602500
H	7.80307800	-1.84982400	0.22074200
H	6.13029800	-2.41521700	-0.14781900
H	6.70404000	-0.84352100	-0.79598300
C	5.97433200	-1.88937700	3.31269400
H	7.00196300	-2.17445500	3.58520300
H	5.51857600	-1.33762100	4.14853200
H	5.37427300	-2.78757200	3.10315300

TS9c_S

E_{elec} (M06/BS1) = -680.46496442 au
H_{corr} (M06/BS1) = 0.266653 au
G_{corr} (M06/BS1) = 0.205321 au
SPE (M06/BS2//M06/BS1) = -680.09001881 au

0 1

C	0.04573200	-0.05836900	-0.01779200
C	0.00053800	0.20347400	1.30361200
C	2.15497500	-0.03706500	0.74478400
N	1.38148700	-0.21284200	-0.36080500
H	-0.73960800	-0.16098700	-0.75335100
H	-0.83495400	0.38120700	1.96606900
N	1.30868300	0.22168200	1.78142000
C	1.91057700	-0.54115400	-1.66670900
H	2.44298900	0.31311800	-2.10052100
H	2.60314100	-1.38567400	-1.58044300
H	1.07892600	-0.81854400	-2.31871300
C	1.67399900	0.59272400	3.14031200
H	2.49111000	1.31903400	3.12367800
H	0.79619200	1.04902300	3.60599500
H	1.98368500	-0.28084700	3.71986300
N	3.47471700	-0.10947700	0.72624000
N	4.10856800	-0.36105300	1.97757600
O	4.94695600	0.72978700	2.18918600
V	5.47123400	-0.21990500	0.69798100
C	7.13107400	0.97656300	0.79478700
H	7.89244100	0.59952800	0.09646000
H	6.83487200	1.98882200	0.48497000
H	7.52764400	1.01210800	1.81746700
C	5.43392300	0.16108900	-1.32051300
H	6.46154700	0.10635000	-1.70717900
H	4.79742400	-0.56461900	-1.84432100
H	5.03814000	1.17170900	-1.49381300
C	6.34351000	-2.00315200	0.96649700
H	7.14281400	-2.10950700	0.21782100
H	6.75500900	-2.09691100	1.97963400
H	5.56893800	-2.76768100	0.80431700

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) for 8M, 9M & $8M_P$ (singlet) in Solvent = THF

8M

E_{elec} (M06/BS1, triplet) = -680.4520571880 au
E_{elec} (M06/BS1, singlet) = -680.4520529980 au
SPE (M06/BS2//M06/BS1, singlet) = -680.07828113 au

C	-4.2619373	-0.8047453	0.2303566
C	-4.1819078	0.5137184	0.5129176
C	-2.1358647	-0.1683652	-0.0953641
N	-3.0005098	-1.2218482	-0.1488488
H	-5.0968999	-1.4905172	0.2633159
H	-4.9366674	1.2171429	0.8358317
N	-2.8674844	0.9154349	0.3126260
C	-2.6108118	-2.5632300	-0.5329110
H	-2.1277434	-2.5466361	-1.5147072
H	-1.9121775	-2.9836395	0.1982498
H	-3.5103735	-3.1815499	-0.5785832
C	-2.4225477	2.2950145	0.4390480
H	-1.8940820	2.6114903	-0.4636058
H	-3.3105623	2.9175495	0.5782448
H	-1.7554033	2.4185155	1.2993510
N	-0.8591455	-0.3300631	-0.4325674
N	-0.1001460	0.7469840	-0.2264061
O	1.1816081	0.5286536	-0.6356339
V	1.3017207	1.0246895	1.1480677
C	1.8504237	2.9300073	1.4993219
H	2.1132107	3.0028351	2.5669877
H	2.7272042	3.2016852	0.8934389
H	1.0232031	3.6222711	1.2803950
C	2.9067493	-0.1221730	1.6287041
H	3.2597652	0.1453763	2.6376526
H	2.6359962	-1.1879162	1.6097417
H	3.7105178	0.0580206	0.8980902
C	0.0754976	0.3595995	2.6304437
H	0.6000661	0.5187237	3.5865698
H	-0.9045412	0.8589092	2.6644751
H	-0.0840706	-0.7210622	2.4876202

9M

E_{elec} (M06/BS1, triplet) = -680.4473542730 au
E_{elec} (M06/BS1, singlet) = -680.4473364440 au
SPE (M06/BS2//M06/BS1, singlet) = -680.07400673 au

C	-4.4225413	1.2309442	-0.4658061
C	-3.4384640	2.0138747	0.0329970
C	-2.6726708	-0.0817456	-0.0070870
N	-3.9443119	-0.0618313	-0.4891961
H	-5.4191114	1.4715123	-0.8092360
H	-3.4000119	3.0801754	0.2068225
N	-2.3536615	1.2023086	0.3208139
C	-4.6840355	-1.2264288	-0.9451700
H	-4.0089736	-2.0844469	-0.9475049
H	-5.5237726	-1.4239718	-0.2708566
H	-5.0590152	-1.0471374	-1.9572458
C	-1.0916721	1.7044399	0.8534691
H	-0.2680969	1.4562116	0.1799700
H	-1.1813566	2.7904414	0.9385238
H	-0.8894447	1.2727442	1.8371755
N	-1.9799882	-1.2321540	0.0505634
N	-0.7862237	-1.1392964	0.6514142
O	-0.2569688	-2.3912835	0.7182386
V	-1.5679594	-2.5469118	2.0488976
C	-0.5669693	-3.7984611	3.3073719
H	-1.1901005	-3.9990435	4.1923835
H	-0.3278188	-4.7510940	2.8094380
H	0.3679007	-3.3219788	3.6378689
C	-3.3200910	-3.5522754	1.8261675
H	-3.5301758	-4.1302053	2.7384806
H	-4.1468451	-2.8485239	1.6482505
H	-3.2462451	-4.2410693	0.9707850
C	-1.8441417	-1.0833467	3.4475220
H	-2.3738470	-1.5288944	4.3053424
H	-0.8696731	-0.7081985	3.7975712
H	-2.4378292	-0.2420860	3.0534373

$8M_P$

E_{elec} (M06/BS1, triplet) = -1638.37752157 au
E_{elec} (M06/BS1, singlet) = -1638.37752187 au
SPE (M06/BS2//M06/BS1, singlet) = -1638.26186146 au

O	1.24177940	0.46710790	-1.30525640
N	-1.88618550	-1.58232900	0.63108160
N	-3.12792760	-0.23108830	-0.57111890
N	-0.83424940	0.25683370	-0.65248320
N	0.34461610	-0.34560390	-0.71202510
C	-1.83848670	-0.49577710	-0.19582260
C	-3.20761570	-2.01064210	0.72987230
H	-3.47988350	-2.83835280	1.36947580
C	-3.96828400	-1.18191250	-0.01286600
H	-5.03613690	-1.15467110	-0.17879340
V	1.02758430	-0.97125450	-2.52219600
C	-0.83187990	-2.13533770	1.42289990
C	0.03049200	-1.30353920	2.13171020
C	-0.73292680	-3.51953750	1.51619030
C	1.02301340	-1.87469820	2.91914780
C	0.25537960	-4.07968000	2.31827760
C	1.13909020	-3.26016440	3.01319440
H	1.70437010	-1.23011490	3.47004780
H	0.33727510	-5.16230250	2.39025050
C	-3.52271120	0.72211700	-1.55838710
C	-3.13293470	2.05393050	-1.44330170
C	-4.31017880	0.29201740	-2.62368030
C	-3.53902390	2.96288980	-2.41340110
C	-4.72207660	1.21397030	-3.58034080
C	-4.33773390	2.54774980	-3.47684970
H	-3.23588720	4.00443860	-2.32991520
H	-5.33843250	0.88469970	-4.41435430
C	0.41971880	-0.03850710	-4.19776880
C	0.80168130	-0.42794680	-5.49192200
C	-0.52796450	0.99330550	-4.07499360
C	0.25496700	0.18670910	-6.61856870
C	-1.08226210	1.60141560	-5.19910380
C	-0.69052700	1.19910300	-6.47530150
H	0.57033050	-0.12824040	-7.61351240
H	-1.82287110	2.39293590	-5.07479690
C	-0.47363210	-2.37902460	-2.49724970
C	-0.18687300	-3.56223250	-1.79667230
C	-1.72955410	-2.29242330	-3.12074050
C	-1.08934250	-4.62522660	-1.74983470
C	-2.65247990	-3.33635150	-3.05047070

C	-2.33044820	-4.51033860	-2.37177680
H	-0.82526750	-5.54238640	-1.22110880
H	-3.62166360	-3.24094530	-3.54290200
C	2.75260390	-1.95331150	-2.88531070
C	2.85415660	-3.06511990	-3.74035460
C	3.94055910	-1.42827860	-2.34614270
C	4.08986060	-3.62871410	-4.04540600
C	5.18024120	-1.99359680	-2.64413410
C	5.25381020	-3.09427590	-3.49344080
H	4.15012910	-4.48857960	-4.71204110
H	6.09008610	-1.57619220	-2.21365900
H	6.22021310	-3.54053530	-3.72528890
H	3.89857540	-0.56436440	-1.67948280
H	-1.11979500	1.67680600	-7.35531510
H	-2.51452710	2.36850110	-0.60689750
H	-0.85352450	1.31762940	-3.08103560
H	-4.65883520	3.26761710	-4.22761210
H	1.53680760	-1.22402580	-5.63185480
H	-1.99226340	-1.39192390	-3.68288290
H	0.76675380	-3.66640850	-1.26874280
H	-3.04203260	-5.33447650	-2.33236090
H	-4.57755620	-0.76093980	-2.70997000
H	-0.07387580	-0.22262850	2.06741830
H	-1.41088400	-4.14785680	0.94048150
H	1.91836090	-3.70066140	3.63192540
H	1.95200150	-3.50060510	-4.17722550