

Insights into the mechanisms of Ag-catalyzed synthesis of CF₃-substituted heterocycles via [3+2]-cycloaddition from α -trifluoromethylated methyl isocyanides: effects of DBU and exploration of diastereoselectivity

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Table S1. Exploring the effects of methods B3LYP, CAM-B3LYP, BLYP, B3PW91, M06 and PBEPBE by comparing the activation free energy barriers from **in3-b** to **ts2-b** (the geometric structures of **in3-b** and **ts2-b** are optimized using B3LYP (CAM-B3LYP, BLYP, B3PW91, M06 and PBEPBE)/6-31G* in gas phase, and the single point energies are obtained at the M06-2x/6-311++G** calculated level in solution phase).

Species	Activation Free Energy Barriers (kJ/mol)					
	B3LYP	CAM-B3LYP	BLYP	B3PW91	M06	PBEPBE
ts2-b	102.6	96.9	103.5	97.7	109.1	96.4

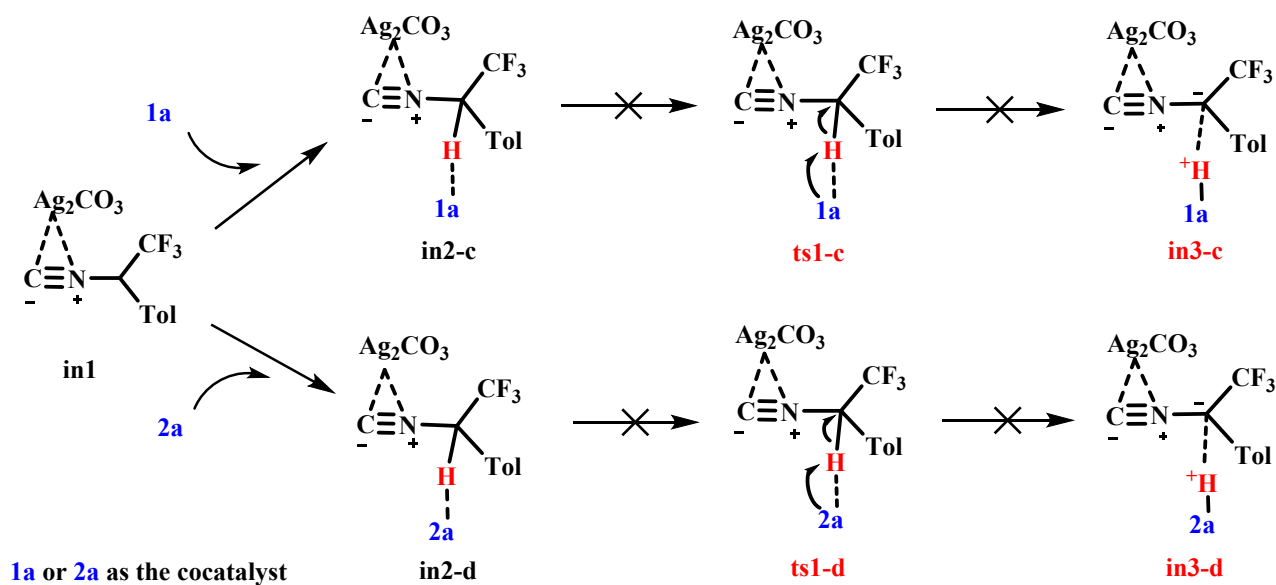
Table S1 shows that the effects of DFT functionals B3LYP, CAM-B3LYP, BLYP, B3PW91, M06 and PBEPBE on the activation free energy barrier are very small.

Table S2. Exploring the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* by comparing the activation free energy barriers from **in3-b** to **ts2-b** (the geometric structures of **in3-b** and **ts2-b** are optimized using B3LYP/6-31G* (6-31G**, 6-31+G* and 6-311G*) in gas phase, and the single point energies are obtained at the M06-2x/6-311++G** calculated level in solution phase).

Species	Activation Free Energy Barriers (kJ/mol)			
	6-31G*	6-31G**	6-31+G*	6-311G*
ts2-b	102.6	104.3	104.9	98.0

Table S2 shows that the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* on the activation free energy barrier are very small.

Scheme S1. **1a**- and **2a**-assisted catalytic reactions, **1a** or **2a** act as the cocatalyst.



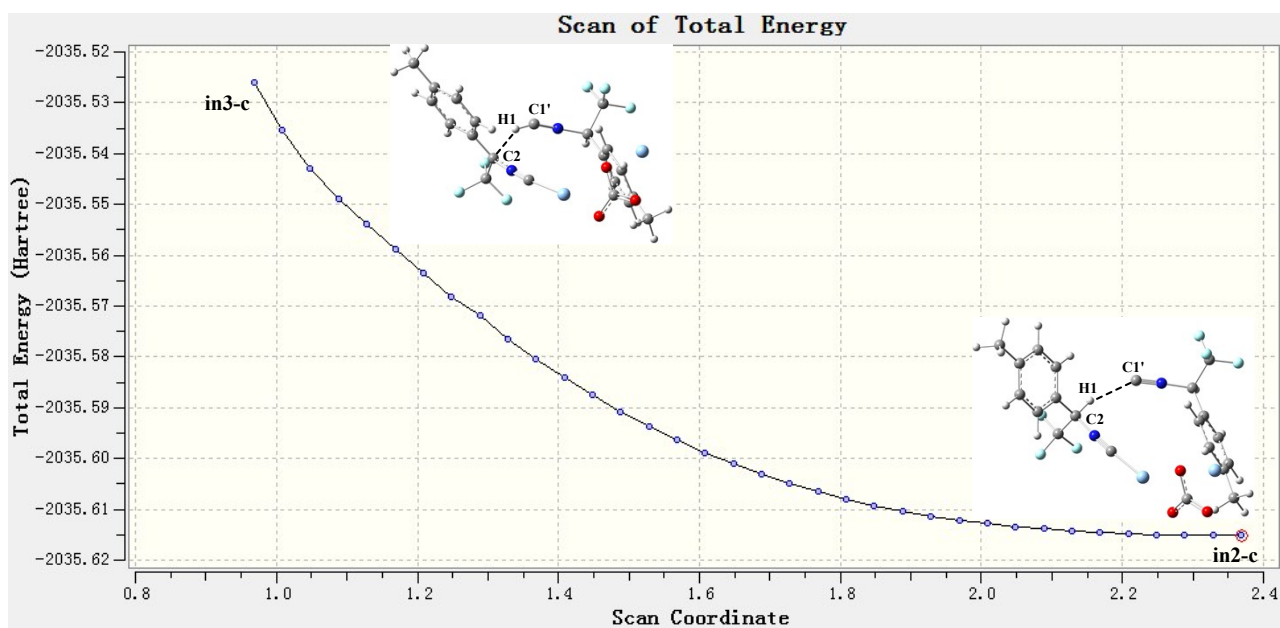


Figure S1. The scan profile from **in2-c** to **in3-c** along with the formation of H1-C1' bond (from 2.368 to 0.968 Å).

The scan profile shows that the energy is rising sharply along with the formation of H1-C1' bond (from 2.368 to 0.968 Å). Obviously, the **1a**-assisted H⁺-shift path (see Scheme S1) is unfavorable for the present catalytic reactions.

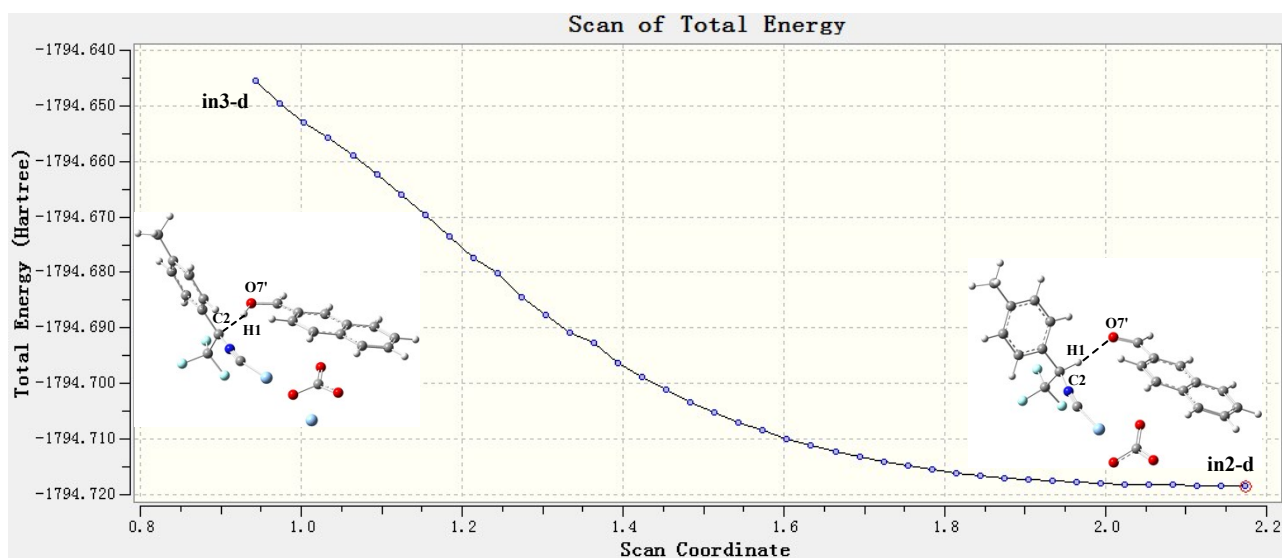


Figure S2. The scan profile from **in2-d** to **in3-d** along with the formation of H1-O7' bond (from 2.174 to 0.944 Å).

The scan profile shows that the energy is rising sharply along with the formation of H1-O7 bond (from 2.174 to 0.944 Å). Obviously, the **2a**-assisted H⁺-shift path (see Scheme S1) is unfavorable for the present catalytic reactions.

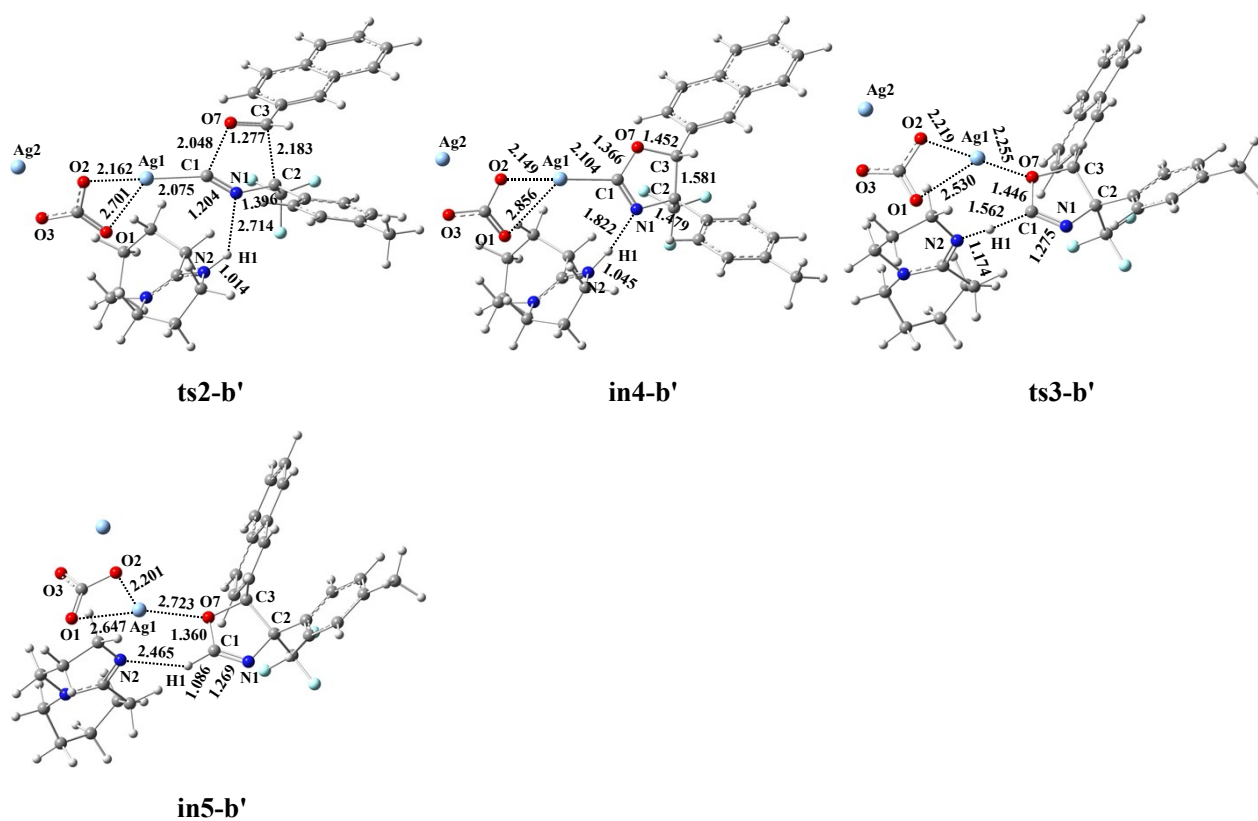


Figure S3. Optimized geometries involved in the Ag_2CO_3 -catalyzed [3+2]-cycloaddition reaction to synthesize the products **P2** with DBU as the cocatalyst in toluene medium. Bond distances are given in Å.

Based on the Arrhenius equation (K. J. Laidler, *J. Chem. Educ.*, 1984, **61**(6), 494-498; S. R. Logan, *J. Chem. Educ.*, 1982, **59**(4), 279-281),

$$P1/P2 = \exp(-\Delta G_{ts2-b}/RT) / \exp(-\Delta G_{ts2-b'}/RT) \dots \text{Eq S1}$$

$$P1/P2 = \exp[(\Delta G_{ts2-b'} - \Delta G_{ts2-b})/RT] \dots \text{Eq S2}$$

$\Delta G_{ts2-b} = 106.7$ kJ/mol; $\Delta G_{ts2-b'} = 110.9$ kJ/mol; $R = 8.314$ J/mol·K; $T = 298.15$ K.

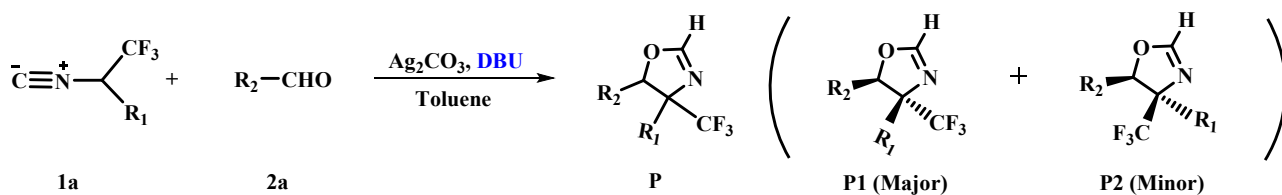
ΔG_{ts2-b} and $\Delta G_{ts2-b'}$ are the rate-determining free energy barriers of **P1**- and **P2**-fomed paths (see Figure 5).

Theoretical calculation result,

$$P1:P2 = 5.4:1.0$$

An **P1:P2**=5.4:1 is predicted by the theoretical calculations based on the energy difference of **ts2-b** and **ts2-b'**, and the similar calculations have been widely reported in previous literatures (H. Han, T. Zhang, S.-D. Yang, Y. Lan and J.-B. Xia, *Org. Lett.*, 2019, **21**, 1749-1754; H. Jiang, Q. Li, Q. Qi, C. Yang and D. Zhang, *Chinese J. Org. Chem.*, 2018, **38**, 825-831; Z. Yu, T. Zhang, R. Bai and Y. Lan, *Catal. Sci. Technol.*, 2019, **9**, 646-651; D. Wei, Q. Liu, L. Sun, S.-J. Li, X. Li, L.-B. Qu and Y. Lan, *Chem-Asian J.*, 2019 (<https://doi.org/10.1002/asia.201900076>)). Therefore, our calculated result is close to the experimental result (**P1:P2** =3.7:1.0, see Scheme 1).

Table S3. Exploring the diastereoselectivity of [3+2]-cycloaddition reaction by changing **R** (**R1** or **R2**) groups of **1a** and **2a** based on the theoretical calculations.



1a R1 groups	2a R2 groups	P1 α ($^\circ$) 	P2 β ($^\circ$) 	$\Delta\Delta G$ (kJ/mol) $\Delta G' - \Delta G =$	Theoretical results (P1:P2)	Experimental results (P1:P2)
		37	25	4.2	5.4:1.0	3.7:1.0
		39	26	6.0	11.0:1.0	3.9:1.0
		40	28	3.4	4.0:1.0	3.7:1.0
		38	30	1.3	1.7:1.0	2.7:1.0
		40	24	7.2	17.5:1.0	4.4:1.0
		44	30	6.6	14.0:1.0	4.0:1.0
		36	26	2.8	3.1:1.0	3.1:1.0

These theoretical calculations reproduce the experimental results to some extent.

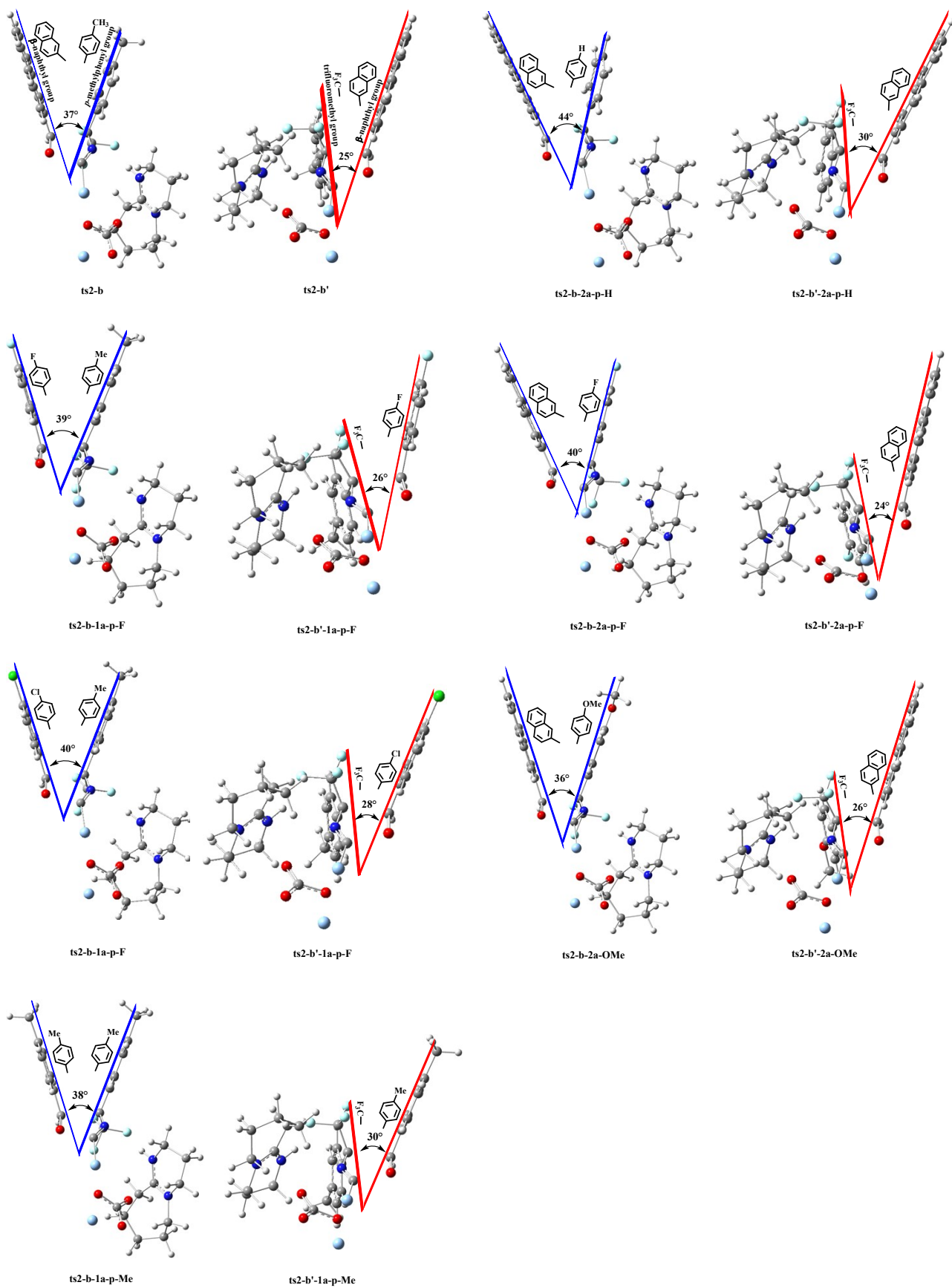


Figure S4. The angles of R1- with R2- vs. R2- with F₃C-.

Intrinsic Reaction Coordinates

When the animation of transition state's vibrations cannot easily confirm the reliability of transition states, the intrinsic reaction coordinate (IRC) calculations is conducted to unambiguously identify the transition states, which are connected with the reactants and the products.

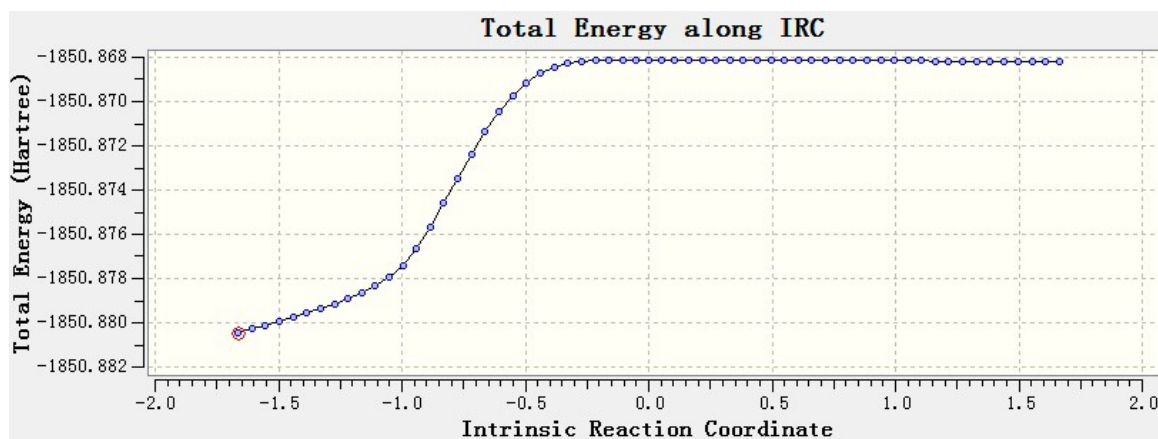


Figure S5. IRC of ts1-a.

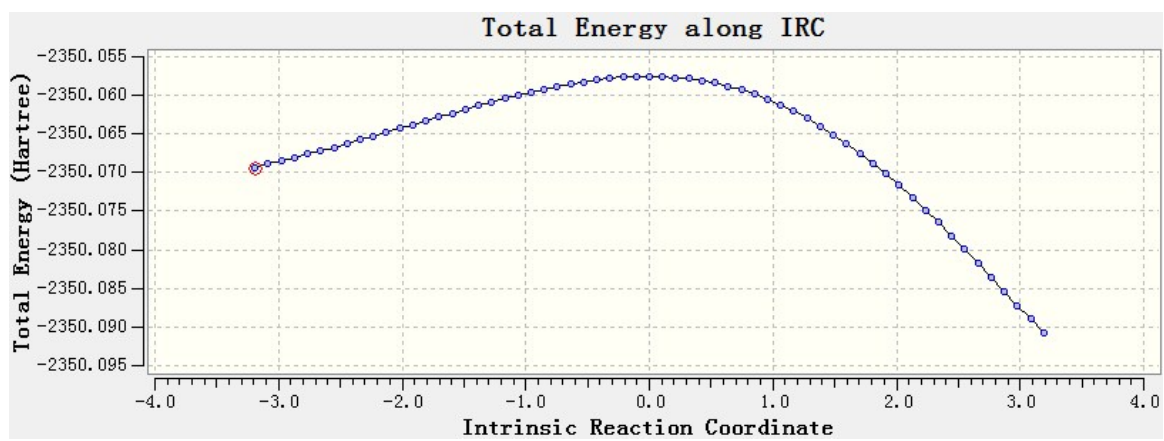


Figure S6. IRC of ts2-a.

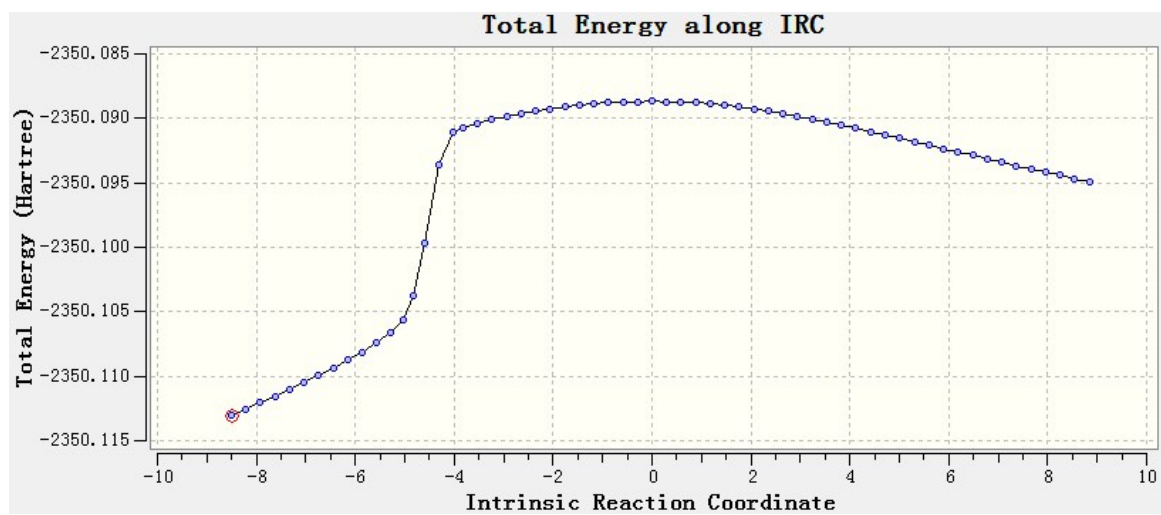


Figure S7. IRC of ts3-a.

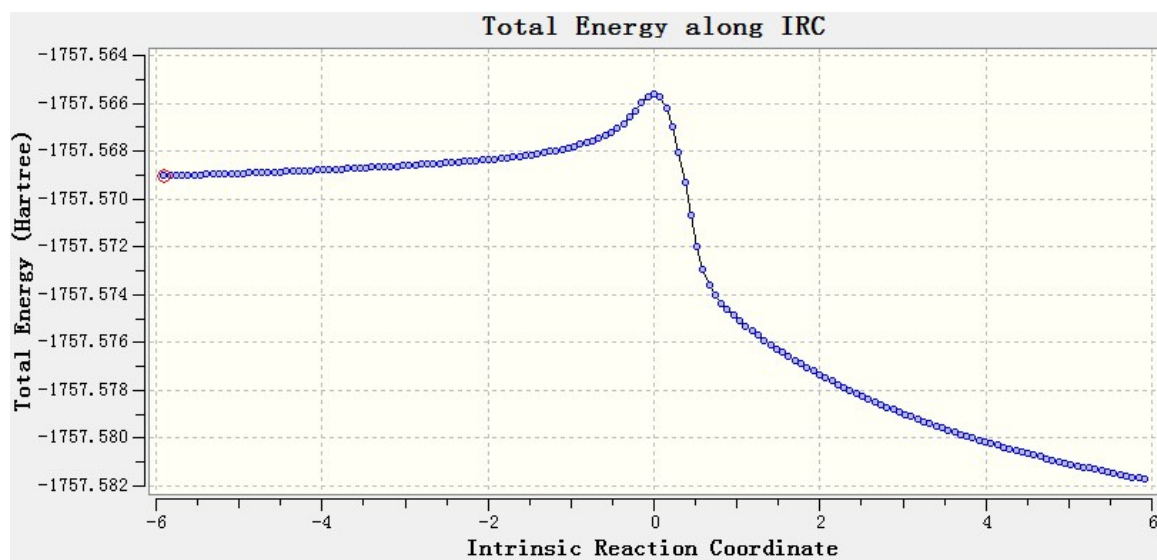


Figure S8. IRC of ts1-b.

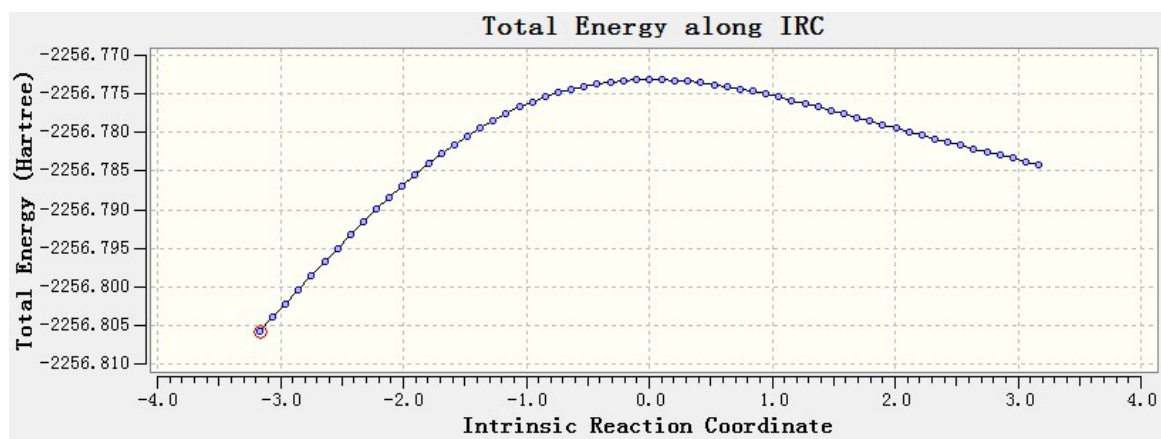


Figure S9. IRC of ts2-b.

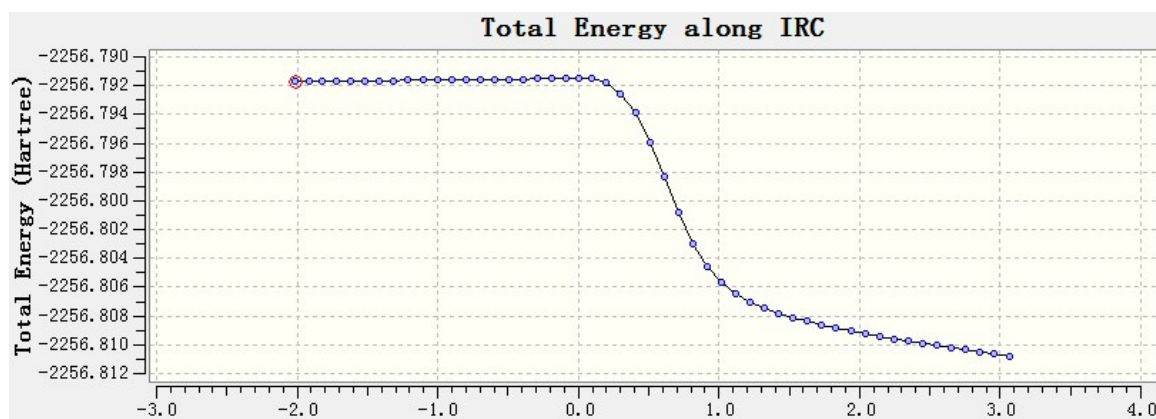


Figure S10. IRC of ts3-b.

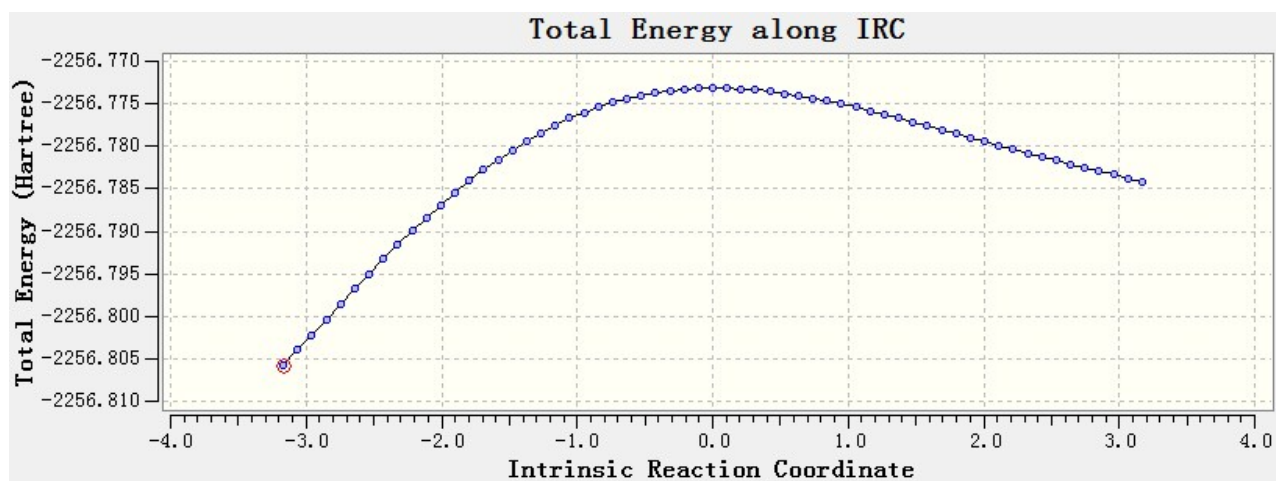


Figure S11. IRC of ts2-b'.

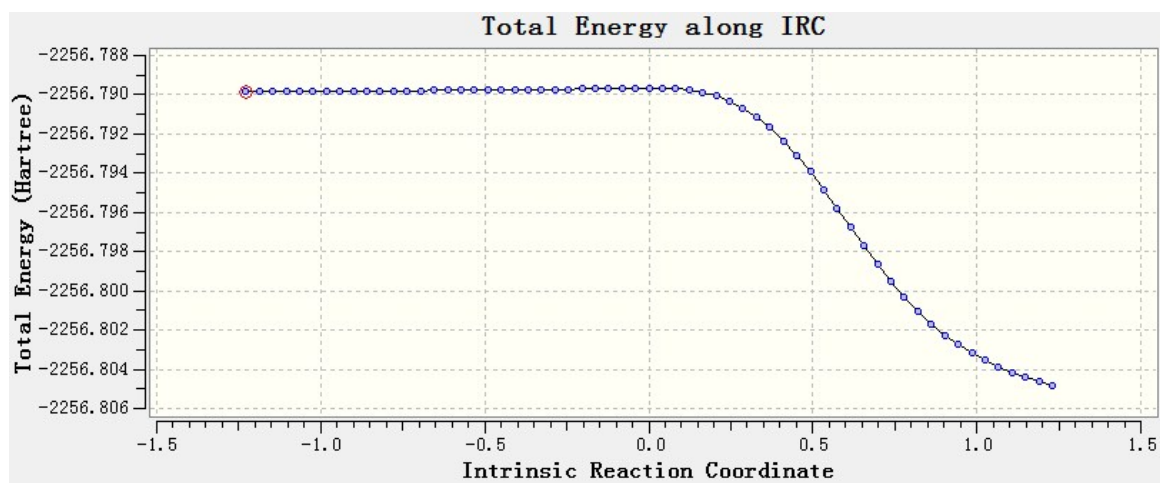


Figure S12. IRC of ts3-b'.

Cartesian coordinates of the optimized stationary points on the optimal reaction channels

The solution-phase Gibbs free energy is determined by adding the solvation single-point energy and gas-phase thermal correction to the Gibbs free energy obtained from vibrational frequency calculation. Unless special emphasis, all the discussed energies are relative solution-phase Gibbs free energies (G_{rel} , kJ/mol) in this paper.

1a

C	1.23159900	0.21823000	-0.69941300
C	2.02222500	-0.66850400	0.28575800
C	-0.26533900	0.16752600	-0.43275300
N	1.75730500	1.53994000	-0.64799100
C	-1.05293100	-0.76679200	-1.10983000
C	-0.86275400	1.00486600	0.51399200
C	-2.22881000	0.91004300	0.76738700
C	-3.03150600	-0.01978900	0.09178300
C	-2.41880700	-0.85854400	-0.84719800
C	-4.51793100	-0.09307500	0.34967900
F	3.33938900	-0.62857300	0.01717000
F	1.84393900	-0.28380700	1.55923200
F	1.61218300	-1.94580800	0.16583800
C	2.18916700	2.63512400	-0.58914200
H	1.44253900	-0.19353000	-1.69291800
H	-0.59970700	-1.43040700	-1.84218800
H	-0.26170400	1.73617300	1.04549500
H	-2.67987300	1.56983600	1.50473000
H	-3.01754800	-1.59068000	-1.38356000
H	-4.91767000	-1.08420300	0.11210500
H	-4.75391200	0.12695400	1.39623400
H	-5.06233900	0.63544600	-0.26569600

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.118129

Sum of electronic and thermal Free Energies = -739.997854

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -740.0656139

No imaginary frequency

2a

C	-0.12610000	2.31758100	0.00000000
C	-1.36736000	2.91294000	0.00000000
C	-2.53881100	2.11710300	0.00000000
C	-2.44972900	0.74199500	0.00000000
C	-1.18665700	0.09601600	0.00000000
C	0.00000000	0.90235300	0.00000000
C	1.26070700	0.25429300	0.00000000

C	1.35512300	-1.12474400	0.00000000
C	0.17579200	-1.92163500	0.00000000
C	-1.05793700	-1.32344700	0.00000000
C	2.68592500	-1.76724500	0.00000000
O	2.87492000	-2.96927500	0.00000000
H	0.77712200	2.92313100	0.00000000
H	-1.45343300	3.99589800	0.00000000
H	-3.51316700	2.59804300	0.00000000
H	-3.34983500	0.13198400	0.00000000
H	2.16652800	0.85896500	0.00000000
H	0.28747700	-3.00123900	0.00000000
H	-1.96247200	-1.92711200	0.00000000
H	3.54270100	-1.05673900	0.00000000

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.123047

Sum of electronic and thermal Free Energies = -499.095217

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -499.1373521

No imaginary frequency

Ag₂CO₃

C	-0.00002100	0.98637900	-0.00016500
O	-0.00004600	-0.35362800	0.00043600
O	-1.12798500	1.59611900	-0.00009700
O	1.12794000	1.59611000	0.00019300
Ag	2.32022900	-0.30453900	-0.00004700
Ag	-2.32021100	-0.30454800	-0.00002300

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = -0.018057

Sum of electronic and thermal Free Energies = -555.352418

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -2119.0429148

No imaginary frequency

DBU

C	0.84271000	1.47411100	0.27465600
C	2.12642700	1.15991500	-0.50360400
N	-0.34261700	0.67727800	-0.07296400
C	2.95865400	0.00495500	0.07769200
C	2.10096800	-1.18765800	0.53038900
C	0.92050000	-1.48180700	-0.41433900
C	-0.37024500	-0.72135200	-0.13317200
C	-1.59389700	1.35774300	0.27655500
C	-2.79477100	0.60668200	-0.28506000
C	-2.72479100	-0.84686200	0.18228700
N	-1.42219000	-1.45953500	-0.03968200

H	0.56361700	2.51177400	0.05971600
H	1.04208800	1.43349300	1.36063800
H	2.74188800	2.06816500	-0.52315200
H	1.85241100	0.95665800	-1.54551400
H	3.55328500	0.36863300	0.92621700
H	3.67962800	-0.32416500	-0.68226500
H	1.71354300	-1.01344600	1.54287800
H	2.73402100	-2.08003500	0.60432100
H	0.62987600	-2.53143300	-0.34369500
H	1.22750300	-1.31056400	-1.45607000
H	-1.54969300	2.37541800	-0.13121000
H	-1.68990500	1.45673300	1.37213900
H	-2.76379800	0.64418100	-1.38114900
H	-3.72447400	1.09143400	0.03630100
H	-3.47768000	-1.45378700	-0.33686000
H	-2.97198900	-0.91162700	1.25380800

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.212154

Sum of electronic and thermal Free Energies = -461.875027

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -462.0017221

No imaginary frequency

in1

C	3.33985800	1.11802300	-0.63058200
C	3.57516200	2.38456200	0.22023800
C	4.20052300	-0.05978600	-0.20712200
N	1.94611800	0.80485500	-0.60005000
C	5.25794900	-0.46439800	-1.02384700
C	3.96079900	-0.74133600	0.99316900
C	4.77059800	-1.81150300	1.35894900
C	5.83888000	-2.22801800	0.54836100
C	6.06817500	-1.53590200	-0.64575900
C	6.70719600	-3.39286900	0.96040100
F	2.81997900	3.40133800	-0.23122100
F	3.27379100	2.18432400	1.51348900
F	4.86533500	2.74242800	0.12948900
C	0.81621800	0.50874000	-0.59403600
H	3.58675200	1.40475100	-1.65839900
H	5.45241600	0.05250200	-1.96046600
H	3.14152500	-0.44027600	1.63877400
H	4.56988200	-2.33452300	2.29079900
H	6.88518900	-1.84090800	-1.29432700
H	7.47376800	-3.60706200	0.20973900
H	7.21545500	-3.19129000	1.91138600
H	6.11040700	-4.30212900	1.10096200

C	-3.69627300	-0.89307700	-0.82173100
O	-4.91998500	-1.27022500	-0.88347500
O	-3.33781500	-0.00727400	0.11490000
O	-2.77902700	-1.31334100	-1.60898700
Ag	-1.15304900	-0.10338000	-0.69333200
Ag	-5.51567600	0.04151300	0.84925400

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.117857

Sum of electronic and thermal Free Energies = -1295.374078

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -1295.2739829

No imaginary frequency

in2-a

C	-2.63135500	-1.85064400	-0.85161700
C	-3.14307600	-2.63164900	-2.06747400
C	-3.53479700	-1.91904700	0.36647700
N	-1.29471000	-2.29698700	-0.56132200
C	-4.07630500	-0.72680300	0.85998400
C	-3.82342900	-3.12891200	1.01177600
C	-4.65258900	-3.14297700	2.13003100
C	-5.21611100	-1.95911000	2.62930100
C	-4.91135600	-0.75797300	1.97832700
C	-6.14041600	-1.98816500	3.82427800
F	-2.32018700	-2.46960900	-3.12080500
F	-3.23196600	-3.96062200	-1.83253300
F	-4.36062200	-2.18596400	-2.40798400
C	-0.16036900	-2.44090400	-0.35141700
H	-2.49425800	-0.79503100	-1.15295600
H	-3.83941300	0.22384000	0.38470800
H	-3.40349600	-4.05951900	0.64282600
H	-4.86692100	-4.08837200	2.62351700
H	-5.32692500	0.17453400	2.35330400
H	-6.17878300	-1.01495500	4.32452300
H	-7.16606800	-2.24305600	3.52530300
H	-5.82320500	-2.73626000	4.55937500
C	3.71898800	0.07214700	-0.25214300
O	4.64707700	0.92572100	-0.05778000
O	3.85067100	-1.14840200	0.26676800
O	2.65817600	0.29735700	-0.93973000
Ag	1.86118000	-1.97830200	-0.12156500
Ag	5.96638400	-0.49304600	1.06996800
C	-1.76149100	1.95665400	-0.63239300
O	-0.78179500	2.86282700	-0.45247900
O	-1.46040900	0.81337900	-1.06726500
O	-2.96166900	2.33497700	-0.32522800

Ag	-2.30701700	4.39323100	0.31429500
Ag	1.02741900	1.70749800	-0.80194400

B3LYP/6-31G* (Lan12DZ for Ag)
 Thermal correction to Gibbs Free Energy = 0.122561
 Sum of electronic and thermal Free Energies = -1850.771572
 M06-2x/6-311++G** (Lan12DZ for Ag)
 Energy = -1850.5058135
 No imaginary frequency

ts1-a

C	-2.43901500	-1.79944500	-1.01645000
C	-3.05325200	-1.85324500	-2.38650200
C	-3.26724100	-2.17311200	0.16427800
N	-1.14826300	-2.30334400	-1.02329700
C	-4.63869500	-1.85488100	0.22873600
C	-2.70030700	-2.79938100	1.28780700
C	-3.46410900	-3.08959400	2.41773600
C	-4.82503600	-2.77445000	2.48263400
C	-5.39186500	-2.15666000	1.35924100
C	-5.64598100	-3.06458800	3.71770900
F	-2.12584000	-1.63145700	-3.34697900
F	-3.65400300	-3.03526200	-2.69446800
F	-4.01342600	-0.90247700	-2.53573500
C	-0.00884900	-2.56999100	-0.97052400
H	-1.96188300	-0.26468200	-0.80750100
H	-5.11982000	-1.36607200	-0.60962200
H	-1.65015500	-3.07505200	1.27875700
H	-2.98729000	-3.58058900	3.26413200
H	-6.45015400	-1.90176300	1.36672000
H	-5.75867100	-2.17166300	4.34862200
H	-6.65617500	-3.40366600	3.45977000
H	-5.17948200	-3.84039300	4.33476300
C	3.64009700	0.18545900	0.06844500
O	4.44354300	0.94251200	0.70974400
O	3.83047600	-1.13025000	0.11324500
O	2.65474500	0.60860500	-0.63831400
Ag	1.96391300	-1.99380100	-0.62050600
Ag	5.69673600	-0.76927100	1.47583700
C	-1.87395700	1.71281400	-0.28412600
O	-1.05184600	2.68937900	0.00025400
O	-1.30766100	0.58523500	-0.63897500
O	-3.12570500	1.86587700	-0.21769700
Ag	-2.97154300	4.03210000	0.44031400
Ag	1.00616100	1.90260500	-0.20989900

B3LYP/6-31G* (Lan12DZ for Ag)
 Thermal correction to Gibbs Free Energy = 0.119889

Sum of electronic and thermal Free Energies = -1850.748220

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -1850.4904308

Number of Imaginary Frequencies = 1

Lowest Frequency = 111.41i

in3-a

C	-2.53385500	-2.12496300	-0.65466500
C	-2.88782500	-2.92036700	-1.86739800
C	-3.52298800	-1.85636100	0.40173700
N	-1.22953500	-2.23432300	-0.28713000
C	-4.91162000	-1.93392200	0.15932700
C	-3.12003700	-1.47190400	1.69638700
C	-4.05297600	-1.17999100	2.68860800
C	-5.42986400	-1.26072700	2.44880800
C	-5.83144900	-1.64352200	1.16113100
C	-6.44078500	-0.98024800	3.53614500
F	-1.80602100	-3.13665800	-2.65000400
F	-3.42744000	-4.14394700	-1.60273100
F	-3.81483900	-2.28074300	-2.63614700
C	-0.09726500	-2.20691400	0.02726200
H	-2.07208700	-0.36819000	-1.41931200
H	-5.27494600	-2.21460400	-0.82205900
H	-2.06181500	-1.40509800	1.93211100
H	-3.69858700	-0.89192900	3.67700500
H	-6.89333000	-1.71724200	0.93336200
H	-6.82111600	-1.90821200	3.98570100
H	-6.00375100	-0.38474800	4.34554500
H	-7.30936100	-0.43416400	3.14907700
C	4.07713500	0.64660300	-0.30782900
O	5.33951300	0.86157700	-0.27265000
O	3.62231900	-0.37847800	0.41424800
O	3.30293100	1.37927500	-1.00806400
Ag	1.74857200	-1.30304700	0.17497100
Ag	5.85680400	-0.85791800	1.04374000
C	-1.78069300	1.49030400	-0.96555800
O	-0.85190800	2.37170400	-0.77077000
O	-1.40070900	0.36959800	-1.56134000
O	-2.97489400	1.68503800	-0.61758700
Ag	-2.59056100	3.73011600	0.26941500
Ag	1.22075400	1.69380500	-0.87506200

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.121449

Sum of electronic and thermal Free Energies = -1850.747013

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -1850.4921635

No imaginary frequency

ts2-a

C	-2.25244200	0.94797800	0.47810200
C	-1.89024100	2.35234500	0.07304900
C	-3.43235400	0.77370200	1.36909000
N	-1.09255200	0.28724200	0.87624200
C	-4.62038900	1.51286700	1.21779500
C	-3.41232400	-0.21333100	2.37142400
C	-4.51998600	-0.44551300	3.18134400
C	-5.70220800	0.29015300	3.03086400
C	-5.72219300	1.27466800	2.03680100
C	-6.91592200	0.01312300	3.88640100
F	-0.79076100	2.38698000	-0.71555700
F	-2.87507100	2.97991200	-0.60040800
F	-1.58996000	3.18131500	1.14683900
C	-0.27371200	-0.43681100	0.38797600
H	-4.69369300	2.28376100	0.46160400
H	-2.50974000	-0.79641900	2.52441900
H	-4.46111700	-1.21294200	3.95070500
H	-6.62160500	1.87000300	1.89285800
H	-7.52600900	0.91328900	4.02119900
H	-7.56111100	-0.74968200	3.42923900
H	-6.63281700	-0.35482700	4.87900400
C	4.49223800	-2.09884700	0.66494200
O	5.38909600	-3.01124100	0.71342600
O	3.38773900	-2.37337100	-0.02942200
O	4.65423100	-0.97822200	1.25638800
Ag	1.54160900	-1.38846800	0.22415300
H	0.28257600	3.06536300	1.74007900
C	1.79072200	3.30501800	0.63319200
O	2.89460500	2.78571200	0.22848800
O	1.19625300	2.72032100	1.67367400
O	1.27614100	4.31952400	0.09020300
Ag	2.71225800	4.37697200	-1.64106500
Ag	3.59800800	0.80808700	0.84002700
C	-7.23947700	-0.48973900	-2.20228600
C	-8.39671900	-1.23644100	-2.17366100
C	-8.37404200	-2.57126100	-1.69941000
C	-7.19256700	-3.13138100	-1.26421500
C	-5.98245900	-2.38887500	-1.28152100
C	-6.00445100	-1.03722500	-1.75961400
C	-4.79352500	-0.29718000	-1.77914600
C	-3.60013300	-0.85113000	-1.35792400
C	-3.58703000	-2.19472000	-0.89188500
C	-4.74209200	-2.93670000	-0.85052000

C	-2.32417900	-0.07952700	-1.42843600
O	-1.20698300	-0.70392100	-1.44311600
H	-7.25510800	0.53549800	-2.56583700
H	-9.33322900	-0.80339100	-2.51574100
H	-9.29282300	-3.15171700	-1.68124800
H	-7.17075900	-4.15653700	-0.90048400
H	-4.81243300	0.72814800	-2.14580200
H	-2.63483800	-2.61762600	-0.58749900
H	-4.72271500	-3.96414200	-0.49238200
H	-2.40782400	0.86025900	-1.99736700
Ag	4.27041300	-4.51640000	-0.49536300

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.268835

Sum of electronic and thermal Free Energies = -2349.788710

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2349.6191180

Number of Imaginary Frequencies = 1

Lowest Frequency = 382.23i

in4-a

C	1.95731900	-1.26014300	-0.80961000
C	2.16073200	0.12223600	-1.47541100
C	2.72339300	-2.33191800	-1.58945000
N	0.49559700	-1.47842500	-0.79447600
C	4.12258800	-2.28363100	-1.70017400
C	2.05100300	-3.39094100	-2.20660500
C	2.75468600	-4.36710500	-2.91515900
C	4.14656100	-4.32100200	-3.03337900
C	4.81675000	-3.26038200	-2.40777700
C	4.90651000	-5.36308600	-3.82031400
F	1.43055000	1.07827300	-0.85764300
F	3.45194800	0.53504800	-1.41548100
F	1.79780200	0.10848500	-2.77048300
C	0.03671800	-1.31605800	0.40702400
H	4.67956400	-1.48239300	-1.22906500
H	0.97205500	-3.45517100	-2.14646400
H	2.20277800	-5.17662900	-3.38749200
H	5.90113400	-3.19858700	-2.47122900
H	5.79781800	-5.70308900	-3.27998400
H	4.28385800	-6.23885200	-4.02991400
H	5.24763400	-4.96345500	-4.78466100
C	-4.59221600	0.35857200	0.91572400
O	-5.72936900	0.66614900	1.42341000
O	-4.04001200	-0.78689400	1.31060400
O	-4.01981700	1.13115100	0.07315100
Ag	-1.97894300	-1.16233700	0.93869200

H	-0.38831700	-1.65280200	-2.07397000
C	-1.27050800	-0.95649800	-3.71762700
O	-1.46232700	0.23767500	-3.21450400
O	-0.86483600	-1.94319900	-2.96134500
O	-1.48085600	-1.17272400	-4.94681800
Ag	-2.07246100	0.93266700	-5.43793500
Ag	-2.58325900	0.57325900	-1.38771400
C	6.43244800	-2.70466300	3.05403600
C	7.17012300	-3.70934500	3.64094700
C	6.65468200	-5.02687700	3.71018700
C	5.41063500	-5.31415900	3.19227600
C	4.62608400	-4.30112500	2.58044300
C	5.14804900	-2.96953800	2.50801600
C	4.35978900	-1.95782000	1.89560200
C	3.11775100	-2.23237000	1.36372100
C	2.60235800	-3.55613200	1.44910500
C	3.33585600	-4.55635800	2.03862100
C	2.30799600	-1.13253600	0.72574000
O	0.98499800	-1.08946100	1.34791900
H	6.82596900	-1.69214000	3.00006900
H	8.15214800	-3.49411800	4.05348800
H	7.24587800	-5.81129700	4.17506300
H	5.01177000	-6.32459900	3.24471400
H	4.75758200	-0.94538900	1.85230100
H	1.61911200	-3.77115900	1.04269100
H	2.93433900	-5.56530100	2.09707500
H	2.78168900	-0.17065300	0.93207700
Ag	-5.91760900	-1.14089800	2.70526300

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.276440

Sum of electronic and thermal Free Energies = -2349.852678

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -2349.6912155

No imaginary frequency

ts3-a

C	1.95731900	-1.26014300	-0.80961000
C	2.16073200	0.12223600	-1.47541100
C	2.72339300	-2.33191800	-1.58945000
N	0.49559700	-1.47842500	-0.79447600
C	4.12258800	-2.28363100	-1.70017400
C	2.05100300	-3.39094100	-2.20660500
C	2.75468600	-4.36710500	-2.91515900
C	4.14656100	-4.32100200	-3.03337900
C	4.81675000	-3.26038200	-2.40777700
C	4.90651000	-5.36308600	-3.82031400

F	1.43055000	1.07827300	-0.85764300
F	3.45194800	0.53504800	-1.41548100
F	1.79780200	0.10848500	-2.77048300
C	0.03671800	-1.31605800	0.40702400
H	4.67956400	-1.48239300	-1.22906500
H	0.97205500	-3.45517100	-2.14646400
H	2.20277800	-5.17662900	-3.38749200
H	5.90113400	-3.19858700	-2.47122900
H	5.79781800	-5.70308900	-3.27998400
H	4.28385800	-6.23885200	-4.02991400
H	5.24763400	-4.96345500	-4.78466100
C	-4.59221600	0.35857200	0.91572400
O	-5.72936900	0.66614900	1.42341000
O	-4.04001200	-0.78689400	1.31060400
O	-4.01981700	1.13115100	0.07315100
Ag	-1.97894300	-1.16233700	0.93869200
H	-0.38831700	-1.65280200	-2.07397000
C	-1.27050800	-0.95649800	-3.71762700
O	-1.46232700	0.23767500	-3.21450400
O	-0.86483600	-1.94319900	-2.96134500
O	-1.48085600	-1.17272400	-4.94681800
Ag	-2.07246100	0.93266700	-5.43793500
Ag	-2.58325900	0.57325900	-1.38771400
C	6.43244800	-2.70466300	3.05403600
C	7.17012300	-3.70934500	3.64094700
C	6.65468200	-5.02687700	3.71018700
C	5.41063500	-5.31415900	3.19227600
C	4.62608400	-4.30112500	2.58044300
C	5.14804900	-2.96953800	2.50801600
C	4.35978900	-1.95782000	1.89560200
C	3.11775100	-2.23237000	1.36372100
C	2.60235800	-3.55613200	1.44910500
C	3.33585600	-4.55635800	2.03862100
C	2.30799600	-1.13253600	0.72574000
O	0.98499800	-1.08946100	1.34791900
H	6.82596900	-1.69214000	3.00006900
H	8.15214800	-3.49411800	4.05348800
H	7.24587800	-5.81129700	4.17506300
H	5.01177000	-6.32459900	3.24471400
H	4.75758200	-0.94538900	1.85230100
H	1.61911200	-3.77115900	1.04269100
H	2.93433900	-5.56530100	2.09707500
H	2.78168900	-0.17065300	0.93207700
Ag	-5.91760900	-1.14089800	2.70526300

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.272503

Sum of electronic and thermal Free Energies = -2349.816183

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -2349.6583777

Number of Imaginary Frequencies = 1

Lowest Frequency = 88.75i

in5-a

C	2.16079600	0.16552400	-0.24207400
C	2.11722900	-1.20655100	0.46666600
C	2.58951500	1.27006300	0.73091300
N	0.80884600	0.40466200	-0.76918600
C	3.77635800	1.17601900	1.47448800
C	1.80725800	2.42137200	0.87922400
C	2.19324500	3.44013000	1.75144900
C	3.36837600	3.34703200	2.50408800
C	4.15348600	2.19722400	2.34295000
C	3.76904000	4.43512500	3.47203800
F	1.55870700	-2.14600100	-0.32095100
F	3.35767500	-1.65234000	0.77917700
F	1.40309900	-1.16174100	1.61346500
C	0.88498600	0.47788500	-2.04413500
H	4.41877200	0.30958900	1.37573300
H	0.89006700	2.52705000	0.31103100
H	1.56345800	4.32153900	1.84632000
H	5.08076600	2.09896700	2.90287000
H	4.85637200	4.56586700	3.50131300
H	3.31786500	5.39590700	3.20376700
H	3.44334900	4.19579200	4.49313400
C	-2.85480600	0.22508500	3.02350100
O	-2.69312800	-0.02987000	4.27028100
O	-1.95028000	-0.27555500	2.18471300
O	-3.84466200	0.92284100	2.60933500
Ag	-1.39249200	0.37054700	0.16613700
H	0.02706400	0.67152200	-2.68383200
C	-3.19276700	1.40593100	-2.34719800
O	-4.25143100	1.59591500	-1.55787600
O	-2.05987600	1.05615900	-1.89450900
O	-3.37706700	1.60299000	-3.60917400
Ag	-5.51381300	2.16245100	-3.47487900
Ag	-4.11605100	1.26261300	0.54300600
C	7.99666200	0.49114800	-1.60368100
C	9.12644700	1.26711700	-1.73984500
C	9.01366200	2.65284300	-2.01238000
C	7.77312900	3.23689900	-2.14450700
C	6.58893200	2.46486800	-2.00895200
C	6.70292100	1.06410800	-1.73194100

C	5.51639800	0.29351800	-1.60446700
C	4.26835200	0.86814900	-1.72740800
C	4.16209400	2.25825800	-2.00708400
C	5.29082100	3.02902300	-2.14511300
C	3.04061100	0.01401900	-1.56961000
O	2.07837600	0.32631700	-2.62579300
H	8.08085600	-0.57300700	-1.39590800
H	10.11069200	0.81803700	-1.63932100
H	9.91259800	3.25389600	-2.11825100
H	7.68386000	4.29982400	-2.35575100
H	5.60760200	-0.77273900	-1.40535800
H	3.18127300	2.70753700	-2.12327400
H	5.20171000	4.09016400	-2.36442100
H	3.30985000	-1.03536200	-1.70975400
Ag	-0.79378100	-1.21021500	3.95536000

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.274198

Sum of electronic and thermal Free Energies = -2349.873226

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -2349.7069577

No imaginary frequency

in2-b

C	3.18314400	-0.18221800	0.77869000
C	3.49336100	-0.03656000	2.27723500
C	4.33069300	-0.80471500	0.00654600
N	1.96101800	-0.91611400	0.64425900
C	5.16450900	0.01939900	-0.75236600
C	4.59427500	-2.17897900	0.06240400
C	5.67138500	-2.71311100	-0.63871000
C	6.51964500	-1.89542300	-1.40155300
C	6.24751800	-0.52338000	-1.44540400
C	7.69531900	-2.48643600	-2.14362000
F	2.46396600	0.54127800	2.92907500
F	3.72919600	-1.22447300	2.86688800
F	4.57814900	0.73724800	2.43616200
C	0.86308900	-1.26425200	0.46533800
H	2.92861500	0.82293800	0.38907700
H	4.96657500	1.08662200	-0.80363000
H	3.95546600	-2.83121700	0.65074000
H	5.85965900	-3.78322300	-0.59178600
H	6.88582200	0.13072300	-2.03411600
H	8.46778400	-2.83674500	-1.44698700
H	7.39317900	-3.34910500	-2.74898900
H	8.15855700	-1.75248600	-2.81017400
C	-3.60879200	-0.24623000	-0.45488500

O	-4.84132600	0.05232500	-0.65854500
O	-3.33929600	-1.51020000	-0.05687900
O	-2.62607800	0.54178500	-0.59417200
Ag	-1.17646300	-1.30561400	0.11816800
Ag	-5.57368400	-2.01185200	-0.11748600
C	-1.80572200	3.73399800	-0.70232400
C	-1.84740700	4.63334500	0.53843100
N	-0.46413900	3.27749400	-1.13511000
C	-1.86893800	3.86560000	1.87002100
C	-0.90579300	2.66922000	1.87010700
C	0.44080100	2.98578800	1.18889400
C	0.50106000	2.73027600	-0.31276900
C	-0.45074100	2.88515300	-2.55010200
C	0.98021500	2.72438100	-3.04703800
C	1.70270400	1.74137300	-2.12939100
N	1.52916100	2.03779900	-0.70954400
H	-2.18644500	4.31555500	-1.54929600
H	-2.46559800	2.86314200	-0.58790700
H	-2.74803200	5.25644100	0.46992700
H	-0.99746300	5.32646100	0.50022100
H	-2.88643900	3.50856900	2.07325500
H	-1.61117500	4.55641200	2.68464300
H	-1.37935200	1.81880700	1.36446100
H	-0.71677900	2.35268600	2.90350700
H	1.23034800	2.36610300	1.61581900
H	0.72536200	4.02825200	1.39113200
H	-0.96746500	3.66655700	-3.11925800
H	-1.02177600	1.95364300	-2.68237900
H	1.48549700	3.69820200	-3.02160800
H	0.98354800	2.37595400	-4.08677700
H	2.77911500	1.73280400	-2.34939200
H	1.34547700	0.71841500	-2.32915600

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.351874

Sum of electronic and thermal Free Energies = -1757.239215

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -1757.2958858

No imaginary frequency

ts1-b

C	2.94616100	-0.23755800	0.93229500
C	3.32597300	0.18775100	2.33501500
C	4.08360700	-0.78856200	0.11005000
N	1.82227200	-1.08114200	0.98787600
C	5.20090400	0.01994400	-0.17026800
C	4.05091800	-2.07286700	-0.44806500

C	5.09443400	-2.53284200	-1.25351100
C	6.21136000	-1.73736200	-1.52583600
C	6.24128200	-0.45173000	-0.96539600
C	7.35163400	-2.23985100	-2.38053500
F	2.22807200	0.52923500	3.05892800
F	3.97498500	-0.75974400	3.05161900
F	4.13267200	1.27515600	2.30544600
C	0.77332100	-1.59365300	0.92946700
H	2.36762100	0.84321200	0.21229300
H	5.25570500	1.02320700	0.23794900
H	3.20519500	-2.72544700	-0.25310900
H	5.03697200	-3.53563600	-1.67143200
H	7.09255000	0.19743100	-1.16077200
H	8.25553000	-2.41184200	-1.78142600
H	7.09702700	-3.18492900	-2.87097800
H	7.61811900	-1.51738600	-3.16158500
C	-3.32632100	-0.16918600	-0.63562200
O	-4.46640600	0.33072300	-0.97140600
O	-3.34513900	-1.38279000	-0.04205400
O	-2.21080700	0.39793100	-0.81238200
Ag	-1.25011500	-1.61219300	0.44746900
Ag	-5.65551900	-1.37778800	-0.15598300
C	-1.45151600	3.49780900	-1.05149300
C	-1.48990000	4.49209900	0.11225800
N	-0.15421200	2.82422800	-1.31380800
C	-1.69840700	3.84363500	1.48914300
C	-0.85812600	2.57018000	1.66350000
C	0.56358200	2.71422400	1.08532200
C	0.70294100	2.34142500	-0.38134300
C	-0.07917900	2.27375200	-2.67898700
C	1.36893000	2.01187900	-3.07277800
C	2.00725500	1.10428800	-2.02925200
N	1.72848800	1.56728600	-0.66835100
H	-1.66616100	4.04961900	-1.97251000
H	-2.21705500	2.71841800	-0.94875600
H	-2.31165500	5.19160700	-0.08482100
H	-0.57409100	5.09689500	0.09749200
H	-2.75873000	3.59655000	1.62382600
H	-1.44488400	4.57411200	2.26923500
H	-1.35873700	1.72623400	1.17470400
H	-0.78049200	2.31955000	2.72788200
H	1.25033500	2.07272100	1.63545500
H	0.93262000	3.73910600	1.22543600
H	-0.53119500	3.00583100	-3.35527100
H	-0.68684600	1.36037800	-2.71881000
H	1.91242000	2.96309500	-3.12804000

H	1.41086500	1.54830200	-4.06440200
H	3.09428600	1.05966700	-2.15253000
H	1.63370700	0.07679300	-2.14067500

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.351171

Sum of electronic and thermal Free Energies = -1757.224787

M06-2x/6-311++G** (Lanl2DZ for Ag)

Energy = -1757.2856725

Number of Imaginary Frequencies = 1

Lowest Frequency = 1298.15i

in3-b

C	-3.04736800	-0.43589600	-1.12026600
C	-3.30770800	0.30284300	-2.38039000
C	-4.12855100	-0.80527300	-0.20007300
N	-1.91149700	-1.18191000	-1.13070900
C	-5.38809100	-0.16159500	-0.22570600
C	-3.94464800	-1.79961100	0.78408300
C	-4.95582700	-2.12248300	1.68844000
C	-6.20032000	-1.48432800	1.66146500
C	-6.38745400	-0.49986100	0.67959200
C	-7.30037700	-1.84131200	2.63390700
F	-2.16101600	0.49842700	-3.08785700
F	-4.18894400	-0.28612100	-3.23573200
F	-3.82754800	1.55097200	-2.14936300
C	-0.89161500	-1.77145300	-1.08849500
H	-1.99209400	0.99700900	0.06635600
H	-5.58627600	0.61091700	-0.95952100
H	-3.00154700	-2.33666200	0.83272700
H	-4.77073000	-2.90076800	2.42678900
H	-7.34310800	0.01853600	0.61899100
H	-8.18271300	-2.24352300	2.11854300
H	-6.96652000	-2.59788700	3.35217900
H	-7.63813900	-0.96735500	3.20647800
C	3.16062500	-0.17611000	0.60645200
O	4.30599900	0.32642100	0.93158700
O	3.17623300	-1.38272100	0.00955100
O	2.05329400	0.39873200	0.80375500
Ag	1.11396500	-1.71517900	-0.53705600
Ag	5.49026700	-1.38054900	0.10594600
C	1.62841400	3.51211700	1.11899700
C	1.57078900	4.52824300	-0.02408700
N	0.38101200	2.75485000	1.40712300
C	1.75883100	3.92442700	-1.42418200
C	0.96603700	2.62321700	-1.61661900
C	-0.43182600	2.67689300	-0.96745100

C	-0.44974100	2.25546700	0.48878500
C	0.39285700	2.17459500	2.76914800
C	-0.98881100	1.68463500	3.18753600
C	-1.52611300	0.73685600	2.12513800
N	-1.38761200	1.37159800	0.81375400
H	1.84205000	4.05132200	2.04657100
H	2.42187600	2.76874800	0.97416800
H	2.36325700	5.26375100	0.16004800
H	0.62824700	5.08675300	0.04022400
H	2.82297000	3.72403000	-1.59849100
H	1.45344100	4.66786200	-2.17214600
H	1.51478200	1.77731900	-1.18840200
H	0.84186700	2.41520600	-2.68489000
H	-1.10849400	2.01058300	-1.50411700
H	-0.86392000	3.68230700	-1.05077900
H	0.73961600	2.95731000	3.45018800
H	1.12874000	1.36252000	2.76065200
H	-1.67106500	2.53405700	3.31131900
H	-0.91663100	1.17301300	4.15230100
H	-2.58272200	0.50113900	2.27189400
H	-0.96636400	-0.20593400	2.11969200

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.354772

Sum of electronic and thermal Free Energies = -1757.232524

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -1757.2996891

No imaginary frequency

ts2-b

C	-2.11470100	0.83567600	-0.43197100
C	-1.78247300	1.85450800	-1.48176400
C	-3.13903000	1.19307500	0.58369600
N	-0.92830300	0.30605000	0.07066000
C	-4.24408000	2.02201900	0.31286600
C	-3.05713600	0.63608600	1.87457400
C	-4.02378800	0.89810800	2.84051000
C	-5.12382600	1.72183900	2.56952200
C	-5.20574700	2.27844600	1.28841600
C	-6.19392300	1.97095800	3.60624600
F	-0.80032200	1.43731600	-2.31631200
F	-2.83454900	2.19977200	-2.24960800
F	-1.29590500	3.05332800	-0.95784800
C	-0.23189000	-0.65905800	-0.11238400
H	-4.36174200	2.47767900	-0.66212800
H	-2.21995600	-0.00946600	2.12094000
H	-3.92129900	0.44907200	3.82668400

H	-6.04387200	2.92684900	1.04074600
H	-5.78580400	1.93371100	4.62268200
H	-6.66805100	2.94920100	3.46828600
H	-6.98899500	1.21497000	3.54869500
C	-7.50895400	-0.84334100	-1.62168800
C	-8.71434300	-1.30883900	-1.14464700
C	-8.74728100	-2.31475400	-0.14722300
C	-7.57242400	-2.83393400	0.35175900
C	-6.31325700	-2.37523500	-0.11780300
C	-6.27873500	-1.35661100	-1.12701600
C	-5.02026600	-0.89964000	-1.59632000
C	-3.83550900	-1.41534000	-1.10643100
C	-3.87896600	-2.42993600	-0.11086900
C	-5.08038900	-2.89188100	0.36905100
C	-2.51888800	-0.95429600	-1.63444900
O	-1.46592300	-1.64379100	-1.42515600
H	-7.48140100	-0.07144100	-2.38781100
H	-9.64635700	-0.90607300	-1.53297900
H	-9.70387400	-2.67583300	0.22164800
H	-7.59384000	-3.60763400	1.11640900
H	-4.99530600	-0.12568000	-2.36210600
H	-2.93568300	-2.83711800	0.23930200
H	-5.10560100	-3.67095100	1.12843700
H	-2.59265400	-0.37195800	-2.56697700
H	0.47600500	2.66822100	0.03105300
C	4.46529600	-0.95811300	0.31035800
O	5.74608000	-1.09529100	0.40775200
O	3.73889600	-2.08511400	0.23442100
O	3.87263700	0.15922100	0.28374300
Ag	1.69258500	-1.41450300	0.06714300
Ag	5.67474900	-3.33637900	0.38636800
C	4.97120400	3.03717800	-0.03470100
C	5.12340000	3.78037800	-1.36378100
N	3.61907200	3.05217200	0.58685000
C	4.67496600	2.98016100	-2.59658300
C	3.35106400	2.23621000	-2.36893900
C	2.33076700	3.07477700	-1.57229500
C	2.46562800	2.94158600	-0.06769700
C	3.66649400	2.71898700	2.02950700
C	2.37127400	3.09427600	2.74147500
C	1.19263500	2.45990800	2.01627600
N	1.32239700	2.73393900	0.58511000
H	5.61778300	3.51718800	0.70560500
H	5.26435000	1.98309700	-0.10880400
H	6.18458600	4.03678900	-1.46731900
H	4.59275900	4.73949100	-1.30286500

H	5.45030900	2.25240200	-2.86413900
H	4.58291600	3.66769500	-3.44769600
H	3.52968300	1.29962700	-1.82954100
H	2.90099700	1.97038100	-3.33150100
H	1.31720100	2.75926900	-1.82844200
H	2.39957400	4.13658200	-1.84232800
H	4.50767500	3.26873600	2.46044400
H	3.87624500	1.64519000	2.09401900
H	2.25527700	4.18438500	2.76470800
H	2.41174100	2.74267100	3.77694800
H	0.23608700	2.87103300	2.35040400
H	1.16513300	1.37509200	2.16591600

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.501 924

Sum of electronic and thermal Free Energies = -2256.271305

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4213091

Number of Imaginary Frequencies = 1

Lowest Frequency = 375.10i

in4-b

C	2.24888300	0.91543300	-0.35839200
C	2.70322200	1.02859700	1.10612100
C	2.75442700	2.09336400	-1.20358200
N	0.77376200	0.87022900	-0.34003900
C	4.05090400	2.61746100	-1.08200100
C	1.91260900	2.65513900	-2.17065200
C	2.34562800	3.70533200	-2.98166100
C	3.63445500	4.23379100	-2.85889500
C	4.47524400	3.66917800	-1.89092100
C	4.11521500	5.35616500	-3.74888700
F	2.08841500	0.10682000	1.88430900
F	4.03774400	0.80585500	1.25347400
F	2.43515600	2.23711100	1.63303400
C	0.35482200	-0.21508600	-0.91495000
H	4.74012800	2.21293000	-0.35126700
H	0.90672800	2.26682100	-2.28573100
H	1.66549600	4.11948400	-3.72328500
H	5.48435800	4.05647400	-1.76647500
H	4.68971800	6.09920100	-3.18375600
H	4.77132300	4.97957500	-4.54492600
H	3.27806600	5.87181600	-4.23094000
C	7.36749900	-1.27146000	-2.24458300
C	8.33868800	-1.36586100	-3.21647800
C	8.00190800	-1.19492900	-4.58231300
C	6.70015200	-0.93348400	-4.94898000

C	5.67515600	-0.82886700	-3.97095100
C	6.01564400	-1.00079800	-2.58994100
C	4.98893100	-0.90240900	-1.61427800
C	3.68122900	-0.63754100	-1.96680400
C	3.34956500	-0.47253600	-3.33866000
C	4.31944000	-0.56700800	-4.30845000
C	2.63095100	-0.52458100	-0.89225000
O	1.35414100	-1.03652800	-1.35495700
H	7.62282500	-1.40330600	-1.19555300
H	9.36881200	-1.57300400	-2.93899400
H	8.77679800	-1.27236400	-5.34034300
H	6.43832900	-0.80362900	-5.99667300
H	5.25076200	-1.03437400	-0.56627600
H	2.31609600	-0.28723600	-3.61075800
H	4.05600300	-0.44492800	-5.35659500
H	2.92792100	-1.14886300	-0.04388600
H	-0.47765400	1.95123600	0.36751300
C	-4.48160600	-0.42058100	-0.51584800
O	-5.75314400	-0.66594100	-0.45989300
O	-3.74991400	-1.25149400	-1.28101200
O	-3.92052300	0.52503500	0.09826300
Ag	-1.67101600	-0.73826400	-1.13417100
Ag	-5.66101300	-2.45731600	-1.78007800
C	-4.22404400	2.09040100	2.88561600
C	-3.67803200	1.62376800	4.23816900
N	-3.24347200	2.66781400	1.93303900
C	-3.07844200	0.20844400	4.22712900
C	-2.20688900	-0.05821800	2.99043900
C	-1.34689200	1.15760600	2.59156200
C	-2.04392600	2.13385300	1.66357800
C	-3.91173300	3.49936600	0.90816400
C	-2.90564500	4.27218200	0.06348100
C	-1.88291900	3.29630600	-0.49975100
N	-1.35234800	2.48074600	0.58911300
H	-4.94390600	2.89473200	3.06392800
H	-4.74908600	1.28587500	2.35522100
H	-4.50865100	1.65724800	4.95375500
H	-2.94611000	2.35793600	4.59806700
H	-3.88633600	-0.53296400	4.26251500
H	-2.48868900	0.07021100	5.14303700
H	-2.83008200	-0.33296900	2.13294900
H	-1.54014100	-0.90602700	3.18293500
H	-0.44681000	0.82064200	2.07506800
H	-1.00515800	1.70227700	3.48139900
H	-4.57671600	4.19059800	1.43568900
H	-4.51383200	2.82320300	0.29061400

H	-2.40277400	5.03360400	0.67197500
H	-3.43128800	4.78735900	-0.74690600
H	-1.04055000	3.81054100	-0.97166600
H	-2.34564100	2.63185500	-1.23917700

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.509257

Sum of electronic and thermal Free Energies = -2256.333449

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4954773

No imaginary frequency

ts3-b

C	-3.29595900	-1.24852900	0.25827600
C	-3.58122700	-1.26228400	1.77769200
C	-4.61076100	-1.42952000	-0.50453900
N	-2.36204600	-2.36349300	0.01173500
C	-5.61889000	-0.45313100	-0.48387500
C	-4.84165800	-2.60375500	-1.22712900
C	-6.03863200	-2.78951900	-1.92154600
C	-7.04309900	-1.81690700	-1.91331400
C	-6.81019800	-0.64576200	-1.17788800
C	-8.33561800	-2.01083100	-2.67195000
F	-2.43602200	-1.18340700	2.49565100
F	-4.33594300	-0.19532100	2.15537800
F	-4.22741000	-2.37065700	2.16216800
C	-1.18162900	-1.94803200	-0.22086000
H	0.16717600	-2.69308200	-0.42556100
H	-5.47839100	0.46421100	0.07665400
H	-4.07525800	-3.37018000	-1.23359600
H	-6.19325100	-3.71244500	-2.47662700
H	-7.57346400	0.12913700	-1.14761300
H	-8.43285200	-1.28522700	-3.49005200
H	-8.39569200	-3.01280800	-3.10902200
H	-9.20770800	-1.87676900	-2.02010000
C	3.56176800	0.57940900	-0.63294000
O	4.82788000	0.82051500	-0.72096600
O	2.72325200	1.59588900	-0.88998700
O	3.07691000	-0.54888900	-0.32534900
Ag	0.80856800	0.54913100	-0.56508700
Ag	4.57633100	2.95260800	-1.30572600
C	4.51399300	-3.21282500	1.06809700
C	4.29234600	-3.68703000	2.50835700
N	3.42940100	-3.50398000	0.10320600
C	3.48237400	-2.71327900	3.38011600
C	2.29113600	-2.09454600	2.63309500
C	1.55613200	-3.10476600	1.73029900

C	2.11983100	-3.24018400	0.32539300
C	3.92167000	-3.49458100	-1.28719900
C	2.86112800	-4.00896200	-2.25351000
C	1.58530100	-3.20229600	-2.05224600
N	1.23158600	-3.15602200	-0.63829200
H	5.38990700	-3.73314700	0.66859500
H	4.72708300	-2.13648500	1.02295800
H	5.27926400	-3.83967400	2.96231000
H	3.81922500	-4.67668100	2.48274700
H	4.13679000	-1.90897500	3.73950000
H	3.13086200	-3.24852900	4.27219200
H	2.62239900	-1.25320600	2.01480800
H	1.57504600	-1.69021000	3.35803700
H	0.51054300	-2.81087500	1.61618400
H	1.54024900	-4.09864200	2.19703800
H	4.81194600	-4.13150700	-1.32404900
H	4.21635500	-2.46753000	-1.53597300
H	2.66615200	-5.07194600	-2.06582400
H	3.22343300	-3.91436000	-3.28287100
H	0.73973000	-3.63942100	-2.59531600
H	1.72335600	-2.17605500	-2.41757200
C	-3.87855200	4.36525100	-2.13717300
C	-4.18518600	5.11901500	-3.24878500
C	-4.12937400	4.54157100	-4.54094300
C	-3.76716100	3.22123600	-4.69683400
C	-3.44569600	2.41753100	-3.57140600
C	-3.50363600	3.00085300	-2.26460900
C	-3.17900800	2.19474000	-1.14023800
C	-2.82247600	0.86870200	-1.27805100
C	-2.76053100	0.29907600	-2.58220100
C	-3.06369700	1.05198200	-3.69034900
C	-2.46289400	0.05422600	-0.06357400
O	-1.12082800	-0.50389200	-0.23900900
H	-3.92149600	4.80600200	-1.14372600
H	-4.47245700	6.16114600	-3.13773600
H	-4.37415500	5.14578600	-5.41037300
H	-3.72302800	2.77541500	-5.68785500
H	-3.21979200	2.64480000	-0.14964500
H	-2.47475700	-0.74248800	-2.69085100
H	-3.01789400	0.60660300	-4.68145800
H	-2.42684900	0.70870800	0.80934500

B3LYP/6-31G* (LanL2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.500642

Sum of electronic and thermal Free Energies = -2256.290456

M06-2x/6-311++G** (LanL2DZ for Ag)

Energy = -2256.4542793

Number of Imaginary Frequencies = 1

Lowest Frequency = 425.20i

in5-b

C	-3.30949700	-1.34751200	0.42322700
C	-3.42899400	-1.06988400	1.94103800
C	-4.70384000	-1.47530900	-0.19050900
N	-2.54163200	-2.59953900	0.30110600
C	-5.58843900	-0.38737400	-0.23832600
C	-5.13285100	-2.70330700	-0.70433000
C	-6.40587900	-2.83623000	-1.26020000
C	-7.29280900	-1.75593600	-1.31330200
C	-6.85748500	-0.52911500	-0.79328600
C	-8.68201000	-1.90720500	-1.88778900
F	-2.20918000	-1.04136100	2.52567000
F	-3.99408400	0.14136400	2.17604300
F	-4.16380900	-1.99519300	2.56768100
C	-1.38649300	-2.28702600	-0.12137900
H	-0.54210400	-2.95153100	-0.28407200
H	-5.29079900	0.57843400	0.15366500
H	-4.46356200	-3.55486700	-0.66287500
H	-6.71394100	-3.80152900	-1.65590500
H	-7.52152700	0.33189700	-0.82423700
H	-8.97591800	-1.02403500	-2.46618500
H	-8.75133900	-2.78072300	-2.54427900
H	-9.42856100	-2.03523700	-1.09253200
C	3.92157000	1.01996500	-0.69531600
O	4.84151800	1.93044000	-0.67229100
O	2.64587400	1.46645100	-0.79388000
O	4.14092800	-0.21776500	-0.62952500
Ag	1.51349600	-0.42208700	-0.75888800
Ag	3.43140900	3.64069400	-0.82715100
C	5.20567800	-3.19349200	0.59206000
C	5.09135600	-3.55026000	2.07947000
N	4.00602600	-3.45990300	-0.23787900
C	4.48724500	-2.43651400	2.95189900
C	3.31113900	-1.71828300	2.27272400
C	2.38659500	-2.67577500	1.49372100
C	2.76668700	-2.96041100	0.04447700
C	4.34931500	-3.70767300	-1.64590900
C	3.12276100	-4.17641200	-2.41547800
C	2.02925900	-3.12832900	-2.24405000
N	1.80472700	-2.77098200	-0.83476200
H	5.99216100	-3.81416800	0.15194500
H	5.49904200	-2.14433600	0.45104900
H	6.09764000	-3.78752100	2.44652700

H	4.51167100	-4.47733700	2.17051400
H	5.26233500	-1.69863200	3.19419800
H	4.16483300	-2.87279500	3.90695000
H	3.68002900	-0.95156100	1.58258400
H	2.71549800	-1.19935400	3.03347100
H	1.37413100	-2.26690700	1.45336100
H	2.30454800	-3.63714700	2.02071600
H	5.13478500	-4.47145500	-1.66593900
H	4.76020600	-2.78907800	-2.08903300
H	2.78679700	-5.14437500	-2.02246700
H	3.37059500	-4.31509600	-3.47391900
H	1.07591300	-3.48390900	-2.65462700
H	2.29934800	-2.22676700	-2.81299800
C	-3.51173500	3.88596900	-2.74676200
C	-3.86843600	4.50958400	-3.92210900
C	-4.03424300	3.75510800	-5.10942300
C	-3.83996100	2.39115700	-5.09976100
C	-3.47323100	1.71839600	-3.90438100
C	-3.30667800	2.48100400	-2.70370200
C	-2.93648000	1.80504400	-1.50989300
C	-2.75094300	0.43853400	-1.48184600
C	-2.91502500	-0.31190200	-2.68023700
C	-3.26304300	0.31231400	-3.85311100
C	-2.35135400	-0.23355500	-0.19580700
O	-1.11467500	-0.98889900	-0.41440900
H	-3.38410900	4.46247000	-1.83347600
H	-4.02461500	5.58463800	-3.94270900
H	-4.31554900	4.25841700	-6.03038800
H	-3.96583800	1.81004100	-6.01021800
H	-2.79983200	2.39038500	-0.60236700
H	-2.77039500	-1.38762300	-2.66195100
H	-3.38764300	-0.26859000	-4.76369800
H	-2.11954800	0.52542600	0.55246400

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.504574

Sum of electronic and thermal Free Energies = -2256.316248

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4820336

No imaginary frequency

ts2-b'

C	2.36440500	0.98505000	-0.35360000
C	2.50293400	0.63336700	1.10060900
C	3.13281000	2.15183100	-0.86660200
N	1.00342000	0.97526400	-0.66383500
C	4.38459000	2.54375200	-0.35338500

C	2.64711900	2.86164900	-1.98248700
C	3.36724400	3.91216900	-2.54371700
C	4.60718900	4.30879500	-2.02598500
C	5.09657500	3.59743400	-0.92467200
C	5.37247800	5.46902400	-2.61838300
F	1.73881700	-0.43108000	1.44358100
F	3.75889000	0.37294100	1.49075000
F	2.05611700	1.65482900	1.94770700
C	0.23499300	0.29932000	-1.29694300
H	4.81532600	2.02665100	0.49436200
H	1.69469600	2.57740600	-2.41874100
H	2.95678800	4.43242400	-3.40708400
H	6.06028100	3.86988200	-0.49866100
H	6.40661700	5.49342100	-2.25742100
H	5.39904100	5.41523700	-3.71252600
H	4.91455100	6.43232400	-2.35332600
C	6.99488000	-2.54421800	0.26743400
C	7.65673200	-3.50611100	0.99831700
C	6.93980600	-4.58202500	1.57777100
C	5.57449400	-4.67293800	1.41361600
C	4.86213600	-3.69744500	0.66748500
C	5.58664100	-2.60758000	0.08064300
C	4.87453800	-1.63431800	-0.66707100
C	3.50503700	-1.71224200	-0.83582400
C	2.79594500	-2.80315300	-0.26042400
C	3.45407400	-3.76160000	0.47026900
C	2.77454400	-0.70776600	-1.66925300
O	1.60911200	-0.98092500	-2.11326200
H	7.54337800	-1.71779900	-0.17935800
H	8.73361000	-3.44358100	1.13246000
H	7.47206300	-5.33629400	2.15154700
H	5.02087000	-5.49871300	1.85559200
H	5.42721800	-0.81042600	-1.11625300
H	1.72615600	-2.85940200	-0.43408700
H	2.90495000	-4.59501400	0.90416400
H	3.43605700	-0.06680300	-2.27436000
H	0.05435000	1.96762800	1.67735600
C	-4.33404100	-0.42827200	-0.39024300
O	-5.54289200	-0.78681000	-0.10916300
O	-3.82262100	-0.87823500	-1.54792400
O	-3.62050700	0.30208500	0.35632800
Ag	-1.75521600	-0.24580700	-1.51889200
Ag	-5.77464300	-2.04992000	-1.94572100
C	-4.13200500	1.32305500	3.23295600
C	-3.79004100	0.56221300	4.51573000
N	-3.02647800	2.08799600	2.59336800

C	-3.12606900	-0.80458700	4.28841500
C	-2.03845700	-0.76056600	3.20508600
C	-1.18353500	0.52150500	3.27783700
C	-1.76136300	1.68561300	2.49684200
C	-3.53424800	3.11180200	1.65110700
C	-2.45781900	4.12648100	1.28099500
C	-1.22505200	3.39418400	0.76971900
N	-0.89596400	2.32084600	1.70729900
H	-4.88565700	2.07945700	3.47110800
H	-4.54225200	0.66667000	2.45587600
H	-4.72997500	0.41916600	5.06221900
H	-3.16921000	1.19981100	5.15843300
H	-3.88700900	-1.53914300	3.99908900
H	-2.70021200	-1.15115000	5.23923900
H	-2.49169900	-0.82086700	2.20938600
H	-1.37291000	-1.62450400	3.30725700
H	-0.19067500	0.32493600	2.86830000
H	-1.03086000	0.83265000	4.31933100
H	-4.37338200	3.61330100	2.14100300
H	-3.90901000	2.57026800	0.77517200
H	-2.19669400	4.73542900	2.15475400
H	-2.84414600	4.80047300	0.51025900
H	-0.35666400	4.05507400	0.69979600
H	-1.39738000	2.95624500	-0.21954800

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.500377

Sum of electronic and thermal Free Energies = -2256.271768

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4181310

Number of Imaginary Frequencies = 1

Lowest Frequency = 385.31i

in4-b'

C	2.24879700	0.82247300	-0.21701500
C	2.49576900	0.92802200	1.30367300
C	2.89872100	1.99614800	-0.95990000
N	0.77737800	0.80611300	-0.36086300
C	4.24701700	2.34011100	-0.78635800
C	2.15730200	2.70945600	-1.91116800
C	2.73806400	3.73698100	-2.65197200
C	4.08220400	4.09116300	-2.47585900
C	4.82117800	3.37244600	-1.53022400
C	4.71022000	5.19686300	-3.29234800
F	1.84083300	-0.04670500	1.98162700
F	3.79438900	0.83650600	1.66300100
F	2.03408000	2.10753100	1.77678700

C	0.38298600	-0.36778600	-0.75130900
H	4.85890300	1.81229200	-0.06506800
H	1.11728000	2.44541500	-2.06856800
H	2.13422200	4.27324400	-3.38161400
H	5.86773700	3.62124300	-1.36807400
H	5.69618800	5.47065000	-2.90327700
H	4.84076100	4.89553800	-4.34007400
H	4.08666500	6.09883000	-3.29351500
C	7.37548700	-2.11835200	-0.34030000
C	8.31436400	-2.92396400	0.26467900
C	7.92598500	-3.84250400	1.27148700
C	6.60582900	-3.93762300	1.65258300
C	5.61342900	-3.11939100	1.04962800
C	6.00583000	-2.18945000	0.03309800
C	5.01135700	-1.37753200	-0.57323600
C	3.68613300	-1.45046500	-0.19220700
C	3.30257300	-2.38527600	0.80818700
C	4.23987000	-3.19315400	1.40675500
C	2.66722500	-0.55856600	-0.86292300
O	1.39695600	-1.24832300	-0.99859500
H	7.67090600	-1.41331900	-1.11404800
H	9.35865900	-2.85864200	-0.02890600
H	8.67582200	-4.47335700	1.74135200
H	6.30432500	-4.64313000	2.42353800
H	5.31291000	-0.68535400	-1.35711900
H	2.25643000	-2.46424000	1.07944400
H	3.93488500	-3.91011200	2.16562600
H	3.01675800	-0.33335200	-1.87550700
H	-0.54849500	1.89089100	0.25903400
C	-4.45047900	-0.69957100	-0.35220800
O	-5.71828400	-0.96549600	-0.30555400
O	-3.68939900	-1.55453200	-1.05971000
O	-3.91896700	0.28966400	0.21838100
Ag	-1.62571500	-0.96743500	-0.93000800
Ag	-5.57373900	-2.80246900	-1.55596600
C	-4.28928600	2.18848500	2.77310300
C	-3.71816800	1.93439500	4.17134000
N	-3.33970500	2.67944300	1.74337800
C	-3.05659200	0.55777100	4.34447200
C	-2.18687200	0.16313500	3.14154400
C	-1.38001000	1.34804000	2.57389000
C	-2.12043200	2.16433900	1.53335700
C	-4.04917600	3.34217400	0.62783400
C	-3.08306100	4.03424500	-0.32631900
C	-2.02201800	3.03538700	-0.76573600
N	-1.44956700	2.39590300	0.41531100

H	-5.04702500	2.97399900	2.84798100
H	-4.77527100	1.29586200	2.35986800
H	-4.54652600	2.02871100	4.88411700
H	-3.01802400	2.74156900	4.42099600
H	-3.83019100	-0.20584500	4.49323400
H	-2.45183600	0.57115700	5.26092400
H	-2.80513100	-0.24886300	2.33666200
H	-1.48305100	-0.62339700	3.43557800
H	-0.47190200	0.97953500	2.09703300
H	-1.05276400	2.01866700	3.37908100
H	-4.73617100	4.07154900	1.06890400
H	-4.63002800	2.56852200	0.11285900
H	-2.60946700	4.89192700	0.16669200
H	-3.63618700	4.41171700	-1.19229600
H	-1.20670500	3.51982400	-1.31098500
H	-2.45769400	2.25925100	-1.40608200

B3LYP/6-31G* (LanL2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.509057

Sum of electronic and thermal Free Energies = -2256.331995

M06-2x/6-311++G** (LanL2DZ for Ag)

Energy = -2256.4932464

No imaginary frequency

ts3-b'

C	-2.99748500	-1.27833800	0.04982800
C	-3.07338400	-1.31116400	1.59349200
C	-4.40416100	-1.45524700	-0.52609100
N	-2.09697800	-2.39043400	-0.31210500
C	-5.38402300	-0.46491200	-0.37086600
C	-4.72966600	-2.60669500	-1.25086000
C	-5.99814400	-2.75810500	-1.81003000
C	-6.98320500	-1.77361700	-1.66073800
C	-6.65052500	-0.62434400	-0.93312600
C	-8.36581900	-1.95792600	-2.24264400
F	-1.83822300	-1.29720900	2.16027800
F	-3.74637500	-0.25388500	2.10638500
F	-3.68788300	-2.42391500	2.02456700
C	-0.96782600	-1.96718200	-0.72759500
H	0.41041600	-2.69383500	-0.84325000
H	-5.16514900	0.43524900	0.19410300
H	-3.97536500	-3.37589500	-1.37181800
H	-6.22581500	-3.66055800	-2.37388900
H	-7.39322400	0.15972600	-0.80100700
H	-8.85976600	-0.99598500	-2.41705300
H	-8.33215800	-2.49861800	-3.19508200
H	-9.00905000	-2.53614500	-1.56550400

C	3.73935400	0.58810700	-0.33423400
O	5.01547800	0.77999800	-0.28682400
O	2.97862300	1.61391700	-0.74979300
O	3.17225600	-0.50101500	-0.02393500
Ag	0.99931000	0.61365300	-0.68387900
Ag	4.88326600	2.90332700	-0.98946400
C	4.38175300	-3.23433000	1.43720600
C	3.89322300	-3.79873500	2.77583800
N	3.52175600	-3.47889700	0.25609300
C	2.89037500	-2.89991800	3.51873400
C	1.84117700	-2.27958700	2.58332700
C	1.35197300	-3.25984200	1.49910800
C	2.18505600	-3.26544500	0.22871400
C	4.28356200	-3.35356000	-1.00084200
C	3.45217000	-3.79283400	-2.20059200
C	2.13825600	-3.02259900	-2.19501300
N	1.50425800	-3.11790700	-0.88563600
H	5.33442900	-3.71420200	1.19238900
H	4.56782500	-2.15392700	1.49835400
H	4.77556100	-3.95210500	3.40942500
H	3.47177400	-4.79691100	2.60379900
H	3.43007200	-2.09726000	4.03733100
H	2.39590100	-3.49485400	4.29809400
H	2.24900400	-1.39034900	2.08972500
H	0.97426900	-1.94974500	3.16756700
H	0.33090200	-3.00954100	1.20680100
H	1.30918000	-4.28313300	1.89457100
H	5.17581200	-3.98209600	-0.90638100
H	4.60315100	-2.30903800	-1.10312200
H	3.25376200	-4.87032000	-2.14601000
H	4.01063400	-3.60421600	-3.12381500
H	1.43509600	-3.41425900	-2.93850400
H	2.31718700	-1.96419900	-2.42629500
C	-3.66295800	4.76027500	-0.16888300
C	-3.56893400	5.99578000	0.43263100
C	-2.68780400	6.19535000	1.52415700
C	-1.91638700	5.15492800	1.99324400
C	-1.99170600	3.86868600	1.39592100
C	-2.88365200	3.66570100	0.29385100
C	-2.95019700	2.38071100	-0.30790900
C	-2.19835500	1.31769500	0.15529800
C	-1.31367200	1.53127700	1.25378400
C	-1.21403100	2.76840400	1.84745400
C	-2.28234800	-0.01098700	-0.55804500
O	-0.94226200	-0.52459300	-0.82090400
H	-4.33814300	4.60502100	-1.00718200

H	-4.17217500	6.82425600	0.07133000
H	-2.62357300	7.17484300	1.99024100
H	-1.23908400	5.30421300	2.83089600
H	-3.61290400	2.24155800	-1.15959600
H	-0.73218900	0.70250500	1.64056000
H	-0.53472200	2.91442200	2.68395100
H	-2.75213500	0.15735400	-1.53211300

B3LYP/6-31G* (Lan12DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.501189

Sum of electronic and thermal Free Energies = -2256.288490

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4537746

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.42i

in5-b'

C	-3.27187200	-1.45614100	0.40605300
C	-3.34957400	-1.22295200	1.93387100
C	-4.68300200	-1.56227400	-0.17281200
N	-2.50879100	-2.70999000	0.24659500
C	-5.54068000	-0.45276100	-0.19676900
C	-5.13510500	-2.76796300	-0.71884100
C	-6.40884100	-2.85844600	-1.28007200
C	-7.27193800	-1.75672700	-1.31003100
C	-6.81187100	-0.55298200	-0.76009000
C	-8.66238400	-1.86795600	-1.89084900
F	-2.11882000	-1.24223900	2.49908500
F	-3.90941900	-0.03357200	2.24294900
F	-4.07621300	-2.18118400	2.52792900
C	-1.37632900	-2.39722300	-0.23371300
H	-0.53288000	-3.05849400	-0.40950400
H	-5.22403800	0.49305400	0.22978500
H	-4.48168200	-3.63278400	-0.70193400
H	-6.73652300	-3.80594000	-1.70223100
H	-7.45865700	0.32163600	-0.76919200
H	-8.98942000	-0.92158300	-2.33516200
H	-8.71298100	-2.64148900	-2.66448300
H	-9.39529600	-2.13338700	-1.11710700
C	3.87446900	1.11018500	-0.50661000
O	4.77120900	2.04217800	-0.44370700
O	2.59276600	1.52717700	-0.63625800
O	4.12329900	-0.12268900	-0.45172700
Ag	1.49806800	-0.38211200	-0.67327800
Ag	3.32615200	3.72065200	-0.63186700
C	5.23946800	-3.09469900	0.66481600
C	5.09754300	-3.52128200	2.13122300

N	4.07302500	-3.36445100	-0.21026000
C	4.43014800	-2.46978000	3.03444900
C	3.24842500	-1.76116600	2.35460200
C	2.38068800	-2.71234900	1.50551600
C	2.81088500	-2.91559800	0.05661000
C	4.46465900	-3.53244700	-1.61749500
C	3.27662300	-4.00101900	-2.44532500
C	2.14538600	-2.99646700	-2.25821000
N	1.86957100	-2.71258500	-0.84125100
H	6.05881800	-3.66840700	0.22090800
H	5.49938900	-2.03095000	0.57761500
H	6.10150800	-3.73878400	2.51643600
H	4.55031800	-4.47174000	2.16531600
H	5.17181900	-1.71797800	3.33209400
H	4.09708400	-2.96010800	3.95915900
H	3.60891900	-0.95084900	1.71123500
H	2.61376600	-1.30021900	3.12131500
H	1.35545600	-2.33776000	1.45370100
H	2.31842100	-3.69940800	1.98551100
H	5.27472800	-4.26967900	-1.64996600
H	4.85823100	-2.58094100	-2.00319700
H	2.96078000	-4.99660800	-2.10869800
H	3.55921100	-4.08097700	-3.50112400
H	1.21608700	-3.36152600	-2.71317100
H	2.40212900	-2.06134400	-2.77705600
C	-3.29544200	4.49851300	-0.62003000
C	-3.06347500	5.78670000	-0.19180800
C	-2.12690000	6.03913400	0.84137000
C	-1.43802600	4.99852500	1.42502200
C	-1.65372800	3.65854000	1.00505900
C	-2.60366200	3.40320400	-0.03592000
C	-2.81242000	2.06369300	-0.45889000
C	-2.14066200	1.00708000	0.12426100
C	-1.19165700	1.27078000	1.15155800
C	-0.95716800	2.55781500	1.57311700
C	-2.39393600	-0.39079800	-0.38482600
O	-1.12578100	-1.09922700	-0.55200900
H	-4.01420400	4.30199500	-1.41215000
H	-3.60015700	6.61601800	-0.64432000
H	-1.95660100	7.05959700	1.17367600
H	-0.72228200	5.18852200	2.22164100
H	-3.51744800	1.87938700	-1.26684400
H	-0.64946500	0.44869100	1.60199200
H	-0.22441700	2.74617500	2.35379200
H	-2.83519100	-0.32173200	-1.38325300

B3LYP/6-31G* (Lanl2DZ for Ag)

Thermal correction to Gibbs Free Energy = 0.503726

Sum of electronic and thermal Free Energies = -2256.315960

M06-2x/6-311++G** (Lan12DZ for Ag)

Energy = -2256.4815380

No imaginary frequency